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Chirality Determination Using Three-Wave Mixing Microwave Spectroscopy

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CHIRALITY DETERMINATION USING THREE-WAVE MIXING MICROWAVE SPECTROSCOPY

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This dissertation consists of the following six articles, formatted in the style used by the Missouri University of Science and Technology.

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ABSTRACT

Rotational spectroscopy has established itself as a reliable gas-phase spectroscopic technique for the structural determination of molecules. This reliability has stemmed from both advancements in microwave technology and a willingness from the community to push the boundaries of the field. In this dissertation, the boundaries are tested in both how well the technique can determine the structure of molecules exhibiting large amplitude motion and through chirality determination. The first half of this dissertation explores the use of deep averaging to determine the structure of silicon containing molecules in collaboration with Dr. Guirgis from the College of Charleston. For each of these molecules, the ground electronic and vibrational state, pure rotational spectrum was analyzed via CP-FTMW spectroscopy. The parent species and singly substituted isotopologues for each molecule were observed in natural abundance and are reported, which allowed for r_s structures to be generated. The second half of this dissertation explores the use of microwave three-wave mixing (M3WM) spectroscopy to determine a molecule's chirality and measure enantiomeric excess. Building off the previous works of Schnell, Patterson, and Pate, a M3WM spectrometer was constructed and demonstrated at Missouri University of Science and Technology for the use of chirality determination. The first molecule studied with this instrument was carvone, whose traditional rotational spectrum is denominated by internal rotation splittings from two non-equivalent methyl rotors. This M3WM experiment marked the first time a M3WM experiment was completely operable in the 6-18 GHz region of the electromagnetic spectrum and also demonstrated the first use of synchronized arbitrary waveform generators for orthogonal pulse generation. Within this work, the design, construction, and demonstration of the M3WM instrument's capabilities using the enantiomers of carvone will be discussed along with the updated spectrum analysis of carvone.

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NOMENCLATURE

Symbol	Description
λ	Wavelength
ω	Angular Frequency
ν	Frequency
h	Planck's Constant
r	Radius
μ	Dipole Moment
$\vec{\mathbf{L}}$	Angular Momentum
I	Angular Moment of Inertia
$\vec{\omega}$	Angular Velocity
J	Total Angular Momentum
$\hat{H}$	Hamiltonian
ψ	Wavefunction
N	Population of Molecules / Population Density
q_r	Rotational Partition Function
χ	Nuclear Quadrapole Coupling Constant
F_c	Centrifugal Force
D, d	Centrifugal Distortion Constants
A, B, C	Rotational Constants
K	Projection of Angular Momentum
κ	Ray's Asymmetry Parameter
V	Potential Energy
F	Rotational Constant for Internal Rotation
α	Linear Sweep Rate / Torsional Angle
T_1	Rate of Decay of Population

T_2	Rate of Decay of Coherence
$\frac{\pi}{2}$ - Pulse	Rabi Angle for $\frac{1}{2}$ Population Invesion
π-Pulse	Rabi Angle for Full Population Inversion
EQ1, EQ2, EQ3	Equitorial Conformers of Carvone
AX1, AX2, AX3	Axial Conformers of Carvone

1. INTRODUCTION

Since its initial discovery by Sir Isaac Newton, spectroscopy has become a fundamental part of the fields of physics, chemistry, and astronomy, among others. Historically, spectroscopy has been defined as a branch of science concerned with how matter interacts with or produces electromagnetic radiation (EMR). Some may say spectroscopists traditionally like to shine a light on the matter. However, over the years, the definition of spectroscopy has been broadened to include interactions between matter and other forms of energy, but these subclassifications will be passed over for the purposes of this work.

Electromagnetic spectroscopy can be divided into two broad classifications: atomic spectroscopy and molecular spectroscopy. As the names suggest, atomic spectroscopy is concerned with how atoms interact with EMR while molecular spectroscopy focuses on the interaction between molecules and EMR. The entirety of this work will focus on molecular spectroscopy. There are traditionally three types of molecular spectroscopy: electronic, vibrational, and rotational. Electronic spectroscopy focuses on the transition of electrons between electronic states. Vibrational spectroscopy is concerned with the vibration of molecules caused by the movement of nuclei. Most importantly for this work, rotational spectroscopy concentrates on the precession of nuclei with respect to one another, or more simply, the rotation of molecules.

Birthed from the technological advancements in microwave RADAR equipment during World War II, the field of rotational spectroscopy has grown tremendously since its humble beginnings. The first rotational spectroscopy experiment was carried out in 1934 by Cleeton and Williams in which they measured the absorption of electromagnetic radiation by ammonia gas [1]. It wasn't until after 1946, however, that the field became more established and took on the secondary name of "microwave" spectroscopy due to the use of EMR within the microwave region to induce rotational transitions. Through advancements in instrumentation brought about by the Balle-Flygare cavity in 1980 [2]

and the chirped pulse Fourier transform microwave (CP-FTMW) spectrometer in 2006 [3], rotational spectroscopy has established itself as a reliable gas-phase spectroscopic technique for the structural determination of molecules. Today, there are over sixty active microwave spectroscopy laboratories around the world, conducting research in a wide variety of areas, including, but not limited to, atmospheric chemistry, synthetic processes, astrochemistry, pharmaceuticals, and instrumentation. Within this work, the use of rotational spectroscopy for chirality determination at the Missouri University of Science and Technology will be presented.

1.1. ELECTROMAGNETIC RADIATION

Light is most commonly represented as a wave comprised of in-phase, oscillating, perpendicular electronic and magnetic fields that propagate in the third mutually orthogonal direction (See Figure 1.1). Since light waves are transverse waves, light can thus be polarized. For the purposes of this work, plane polarized light, in which all oscillations of either the electronic or magnetic field lie in a singular plane, will be the focus. Light can thus be represented by the plane wave equation [4]

$$E(r,t) = E_o cos(k \cdot r - \omega t + \phi). \tag{1.1}$$

In this equation, E is the electric field that propagates in the $\mathbf{k}$ ($|\mathrm{k}| = 2\pi/\lambda$) direction, ω is the angular frequency ($\omega = 2\pi\nu$), t is time, and ϕ is the arbitrary initial phase angle. The wavelength, λ, and frequency, ν, are related by the equation

$$c = \frac{\lambda\nu}{n}, \tag{1.2}$$

where c is the speed of the electromagnetic wave and n is the index of refraction for the medium.

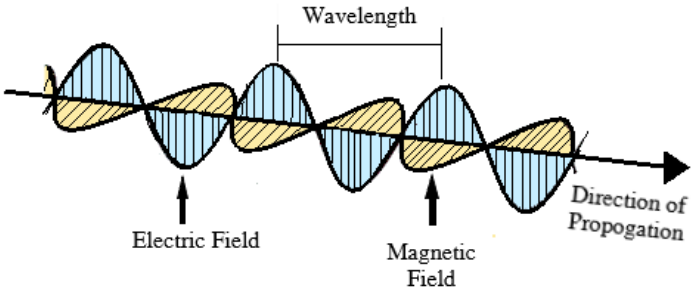


Figure 1.1. Diagram of a light wave.

While the wave representation is the most commonly used for light, light is also found to have properties more associated with that of a particle, such as its ability to induce absorption or emission of radiant energy within atomic systems [5]. As a result, light displays wave-particle duality. When described as a particle, light is more commonly referred to as a photon, whose definite energy, E, and momentum, p, are defined as [4]

$$E = h\nu = \hbar\omega = \frac{hc}{\lambda}, \tag{1.3}$$

and

$$p = \frac{h}{\lambda} = \hbar k, \tag{1.4}$$

respectively.

1.2. ELECTROMAGNETIC SPECTRUM

Due to light's ability to vary drastically in terms of frequency, light itself makes up an electromagnetic spectrum (See Figure 1.2). The traditional regions of the electromagnetic spectrum are defined as radio, microwave, infrared, visible, ultra-violet, X-ray, and gamma ray. The radio frequency region consists of waves with the longest wavelengths but lowest energies, while the gamma ray region is comprised of waves with the highest energies

but shortest wavelengths. While general parameters are defined for each region, it should be noted that different regions do not possess sharp boundaries. Therefore, spectroscopic properties associated with a given region are not limited to that region alone but may be found in nearby regions as well, the most notable example of which is ro-vibrational transitions. The general properties of each region are defined as follows [4]:

- Radio Wave Region: Consists of light between 3 MHz and 3 GHz whose photons have sufficient energy to flip nuclear spins in magnetic fields of a few Tesla.

- Microwave Region: Consists of light between 3 GHz and 3000 GHz whose energy corresponds to rotational transitions in molecules.

- Infrared Region: Consists of light between 100 cm^{-1} and 13,000 cm^{-1} whose energy can excite vibrational motion in molecules. The infrared region is broken down further into far- (33 - 333 cm^{-1}), mid- (333 - 3,333 cm^{-1}) and near- (3,333 – 13,000 cm^{-1}) IR regions.

- Visible Region: Corresponds to light visible to the human eye between about 7,800 Å and 4,000 Å . It is divided into colors of the rainbow starting with red at 7,800 Å and ending with violet at 4,000 Å.

- Ultra-Violet Region: Consists of light between 4,000 Å and 100 Å whose energy can promote valence electron rearrangements in molecules. The UV region is broken down further into near- (4,000 - 2,000 Å) and vacuum- (2,000 - 100 Å) UV.

- X-Ray Region: Consists of light between 100 Å and 0.1 Å whose energy promotes core electronic transitions.

- Gamma Ray Region: Consist of light below 0.1 Å whose energy is associated with nuclear processes.

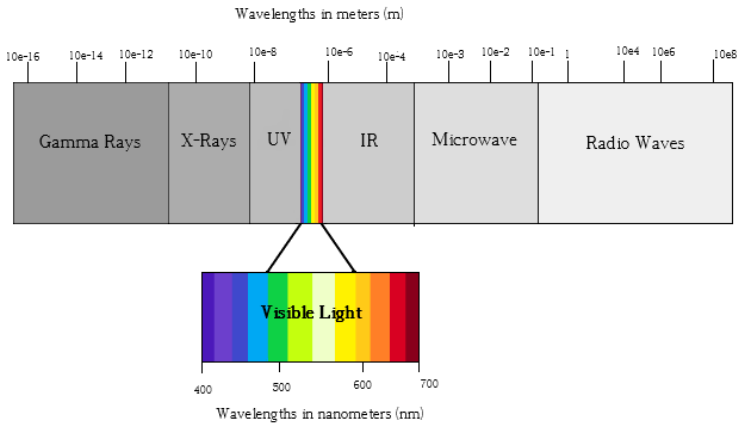


Figure 1.2. Components of the electromagnetic spectrum.

1.3. GENERAL MICROWAVE SPECTROSCOPY THEORY

As briefly mentioned, rotational spectroscopy is a gas-phase spectroscopic technique that is useful for the structural determination of molecules. It involves the transition from one rotational state to another through the interaction of the electromagnetic wave with the permanent electric dipole moment of the molecule. The rotational spectrum thus measures the difference in transitional energy between the rotational states. This information allows one to derive physical constants that can be used to determine the molecular structure of gas-phase molecules, such as the bond lengths and bond angles, electronic structure, Stark and Zeeman effects, and hyperfine structure. Based on this, the basic requirements for a molecule to be studied via microwave spectroscopy is that the molecule must 1.) contain a permanent electric dipole moment and 2.) be in the gas phase. The first requirement is a direct consequence of the selection rules derived from quantum mechanics, and will be discussed further within the *Selection Rules for the Rigid Rotor* section. The second requirement comes from the fact that the gas phase allows for the greatest amount of rotational freedom within the molecule and as a result, provides the resolution needed to observe these transitions. However, this does not mean that only light molecules traditionally in the gas phase at

standard temperature and pressure can be studied via rotational spectroscopy. Over the years, advancements in sourcing techniques have allowed for more than just traditional gas phase molecules to be studied (more on this in Section 2).

It is useful when describing the theory of rotational spectroscopy to start with the most basic case of a molecule rotating end-over-end. To simplify the initial theory, an important assumption will be made that the rotating body is rigid. As a result, the rigid rotor will be explored first.

1.3.1. The Rigid Rotor. All molecules have three types of nuclear freedom: translational, rotational, and vibrational. The simplest molecular system which possesses rotational motion is a diatomic molecule, which can be thought of as a rigid rotor. A rigid rotor can be visualized as two spheres connected by a solid rod. The axis of rotation for the rigid rotor is perpendicular to the plane of rotation and passes through the rotor's center of mass. In a sense, the rigid rotor can be said to be equivalent to a single mass moving on a ring with a fixed radius, which is equal to the bond length between the atoms. The single mass can be expressed by using the reduced mass formula where m_1 and m_2 are the respective masses of the two atoms:

$$\mu = \frac{m_1 m_2}{m_1 + m_2}. \tag{1.5}$$

It is useful at this point to introduce the principal axis system (PAS), which is drawn within the molecular frame. Within the PAS, the origin of the coordinate system is chosen as the center of mass so that the total kinetic energy can be written as the sum of the kinetic energy of translational motion and the kinetic energy of the motion relative to the center of mass [6]. Thus, the translational and rotational motions can be treated separately. From here, the axis a is chosen to lie along the axis with the most amount of molecular mass\inertia. Axis b is chosen to lie along the axis with the second most amount of molecular mass\inertia. Finally, axis c is chosen to lie along the axis with the least amount of molecular mass\inertia. The axes are chosen this way in order for the rotational constants (to be defined later within Section 1) to have the form of $A \geq B \geq C$. Figure 1.3

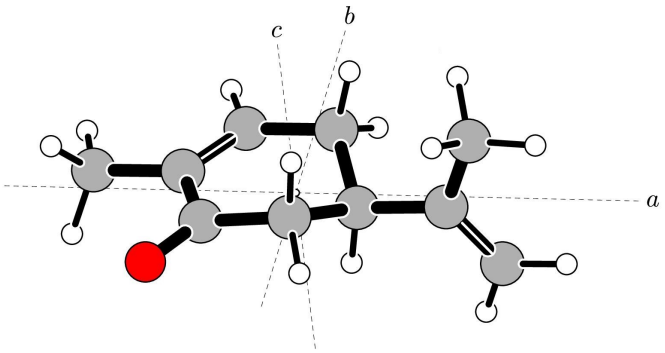


Figure 1.3. Example of the principal axis system for carvone.

shows an example the PAS for a molecule of carvone. For the remainder of this work, when the axis a, b, or c is mentioned, it refers to the PAS within the molecular frame, while the axis X, Y, or Z will refer to the standard cartesian coordinate system within the laboratory frame.

Before the rotational kinetic energy can be derived, the classical angular momentum of a rigid system must first be defined, which can be written as:

$$\vec{\mathbf{L}} = \mathbf{I}\vec{\omega}, \tag{1.6}$$

where $\vec{\omega}$ is the angular velocity and $\mathbf{I}$ is the angular moment of inertia tensor. $\mathbf{I}$ can be represented in dyadic notation as [6]

$$\mathbf{I} = I_{aa}\mathbf{ii} + I_{ab}\mathbf{ij} + I_{ac}\mathbf{ik} + I_{ba}\mathbf{ji} + I_{bb}\mathbf{jj} + I_{bc}\mathbf{jk} + I_{ca}\mathbf{ki} + I_{cb}\mathbf{kj} + I_{cc}\mathbf{kk}, \tag{1.7}$$

where

$$I_{aa} = \sum m(b^2 + c^2), \tag{1.8}$$

$$I_{bb} = \sum m(c^2 + a^2), \tag{1.9}$$

$$I_{cc} = \sum m(a^2 + b^2), \tag{1.10}$$

$$I_{ab} = I_{ba} = \sum mba, \tag{1.11}$$

$$I_{ac} = I_{ca} = \sum mac, \tag{1.12}$$

$$I_{bc} = I_{cb} = \sum mbc. \tag{1.13}$$

In the above equations, m is the mass of a particular particle while a, b, and c are its positional coordinates in the PAS. The first three terms of I_{aa}, I_{bb}, and I_{cc} are referred to as the moments of inertia and, for a diatomic rigid rotor, can more simply be expressed as $I = \mu r^2$. The remaining terms are referred to as the products of inertia.

The components of angular moment then become:

$$L_a = I_a \omega_a, \tag{1.14}$$

$$L_b = I_b \omega_b, \tag{1.15}$$

$$L_c = I_c \omega_c. \tag{1.16}$$

From this information, the rotational kinetic energy can be derived as:

$$E_r = \frac{1}{2}\vec{\boldsymbol{\omega}}\mathbf{I}\vec{\boldsymbol{\omega}} = \frac{1}{2}I_a\omega_a^2 + \frac{1}{2}I_b\omega_b^2 + \frac{1}{2}I_c\omega_c^2 = \frac{1}{2}(\frac{L_a^2}{I_a}) + \frac{1}{2}(\frac{L_b^2}{I_b}) + \frac{1}{2}(\frac{L_c^2}{I_c}), \tag{1.17}$$

where

$$L_i^2 = I_i^2\omega_i^2. \tag{1.18}$$

When written in terms of the total angular momentum, J, the total rotational kinetic energy becomes

$$E_r = \frac{1}{2}(\frac{J_a^2}{I_a}) + \frac{1}{2}(\frac{J_b^2}{I_b}) + \frac{1}{2}(\frac{J_c^2}{I_c}). \tag{1.19}$$

The total angular momentum, J, is defined as

$$J = L + S, \tag{1.20}$$

where L is the orbital angular momenum S is the spin angular momentum. For convenience, in this work, it will be assumed $S = 0$, thus $J = L$.

1.3.2. Rotational Eigenvalues for the Rigid Rotor. In order to describe the characteristic rotational energy levels of a system, the eigenvalues of the Hamiltonian operator for rotational motion must be known. For a rigid rotor in isotropic space, the rotational Hamiltonian is given by [4]

$$\hat{H} = \hat{E}_r = \frac{\hat{J}^2}{2I}, \tag{1.21}$$

which is similar to the total rotational kinetic energy derived in Equation 1.19, except that the classical terms have now been replaced with equivalent operators. In operator form,

$$\hat{J}^2 = \hbar^2 J(J+1). \tag{1.22}$$

In order to derive the rotational eigenvalues, the time independent Schrödinger equation,

$$\hat{H}\psi = E\psi, \tag{1.23}$$

where ψ is one of the spherical harmonics ($\psi = \Theta(\theta)\,\Phi(\phi)$), must be solved. Equation 1.23 can be solved immediately using the information from Equation 1.21 and 1.22.

$$\hat{H}\psi = \frac{\hat{J}^2}{2I}\psi = \frac{\hbar^2 J(J+1)}{2I}\psi = BJ(J+1)\psi, \tag{1.24}$$

where

$$B = \frac{\hbar^2}{2I} = \frac{h^2}{8\pi^2 I} \tag{1.25}$$

is known as the rotational constant. Thus, the rotational energy eigenvalue is given as

$$W(J) = BJ(J+1). \tag{1.26}$$

1.3.3. Selection Rules for the Rigid Rotor. While Equation 1.26 derives the possible rotational levels a given system may have, it does not indicate which types of transitions are allowed between the rotational levels. These transitions are instead governed by the rotational selection rules. To derive the selection rules, the frequency observed when a molecule makes a rotational transition between a lower state, W_1, and an upper state, W_2, will first be determined using the equation [7]

$$\nu_{W_1 \leftarrow W_2} = \frac{E}{h} = \frac{W_2 - W_1}{h} = \frac{h}{8\pi^2 I}[J_2(J_2+1) - J_1(J_1+1)]. \tag{1.27}$$

Remembering that $\omega = 2\pi\nu$ and $J = I\omega$, it can be determined that the frequency of the transition should take the form of

$$\nu = \frac{Jh}{4\pi^2 I}, \tag{1.28}$$

where J must be a positive integer. This is only possible when $J_2 = J_1 \pm 1$. As a result, $\Delta J = \pm 1$ is the rotational transition selection rule, and the observed frequency then takes the form of

$$\nu_{W_1 \leftarrow W_2} = 2B(J+1). \tag{1.29}$$

This derivation of the selection rule assumes that there is no additional vibrational, orbital, or spin angular moment present. If additional angular moment is present, then $\Delta J = 0$ would also be allowed [4].

The intensity of the allowed rotational transition is governed by both the transition dipole moment and the population difference in the two rotational levels. The transition dipole moment is given by [4]

$$M = \int \psi_{J',M'} \boldsymbol{\mu} \psi_{J",M"}, \tag{1.30}$$

where the dipole moment, $\boldsymbol{\mu}$, has the form

$$\boldsymbol{\mu} = \mu_a \hat{e}_1 + \mu_b \hat{e}_2 + \mu_c \hat{e}_3. \tag{1.31}$$

The population of molecules, N_J, within a particular rotational energy level, J, is given by

$$N_J = N(2J+1)\frac{e^{\frac{-BJ(J+1)}{kT}}}{q_r}, \tag{1.32}$$

where N is the total population of molecules, k is the Boltzmann constant, and q_r is the rotational partition function defined as

$$q_r = \sum_J (2J+1) e^{\frac{-BJ(J+1)}{kT}}. \tag{1.33}$$

Since the intensity of all possible transitions would be zero if the dipole moment equaled zero, a second selection rule for rotational spectroscopy is that the molecule must possess a permanent electric dipole moment, as previously mentioned.

1.3.4. Forbidden Transitions. While $\Delta J = 0, \pm 1$ are the only transitions allowed by the selection rules, it is possible to observe in practice rotational transitions originating from $\Delta J = \pm 2, \pm 3 \ldots$, etc. These are known as electric dipole forbidden, nuclear quadrupole allowed transitions and are typically weaker in intensity than electric dipole allowed transitions. First theorized by Javan [8] and observed by Oka [9], these transitions occur when atoms containing large nuclear quadrupole moments (such as Br or I) are combined with

relatively small or approximately equal size rotational constants. The forbidden transitions arise from transition pathways made through an off-diagonal nuclear electric quadrupole containing tensor component.

More specifically, these transition pathways are part of a three-state system in which the electric dipole forbidden transition type and the electric dipole allowed transition type are linked by the χ tensor off-diagonal component in question. The mixing of states is then done by a third electric dipole allowed transition type not contained in the off-diagonal component. For example, if the forbidden and allowed transitions are *b*-type and *a*-type transitions (to be defined shortly), respectively, then the mixing states are connected via a *c*-type transition and the off-diagonal nuclear electric quadrupole tensor component providing the mixing is χ_{ab}.

Due to the similarities in mixing schemes, it has been hypothesized if microwave three-wave mixing spectroscopy (Section 3) could be utilized to study chiral molecules that exhibit electric dipole forbidden, nuclear quadrupole allowed transitions [10]. While preliminary work has been undertaken for this purpose, the results are still inconclusive. As a result, these types of transitions and their connection to microwave three-wave mixing will not be explored further within the remainder of this work.

1.3.5. Centrifugal Distortion. In the discussion thus far, molecules have been treated as rigid rotors. Within this model, the distance between the atoms does not change while the molecule rotates. However, in reality, the distance between the atoms will in fact change during rotation. As a molecule rotates, the atoms will experience a centrifugal force in the rotating molecular frame that will change the internuclear positions. For a diatomic molecule, like the ones that have been described thus far, the expression for the stretching of the radius, r, between the nuclei can be obtained by allowing the bond to stretch from r_e to r_c when acted upon by the centrifugal force [4]:

$$F_c = \frac{\mu v^2}{r} = \mu\omega r^2 = \frac{J^2}{\mu r^3}. \tag{1.34}$$

The centrifugal force is then counteracted by the Hooke's law restoring force:

$$F_k = k(r_e - r_c), \tag{1.35}$$

where k is the spring constant and is a measure of the bond strength. Centrifugal distortion is accounted for in the eigenvalue expression through the equation:

$$W(J) = B(J+1) - D(J(J+1))^2 = (B - DJ(J+1))J(J+1), \tag{1.36}$$

where D is the centrifugal distortion constant given by

$$D = \frac{4B^3_{equilibirum}}{\omega^2_{equilibrium}}. \tag{1.37}$$

Within the equation, $\omega_{equilibrium}$ is the equilibrium vibrational frequency.

It should be noted that while centrifugal distortion results in an increase in the internuclear distance or radius, r, it also results in a decrease in the rotational constant, B, compared to that of a true rigid rotor. The effective rotational constant thus becomes

$$B_{eff} = B - DJ(J+1). \tag{1.38}$$

This then changes the observed transition frequency to

$$\nu_{W_1 \leftarrow W_2} = 2(B - 2D(J+1)^2)(J+1). \tag{1.39}$$

1.4. MOLECULAR TOPS

Within rotational spectroscopy, there are two guiding rules that help dictate what a molecule's rotational spectrum will look like. The first is the fact that what is being measured by the spectrum is the distribution of mass with respect to a molecule's (or

system of molecules') center of mass. This distribution of mass will be reflected within the molecule's rotational constants of A, B, and C where $A \propto 1/I_a$, $B \propto 1/I_b$, and $C \propto 1/I_c$. These rotational constants will be defined further within the following sections.

The second guiding rule, similar to the first, is that the spectrum is measuring the distribution of mass through the rotations about the a-, b-, and c-axis. Two fundamental questions arise from this statement. The first is: what is providing this rotation? As briefly mentioned, the molecule's rotation is provided by the coupling between the molecule's dipole moment and the electric field, which, in the case of rotational spectroscopy, is generated by the use of microwave radiation. Since molecules can only rotate with respect to the a-, b-, and c-axis, this leads to three possible types of rotations: a-type, b-type, or c-type rotations in which the electric field is coupled to μ_a, μ_b, or μ_c, respectively. However, it should be clarified that a rotation about the a-axis is not necessarily an a-type transtion. Instead, it simply means that the a-axis is rotating. This will be explained further within this section.

The second fundament question is: what is governing the rotation of the molecule? The shape of the molecule governs its dipole moments and therefore governs how the molecule will rotate. As a result, it is important to have a firm grasp of molecular shapes, also referred to as molecular tops, in order to study rotational spectroscopy. In general, there are four different types of molecular tops that molecules possessing an electric dipole moment can belong to: linear, prolate symmetric, oblate symmetric, or asymmetric.

1.4.1. Linear. The simplest molecular top is a linear top. Typical molecules that fall into this category are diatomic molecules, such as hydrogen chloride (HCl), as well as linear polyatomic molecules, such as carbonyl sulfide (OCS). Linear tops are characterized by only possessing rotations about the b- or c-axis and having rotational constants with the following property: $A > B = C$. In this case, the dipole moment lies along the μ_a.

Since linear tops are the closest physical molecules to the rigid rotor, many of the parameters derived previously for the rigid rotor will apply to linear tops. Linear tops will obey the $\Delta J = +1$ selection rule and have a transition frequency of $\nu = 2B(J + 1)$, when not experiencing centrifugal distortion. As a result, within a linear top's spectrum, a set of R-branch ($\Delta J = +1$) transitions should occur at frequency spacings of 2B, 4B, 6B, . . . , etc. These frequencies will correspond to the transitions of $J = 1 \leftarrow 0$, $J = 2 \leftarrow 1$, $J = 3 \leftarrow 2$, . . . , etc., respectively [11].

Linear polyatomic molecules will experience deviations from the rigid rotor approximation more frequently than diatomic molecules. This is mostly due to the additional bonds allowing more vibrational modes of freedom. These additional vibrational modes of freedom can be considered by modifying the rotational constant to [7]

$$B = B_e - \sum_i a_i(v_i + \frac{1}{2}) - J(J + 1)D, \tag{1.40}$$

where a_i is the change in the equilibrium value B_e due to excitation of the i^{th} vibration, and v_i is the quantum number to the vibrational excitation. For most experiments, the molecules will be within the vibrational ground state, and, as a result, the summation will be simply $-\sum_i a_i/2$.

In addition, linear polyatomic molecules are more likely to experience Coriolis forces, represented in Hamiltonians by Coriolis constants which are vibrational-rotational interaction terms. When a non-rigid molecule rotates, the molecule will stretch causing its rotation to slow. As the molecule contracts back to its original dimensions, its rotation is sped up by Coriolis forces. The Coriolis forces can be represented by: [4]

$$F_{cor} = -2\mu\omega\nu', \tag{1.41}$$

where μ is the mass of the molecule, ω is the angular velocity, and v' is the velocity of the rotating frame. Its magnitude is thus given by:

$$| F_{cor} |= 2\mu\omega v_{radial}. \tag{1.42}$$

These changes in rotational velocity are usually attributed to the law of conservation of angular momentum – as the molecule expands its moment of inertia increases, thus it must slow down in order to conserve angular momentum [7].

1.4.2. Symmetric. The next type of molecular top—from which linear tops are sometimes considered a special case—is symmetric tops. As the name suggests, symmetric tops are defined by possessing a symmetry of C_3 or greater. An axis of symmetry is considered to be present if the distribution of atoms in space is unchanged when the molecule is rotated about some axis by an angle of $2\pi/n$. The molecule is said to have an n-fold symmetry axis.

For a linear top, no angular moment occurrs in the direction of the molecular axis due to the moment of inertia about the axis being so small. However, for more general types of molecules such as symmetric and later asymmetric tops, there is no axis about which the moment of inertia is extremely small. As a result, the normal rotational states for these molecules may involve rotations about any molecular axis [7]. However, it should be noted, that in a true symmetric top, any permanent dipole moment must necessarily lie along the symmetry axis, and as a result, all rotations observed in the spectrum will arise from the coupling of this dipole moment with the generated electric field [6].

In a symmetric top, one of the principal axes of inertia must lie along the molecular axis of symmetry. In addition, the other principal moments of inertia perpendicular to the axis of symmetry must be equal [6]. Depending on what axis possesses the axis of

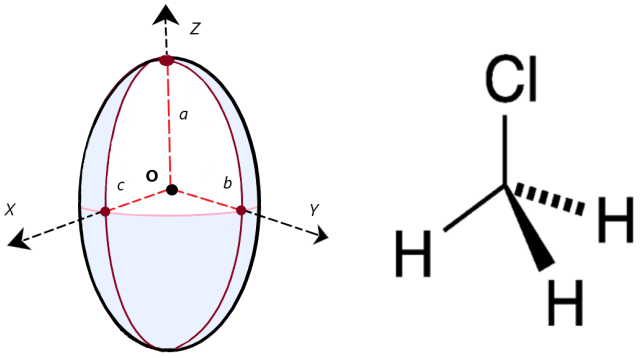


Figure 1.4. Prolate top example using chloromethane.

symmetry, a symmetric top can fall into two categories: prolate or oblate symmetric tops. Since most of the symmetric top molecules observed in the microwave region are prolate, this subcategory will be described first.

1.4.2.1. Prolate. A prolate symmetric top is a molecule, such as chloromethane shown in Figure 1.4, that possess a cigar or football like shape. It is characterized by having mass distributed about the a-axis–which is also the symmetry axis–and the moment of inertia about the symmetry axis being smaller than the moment of inertia about the other two axes ($I_a < I_b = I_c$). In other terms, the rotational constant A for a prolate top will be the greatest while B and C will be equal ($A > B = C$) [7].

The classical energy-level expression for a rigid prolate symmetric top is given by [4]

$$E = \frac{J_a^2}{2I_a} + \frac{1}{2I_b}(J_b^2 + J_c^2). \tag{1.43}$$

To simplify the equation, the following equalities will be used:

$$J_a^2 + J_b^2 + J_c^2 = J^2, \tag{1.44}$$

$$J_b^2 + J_c^2 = J^2 - J_a^2. \tag{1.45}$$

Thus,

$$E = \frac{1}{2I_b}J^2 + (\frac{1}{2I_a} - \frac{1}{2I_b})J_a^2. \tag{1.46}$$

As a result, the corresponding Hamiltonian operator is given by

$$\hat{H} = \frac{1}{2I_b}\hat{J}^2 + (\frac{1}{2I_a} - \frac{1}{2I_b})\hat{J}_a^2. \tag{1.47}$$

One can solve for the symmetric top rotational eigenvalues by inserting the above Hamiltonian into the Schrödinger equation along with the symmetric top wavefunction, which has the form of

$$|J, K, M\rangle = (\frac{2J+1}{8\pi^2})^{\frac{1}{2}} e^{iM\phi} d_{MK}^{(J)}(\theta) e^{ik\chi}. \tag{1.48}$$

Within this equation, K is the quantum number associated with the projection of angular moment on the symmetry axis ($K = J, J\text{-}1, \ldots, -J$), M is the magnetic quantum number, and $d_{MK}{}^{(J)}$ functions are hypergeometric functions of $\sin^2(\theta/2)$ that are related to the rotation matrices of angular moment theory.

Solving the Schrödinger Equation, one gets

$$\hat{H}\psi = (\frac{1}{2I_b}\hat{J}^2 + (\frac{1}{2I_a} - \frac{1}{2I_b})\hat{J}_a^2)|J, K, M\rangle \tag{1.49}$$

$$= (\frac{1}{2I_b}\hat{J}^2)|J, K, M\rangle + (\frac{1}{2I_a} - \frac{1}{2I_b})\hat{J}_a^2)|J, K, M\rangle \tag{1.50}$$

$$= (\frac{1}{2I_b}(J(J+1)\hbar^2)|J, K, M\rangle + (\frac{1}{2I_a} - \frac{1}{2I_b})K^2\hbar^2|J, K, M\rangle \tag{1.51}$$

$$= [\frac{1}{2I_b}(J(J+1)\hbar^2) + (\frac{1}{2I_a} - \frac{1}{2I_b})K^2\hbar^2]\psi \tag{1.52}$$

Thus, the rotational eigenvalues for a symmetric prolate top are given by

$$E_{JK_a} = BJ(J+1) + (A - B)K_a^2, \tag{1.53}$$

where

$$A = \frac{h^2}{8\pi^2 I_a}, \tag{1.54}$$

$$B = \frac{h^2}{8\pi^2 I_b}, \tag{1.55}$$

and

$$C = \frac{h^2}{8\pi^2 I_c}. \tag{1.56}$$

It is standard to classify the energy levels of symmetric tops by their K quantum number. It should be noted that all K levels, except $K = 0$, are doubly degenerate and this degeneracy cannot be removed by either external or internal fields. In addition, as the level of a given J value increases in energy, the value of K also increases for that of a prolate top.

Following the methods shown for those of a rigid rotor, one will find that the selection rules for prolate symmetric tops are $\Delta J = 0, \pm 1$ and $\Delta K = 0$. The selection rule of $\Delta K = 0$ arises from the fact that due to the symmetry within the molecule, there can be no dipole moment perpendicular to the axis of symmetry, and hence no torque along the axis due to coupling with the generated electric field. As a result, angular momentum along the molecular axis cannot change [7]. Based on these selection rules, the frequency of the rotational transition is given by

$$\nu_{W_1 \leftarrow W_2} = 2B(J + 1). \tag{1.57}$$

Therefore, as long as the centrifugal distortion or other effects are neglected, the frequencies observed do not depend on K.

If centrifugal distortion is considered, which for a symmetric top is given by [4]

$$F(J, K) = BJ(J + 1) - D_J(J(J + 1))^2 + (A - B)K^2 - D_K K^4 - D_{JK} J(J + 1)K^2, \tag{1.58}$$

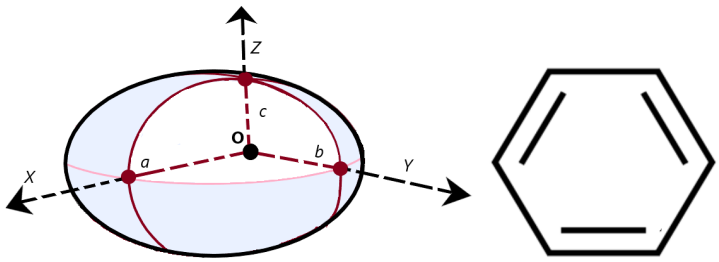


Figure 1.5. Oblate top example using benzene.

the frequency of the rotational transitions becomes

$$\nu_{W_1 \leftarrow W_2} = 2B(J+1) - 4D_J(J+1)^3 - 2D_{JK}(J+1)K^3. \tag{1.59}$$

Note that unlike that of a linear molecule, the centrifugal force now contains three separate centrifugal distortion constants: D_J, D_K, and D_{JK}.

1.4.2.2. Oblate. The second type of symmetric top is an oblate top, such a benzene shown in Figure 1.5, which possess a disk or pancake like shape. It is characterized by having mass distributed around the c-axis–which is also the symmetry axis–and the moment of inertia about the symmetry axis being greater than the moment of inertia about the other two axes ($I_a = I_b < I_c$). In other terms, the rotational constant C for an oblate top will be the smallest while B and A will be equal ($A = B > C$) [7].

The classical energy-level expression for a rigid oblate symmetric top is given by [4]

$$E = \frac{1}{2I_b}(J_a^2 + J_b^2) + \frac{J_c^2}{2I_c}, \tag{1.60}$$

which, using the same method as that for the prolate top, can be simplified to

$$E = \frac{1}{2I_b}J^2 + (\frac{1}{2I_c} - \frac{1}{2I_b})J_c^2. \tag{1.61}$$

As a result, the Hamiltonian operator is given by

$$\hat{H} = \frac{1}{2I_b}\hat{J}^2 + (\frac{1}{2I_c} - \frac{1}{2I_b})\hat{J}_c^2. \tag{1.62}$$

Following the same procedure shown for the prolate top, one discovers that the rotational eigenvalues for the oblate top are given by

$$E_{JK_c} = BJ(J+1) + (C-B)K_c^2. \tag{1.63}$$

Note that unlike the prolate top, as the level of a given J value increases in energy, the value of K decreases for an oblate top. All other characteristics, such as the selection rules, observed frequency, and centrifugal force are the same for the oblate top as they were for the prolate top.

1.4.3. Asymmetric. The last type of top—and the most important type for the research presented within this work—is an asymmetric top. As the name suggests, an asymmetric top is a molecule that has less than a three-fold axis of symmetry or processes no symmetry at all. Due to this, no two principal moments of inertia will be equal ($I_a \neq I_b \neq I_c$). Instead, due to the fall outs of the principal axis system, the principal moments of inertia and rotational constants will follow the trends of $I_a < I_b < I_c$ and $A > B > C$, respectively.

For an asymmetric top, the classical energy for a rigid rotor is given by [4]

$$E = \frac{J_a^2}{2I_a} + \frac{J_b^2}{2I_b} + \frac{J_c^2}{2I_c}, \tag{1.64}$$

and as a result, the Hamiltonian operator is

$$\hat{H} = \frac{\hat{J}_a^2}{2I_a} + \frac{\hat{J}_b^2}{2I_b} + \frac{\hat{J}_c^2}{2I_c}. \tag{1.65}$$

It should be noted that the Schrödinger equation for the asymmetric top has no general analytical solution and therefore must be solved numerically. Due to this, rotational eigenvalues and frequencies cannot be expressed in convenient equations that represent asymmetric top molecules as a whole, such as what has been done for linear or symmetric tops. However, depending on how asymmetric a molecule is, it may follow closely with the parameters outlined for the prolate or oblate top.

The degree of asymmetry within a molecule can be quantified using Ray's asymmetry parameter, κ, given by [4]

$$\kappa = \frac{2B - A - C}{A - C}. \tag{1.66}$$

The value of κ runs from -1 (prolate top) to +1 (oblate top). The closer κ is to -1 or +1, the closer the molecule behaves like a prolate or oblate top, respectively. Though it should be noted that even a slight asymmetry will split the levels $\pm K$, which are degenerated for a symmetric top. The closer to 0 the value of κ lies, the greater asymmetry the molecule will process and the further it will differ from the parameters derived thus far.

An asymmetric top molecule may have up to three non-vanishing dipole moment components–μ_a, μ_b, and μ_c–along the principal axes. Each non-vanishing dipole moment component makes a certain set of transitions possible and thus there will be a certain set of selection rules for each transition type. These types of transitions include a-type, b-type, and c-type transitions. All transitions will follow the selection rules of $\Delta J = 0, \pm 1$, as was the case with linear and symmetric top molecules. The individual selection rules for a-type, b-type, and c-type transitions are presented in Table 1.1. See the *Asymmetric Ladder* discussion below for a definition of K_a and K_c. It should be noted, however, that for a molecule with high asymmetry, all three types of transitions can occur together. As a result, the energy levels may not form any obvious patterns and the resulting spectrum can become quite complex.

Table 1.1. Selection rules for asymmetric tops.

Transition Type	**Dipole Moment Component**	**Allowed Transitions ($\mathbf{K}_a\ \mathbf{K}_c \rightarrow \mathbf{K}_a\ \mathbf{K}_c$)**	**$\Delta\mathbf{K}_a$ Selection Rules**	**$\Delta\mathbf{K}_c$ Selection Rules**
a- type	μ_a	Even Even → Even Odd, Odd Odd → Odd Even	0, ±2, etc.	±1, ±3,etc.
b- type	μ_b	Even Even → Odd Odd, Odd Odd → Even Even	±1, ±3, etc.	±1, ±3, etc.
c- type	μ_c	Even Even → Odd Even, Odd Odd → Even Odd	±1, ±3, etc.	0, ±2, etc.

Furthermore, centrifugal distortion is greatly more important for an asymmetric top spectrum than in the spectra of symmetric tops. This is because within asymmetric tops, centrifugal distortion may change the rotational frequencies by hundreds of megahertz comparably to one megahertz or less for symmetric tops [7]. This is due to the fact that microwave transitions within an asymmetric top may occur between states of rather large angular moment and of very large rotational energies. Similar to the rotational frequencies, there is not a singular equation that can represent the centrifugal distortion observed in each asymmetric top.

When fitting centrifugal distortion in asymmetric tops, Watson *A*- or *S*-reduced Hamiltonians are used. Originally, Watson *A* or *S* were named for their ease of mathematics in fitting asymmetric tops based on a molecule being closer to a symmetric top (Watson *S*) or being more asymmetric (Watson *A*). However, with the emergence of fitting programs easing the programing and mathematical burden, it is widely acceptable and generally practiced to use either a Watson *A*- or Watson *S*-reduced Hamiltonian for fitting of either case. Depending on the degree of accuracy needed in the centrifugal distortion analysis, Watson's two sets of reduced Hamiltons can possess quartic, sextic, or octic centrifugal distortion terms [12]. For the work presented within this study, only the quartic terms are reported. Thus, the Watson *A*-reduced Hamiltonian with quartic centrifugal distortion

terms is given, in the laboratory frame, by [12]:

$$\hat{H} = \frac{\hat{J}_x^2}{2I_x} + \frac{\hat{J}_y^2}{2I_y} + \frac{\hat{J}_z^2}{2I_z} - D_J\hat{J}^4 - D_{JK}\hat{J}^2\hat{J}_z^2 - D_K\hat{J}_z^4 - \frac{1}{2}[\delta_J\hat{J}^2 + \delta_K\hat{J}_z^2, \hat{J}_+^2 + \hat{J}_-^2]_+, \quad (1.67)$$

where D_J, D_{JK}, D_K, d_J, and d_K are the quartic centrifugal distrotion terms, δ_J and δ_K are higher order centrifugal distortion terms, and J_+ and J_- are operators defined as:

$$J_+ = J_x + iJ_y, \quad (1.68)$$

and

$$J_- = J_x - iJ_y, \quad (1.69)$$

respectively. In a similar fashion, the Waston *S*-reduced Hamiltonian with quartic centrifugal distortion terms is given by:

$$\hat{H} = \frac{\hat{J}_x^2}{2I_x} + \frac{\hat{J}_y^2}{2I_y} + \frac{\hat{J}_z^2}{2I_z} - D_J\hat{J}^4 - D_{JK}\hat{J}^2\hat{J}_z^2 - D_K\hat{J}_z^4 + d_J\hat{J}^2(\hat{J}_+^2 + \hat{J}_-^2) + d_K\hat{J}^2(\hat{J}_+^4 + \hat{J}_-^4). \quad (1.70)$$

1.4.4. Asymmetric Ladder. As mentioned above, the degree to which a molecule is asymmetric influences its principal moments of inertia, rotational energy levels, and observed frequencies. Since there are two limiting cases, prolate symmetric and oblate symmetric, these two limits must be linked through asymmetry in some way. The asymmetric ladder provides this link by connecting oblate symmetric, prolate symmetric, and asymmetric top energy levels. It also dictates the types of transitions allowed for each molecular top and provides a useful labeling technique for asymmetric top levels.

Shown in Figure 1.6, the asymmetric ladder contains three main components. The first component is the prolate symmetric energy levels presented on the left side of the ladder. For every J value in a prolate symmetric top, there are J+1 K levels. These K levels increase in value as one moves up the ladder. The second component is the oblate

symmetric energy levels, presented on the right side of the ladder. In similar fashion, for every value of J in an oblate symmetric top, there are J+1 K levels. However, the K levels decrease in value as one moves up the ladder.

These two limiting cases are then connected through the asymmetric energy levels presented in the middle of the ladder. The connections are built in such a way that K = 0 levels only connect to one other level. The K = 1, 2, 3, . . . , etc., levels, however, connect to two other levels due to their degeneracy. This results in $2J$+1 K_aK_c levels per J level. In general, the effects of asymmetry are strongest at low K_a or K_c values [11]. The asymmetric top energy levels are labeled as J_{KaKc}, where J is the total angular moment quantum number, K_a (or K_p) is the projection quantum number for the associated prolate top, and K_c (or K_o) is the projection quantum number for the associated oblate top. Note, that the sum of K_a and K_c is either J or J+1.

For an asymmetric top, J is the only good quantum number and as a result, K_a and K_c are simply labels. This is due to the fact that in both the classical motion and quantum mechanical solution for a rotating asymmetric molecule, the components to the angular momentum along any direction are not constant. As a result, there is no projection of J on the symmetry axis and K can not be used to specify the rotational state. Therefore, K_a and K_c are only good quantum numbers in the prolate or oblate symmetric top limit, respectively [7].

1.5. LARGE AMPLITUDE MOTION

Like centrifugal distortion and Coriolis coupling, another phenomenon that complicates the rotational spectrum of a molecule is large amplitude motion. The first case of large amplitude motion reported in rotational spectroscopy was in 1934 with the observation of inversion tunneling within ammonia [1]. While often leading to an involved analysis process, a great variety of molecular systems of interest for astrophysics, atmospheric studies, and molecular biology contain large amplitude motion. As a result, it is becoming increas-

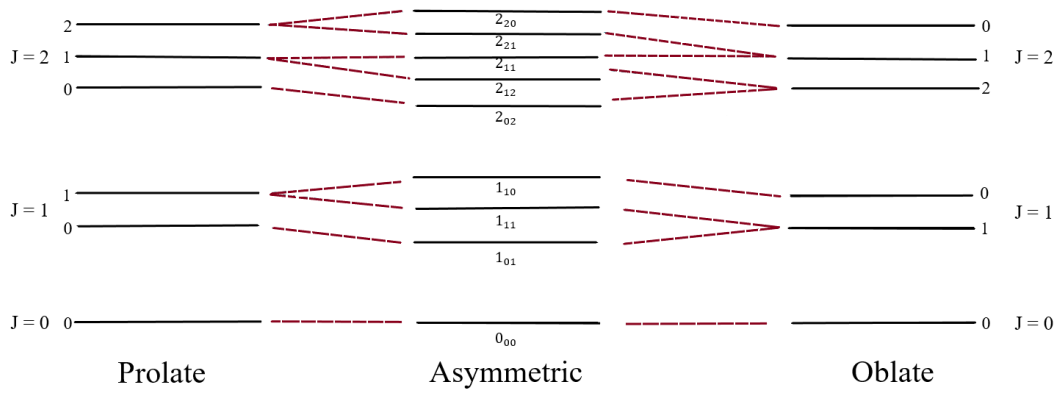


Figure 1.6. Representation of the asymmetric ladder.

ingly more important to be able to study these complex species thoroughly. However, it has only been within the last few decades that program analysis has improved to allow for the study of large amplitude motion to become more routine.

The two most common types of large amplitude motion (LAM) are internal rotation and inversion tunnelling, both of which result in tunneling splitting within the rotational spectrums where they are present. This is due to the effect of intramolecular dynamics which causes all rotational energy levels to split into several levels on account of tunneling effects [13]. Other types of LAMs include ring puckering, pseudorotation, and interactions between weakly bounded complexes. The two types of large amplitude motion observed within this work are ring-puckering and internal rotation. As a result, both types will be described below. However, since internal rotation is more central to this work, it will receive a deeper analysis than ring-puckering.

1.5.1. Ring-Puckering. In small ring molecules, a ring-puckering motion (which ring-twisting is a specific case of) can occur if the rings are flexible enough to adopt different conformations due to out-of-plain bending motions. These conformations are caused by changes in the rotatable ring bonds and usually involve an inversion though a plane. Typically, the ring puckers can be classified into different canonical forms (such as chair or boat) and are usually low-energy conformations [14]. The large amplitude motion

that connects the two conformers leads to vibrational-rotational coupling of energy levels. For four-membered rings and five-membered rings with a double bond, this results in two equivalent vibrational energy minima separated by low-lying barriers. Six-membered rings, on the other hand, tend not to show ring-puckering due to a higher energy barrier between conformers [11].

The potential energy for this type of motion can be described with good accuracy by:

$$V = ax^4 + bx^2. \tag{1.71}$$

Depending on the molecule, b may vary in relative magnitude and sign to a. Within the rotational spectra, such potential functions give rise to inversion splitting often less than 1 cm^{-1} [15]. In general, one observes a rotational spectrum where each line is accompanied by several vibrational satellites [11].

1.5.2. Internal Rotation. Internal rotation is a phenomenon in which an internal rotor rotates with respect to the rest of the molecule, referred to as the molecular frame. The internal rotor can be symmetric – as in a methyl group – or asymmetric – such as -OH, -SH, and -NH_2 groups. One of the earliest molecules observed that contained internal rotation was methanol, which was first observed by Koehler and Dennison in 1940 [16].

To determine if a given rotor will produce internal rotation, its energy potential must first be calculated. For an internal rotor with C_3 symmetry (such as a methyl rotor) attached to an asymmetric frame, a threefold energy potential (seen in Figure 1.7) is present, which can be described by [13]

$$V(\alpha) = \frac{1}{2}V_3(1 - \cos(3\alpha)) + \frac{1}{2}V_6(1 - \cos(6\alpha)) + \frac{1}{2}V_9(1 - \cos(9\alpha)), \tag{1.72}$$

where V_3, V_6, and V_9 are the potential barrier heights and α is the torsional angle. It should be noted that due to the very low rotational temperatures of supersonic jets now present in most microwave spectrometers, it is often not possible to determine contributions to higher

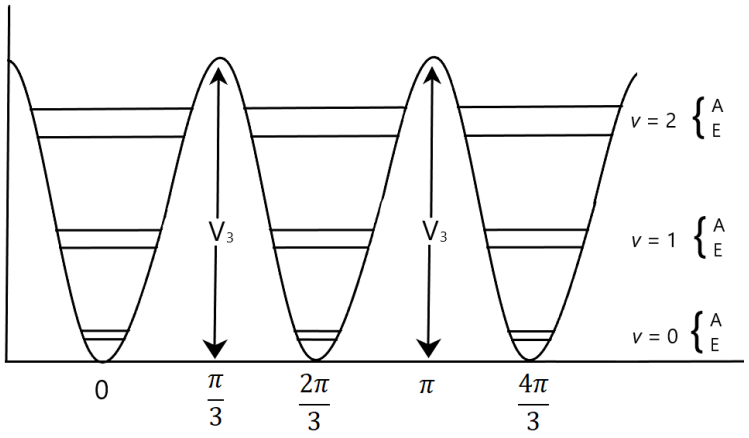


Figure 1.7. Schematic representation of the potential function and torsional energy levels. The torsional sublevels are denoted by their symmetry A or E under the C_3 group.

order terms such as V_6 and V_9. The height of the potential in Equation 1.72, specially V_3, can vary drastically between molecular species. This value is influenced by the symmetry of the rotor and any steric hinderance produced by the frame. In the case of very high barriers ($V_3 \rightarrow \infty$), the internal motion will be restricted to small oscillations – specifically torsional oscillations – about the minimum of the barrier [6]. If the barrier was very low ($V_3 \rightarrow 0$), on the other hand, the internal motion would be essentially free rotation about the C-C bond. For reference, methanol possesses a barrier heigh of about 380 cm^{-1} [16].

For barrier heights between these two extremes, the quantum mechanical tunneling effect leads to a splitting of the three-fold degeneracy because the probability of tunneling through the barrier is finite since V_3 is finite. The effect of tunneling through the potential barrier is to split the triply degenerate torsional level into two levels, a non-degenerate level referred to as an A level and a doubly degenerate level referred to as an E level. This will lead to characteristic spectral splittings within the molecule's rotational spectrum that can be analyzed to yield information about V_3. The smaller the barrier to internal rotation is, the larger the splitting in the spectrum will be and the more complicated the spectrum analysis will become. To aid in the analysis, potential energy barriers are often calculated from potential energy scans where the LAM coordinates are varied systematically while all other

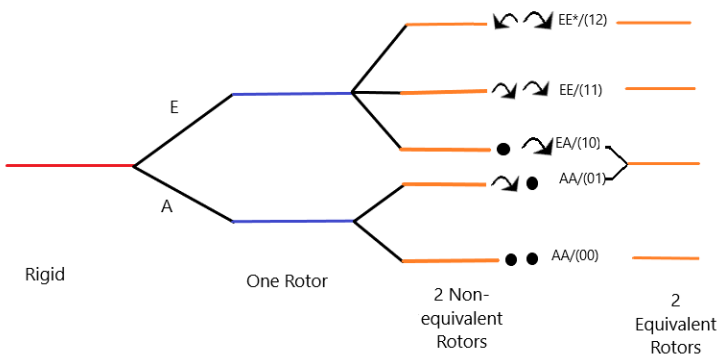


Figure 1.8. Schematic splittings due to internal rotation. In the figure, the dots represent the non-rotating states of the rotors, while the rounded arrows symbolize the two rotating states.

geometry parameters are relaxed [13]. Though, it should be noted that calculating highly accurate energy barriers still remains a great challenge for internal rotation analysis. Based on the resolution of the microwave spectrometer utilized, splittings will traditionally only be observed for barrier heights less than 1,000 cm^{-1}.

Table 1.2. The character table for a C_{3V} group.

C_{3V}	E	$2C_3$	$3\sigma_v$
A_1	1	1	1
A_2	1	1	-1
E	2	-1	0

The type of splitting and its frequency location are determined by the type of internal rotor present and the barrier height. If only one internal rotor is present, all rotational transition lines will split into an A and an E component. These splittings result from invoking the A_1 and E irreducible representations in the C_{3V} character table, which is depicted in Table1.2. If two rotors are present, the rotational lines will split into either quartets or quintets depending on if the rotors are equivalent or non-equivalent. In the case of two non-equivalent internal rotors, all A components split into AA-AE doublets, and all E components split into the EA-EE-EE$*$ triplets. This particular notation is based on

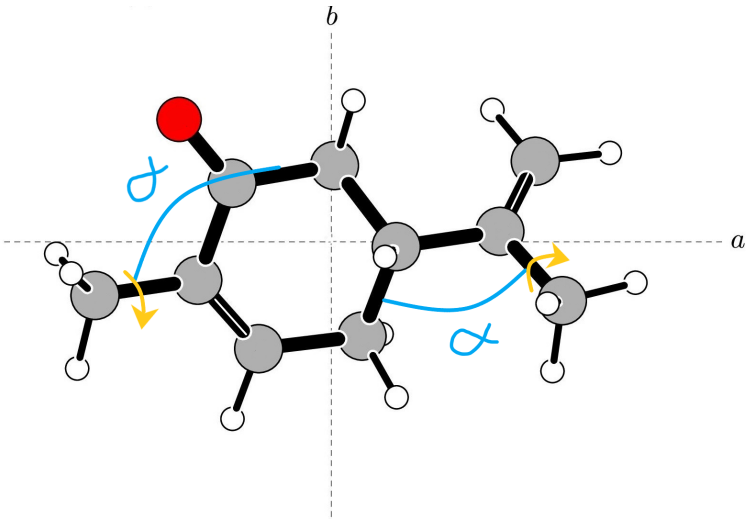


Figure 1.9. Torsisonal angle α for the two methyl rotors of carvone. Torsisonal angle α is shown in blue while the internal rotation of the bond is shown in yellow.

the worked by Driezler in accordance with the direct product ${C_{3v}}^{(1)} \otimes {C_{3v}}^{(2)}$ [17]. The E components split into a triplet due to degeneracies within the E state. However, if the two rotors were instead equivalent, AA-AE-EE-EE$*$ quartets would arise due to the degeneracy of the AE and EA torsional components collapsing in on themselves [13]. All energy level splitting's mentioned above are depicted within Figure 1.8. In the figure, the dots represent the non-rotating states of the rotors (*i.e.* rigid rotors), while the rounded arrows symbolize the two rotating states. It should also be noted that recently a new labeling scheme that uses semi-direct products has been created for molecules with frames that have C_s symmetry. Within this labeling scheme, species are denoted as (00), (01), (10), (11), and (12) instead of AA, AE, EA, EE, and EE$*$, respectively [18].

For the molecular tops mentioned previously, it was sufficient to analyze the rotational spectrum classically using the rigid rotor Hamiltonian, H_r, and supplementing it with centrifugal distortion terms, H_{cd}. However, since the rotational spectrum of a molecule processing methyl internal rotation features splittings in each rotational transition, the rigid rotor model can no longer be used to analyze the spectrum and as a result, the classical Hamiltonian cannot be used. Instead, if one wants to solve the system classically, a rigid

frame–rigid top Hamiltonian must be used. There exist two methods to solve this type of Hamiltonian, and each has its own advantages and disadvantages. The optimal method of choice is dependent on the barrier height, the geometry of the system, and the mass distribution. One method, developed by Nielsen [19], is known as the Internal Axis Method (IAM). This method is preferred for slightly asymmetric molecules with light frames. IAM uses a coordinate system in which the symmetry axis of the rotor is chosen as one of the coordinate axes. The other two axes are then fixed with respect to the molecular framework [11]. One or more coordinate transformations may be employed to eliminate or minimize the rotational-torsion coupling. This is the method utilized by the XIAM fitting program [20]. An issue that is encountered while working with IAM is that the axes do not coincide with the principle axes, which introduces terms involving the products of inertia that do not vanish [6].

The second method – which was developed by Kilb, Lin, and Wilson [21] – is known as the Principle Axis Method (PAM). This method is more widely applicable if a fitting program is not utilized. Within PAM, the reference axes are the principal axes of the whole molecule, which helps simplify the calculations. For the sake of simplicity, PAM will be utilized within the following derivation. For an asymmetric molecule with a methyl top in the principle axis system, the rigid frame–rigid top Hamiltonian takes the form of [13]

$$\hat{H} = A\hat{J}_a^2 + B\hat{J}_b^2 + C\hat{J}_c^2 + F(p_\alpha - \rho_a\hat{J}_a - \rho_b\hat{J}_b - \rho_c\hat{J}_c)^{\frac{1}{2}} + \hat{H}(\alpha), \tag{1.73}$$

where p_α is the internal rotation angular momentum associated with the torsional angle α (shown in Figure 1.9), F is the rotational constant for the internal rotor,

$$F = \frac{\hbar^2}{2rI_a}, \tag{1.74}$$

and ρ_i are the components of the $\vec{\boldsymbol{\rho}}$ vector given by

$$\vec{\boldsymbol{\rho}} = \frac{\lambda_i I_\alpha}{I_i}. \tag{1.75}$$

Within Equation 1.75, λ_i are the direction cosines of the internal rotation axis of the top. By adding the above effective terms into the Hamiltonian and considering all A and E species, a standard fit close to the measurement accuracy can be achieved for molecules exhibiting internal rotation.

2. INSTRUMENTS AND TECHNIQUES

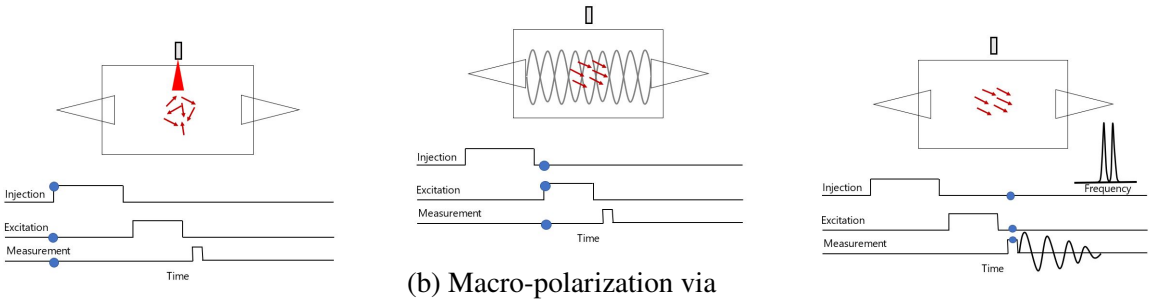
Through continuous advancements in microwave technology and computer processing, microwave spectrometers have become more refined since their initial introduction, allowing for more complex systems and intricate projects to be studied. Post WWII, the most common instruments used by rotational spectroscopists were waveguides, or microwave Stark spectrometers, developed by McAfee et al. [22] as well as Hughes and Wilson [23]. However, these instruments were limited not only by their low sensitivity and substantial background noise, but also by their need for substantial vapor pressure in the sample cell, which restricted the range of molecules that could be studied [3]. By 1980, many of these initial challenges were able to be overcome with the introduction of Fabry-Péroit cavity, pulsed Fourier transform microwave (FTMW) spectrometer by Balle and Flygare [2]. This new design allowed for high frequency resolution spectroscopy to be performed without the power broadening seen in waveguides and also introduced the use of pulsed molecular beam sources. However, though the FTMW provided the higher resolution needed to advance the field, it lacked the ability to take broadband measurements quickly. This would not come until the introduction of the chirped pulse Fourier transform microwave (CP-FTMW) spectrometer by Pate et al. in 2006 [3]. Today, most microwave studies are performed on either a cavity FTMW or CP-FTMW, with the cavity FTMW still being considered as having the higher sensitivity and resolution of the two. Though these two instruments may dominate the field, this has not stopped research and development in instrumentation as shown by the introduction of microwave three-wave mixing spectrometers [24] and multiple antenna detection [25] over the last ten years. As microwave components continue to become more accessible and refined, advancements will continue within the instrumentation.

2.1. EXPERIMENTAL PROCESS AND INSTRUMENTATION THEORY

A thorough rotational spectroscopy investigation is a union between quantum chemical calculations, experimentally collected spectra, and analysis. As a result, the experimental processes and instrumentation theory needed to complete these three objectives will be briefly presented.

2.1.1. Calculations. Most rotational spectroscopy investigations start with quantum chemical calculations in order to obtain theoretical transition frequencies to investigate. While many types of quantum chemical calculations can be performed, the typical starting point for rotational spectroscopy is the geometric optimization of the molecule in question. This type of calculation determines the equilibrium structure for the molecule, from which its theoretical rotational constants can be determined. By altering the starting structure incrementally between calculations, structural conformers can be determined. Computer programs, such as Gaussian [26], are often utilized for these types of calculations and work by minimalizing the molecule's total energy through varying the atoms' positions in small steps until convergence on an optimal molecular structure is obtained [13].

These calculations can be performed utilizing different method and basis sets depending on the level of accuracy needed and the computation time one is willing to spend. The method set defines the way in which the electronic Schrödinger equation will be solved. The two most common method sets used by rotational spectroscopists are the density functional theory (DFT) method in conjunction with the B3LYP (Becke, 3-parameter, Lee-Yang-Parr) functional and the Møller-Plesset perturbation theory (MP2) method. The two methods mainly differ by what is optimized, which is the electron density for DFT and the wavefunction in *ab initio* MP2. The basis set, on the other hand, determines–by a series of linear combination functions–the space in which the Schrödinger equation is numerically solved. In essence, the basis set is a recipe to construct the one-electron orbitals. Typically, in combination with either of these methods, the Pople valence double-zeta (6-31++G(d,p)) or tiple-zeta (6-311++G(d,p)) basis set is utilized due to its description of the valence shell



(a) Introduction of Sample

(b) Macro-polarization via Microwave Radiation

(c) Detection of FID

Figure 2.1. Experimental process for a rotational spectroscopy experiment using a CP-FTMW.

electrons [13]. Though, the Grimme dispersion basis set can also be used. These calculations are then commonly run on computer clusters, such as the Foundry at Missouri S&T.

A second type of calculation performed throughout this work is a barrier height to internal rotation calculation. These are performed by scanning the dihedral angle made between the internal rotor and the molecular frame of a geometrically optimized molecule. Typically, all 360° of rotation are scanned in several increments. The most common incrementation utilized is 72 steps with 5° of rotation between steps. The output of the scan is the three-fold energy potential from which the barrier height, or V_3, can be determined.

2.1.2. Instrumentation Theory. Though both cavity FTMWs and CP-FTMWs are utilized commonly in microwave spectroscopy laboratories, the following discussion will focus solely on the CP-FTMW, as it is more pertinent to this work. A depiction of a standard rotational spectroscopy experiment process in terms of a CP-FTMW can be seen in Figure 2.1. The experiment first begins when the sample molecule in the gas phase is pulsed into the vacuum chamber, resulting in a supersonic expansion. In order for the equilibrium expansion properties to be achieved quickly, the gas nozzle is kept open for only a very short period of time (on the order of μs). As the gas plume expands, the random translational

kinetic energy and internally stored rotational and vibrational energy are converted to mass flow through collisions [2]. This results in effective rotational and vibrational temperature drops to roughly 3 Kelvin as well as a narrowing of the distribution of molecular velocities.

When the molecules first enter the chamber, their dipoles are oriented randomly. However, in order to induce a rotational transition, a macroscopic polarization of the molecules in a given direction must take place. This process is made possible due to the fast-passage technique developed by J. C. McGurk and Flygare [27] and is governed by the Bloch Equations (described in Section 3). Physically, microwave radiation within the 2-20 GHz range is first introduced into the chamber via one of the horn antennas (or dipole antennas in a cavity FTMW). The electric field component of this pulse can be described as [3]

$$E(t) = E_{max} e^{i(\omega t + \frac{1}{2}\alpha t^2)}, \tag{2.1}$$

where E_{max} is the peak electric field of the pulse, α is the linear sweep rate, and the instantaneous frequency is given by

$$\omega_{int} = \frac{\delta}{\delta t}(\omega_o t + \frac{1}{2}\alpha t^2) = \omega_o + \alpha t. \tag{2.2}$$

As this electric field passes through the gas plume, it interacts with the molecule's permanent electric dipole moment via the fast passage process and the two become aligned. The fast passage process arises when a frequency is swept through a two level resonance in a time short relative to the relaxation process [27]. As the frequency of the microwave pulse approaches that of an allowed rotational transition, the molecules begin to rotate uniformly, resulting in the desired macroscopic polarization.

Once the microwave pulse decays or sufficiently passes the desired frequency, the molecules fall out of their alignment and begin to rotate randomly again. As they do this, they will relax from the excited rotational state through a free induction decay (FID), an example of which can be seen in Figure 2.2. Physically, the FID is produced by the

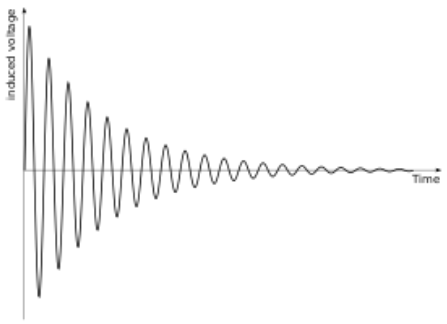


Figure 2.2. Example of a free induction decay.

oscillation of electric field lines within the molecule as it rotates, which can be recorded by the detection antenna as a voltage. The strength of the FID is dependent on three things: the strength of the coupled dipole moment, the polarization power of the microwave pulse (which can be increased by shortening sweep durations), and the population of molecules present. The signal strength has the form of [3]

$$S \propto \omega \cdot \mu^2 \cdot E_{pulse} \cdot \Delta N_o (\frac{\pi}{\alpha})^{\frac{1}{2}}, \tag{2.3}$$

where ω is the frequency, μ is the transition dipole moment, E_{pulse} is the electric field strength, and ΔN_o is the population difference at equilibrium, which is assumed to be unchanged by the pulse.

For spectral analysis, the FID, which is recorded in the time-domain, must be Fourier transformed into the frequency domain. A standard Fourier transform is represented by the equation

$$F(\omega) = \int_{-\infty}^{\infty} f(t) e^{-i\omega t} dt. \tag{2.4}$$

Oftentimes, however, the Fourier transform must be solved numerically and Equation 2.4 cannot be used. In these cases, a Fast Fourier Transform (FFT) through the Cooley-Tuckey algorithm must instead be used [28]. Regardless of how the Fourier transform is achieved, it

produces a spectrum comprised of different frequencies and intensities. Typical resolutions for these spectrums are on the order of kHz with line widths falling between 80 to 100 kHz at full width half max (FWHM).

2.1.3. Analysis. Once the rotational spectrum has been collected, it must be analyzed through a process referred to by rotational spectroscopists as "fitting". In this process, experimentally observed rotational frequencies are assigned to quantum numbers related to predicted transitions between specific rotational energy levels. This information is then used to build and diagonalize the rotational Hamiltonian, from which the experimental rotational constants can be obtained. To facilitate this process, many spectroscopist utilize computational tools such as Pickett's SPFIT/SPCAT [29], XIAM [20], PGOPHER [30], or any number of programs found on the PROSPE website [31]. It is also not uncommon for research groups to design their own computational packages to facilitate the fitting process.

2.1.4. Structure Determination. One of the strengths of microwave spectroscopy is its ability to determine molecular structures accurately and precisely. This is only possible though if a suitable number of isotopologues of the molecule are first experimentally detected. This can be facilitated either through their detection in natural abundance within the spectrum or by using an enriched sample designed at targeting a specific isotope at a specific location in the molecule. This analysis of the isotopologues' rotational spectrum can be accomplished by obtaining the ratio of the theoretical rotational constants for the parent species (molecule consisting of the most abundant isotope of each atom) to the experimentally determined one. This ratio is then used to adjust the theoretical isotopologue rotational constants–which are acquired by simply changing the atomic mass of the specific nuclei in question. This yields isotopic rotational constant predictions with great accuracy and ease, making traditional assignments for these species much simpler.

Once experimental rotational constants for the isotopologues have been obtained, then the experimental molecular structures can be determined through Kraitchman substation [32]. This method works by measuring the changes in mass due to isotopic substitution

to determine the position coordinates for each substituted atom. Through rotational spectroscopy analysis, the rotational constants for a molecule can be determined. As described in Section 1, these rotational constants are inversely proportional to the moments of inertia, which are proportional to the mass distribution along a given axis. The moment of inertia tensor, given in Section 1, is defined by the coordinates of an atom as well as the mass of the atom. As a result, the tensor is directly affected by the changes in mass from isotopic substitution.

By comparing the changes in these moments of inertia with the location of the substitution in the molecule, an exact coordinate system–within experimental uncertainties–can be derived. This derived structure is referred to as an r_s structure, where the s stands for substitution. From this, the desired bond lengths between atoms can be determined by using the three-dimensional Pythagorean Theorem. Once the bond lengths are known, the desired angles and dihedrals can be calculated using basic trigonometry.

2.2. MICROWAVE SPECTROSCOPY AT MISSOURI S&T

2.2.1. Multi-Antenna Detection Chirped Pulse Fourier Transform Microwave Spectrometer. The multi-antenna detection, chirped pulse Fourier transform microwave (MAD-Chirp) spectrometer at Missouri S&T was designed to be a low noise, high precision instrument. It's design is based off of a traditional CP-FTMW [3] and the microwave three-wave mixing spectrometer presented by Pate et al. [33]. A schematic of the instrument is presented in Figure 2.3 along with operational pictures shown in Figure 2.4. The sampling source (component 3) will be described within the *Sourcing Techniques* subsection. All other components will be described below. The three basic sections of this instrument – like those of any CP-FTMW – are 1.) the chirped microwave pulse generator, 2.) the vacuum chamber, and 3.) the FID detection.

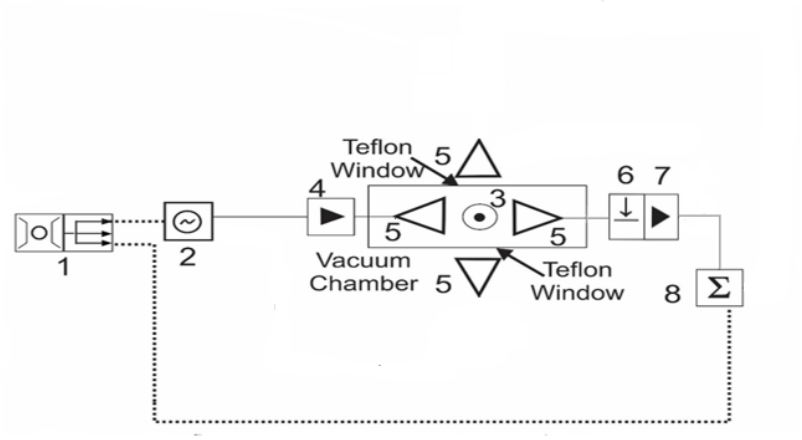


Figure 2.3. Schematic of the multi-antenna detection, chirped pulse Fourier transform microwave spectrometer at Missouri S&T in traditional CP-FTMW configuration. See text for details.

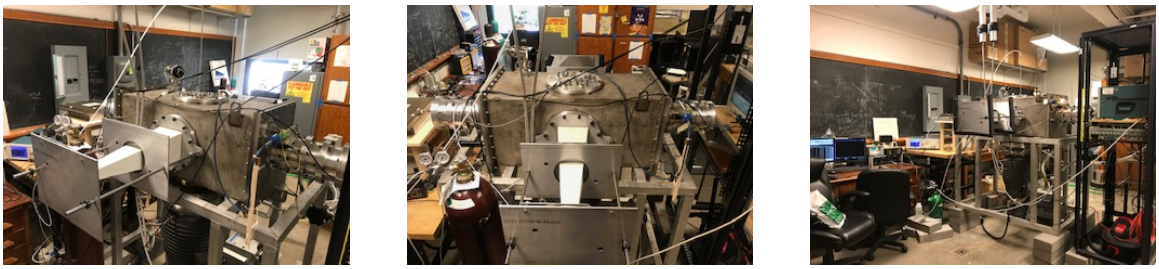


Figure 2.4. Photos of the fully operational MAD-Chirp spectrometer at Missouri S&T.

All components are kept in synchronization through the use of components 1 in Figure 2.3, which are a 5 and 10 MHz frequency Rubidium standard clock with an amplifier, produced by Stanford Research Systems (model F2725). Component 2 is a Tektronix® Arbitrary Waveform Generator, model AWG70001A, which has a 50 GS/s digitization rate and is capable of producing waveforms up to 20 GHz. The linear frequency sweeps, or chirps, used to define the experimental microwave pulses are generated by MATLAB scripts and are imported into the Arbitrary Waveform Generator utilizing the program TekVISA®. Typical chirps utilized are 4 μs in length and 4.75 GHz in bandwidth. Three overlapping frequency ranges of 5.5-10.25 GHz, 9.75-14.5 GHz, and 14-18.75 GHz are typically used to obtain spectra in the 6-18 GHz region of the electromagnetic spectrum. These chirps are fed into component 4 which is a 40 W TTL controlled Microsemi® (model L0618-46-T680) solid state amplifier for the 6-18 GHz range.

The signal is then broadcasted into the vacuum chamber and detected via components 5, which are Qpar 2-18 GHz high gain ridged horn antennae (Steatite® QWH-SL-2-18-S-HG-R). The four-antennae orthogonal design was inspired by the CP-FTMW/microwave three-wave mixing (M3WM) instrument of Pate et al. to allow for the performance of chirality experiments [33]. One difference from Pate's design, however, is that for the Missouri S&T spectrometer, two antennae reside outside the chamber and are set up on a bracketing system which allow for the antennae to rotate clockwise up to 270° with hard stops at 90°. This idea was inspired by the M3WM experiment of Schnell et al. where one antenna is rotated approximately 45° in comparison to the other and was enough to produce the chiral signal effect [24]. The antennae outside the vacuum chamber detect signals through a 0.32 cm thick Teflon – which is invisible to microwaves – window that resides in a flange specifically designed for the aperture of the antennae. Comparison of data has shown that the measured transition line centers are unaffected by the use of the external antennae with the Teflon windows with respect to the internal antennae.

The vacuum chamber itself is a stainless-steel vacuum chamber acquired from Brian Howard's group at Oxford that is connected to a diffusion pump and rotary vein pump to maintain a vacuum of roughly 1^{-6} torr. The diffusion pump is a Varian® VHS-10 diffusion pump which is backed by an Edwards® 40 rotary pump.

After the FID has been collected by component 5, it is passed to component 6, which is a TTL controlled, single pole, single throw (SPST) switch purchased from ATM® (PNR S1517D). The purpose of this switch is twofold. First, it helps protect components 7 and 8 from the excitation pulse which has the power to destroy the sensitive electronics. Secondly, it allows for the FID signal to pass after the excitation pulse has been turned off. The signal is then amplified by component 7 which is a RF-Lambda® (RLNA06G18G45) low noise amplifier in the 6-18 GHz range. Lastly, component 8 is the Tekronix® DPO 72304DX Digital Phosphor Oscilloscope, capable of 50 GS/s and 23 GHz bandwidth. It is responsible for analyzing and saving the collected data. The FastFrame software available on this oscilloscope allows for multiple data acquisitions per nozzle pulse. More importantly, the oscilloscope allows for multiple FIDs (up to 2 million) to be averaged together. This is beneficial as averaging spectra will improve the signal-to-noise ratio as a function of $\sqrt{n}$, where n is the number of averages. This is due to the fact that background noise will not be consistent at a specific frequency. Thus, by averaging multiple FIDs together, one is able to reduce the background noise while increasing the signal for consistent frequencies that may be too weak to see in a single FID.

2.2.2. Microwave Three-Wave Mixing. For chiral analysis via microwave three-wave mixing (M3WM) spectroscopy (the theory of which is described in Section 3), the above spectrometer is utilized, but in a secondary configuration. A schematic of the M3WM configuration can be seen in Figure 2.5. Terms such as π-pulse and $\frac{\pi}{2}$-pulse will be further defined in Section 3. Since M3WM was the original intent for the MAD-Chirp, its four, orthogonal antenna design was inspired by the previous M3WM spectrometers designed by Pate et al. [33] and Schnell et al. [24, 34], as mentioned previously. However, one addition

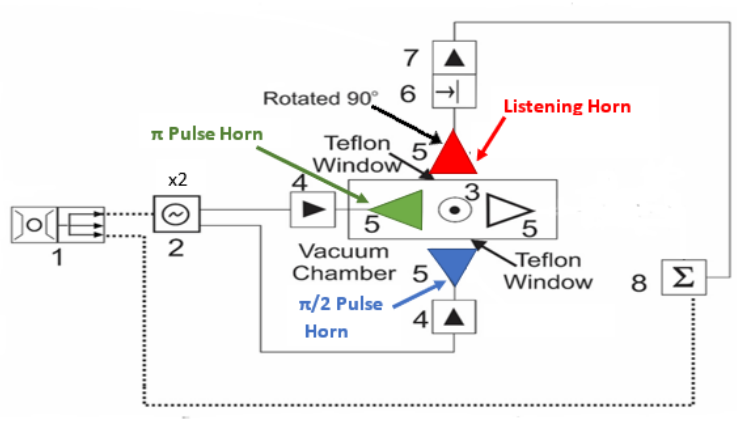


Figure 2.5. Schematic of the MAD-Chirp at Missouri S&T in the microwave three-wave mixing configuration.

unique to this spectrometer is the use of two, synchronized arbitrary waveform generators to generate the two orthogonal microwave pules utilized within the experiment. The overall circuit design and unique additions to this spectrometer will be elaborated on below.

In similar fashion to the traditional set up, all components are kept in synchronization through the use of components 1 in Figure 2.5, which are a 5 and 10 MHz frequency Rubidium standard clock. One of the biggest differences in the M3WM set up is component 2, which now consists of two Tektronix® Arbitrary Waveform Generators (model AWG70000) and a Tektronix® AWGSYNC01 synchronization hub. The decision to include two arbitrary waveform generators (AWGs) was due in part to initial testing that indicated power losses would occur if a switch was used to separate the two needed microwave pulses, resulting in problems properly polarizing the molecules. Therefore, it was decided that two AWGs would be used instead to simultaneously generator the two desired microwave pulses which eliminated the need for a switch. During standard M3WM operations, one AWG, dubbed the "master", controls the first microwave pulse ($\frac{\pi}{2}$-pulse), the flags for the TTL switches, and the gas pulse. The second AWG, dubbed the "servant", controls only the second microwave pulse (π-pulse).

The benefit of using two AWGs is that they allow for the production of multiple pulses across multiple channels. These pulses can even be broadcast simultaneously with overlap. Previously, with only one AWG, two pulses were only possible if they were run one after the other on a singular channel with a switch further in the circuit to direct the correct pulse to the correct horn. Thus, having two AWGs simplified this. However, it should be noted that if the AWG had been comprised of multiple channels, there would have been no need to have two as running the pulses on separate channels would have achieved the same objective.

The $\frac{\pi}{2}$-pulse is then directed from the master AWG to component 4, which for this pulse is comprised of a 1 W Avantek® power amplifier (model APT-18649). The amplified pulse is then directed to component 5, which is one of the external Qpar 2-18 GHz high gain ridged horn antennae shown in blue. As for the π-pulse, it is directed from the servant AWG to component 4, which for this pulse is the 40 W TTL controlled Microsemi® (model L0618-46-T680) solid state amplifier. The amplified pulse is then directed to component 5, which is one of the internal horn antennae shown in green. The resulting FID is detected by the other external horn antennae, shown in red, which is rotated 90° to maintain the orthogonality needed for chiral detection (explained further in Section 3). The rest of the circuit is the same for the M3WM as it for a standard MAD-Chirp experiment as components 6, 7, and 8 are the SPST switch, low noise amplifier (LNA), and oscilloscope, respectively. One downfall of the M3WM set up is the need for 10-foot-long microwave cables between the LNA and the oscilloscope. This is due to the fact that there is roughly a 0.4 db loss in power per foot of microwave cable. As a result, signal-to-noise ratios may be lower throughout the acquired spectrum due to the cable length.

To account for this, a second configuration of the M3WM experiment was later designed, and can be seen in Figure 2.6. Within this design, the two side horns (shown in blue and green) operate as a the broadcasting antennae for the $\frac{\pi}{2}$- and π-pulses. The horn associated with the π-pulse (shown in green) is rotated 90°to maintain the mutual orthogonal

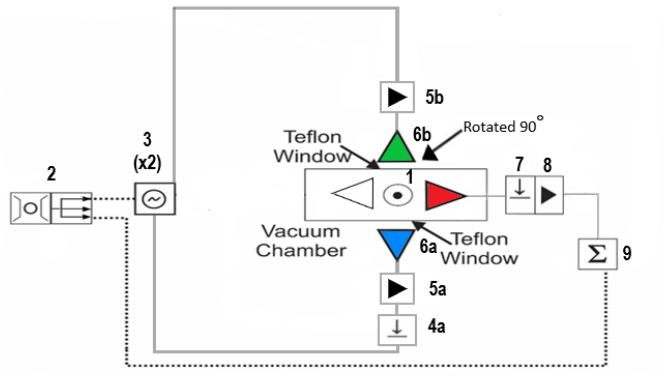


Figure 2.6. Schematic of the MAD-Chirp at Missouri S&T in the second microwave three-wave mixing configuration.

directions. The second internal horn (shown in red) now operates as the receiving horn as it can be connected directly to the oscilloscope via microwave unions, eliminating the need for the 10-foot-long microwave cable at the receiving end. This has improved the single-to-noise ratio of M3WM experiments performed by this instrument by a factor of 5.

2.2.3. Development of a Broadband Spectrometer with Multiple Antenna Detection and Chiral Coherent Quantum Control for Rotational Spectroscopy. Shortly after the demonstration of the MAD-Chirp at Missouri S&T, the design and construction of a second broadband spectrometer with multiple antenna detection and chiral coherent quantum control was undertaken with support from the National Science Foundation's Major Research Instrumentation (MRI) grant. The goals of this particular instrument design were four-fold. First, as with the MAD-Chirp, the aim of this design was to build a new, state-of-the-art, rotational spectrometer with both traditional chirped pulse and M3WM capabilities. Secondly, this new instrument would have five possible detection points (with space to add two more in future years) to increase sensitivity by up to a factor of 2.25 as shown in Reference [25]. Thirdly, this microwave spectrometer was to be equipped with four types of sourcing techniques and multiple sample introduction nozzles to allow for the investigation of exotic, unstable, or nonvolatile species. Each of these four sourcing

Figure 2.7. The new, state-of-the-art rotational spectrometer under construction at Missouri S&T as part of an NSF MRI grant. From left to right: Figure 1.) Initial CAD design for the chamber and stand. Figure 2.) The chamber as of the time of writing. Figure 3.) The stand as of the time of writing.

techniques—traditional gas nozzle, heated nozzle, laser ablation source, and direct current discharge source—were designed by separate research groups in collaboration with the microwave spectroscopy team at Missouri S&T–Dr. Donnell's electrical engineering group at Missouri S&T, Dr. Sedo's group at University of Virginia-College at Wise, Dr. Cooke's group at SUNY-Purchase, and Dr. Raston's group at James Madison University, respectively. Lastly, the instrument would process remote access capabilities and online control to allow instrument access to both the national and international scientific communities who may not otherwise have access to microwave spectroscopy techniques.

The vacuum chamber and stand for the new instrument, lovingly nicknamed "Octo", was designed by this author in collaboration with Independent Steel and Machine in Rolla, Missouri. The vacuum chamber itself is a stainless-steel vacuum chamber with aluminum ports, originally acquired from Independent Steel and Machine, that has been retrofitted for multiple antenna detection. The chamber is connected to an Agilent Technologies® HS-20 oil diffusion pump (P/N 84341319) and Edwards® rotary vein pump (P/N E2M275) to

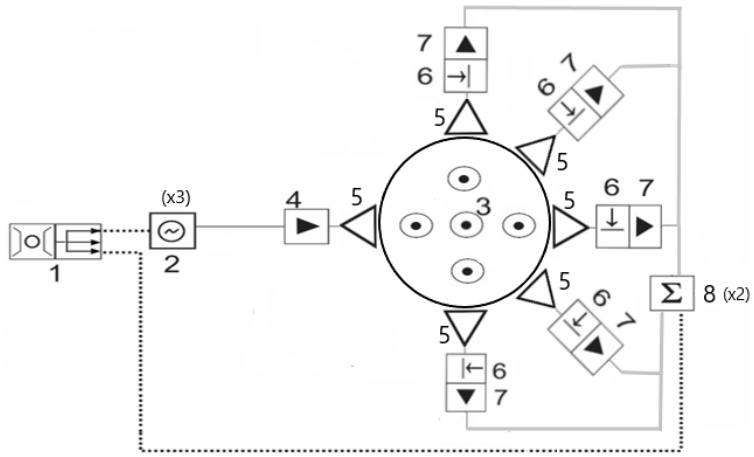


Figure 2.8. Schematic of the new spectrometer's circuit design at Missouri S&T.

maintain a vacuum pressure of up-to 1^{-7} torr. The original CAD design for the chamber as well as photos from the time of writing can be seen in Figure 2.7. In addition, a schematic of the instrument can be seen in Figure 2.8.

All components are kept in synchronization through the use of components 1 in Figure 2.8, which are a 5 and 10 MHz frequency Rubidium stand clock oscillator, produced by Stanford Research Systems (model F2725). Components 2 are three, synchronized Tektronix® Arbitrary Waveform Generators (model AWG7001-B) and a Tektronix® Synchronization Hub (model AWGSYNW1). The arbitrary waveform generators have a 50 GS/s digitization rate and are capable of producing waveforms up to 20 GHz. The linear frequency sweeps, or chirps, used to define the experimental microwave pulses are generated by MATLAB scripts and are imported into the arbitrary waveform generators utilizing the program TekVISA®. The chirps produced by these arbitrary waveform generators are fed into component 4 which is a 120-Watt, TTL controlled RF-Lambda® (model REMC06G18GF) solid state power amplifier for the 6-18 GHz range.

The signal is then broadcasted into the vacuum chamber and detected via components 5, which are the Qpar 2-18 GHz high gain, ridged horn antennae (Steatite® QWH-SL-2-18-S-HG-R). The six horn design (with space for two more) was influenced by the quadrature

detection results obtained within Reference [25]. The antennae reside outside the chamber and are set up on a bracketing system which allows for the antenna to rotate clockwise up to 270° with hard stops at 90° for M3WM purposes. The antennae detect signals through a 0.32 cm thick Teflon window which resides in a flange specifically designed for the aperture of the antenna.

All detection horns are equipped with a reflective coaxial SPST switch within the 2-18 GHz region purchased from RF-Lambda® (model RFSPSTR0218G), which is component 6 in the schematic. The signal is then amplified by component 7 which is an RF-Lambda® low noise amplifier (model RLNA06G18G45D) in the 6-18 GHz region. The signal is then recorded and averaged by component 8: one of the two Tektronix® DPO 72304DX Digital Phosphor Oscilloscope, capable of 50 GS/s and 23 GHz bandwidth. The FastFrame software available on these oscilloscopes allows for multiple data acquisitions per nozzle pulse.

At the time of this writing, the instrument has been 90% designed and constructed, though no formal testing has commenced. Yet, this author is excited to see what the future holds for this instrument and the discoveries it will facilitate.

2.2.4. Sourcing Techniques. As mentioned previously, microwave spectroscopy is a gas phase technique. Over the years, however, the introduction of various sourcing techniques has broadened the field of possible molecular systems away from just those that are gases at standard temperature and pressure to solids and liquids as well. Within Figure 2.3, Figure 2.5, and Figure 2.8, component 3 represents the entrance of the sourcing technique into the vacuum chamber. Most often, the sourcing technique utilized is a pulsed nozzle source, specifically Parker Hannifin® Series 9 supersonic nozzle with a 0.8 mm orifice that is controlled by a Parker Hannifin IOTA ONE® pulse driver and Quantum Composers® 9520 Series pulse generator. This sourcing technique is preferred for gas phase samples as it promotes the supersonic expansion of the gaseous sample into the vacuum chamber.

For liquid or solid samples, additional components can be added to the supersonic nozzle to aid the sample into the gas phase. For liquids and solids with low boiling points, a heated reservoir can be added to promote vaporization [35]. The apparatus itself is comprised of a 3 mL reservoir that holds the desired sample and a Chromalox MB1A1A1A1 clam shell heater. The heater applies heat to the exterior of the revisor and is controlled by varying the 120 V power supply through the use of a VaryAC. The temperature is monitored through the use of a MAX31855 K-type thermocouple that feeds into an AD595 thermocouple interface chip that collects, amplifies, and converts the signal to a voltage. This voltage is then monitored by an Arduino Uno and converted to a temperature.

For solids with high boiling points, such as metal rods, a laser ablation source can be implemented. This sourcing technique works by focusing a high-power laser onto the surface of a solid rod and ablating away small fractions of the surface, which can then interact with a plume of either a backing gas or complex mixture. Lastly, for radical species, a DC discharge nozzle can be utilized, which forces the sample molecule though an electric field, promoting radicalization. Since neither the laser ablation source nor the DC discharge nozzle were employed in the following work, they will not be described further.

3. MICROWAVE THREE-WAVE MIXING THEORY

Chirality is the property some molecules have in which they are non-superimposable with their mirror image. While chirality has been known for over a century, it has remained a focal point of research due to its implications in the realm of biology, pharmaceuticals, material development, and even quantum mechanics to name a few. Though chirality is important, it is also difficult to study since chiral molecules have identical chemical and physical characteristics, and, traditionally, are only distinguishable by how they rotate polarized light. While some methods have been developed over the years to study chiral species more quantitatively—such as circular dichroism (CD), vibrational circular dichroism (VCD), and Raman optical activity (ROA) spectroscopy—many require a large amount of sample to be destroyed or require long acquisition times. Both of which are counterproductive for both academic and industrial applications. Yet, a new detection method developed within the last ten years, known as microwave three-wave mixing (M3WM), has the potential to solve these two issues.

In its traditional form, microwave spectroscopy cannot be used as a chirality determination technique due to both enantiomers producing identical microwave spectra. This is a consequence of the fact that both enantiomers have identical moments of inertia, which leads to identical rotational constants, and as a result, identical spectra. However, this all changed in 2013, when Schnell and colleagues first introduced the technique of M3WM in their revolutionary *Nature* paper [24]. In their initial paper, they described the use of microwave spectroscopy to distinguish between enantiomers through orthogonal microwave pulses. This technique can be viewed as a polarization-sensitive double resonance technique that relies on the fact that the dipole moments for enantiomers are mirror images of each other [34]. This approach to chirality determination is advantageous compared to other techniques due to the resolution afforded by FTMW spectroscopy, which allows for the discernment of specific molecules even in complex mixtures. In addition, the measurement

times can be as quick as mere seconds compared to the minutes or hours of traditional chiral determination techniques. Therefore, this technique is excellent for chiral molecules that can be easily brought into the gas phase. Since 2013, the advantages of M3WM have been demonstrated through numerous research studies with many more projects currently in development [24, 33, 34, 36, 37, 38, 39].

3.1. CHIRALITY DETERMINATION VIA MICROWAVE SPECTROSCOPY

The basis of M3WM is dependent on the parity conserving Hamiltonian of an asymmetric top molecule in an external electric field. This can be represented by the equation [24]

$$\hat{H}(t) = \hat{H}_o - E_a(t)\mu_a - E_b(t)\mu_b - E_c(t)\mu_c, \tag{3.1}$$

where $\hat{H}_o$ is the asymmetric top Hamiltonian before the electric field is applied and $E_i(t)$ is the time dependent electric field in a given direction. For this type of molecule, the three rotational constants A, B, and C, and the corresponding dipole moment component magnitudes $|\mu_a|$, $|\mu_b|$, and $|\mu_c|$ determine the allowed rotational energy levels as described in Section 1. More importantly, the specific signs of μ_a, μ_b, and μ_c fully determine the chirality of the molecule in question. While the sign of any two of the three dipole moment components for a molecule is arbitrary and changes with the choice of axes, the sign of the product of all three dipole moments,

$$\mu_a\mu_b\mu_c = \vec{\mu_a} \bullet (\vec{\mu_b} \times \vec{\mu_c}), \tag{3.2}$$

is axis independent and changes with enantiomer. This enantiomer specific sign change can be accurately predicted via numerical integration of the asymmetric top Hamiltonian if one knows the rotational constants and dipole moment components. In addition, chiral

molecules, by definition, have a dipole moment component along each axis. Thus, the product $\mu_a\mu_b\mu_c$ will never equal zero. Instead, it will either be a positive or negative value depending on the handedness of the enantiomer in question.

Thus, by mapping the enantiomer-dependent sign of an electric dipole Rabi frequency (to be defined shortly) onto the phase of emitted microwave radiation, one can determine the enantiomer present. In more simplified terms, if microwave radiation is used to probe a rotational transition involving dipole moment a (μ_a) and dipole moment c (μ_c) with orthogonal microwave fields, for example, then the phase of the molecule signal involving dipole moment b (μ_b) in their mutually orthogonal direction differs by π radians between the two enantiomers. As a result, the resulting FID for each enantiomer will be 180° out of phase from each other allowing for the determination of chirality.

In addition to chriality discernment, the determination of enantiomeric excess (*ee*) is also possible via M3WM. This is due to the fact that M3WM is strictly forbidden for a racemic mixture under any geometry present in the electric dipole approximation, which yields no signal for a racemic sample [34]. In more simplified terms, the 180° phase difference in the FIDs of the two enantiomers causes destructive interference that results in a net zero signal since the two enantiomers have coherent emission at the same frequency. As a result, any signal detected by M3WM is due to *ee* within the mixture. In fact, the intensity of a signal produced by M3WM is proportional to the amount of *ee* within the mixture.

3.2. THE BLOCH EQUATIONS

As mentioned in Section 2, the macroscopic polarization needed for microwave spectroscopy experiments is made possible due to the fast-passage technique developed by McGurk and Flygare and is governed by the Bloch equations [27]. As a result, in order to fully present the requirements of a M3WM scheme, the Block equations must first be

introduced. The optical Bloch equations used in microwave spectroscopy are analogous to the Bloch equations used to describe magnetic polarization in nuclear magnetic resonance (NMR) spectroscopy.

In order to describe the equations, the phenomenon of fast passage will be treated using the theory of the interaction of coherent electromagnet radiation with a two-level quantum system through the electric dipole interaction. The macroscopic polarization in the two-level system can be written in the form [27]

$$P = (P_r + iP_i)e^{i(\omega t - kz)} + cc, \tag{3.3}$$

where cc is the complex conjugate, P_r is the real component of the polarization, and P_i is the imaginary component of the polarization. These values can be determined through the Bloch equations, which are three coupled differential equations given by

$$\frac{dP_r}{dt} + \Delta\omega P_i + \frac{P_r}{T_2} = 0, \tag{3.4}$$

$$\frac{dP_i}{dt} - \Delta\omega P_r + \kappa^2 \xi (\frac{\hbar \Delta N}{4}) \frac{P_i}{T_2} = 0, \tag{3.5}$$

and

$$\frac{d}{dt}(\frac{\hbar \Delta N}{4}) - \xi P_i + \frac{\hbar}{4} \frac{(\Delta N - \Delta N_o)}{T_1} = 0. \tag{3.6}$$

Within these equations, $\Delta\omega$ is the difference between the molecular transition frequency and the frequency of radiation, and ΔN is the population difference. κ is given by

$$\kappa = (\frac{2}{\hbar}) |\langle a | \boldsymbol{\mu} | b \rangle|, \tag{3.7}$$

where $\boldsymbol{\mu}$ is the dipole moment operator, while a and b denote the lower and upper levels, respectively. The optical Block equations also include the phenomenological relaxation rates of T_1 (for decay of the populations different to its equilibrium value) and T_2 (for decay of the coherence) [40]. These two values limit the duration of the FID.

Equations 3.4 - 3.6 can be solved for the case where $\Delta\omega$ is swept from $\Delta\omega_i$ to $\Delta\omega_f$ in a time short compared to the relaxation times T_1 and T_2. The equations then become [27]

$$\alpha\frac{dP_r}{d(\Delta\omega)} + \Delta\omega P_i = 0, \tag{3.8}$$

$$\alpha\frac{dP_i}{d(\Delta\omega)} - \Delta\omega P_r + \frac{\kappa^2\xi\hbar}{4}\Delta N = 0, \tag{3.9}$$

and

$$\alpha\frac{d}{d(\Delta\omega)}(\frac{\hbar\Delta N}{4}) - \xi P_i = 0, \tag{3.10}$$

where α is the sweep speed defined by

$$\alpha = \frac{d(\Delta\omega)}{dt}. \tag{3.11}$$

Solving these equations further yield mathematical expressions for the pulse polarization and signal at the detection site, which is explained in detail within Reference [27]. Note that the above equations indicated that the excitation response of a rotational transition using fast passage is depended on the frequency range, $\Delta\omega$, and the time spent sweeping through the frequency range. The requirements for a M3WM mixing schemes are also dependent on these three values.

3.3. REQUIREMENTS FOR A M3WM SCHEME

In order to determine chirality via M3WM, a mixing scheme must be created involving three rotational energy levels connected to one another through allowed rotational transitions. An example of such a scheme is shown in Figure 3.1. In addition to the energy

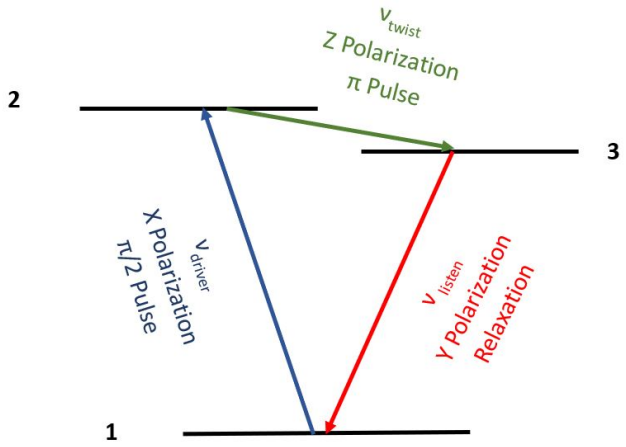


Figure 3.1. Example of a M3WM scheme.

levels themselves, the microwave pulses that promote population transfers between these states must also meet certain criteria in order for the enantiomer-dependent sign of $\mu_a\mu_b\mu_c$ to be mapped onto the phase of the FID properly. A brief description is presented here for the creation of a M3WM scheme to produce an enantiomer-specific chiral signal. More detail descriptions are presented in Reference [24] and [33].

The scheme begins with a resonate, single-frequency microwave pulse with X polarization. (Polarization is dependent on the dipole moment of the starting transition. In this case, X is simply a placeholder.) This pulse transforms the population difference into coherence, creating a superposition state with the form [33]

$$|\Psi\rangle = \cos(\frac{\Theta_{Rabi}}{2})e^{-\frac{iE(1)t}{\hbar}}|1\rangle + i\sin(\frac{\Theta_{Rabi}}{2})e^{-\frac{iE(2)t}{\hbar}}|2\rangle, \tag{3.12}$$

with the Rabi flip angle defined as

$$\Theta_{Rabi} = \omega_{Rabi}t_{pulse} = \frac{\langle\boldsymbol{\mu}\rangle E}{\hbar}t_{pulse}, \tag{3.13}$$

where E is the electric field strength of the resonant microwave pulse, $\langle \boldsymbol{\mu} \rangle$ is the transition dipole moment element between the initial and intermediate states, and t_{pulse} is the length of the excitation pulse. In this way, the superposition state coefficients contain the signed dipole moment information. The optimal coherence in Equation 3.12 is created by a Rabi flip angle of $\frac{\pi}{2}$. This results in a $\frac{1}{2}$ population inversion between states 1 and 2 within the M3WM scheme.

The second transition is induced by a resonant field with Z polarization. (Once again, polarization is dependent on the dipole moment of the transition. In this case, Z is simply a placeholder to indicate this polarization is different than the starting polarization.) In addition to creating a coherence between the states 2 and 3, this pulse also transfers some of the existing coherence between states 1 and 2 into a coherence between states 1 and 3. This coherence is optimized when the Rabi flip angle for the second pulse is equal to π [33]. This specific Rabi flip angle results in a full population inversion between states 2 and 3 within the M3WM scheme. Following the π-pulse, the wave function for the system has the form [33]

$$|\Psi\rangle = c_1(t)|1\rangle + c_2(t)|2\rangle + c_3(t)|3\rangle, \tag{3.14}$$

and it will generate a coherent emission at the frequency of the $3 \leftarrow 1$ rotational transition with Y polarization.

An optimal M3WM mixing scheme also takes into consideration the following points, though they are not exclusively required. First, since the chiral signal is proportional to the population difference between the pair of states first pumped, it is optimal if the transition with the largest population difference (highest frequency) is designated as the $\frac{\pi}{2}$-pulse. It is also optimal to choose an R-branch ($\Delta J = +1$) transition with the smallest dipole moment projection for this pulse since the $\frac{\pi}{2}$ Rabi flip angle will provide the most power. Secondly, since the chiral signal is also proportional to the strength of transition dipole moment component, it is suitable to choose a rotational transition with the largest dipole

moment at a high molecular frequency (ΔJ = -1, P-branch transition) for the relaxation transition [33]. By default, the π-pulse consists of a Q-branch (ΔJ = 0) transition with the remaining dipole moment component.

3.4. LIMITING FACTORS TO M3WM SCHEME'S EFFICIENCY

The efficiency of the M3WM scheme mentioned above can be limited by three factors. The first factor is the temperature of the sample or, specifically, the thermal population in the excited states targeted by the three-wave mixing scheme [41]. Since M3WM schemes only consisted of rotational transitions within the microwave region of the electromagnetic spectrum, the population in the three levels – at the typical effective rotational temperature of approximately 10 K – will be roughly of the same order of magnitude according to the Boltzmann distribution. This limits the effectiveness of the excitation pulses meant to arouse population transfer between these three states. One solution to this limitation is to focus on energy levels which are sufficiently highly excited such that the thermal population vanishes [41]. The super-sonic expansion of the sample into the vacuum chamber also helps to alleviate this issue to some extent by cooling the molecules into the vibrational ground state.

The second factor is due to the fact that chiral molecules are typically asymmetric top rotors, as described in Section 1. For rigid asymmetric top rotors, every rotational level consists of $2J + 1$ states with a different orientation of the magnetic quantum number M, often referred to as M-degeneracies. Due to this, transfer efficiencies between the three rotational states are only predicted correctly for cycles which start from the non-degenerate rotational ground state (J = 0). If not, the cyclic excitation involves a number of coupled, partially incomplete three-level systems. This limits the efficiency of the population transfer between the three states even in the absence of thermal population [42].

The last factor is currently only theorized, but preliminary work has been undertaken to understand it more fully and is presented within this dissertation. Specifically, this factor is internal rotation. As mentioned in Section 1, internal rotation breaks the symmetry of the molecule and causes degeneracies to form within its rotational states. With two non-equivalent methyl rotors, for example, each rotational state is split into five symmetry states. Thus, the cyclic excitation would now involve a number of coupled, partially incomplete, three-level systems, just like in *M*-degeneracies. Since many M3WM works to date ignore this factor, it is imperative that more work be done to understand its effect on the efficiency of standard M3WM schemes and what can be done to alleviate it.

3.5. ANALYSIS OF THE FREE INDUCTION DECAY

After the FID induced by the M3WM scheme has been collected, it must be analyzed in order to deduce the recorded phase produced by the enantiomer in question. The FID itself can be represented by [39]

$$\varepsilon_{listen}(t) \propto |\mu_a\mu_b\mu_c| \cdot \cos(2\pi\nu t + \frac{\mu_a\mu_b\mu_c}{|\mu_a\mu_b\mu_c|}\frac{\pi}{2}), \tag{3.15}$$

where ε_{listen}(t) is the observed FID signal at the listening frequency. Based upon Equation 3.15, the overall phase of the FID is dependent on the sign of $\mu_a\mu_b\mu_c$, as mentioned previously. Thus, if one knows the sign of $\mu_a\mu_b\mu_c$ for the two enantiomers via *ab initio* calculations, the absolute configuration can be determined directly from the FID measurement. However, it is also necessary to know the time between when the excitation occurred, and when the recording of the FID began in order to deduce the absolute phase of the enantiomer as explained in Reference [34].

An important clarification to make at this point is that it is crucial to know either the sign of $\mu_a\mu_b\mu_c$ for the two enantiomers from *ab initio* calculations or to analyze the FID of the two known and pure enantiomers first before analyzing unknown or mixed samples.

This is due to the fact that not every R-enantiomer will have a negative $\mu_a\mu_b\mu_c$ nor every S-enantiomer will have a positive $\mu_a\mu_b\mu_c$, for example. The exact sign of $\mu_a\mu_b\mu_c$ for a given enantiomer is molecule dependent. Since the phase of the FID is influenced by the sign of $\mu_a\mu_b\mu_c$ and the sign of $\mu_a\mu_b\mu_c$ is molecular dependent, it is not possible at the present time to determine solely by the phase of the FID which enantiomer is present without the additional information mention above. Many groups are currently trying to tackle this problem [43], but much work is still left to be done.

3.6. CHIRAL TAGGING

It's inappropriate to discuss microwave three-wave mixing in-depth without acknowledging the second chirality determination method that has been developed for rotational spectroscopy, known as chiral tagging. Developed five years after M3WM by Pate et al. [44], this method works on the principle of complexing the enantiomers of interest with well-characterized chiral molecules of known handedness, referred to as chiral tags. By complexing the two types of enantiomers together, diastereomeric complexes (non-mirror image, non-identical stereoisomers) are formed. These complexes can then be studied directly using rotational spectroscopy as the diastereomers will have distinct three-dimensional structure and thus have separate, distinct rotational constants. Since the handedness of the chiral tag is known, this allows for the determination of the handedness of the enantiomers of interest. In addition, by analyzing the transitions intensities for the two diastereomers, one can obtain information on the enantiomeric excess of the sample.

While chiral tagging has been shown to perform equally with M3WM in terms of determining the handedness of an enantiomer and its enantiomeric excess [45], it does have its drawbacks. The most notable being that the enantiomer in question must be fundamentally changed though complexation before it can be analyzed. Certain research focuses, such as pharmaceutical matters, may wish to study the enantiomer in its unaltered form. In addition, not all chiral molecules are excellent candidates for complexation, and

effective chiral tags must also follow strict guidelines (i.e., must be small enough for the complex to not have inconveniently small rotational constants, but large enough so that the rotational constant between the two complexes are distinct [45]). However, for research groups not possessing a M3WM spectrometer, this is a suitable alternative.

PAPER

I. PURE ROTATIONAL SPECTRUM AND STRUCTURAL DETERMINATION OF 1,1-DIFLUORO-1-SILACYCLOPENTANE

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ABSTRACT

The ground state, pure rotational spectrum of 1,1-difluoro-1-silacyclopentane has been studied using chirped-pulse, Fourier transform microwave (CP-FTMW) spectroscopy and observed in the 6-20.3 GHz region of the electromagnetic spectrum. This spectrum was acquired leveraging the deep averaging capability of the technique. The parent species, ^{13}C, ^{29}Si, and ^{30}Si singly substituted isotopologues were observed in natural abundance and are reported. Only one conformer, the C_2 conformer (half-chair), was observed. This is confirmed with a determined CCCC dihedral angle of -48.1(11)°. The spectrum is comprised of entirely *a*-type transitions in accordance with quantum chemical calculations. Multiple split transitions are present in the spectrum which have been attributed to a ring-twisting of the carbon atoms attached to the silicon atom in the ring. This motion has the carbons crossing the *a*-axis in the *bc*-plane leading to an inversion potential. Potential energy surfaces for

the ring-twisting motion were undertaken and the experimentally determined energy level difference observed in comparison to these surfaces is reasonable. A Kraitchman analysis of the experimentally determined, singly substituted isotopologues is in agreement with the optimized, twisted (nonplanar) equilibrium structure. This structure has been compared to other similar silicon-containing ring molecules using second moment arguments and these comparisons are discussed.

1. INTRODUCTION

Ever since the chirped-pulse, Fourier transform microwave (CPFTMW) spectrometer was introduced to the scientific community over fifteen years ago [1], it has repeatedly demonstrated its advantages as a microwave technique. At the time of its debut, the main strength of the CP-FTMW was its ability to collect broadband spectra in a fraction of the time it took the traditional Balle-Flygare cavity experiment [2]. However, the Balle-Flygare cavity was still considered superior in its sensitivity. As technology has improved, however, the time advantage provided by the CP-FTMW can be leveraged to bridge the gap in sensitivity by collecting and averaging very large (100k or more) amounts of time domain molecular signals. This is known as deep averaging [1, 3].

Highly accurate experimental molecular geometric structures from pure rotational spectroscopy rely heavily on the ability to collect isotopic substitution data. Ideally, this data can be collected from the molecule of study in natural abundance. For many organic molecules, the most abundant isotopologue species are ^{13}C substituted, which are approximately 1% abundant (or some multiple of 1% depending on symmetry). Because the sensitivity in CP-FTMW spectra is traditionally lower than the Balle-Flygare FTMW instrument, collecting such data in natural abundance has been a challenge. If this barrier is overcome, though, the correct relative intensity information is useful for quick isotopologue assignment [4]. The ability to quickly average many free induction decays (FIDs) per gas pulse with very fast digitizers on broadband spectra has led to the use of deep

averaging. Deep averaging makes up for the direct lack of sensitivity in the CP-FTMW technique compared to that of the cavity FTMW technique by leveraging the increased acquisition speed of the broadband spectrometer. This averaging capability – which decreases the noise floor and, thus, increases signal-to-noise (S:N) – has been utilized on the CP-FTMW instrument at the Missouri University of Science and Technology (Missouri S&T) before. The increased S:N makes it possible to garner much more information from a single broadband spectrum, particularly in regards to weaker isotopologue data [5, 6]. This is especially useful for molecules like those of the silacyclopentane family which (a) can only be synthesized in limited quantities, (b) likely possess isotopologues that only have limited natural abundances, and (c) may possess splitting observable on only a few weaker transitions. Deep averaging, therefore, allows for a more complete understanding of a rotational spectrum of a molecular system with less sample consumption and less time.

The rotational spectrum of silacyclopentane (c-$C_4H_8SiH_2$) was first observed using microwave spectroscopy in 1976 [7]. At the time, only the parent and one isotopologue — the ^{29}Si isotopologue — were observed, resulting in an incomplete substitution structure. In addition, while it is generally accepted that saturated five-membered carbon rings —like that of c-$C_4H_8SiH_2$ —exist in a non-planar configuration due to torsional forces related to the carbon-carbon bonds [8, 9], the splitting often observed in microwave spectra due to this was not reported in the original work. However, in 2011, the rotational spectrum of c-$C_4H_8SiH_2$ was collected again using a Balle-Flygare type, pulsed-jet Fourier transform microwave (FTMW) spectrometer as well as a CP-FTMW [10]. This work observed and reported the parent and all corresponding unique heavy atom, singly substituted isotopologues, resulting in a heavy atom structure. Since then, numerous other members of this family of molecules have been accurately studied using CP-FTMW along with IR and Raman spectroscopy including 1-fluoro-1-silacyclopentane [11], 1-bromo-1-silacyclopentane [12], 1,1-difluoro-1-silacyclopent-2-ene [13, 14], 1-chloro-1-silacyclopentane [15], 1,1-dimethyl-

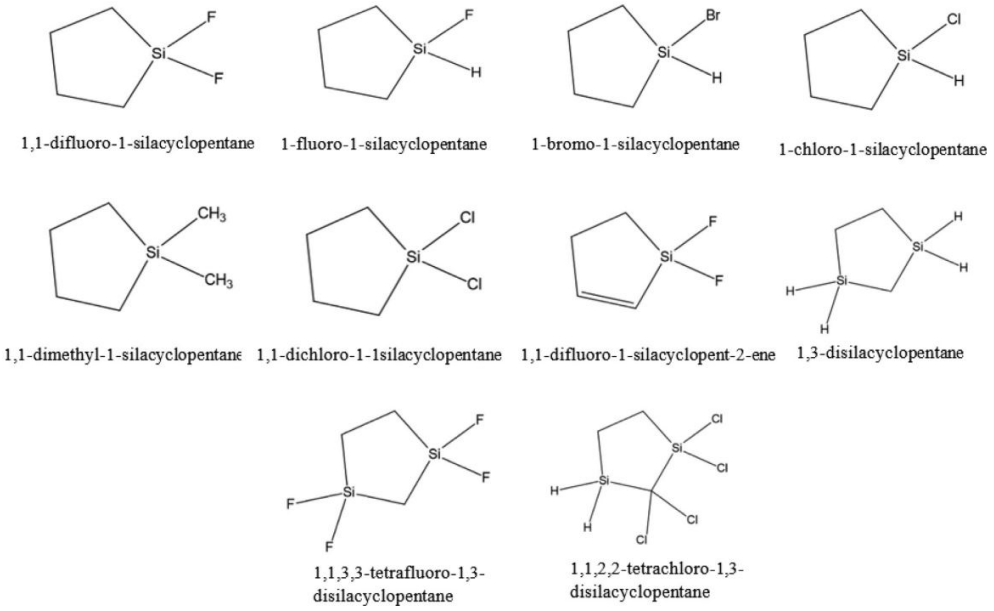

Figure 1. Members of the silacyclopentane family previously observed.

1-silacyclopentane [16], 1,1-dichloro-1-silacyclopentane [17], 1,3-disilacyclopentane [13], 1,1,2,2-tetrachloro-1,3-disilacyclopentane [18], and 1,1,3,3-tetrafluoro-1,3-disilacyclopentane [19]. The structures of these molecules can be seen in Fig. 1.

In this work, therefore, the sensitivity advantage of CP-FTMW spectroscopy due to deep averaging is demonstrated on a member of the silacyclopentane family, 1,1-difluoro-1-silacyclopentane (*c*-$C_4H_8SiF_2$). The microwave spectrum of *c*-$C_4H_8SiF_2$ parent as well as the ^{13}C, ^{29}Si, and ^{30}Si isotopologues in natural abundance have been observed and are reported, resulting in an experimentally determined ring structure (r_s). Splitting due to ring-twisting motions in the molecule have been observed, analysed, and reported. Quantum chemical calculations were undertaken to fully interpret the observed spectra and are reported. The calculations indicate that the barrier to the ring-twisting motion is high, resulting in twisting levels in the ground state which are degenerate (or near degenerate). Observation of the ring-twisting motion splitting, therefore, is owed to the high-resolution and deep averaging capabilities of the CP-FTMW technique. Additional quantum chemical calculations were carried out on the parent *c*-$C_4H_8SiH_2$ molecule for the sake of comparison.

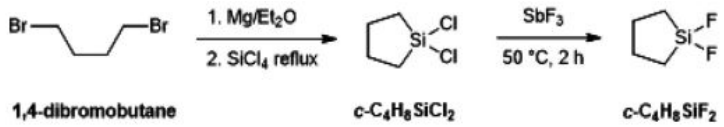

Figure 2. Reaction conditions for the synthesis of c-$C_4H_8SiCl_2$ and c-$C_4H_8SiF_2$.

2. EXPERIMENTAL

2.1. SYTHETIC WORK

The synthetic work was carried out at the College of Charleston in two steps. First, 1,1-dichloro-1-silacyclopentane (c-$C_4H_8SiCl_2$) was prepared by adding a double Grignard reagent of 1,4-dibromobutane in anhydrous ethyl ether to a solution of silicon tetrachloride in additional ethyl ether under argon. The method for the synthesis of c-$C_4H_8SiCl_2$ is the same as that reported by Tacke [20] and Charette [21]. The NMR data for c-$C_4H_8SiCl_2$ ^{1}H NMR (400MHz, $CDCl_3$): δ (ppm) 1.47 (p, 4.32 Hz, 4H, CH_2) 0.43 (t, 1.21 Hz, 4H, CH_2). ^{13}C NMR (400 MHz, $CDCl_3$): δ (ppm) 28.88 (s), 14.70 (s). ^{29}Si NMR (400 MHz, $CDCl_3$): δ (ppm) 16.52 (s). The sample of c-$C_4H_8SiF_2$ was prepared by fluorination of c-$C_4H_8SiCl_2$ with freshly sublimed antimony trifluoride without solvent (Figure 2).

The synthesis of c-$C_4H_8SiF_2$ has been reported previously [22], but a new procedure was developed which uses more readily available commercial compounds and it is reported below. A liquid sample of c-$C_4H_8SiCl_2$ (2.00 g, 16.4 mmol) was added to a 50 mL Schlenk tube, 20 cm in length, and equipped with a stir bar. The tube was fitted with a vacuum adapter and the sample with frozen with liquid nitrogen. Antimony trifluoride (3.22 g, 18.0 mmol) was added while purging with argon. The tube containing the reaction mixture was sealed, frozen with liquid nitrogen, and evacuated to 0.20 Torr. The mixture warmed to room temperature, stirred for 30 minutes, and then was heated to 50°C for two hours while stirring. Volatile components were removed from the flask using vacuum transfer and the product was purified using trap-to-trap distillation. The purity of the sample was checked

using nuclear magnetic resonance spectroscopy and infrared spectroscopy. For the infrared spectrum, the SiF_2 symmetric and antisymmetric stretching frequencies were observed at 871 and 877 cm^{-1} as previously reported [14]. A total of 1.76 g, 11.5 mmol of isolated product was collected. Yield: 69%. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 1.70 (m, 1.6 Hz, 4H, CH_2) 0.72 (m, 2.9 Hz, 4H, CH_2). ^{13}C NMR (400 MHz, $CDCl_3$): δ (ppm) 23.64 (t, 2.9 Hz), 7.48 (t, 14.0 Hz). ^{19}F NMR (400 MHz, $CDCl_3$): δ (ppm) -138.59. ^{29}Si NMR (400 MHz, $CDCl_3$): δ (ppm) 18.79.

2.2. MICROWAVE SPECTRA

The microwave experiments were carried out at Missouri S&T using a CP-FTMW. The details of this spectrometer are reported elsewhere [5, 6, 23, 24]. The sample of *c*-$C_4H_8SiF_2$—a liquid under standard conditions—was made into a gas mix by utilizing the vapor pressure of the molecule at room temperature. A gas tank was evacuated and attached to the sample, which then allowed the sample to vaporize. The vapor in the tank was then mixed with industrial grade argon gas until the sample was 3% in concentration. The 3% gas tank was then attached to the CP-FTMW, and sample was introduced at a sub-atmospheric pressure of 0.66 atm relative to vacuum.

Spectra of *c*-$C_4H_8SiF_2$ were then acquired in the 6-12 GHz and 12-18 GHz regions of the electromagnetic spectrum using 4 μs chirp widths. A Parker Hannifin® Series 9 supersonic nozzle pulsed sample into the chamber at a rate of 5 Hz with 5 FIDs per gas pulse. In total, 168,000 FIDs, each FID being 20 μs in length, were averaged together in each frequency range before the sample was completely depleted. Spectra for the 6-12 GHz and 12-18 GHz ranges can be seen in Figs. 3 and 4, respectively. Typical linewidths for the spectra were 70-80 kHz with an attributed 10 kHz uncertainty in the line centers.

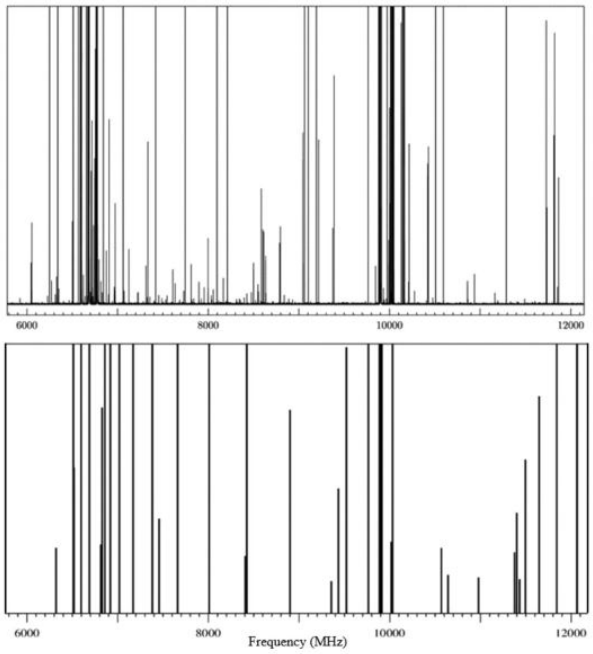

Figure 3. The top image depicts the 6-12 GHz spectra for 1,1-difluoro-1-silacyclopentane (c-$C_4H_8SiF_2$). The bottom image depicts the predicted spectra within the 6-12 GHz region. Intensities of the strongest transitions are cut off so that less intense transitions are visible.

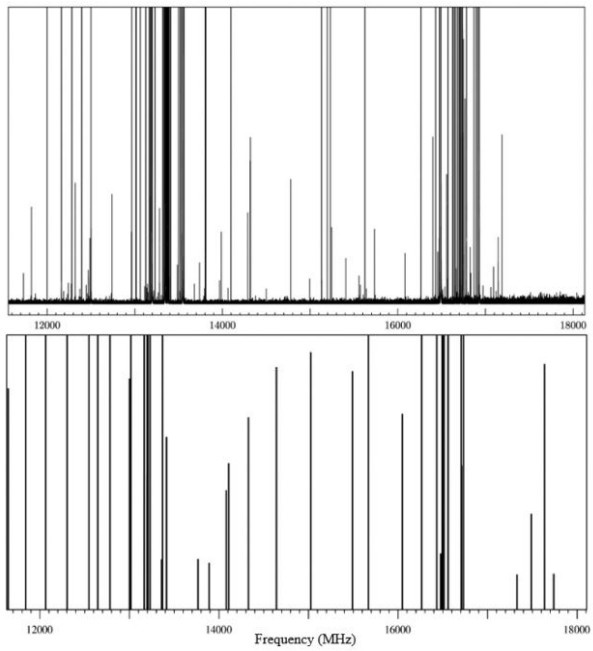

Figure 4. The top image depicts the 12-18 GHz spectra for c-$C_4H_8SiF_2$. The bottom image depicts the predicted spectra within the 12-18 GHz region. Intensities of the strongest transitions are cut off so that less intense transitions are visible.

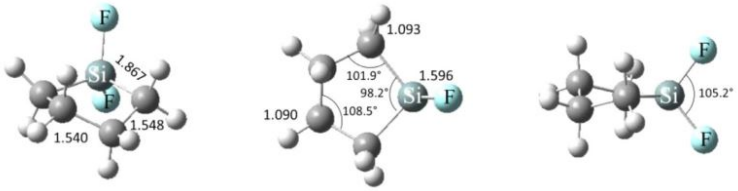

Figure 5. Calculated geometrical parameters from CCSD/cc-pVTZ computations of the twisted conformation of *c*-$C_4H_8SiF_2$.

3. QUANTUM CHEMICAL CALCULATIONS

3.1. STRUCTURE CALCULATIONS

The geometric structure of *c*-$C_4H_8SiF_2$ was optimized at the B3LYP/cc-pVTZ level at Missouri S&T. The optimized structure provided the rotational constants utilized in the initial experimental analyses. In order to carry out the calculations, Gaussian09 [25] was used in conjunction with GaussView 5.0 [26] for visualizing structures. The results from this optimized equilibrium structure can be found in Table 1.

In addition, optimized geometries and conformational energies of *c*-$C_4H_8SiF_2$ were calculated at the MP2/cc-pVTZ and CCSD/ccpVTZ *ab initio* level of theory at Texas A&M University. For these calculations, Gaussian16 [27] was used in conjunction with GaussView 6.1.1 [26] in order to visualize the structures.

The calculated geometrical structures of the molecule are shown in Fig. 5. The twisted structures have C_2 symmetry. This was the only conformer observed in the spectra.

Table 1 presents the calculated geometrical parameters of *c*-$C_4H_8SiF_2$ and the microwave values to be discussed within the Discussion section. Similarly, Table 2 presents the second moment values to be discussed within the Discussion section.

Table 1. Geometric parameters for c-$C_4H_8SiF_2$.

	Experimental (r_s)	Theoretical (r_e)		
	microwave[a]	B3YLP/cc-pVTZ	MP2/cc-pVTZ	CCSD/cc-pVTZ
	Bond Lenghth, Å	*Bond Length, Å*		
Si-C1	1.85(6)[b]	1.864	1.866	1.867
C1-C2	1.56(5)	1.548	1.646	1.548
C2-C3	1.54(1)	1.542	1.537	1.540
C3-C4	1.56(5)	1.548	1.646	1.548
	Bond Angle, deg	*Bond Angle, deg*		
C1-Si-C4	99.84(44)	98.5	98.1	98.2
C2-C1-Si	101.7(26)	102.1	113.3	101.9
C3-C2-C1	109.1(30)	108.9	99.0	108.5
C4-C3-C2	109.1(30)	108.9	108.3	108.5
C4-Si-C1	99.84(44)	98.5	98.1	98.2
	Dihedral Angles, deg	*Dihedral Angles, deg*		
Si-C1-C2-C3	34.8(85)	35.6	37.8	37.0
C1-C2-C3-C4	-48.1(11)	-49.2	-52.3	-51.1
C2-C3-C4-Si	34.8(85)	35.6	37.8	37.0
C3-C4-Si-C1	-12.3(50)	-12.7	-13.4	-13.2
C4-Si-C1-C2	-12.3(50)	-12.7	-13.4	-13.4

[a] Parameters obtained through Kisiel's EVAL program [28].
[b] Uncertainties obtained from Costain errors given in values of the least significant figure.

Table 2. c-$C_4H_8SiF_2$ second moments from experiment.

	Parent	^{29}Si	^{30}Si	^{13}C1 / ^{13}C4	^{13}C2 / ^{13}C3
$\mathbf{P}_{aa}$(amu-Å^2)	227.27110(12)	227.598(13)	227.913(11)	227.658(11)	231.1328(56)
$\mathbf{P}_{bb}$(amu-Å^2)	83.037692(12)	83.00(13)	83.035(11)	84.651(11)	83.6112(56)
$\mathbf{P}_{cc}$(amu-Å^2)	67.164670(12)	67.159(13)	67.161(11)	67.540(11)	67.1653(56)

3.2. KINETIC ENERGY AND POTENTIAL ENERGY CALCULATIONS

The one-dimensional Schrödinger equation in terms of the ring-twisting coordinate χ_2 (as shown in Fig. 6) is

$$H(\chi_2)\Psi(\chi_2) = E\Psi(\chi_2) \tag{1}$$

where the Hamiltonian is given by

$$H(\chi_2) = (\frac{\hbar}{2})\frac{\partial}{\partial\chi_2}g_{55}(\chi_2)\frac{\partial}{\partial\chi_2} + (\chi_2). \tag{2}$$

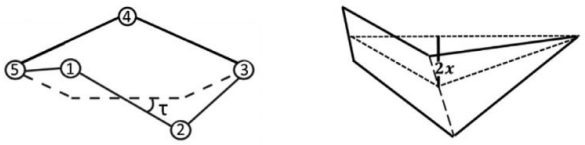

Figure 6. Definition of the ring-twisting angle $\tau = \chi_2$ and the ring-puckering coordinate, $\chi = \chi_1$.

$V(\chi_2)$ is given in

$$V(\chi_2) = a\chi_2^4 + b\chi_2^2 \tag{3}$$

and the reciprocal reduced mass expansion $g_{55}(\chi_2)$ reflects the fact that the reduced mass value changes with the ring-twisting coordinate is given by

$$g_{44}(\chi_2) = \sum_{i=0}^{6} g_{55}^i \chi_2^i. \tag{4}$$

These $g_{55}(\chi_2)$ terms were calculated by methods previously described [29, 30, 31].

The Laane group TWISTANE program [32], which is based on vector and numerical methods, was used to calculate the coordinate dependent kinetic energy functions $g_{55}(\chi_2)$ for the ring-twisting. The geometrical parameters for the computed planar structures of these molecules provided the input for the programs. The vibration was assumed to be curvilinear and the magnitude of the reciprocal reduced mass g_{55} was calculated for different values of the ring-twisting coordinate χ_2 so that the full $g_{55}(\chi_2)$ function could be determined. (Subscripts 1 to 3 on g are reserved for the molecular rotations and 4 for the ring-puckering vibration).

Using these potential energy parameters in Eq. 3, the DA1OPTN Meinander-Laane potential energy program [33] was used to calculate the theoretical energy levels and energy level spacings, seen in Fig. 9.

The theoretical equations for the 1-D potential energy functions and the calculated potential energy surface which as coordinates the ring-twisting angle, and the ring-twisting coordinate were obtained using the MAPLE 2015.1 computing environment [34].

3.3. POTENTIALl ENERGY SURFACES

The potential energy surface (PES) based on the calculated MP2/cc-pVTZ energies of 34 different configurations calculated for *c*-$C_4H_8SiF_2$ is:

$$V(cm^{-1}) = 3.297 \times 10^5 \chi_1^4 - 2.971 \times 10^4 \chi_1^2 + 4.080 \times 10^4 \chi_2^4 - 2.007 \times 10^4 \chi_2^2 + 2.854 \times 10^5 \chi_1^2 \chi_2^2 + 4.337 \times 10^5 \chi_1^4 \chi_2^4 + 2328. \quad (5)$$

For the sake of comparison, the potential energy surface (PES) based on the calculated MP2/cc-pVTZ energies of 28 different configurations calculated for *c*-$C_4H_8SiH_2$ is:

$$V(cm^{-1}) = 3.928 \times 10^5 \chi_1^4 - 4.039 \times 10^4 \chi_1^2 + 4.433 \times 10^4 \chi_2^4 - 2.124 \times 10^4 \chi_2^2 + 2.929 \times 10^5 \chi_1^2 \chi_2^2 + 9.540 \times 10^5 \chi_1^4 \chi_2^4 + 2328. \quad (6)$$

The calculated PES for *c*-$C_4H_8SiF_2$ and *c*-$C_4H_8SiH_2$ and the plot of their contour maps are shown in Figs. 7 and 8.

Numerically and graphically it is seen on Table 3 and Figs. 7 and 8 that the calculated geometric parameters for the twisted conformers are quite similar for 1,1-difluorosilacyclopentane and silacyclopentane. However, the energy for the pure bent conformation for 1,1-difluorosilacyclopentane is 669 cm^{-1} lower in energy than its planar form and the pure bent conformation for silacyclopentane is 1036 cm^{-1} lower in energy than its planar form leading the visualization of this local minimum closer to the respective global maximum.

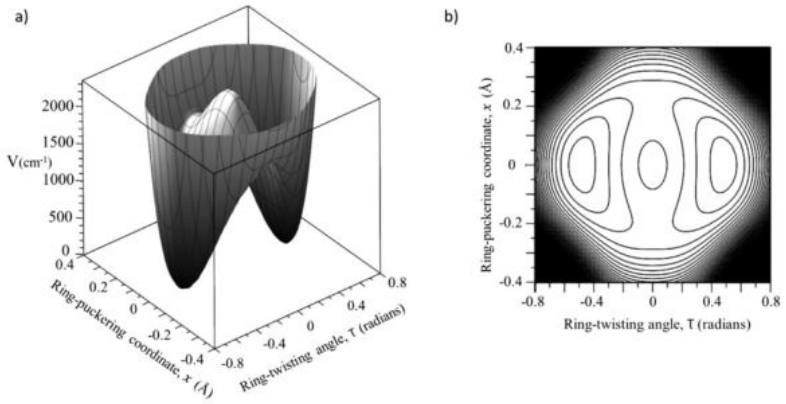

Figure 7. a) PES and b) contour map for *c*-$C_4H_8SiF_2$ from MP2/cc-pVTZ computations. The maximum calculated energy corresponds to the planar structure at 2338 cm^{-1}.

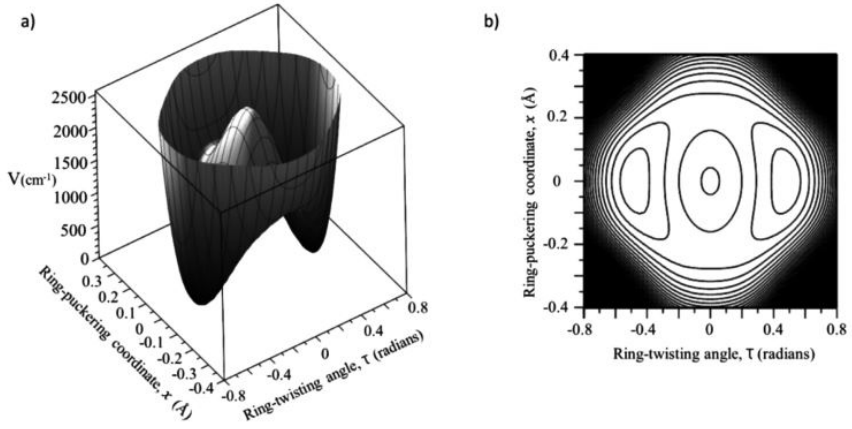

Figure 8. a) PES and b) contour map for *c*-$C_4H_8SiH_2$ from MP2/cc-pVTZ computations. The maximum calculated energy corresponds to the planar structure at 2544 cm^{-1}.

Table 3. Calculated energies and ring parameters of selected conformations of c-$C_4H_8SiH_2$ (top) and c-$C_4H_8SiH_2$ (bottom) at the CCSD and MP2 levels of theory.

	c-$C_4H_8SiH_2$					
	Twisted, C_2		Bent, C_2		Planar (TS)	
	CCSD/cc-pVTZ	MP2/cc-pVTZ	CCSD/cc-pVTZ	MP2/cc-pVTZ	CCSD/cc-pVTZ	MP2/cc-pVTZ
Energy, cm^{-1}	0	0	1566	1659	2136	2338
τ, radians	+/-0.48	+/-0.48	0	0	0	0
χ, Å	0	+/-0.0204	+/-0.0204	0	0	0
	c-$C_4H_8SiF_2$					
	Twisted		Bent		Planar (TS)	
	CCSD/cc-pVTZ	MP2/cc-pVTZ	CCSD/cc-pVTZ	MP2/cc-pVTZ	CCSD/cc-pVTZ	MP2/cc-pVTZ
Energy, cm^{-1}	0	0	1451	1508	2338	2544
τ, radians	+/-0.48	+/-0.49	0	0	0	0
χ, Å	0	+/-0.224	+/-0.232	0	0	0

3.4. POTENTIAL ENERGY FUNCTIONS FOR THE RING-TWISTING

The potential energy functions (PEFs) for c-$C_4H_8SiF_2$ and c-$C_4H_8SiH_2$ were obtained according to both MP2/cc-pVTZ and CCSD/cc-pVTZ computations.

The calculated reduced mass for c-$C_4H_8SiF_2$ is 33.31 amu from the CCSD/cc-pVTZ computations and 33.41 amu from the MP2/cc-pVTZ computations. The $g_{55}(\chi)$ kinetic energy functions are done using the geometrical parameters of the planar structures. The g_{55} kinetic energy function for c-$C_4H_8SiF_2$ from the CCSD/cc-pVTZ computations is:

$$g_{55}(\chi) = 3.002 \times 10^{-2} - 9.597 \times 10^{-2}\chi_2^2 + 3.002 \times 10^{-2}\chi_2^4 \tag{7}$$

and the theoretical 1-D PEF is:

$$V(cm^{-1}) = 4.199 \times 10^4\chi_2^4 - 1.894 \times 10^4\chi_2^2 \tag{8}$$

The $g_{55}(\chi)$ kinetic energy function for c-$C_4H_8SiF_2$ from the MP2/cc-pVTZ computations is:

$$g_{55}(\chi) = 2.993 \times 10^{-2} - 9.638 \times 10^{-2}\chi_2^2 + 1.401 \times 10^{-1}\chi_2^4 \tag{9}$$

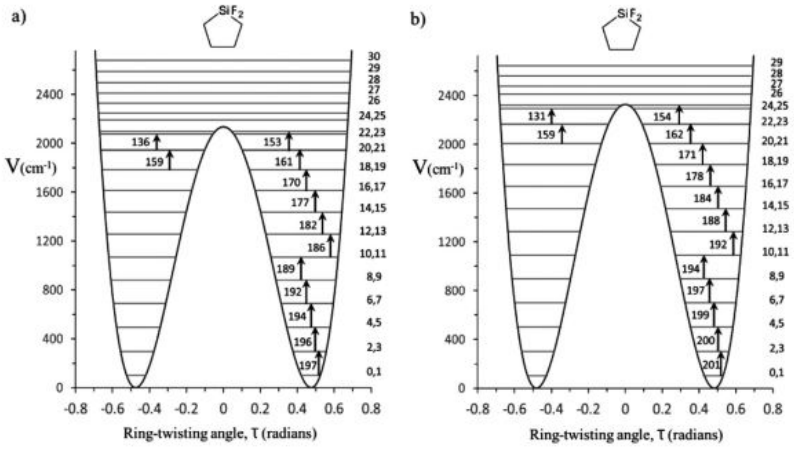

Figure 9. a) Calculated one-dimensional ring-twisting PEF and energy levels for c-$C_4H_8SiF_2$ from CCSD/cc-pVTZ computations (Reduced mass: 33.31 amu). b) Calculated PEF and energy levels for c-$C_4H_8SiH_2$ from MP2/cc-pVTZ computations for c-$C_4H_8SiH_2$ (Reduced mass: 33.41 amu). All the lowest energy levels in a) and b) appear as degenerate.

and the theoretical 1-D PEF is:

$$V(cm^{-1}) = 4.324 \times 10^4 \chi_2^4 - 2.007 \times 10^4 \chi_2^2 \tag{10}$$

Fig. 9 shows the calculated energy levels for c-$C_4H_8SiF_2$ using the $g_{55}(\chi)$ functions and the calculated potential energy parameters in the DA1OPTN Meinander-Laane potential energy program [33].

Previously two-dimensional fits for the calculation of the energy levels taking in account the ring-puckering parameter, ring-puckering parameter, χ_1 and the ring-twisting parameter, χ_1 based on experimental data have been reported for the parent c-$C_4H_8SiH_2$ molecule [35]. Utilizing the calculated reduced mass and the $g_{55}(\chi)$ values from our present work, we have calculated a one-dimensional experimentally fitted PEF that is shown in Fig. 10. Table 4 shows a comparison of the observed and calculated ring-twisting frequencies, and the agreement is very good. This PEF may be compared to the theoretically determined PEFs in Fig. 10. These are presented to provide a perspective on the accuracy that can be expected for the difluoride PEF presented in this work.

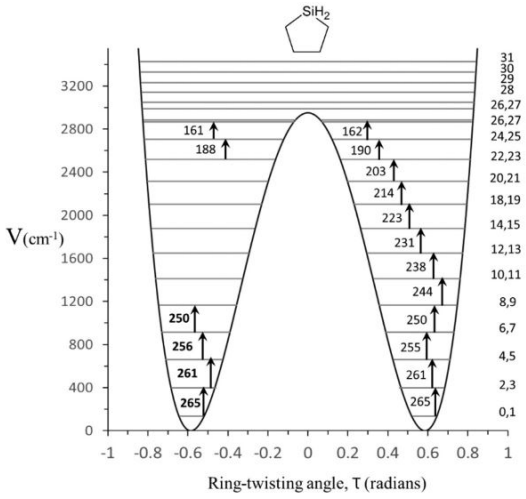

Figure 10. 1-D PEF from experimental fit for the ring-twisting vibration of c-$C_4H_8SiH_2$. The observed values [35] are indicated in bold.

The 1990 paper [35] reported a 1-D PEF fit barrier of 3250 cm^{-1}. Our experimental 1-D barrier is 2951 cm^{-1}. The paper also shows an optimal two-dimensional fit with a barrier of 2110 cm^{-1}, which is very similar to that obtained from our theoretical CCSD/cc-pVTZ computations, which is 2338 cm^{-1}.

The experimentally 1-D PEF for c-$C_4H_8SiH_2$ obtained in this work is:

$$V(cm^{-1}) = 2.518 \times 10^4 \chi_2^4 - 1.724 \times 10^4 \chi_2^2 \tag{11}$$

The calculated reduced mass for the parent c-$C_4H_8SiH_2$ molecule is 30.17 amu according to our CCSD/cc-pVTZ computations. This calculated reduced mass along with its complete $g_{55}(\chi)$ expression was used to perform the experimental fit. The value of the reduced mass from our MP2/cc-pVTZ computations is 30.19 amu. Previously the reduced mass was reported to be 31.38 amu by Laane et al. in 1990 [35]. The $g_{55}(\chi)$ kinetic energy function for c-$C_4H_8SiH_2$ from the CCSD/cc-pVTZ computations is:

$$g_{55}(\chi) = 3.315 \times 10^{-2} - 7.484 \times 10^{-3} \chi_2^2 + 6.427 \times 10^{-3} \chi_2^4, \tag{12}$$

Table 4. Observed and calculated ring-twisting transitions (cm^{-1}) for c-$C_4H_8SiH_2$ from experimental fitted PEF.

	Observed[a]	Experimental Fit					
	FIR	This Work		Literature[a]			
Transition	V(cm^{-1})	V(cm^{-1})[b]	Δ	V(cm^{-1})[c]	Δ	V(cm^{-1})[d]	Δ
FIR[a]							
0-2	265.2	265.3	-0.1	265.2	0.0	267.9	-2.7
2-4	260.5	260.5	0.0	260.5	0.0	260.5	0.0
4-6	255.8	255.5	0.3	255.7	0.1	252.3	3.5
6-8	249.8	250.0	-0.2	250.6	0.8	243.4	6.4

[a] From reference [35].
[b] V(cm^{-1}) = 2.518 x $10^4{\chi_2}^4$ - 1.724 x $10^4{\chi_2}^2$
[c] V(cm^{-1}) = 2.46 x $10^4{\chi_1}^4$ - 1.26 x $10^4{\chi_1}^2$ + 2.28 x $10^4{\chi_2}^4$ - 1.70 x $10^4{\chi_2}^2$ + 9.47 x $10^4{\chi_1}^2{\chi_2}^2$
[d] V(cm^{-1}) = 1.10 x $10^4{\chi_1}^4$ - 5.14 x $10^3{\chi_1}^2$ + 3.68 x $10^4{\chi_2}^4$ - 1.76 x $10^4{\chi_2}^2$ + 1.17 x $10^5{\chi_1}^2{\chi_2}^2$

and the related theoretical PEF is:

$$V(cm^{-1}) = 4.199 \times 10^4 \chi_2^4 - 1.894 \times 10^4 \chi_2^2. \tag{13}$$

The $g_{55}(\chi)$ kinetic energy function for c-$C_4H_8SiH_2$ from the MP2/cc-pVTZ computations is:

$$g_{55}(\chi) = 3.312 \times 10^{-2} - 7.460 \times 10^{-3} \chi_2^2 + 6.413 \times 10^{-3} \chi_2^4, \tag{14}$$

and the related theoretical PEF is:

$$V(cm^{-1}) = 4.433 \times 10^4 \chi_2^4 - 2.124 \times 10^4 \chi_2^2. \tag{15}$$

Fig. 11 shows the theoretical PEFs along with their calculated energy levels for the parent c-$C_4H_8SiH_2$ using the $g_{55}(\chi)$ functions.

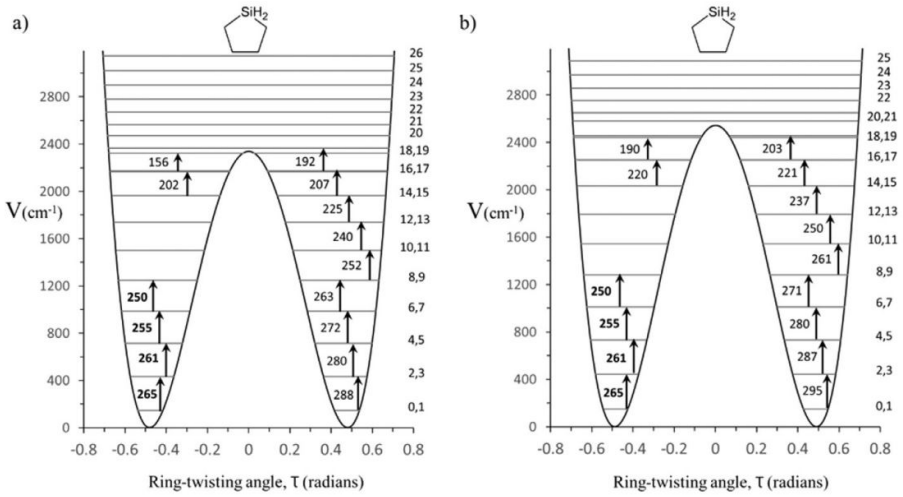

Figure 11. a) Calculated one-dimensional ring-twisting PEF and energy levels for *c*-$C_4H_8SiH_2$ from CCSD/cc-pVTZ computations (Reduced mass: 33.3 amu). b) Calculated PEF and energy levels for *c*-$C_4H_8SiH_2$ from MP2/cc-pVTZ computations. (Reduced mass: 33.4 amu). All the lowest energy levels in a) and b) appear as degenerated. The observed values [33] are indicated in bold.

4. RESULTS AND ANALYSIS

4.1. MICROWAVE SPECTRA AND ANALYSIS

Analysis of the spectra was performed using SPFIT and SPCAT [36] in combination with Kisiel's AABS package [37]. An *S*-reduced Hamiltonian in the I^r representation was employed while fitting the spectra. Using the calculated rotational constants, which can be seen in Table 5, a total of 50 lines for the parent species were observed. Although the experiment was only powered for 6-18 GHz, transitions up to 20.3 GHz for the parent isotopologue were observed and assigned. Fig. 12 shows the location of the *a*, *b*, and *c* axes for *c*-$C_4H_8SiF_2$. In addition, the isotopologues corresponding to each ^{13}C, ^{29}Si, and ^{30}Si were observed and their corresponding rotational constants can be found in Table 5. For the isotopologues 26, 22, 24, and 24 transitions were observed for $^{13}C1$ / $^{13}C4$, $^{13}C2$ / $^{13}C3$, ^{29}Si, and ^{30}Si, respectively. It should be noted that some of the Microwave RMS values for these isotopes are larger than traditional values due to the parameters added for

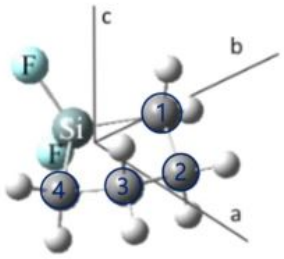

Figure 12. Principal axes a, b, and c of the c-$C_4H_8SiF_2$ twisted structure.

the splitting but are of usual magnitude for similar large amplitude motion spectroscopic fits. Table 5 also shows the calculated rotational constants from the theoretical calculations. Overall, the theoretical calculations appear to be in good agreement with the experimental data since the values differ by roughly 1%. The quantum number assignments and fits can be found in the Supporting Information.

Table 5. c-$C_4H_8SiF_2$ experimental parameters compared to theory (DFT).

Ground Vibrational States	c-$C_4H_8SiF_2$ Splitting Fit Separately	c-$C_4H_8SiF_2$ Splitting Fit Together	^{29}Si	^{30}Si	^{13}C1 / ^{13}C4	^{13}C2 / ^{13}C3
A_0 (MHz)	3364.6527(41)[a]	3364.654176(50)	3364.86(57)	3364.80(47)	3320.69(50)	3351.84(25)
B_0 (MHz)	1716.4316(12)	1716.4320798(82)	1714.5574(31)	1712.7135(30)	1712.0044(36)	1694.2075(18)
C_0 (MHz)	1628.6318(12)	1628.6325533(77)	1626.9383(31)	1625.2808(30)	1618.2019(37)	1605.6823(18)
A_1 (MHz)	3364.6453(57)	—	—	—	—	—
B_1 (MHz)	1716.4204(53)	—	—	—	—	—
C_1 (MHz)	1628.6278(45)	—	—	—	—	—
D_J (kHz)	0.145(23)	0.17637(31)	[0.17637][c]	0.122(50)	0.140(64)	0.090(31)
D_{JK} (kHz)	0.911(56)	1.00210(59)	[1.0021]	1.11(16)	1.07(20)	1.54(10)
D_K (kHz)	1.07(45)	0.6148(68)	[0.6148]	[0.6148]	[0.6148]	[0.6148]
F_{BC} (MHz)	0.930(52)	0.83595(75)	[0.93595]	[0.93595]	[0.93595]	[0.93595]
$\Delta E_{0,1}$ (MHz)	39755.59(64)	39456.547(79)	[39456.547]	[39456.547]	[39456.547]	[39456.547]
ν_{RMS} (kHz)[b]	16.6	25.3	29.7	21.4	27.7	12.9
Number of Transitions	47	47	24	24	26	22
Theoretical Equilibrium Parameters *B3LYP/cc-pVTZ*						
A_e (MHz)	3340	3340	3340	3340	3300	3300
B_e (MHz)	1700	1700	1640	1700	1700	1680
C_e (MHz)	1620	1620	1610	1610	1610	1590

[a] Numbers in parentheses give standard errors at 1σ (67% confidence) level to the least significant figure.
[b] MW RMS is defined as $\sqrt{(\sum[(obs-calc)^2]/n)}$.
[c] Values in brackets there were held to the parent value.

All observed lines are *a*-type transitions. No *b*-type or *c*-type transitions were observed. These observations are in accordance with the predicted dipole values of 2.47, 0.00, and 0.00 D for μ_a, μ_b, and μ_c, respectively, at the B3LYP/def2TZVP with gd3bj level of theory. In addition, the majority of transitions were *R*-branch transitions with the second most abundant transitions being *Q*-branch. No *P*-branch transitions were observed.

As mentioned previously, splitting in the spectra due to the ring puckering motion was observed. An example of one such transition exhibiting this splitting is the $6_{06} \leftarrow 5_{05}$ transition shown in Fig. 13. Fifteen such transitions exhibited this type of splitting. Thus, to fit those transitions, a rotation-vibration term, $F_a P_A \rho_Z$, was required, where F_a is the Coriolis parameter, P_A is the angular momentum about the *a*-axis, and ρ_Z is the linear momentum resulting from the inversion moment. This Coriolis parameter has been chosen because the two equivalent structures of *c*-$C_4H_8SiF_2$ going through the planar maximum energy of the motion arise from the twisting motion about the *a*-axis. As described by Pickett [38], a better fit of the vibration-rotation interaction results from using the equivalent operator, F_{bc}, $(P_B P_C + P_C P_B)\rho_Z$. $\Delta E_{0,1}$ is also necessary to account for the inversion frequency of the ring-twisting motion. Although fitting this type of spectra is described as a tunnelling motion in Pickett, it is fit using vibrational states as labels. Therefore, $v = 0$ and $v = 1$ correspond to an A and E of a methyl rotor or + and – of a ring-twisting motion. As a check for self-consistency, two fits were undertaken as noted in Table 5. One is labelled "Fit Separately", and the other is labeled "Fit Together". In the "Fit Separately" approach, three rotational constants and three quartic centrifugal distortion constants—D_J, D_{JK}, and D_K—were fit to each individual ring-twisting state, labeled $v = 0$ and $v = 1$. In the "Fit Together" approach, only three rotational constants are used with all other constants remaining the same. Both approaches yielded very similar spectroscopic outcomes as shown in Table 5, providing some assurance this was accurately describing the

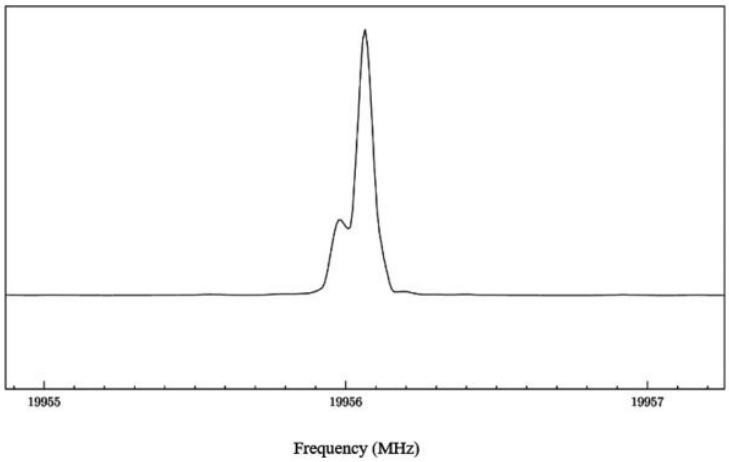

Figure 13. Example of doubling seen in spectrum due to ring-twisting for the $6_{06} \leftarrow 5_{05}$ transition.

observed splitting. The "Fit Together" approach was used for analysis as that fitting method utilized fewer Hamiltonian parameters with a similar magnitude uncertainty in the fit (within a factor of 2). A list of the split transitions is located in the Supporting Information.

The identification of ^{13}C, ^{29}Si, and ^{30}Si isotopologues was accomplished by obtaining the ratio of the calculated rotational constants of the parent to the experimentally determined ones and using this ratio to adjust the "calculated" isotopologue rotational constants acquired by simply changing the atomic masses of the specific nuclei in question. This yielded isotopologue rotational constant predictions with great accuracy and ease, making traditional assignments for these species much simpler. Then, the correct relative intensity aspect of the CP-FTMW technique was utilized in order to accurately identify each singly substituted species in natural abundance. An example of this relative intensity profile can be found in Fig. 14 for the $5_{15} \leftarrow 4_{14}$ transition. After successfully assigning the spectra associated with each isotopologue, a Kraitchman [39] substitution structure for the ring was determined. This process was carried out using Kisiel's KRA program [40]. The results from the Kraitchman analysis can be seen in Table 6. Then, Kisiel's EVAL program [28] was utilized to determine the corresponding bond angles, bond lengths, and dihedral angles

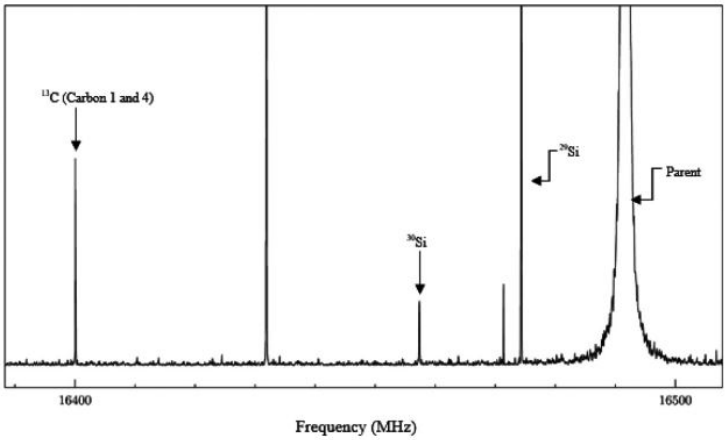

Figure 14. Example of the relative intensity profile for the isotopic species observed for the $5_{15} \leftarrow 4_{14}$ transition. All species are labeled within the figure.

for the elements contained within the ring. Both the KRA and EVAL program were obtained from the PROSPE website [40]. Because magnitudes and not absolute atom positions are given in the Kraitchman analysis, experimental structure determinations were aided by substitution of the computational sign values for the experimentally determined positions. From this analysis, the experimental substitution structure for the ring was determined to be nonplanar with a nonzero dihedral angle for every combination in the ring.

Table 6. Kraitchman atomic coordinates with Costain errors [39].

	^{29}Si (Å)	^{30}Si (Å)	^{13}C1 / ^{13}C4 (Å)	^{13}C2 / ^{13}C3 (Å)[a]
a	0.57 ± 0.11	0.57 ± 0.01	0.62 ± 0.01	2.0 ± 0.01
b	0.00[b] ± 0.10	0.00 ± 0.08	(-/+)[c] 1.3 ± 0.01	$(-/+)_d$ 0.77 ± 0.01
c	0.00 ± 0.09	0.00 ± 0.07	(+/-)[c] 0.65 ± 0.01	$(+/-)_d$ 0.03 ± 0.13

[a] Kraitchman Analysis only reports magnitude, but signs of coordinates were assigned by authors to correspond to their computed position values.[b] Values reported as 0.00 are imaginary values. [c] The first sign in parentheses represents C_1 while the second represents C_4. [d] The first sign in parentheses represents C_2 while the second represents C_3 .

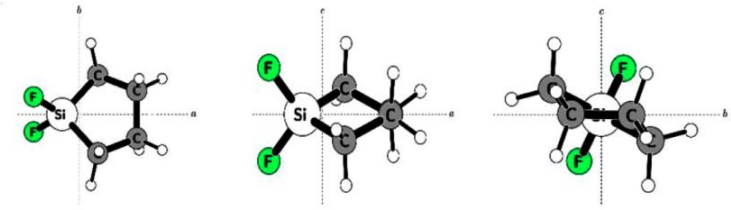

Figure 15. Calculated geometrical structure of *c*-$C_4H_8SiF_2$ within the *ab*-, *ac*- and *bc*-planes.

5. DISCUSSION

From the results of the high-level *ab initio* calculations and microwave spectroscopy experiments, *c*-$C_4H_8SiF_2$'s minimum energy structure has C_2 symmetry as shown in Fig. 5.

Fig. 15 shows the molecule in the *ab*-, *ac*-, and *bc*-molecular planes. As is shown in this view, the minimum energy C_2 structure distributes the twisted carbons out of the *ab*-molecular plane with their mass now distributed in the *ac*-molecular plane. This is consistent with other works performed previously on members of the silacyclopentane family [7, 10]. Inversion splitting due to the ring motion in the molecule was observed and analysed via potential energy calculations described previously. Based on these calculations, it was determined that there are two equal conformations for the minimum energy structure that were separated by an energy barrier corresponding to the planar conformation. The potential energy barrier between these two minimum energy structures, accessible by a ring-twisting motion, is calculated to be 2,338 cm^{-1}. From this potential energy surface, the lowest energy levels appear degenerate. There is still enough nondegeneracy, however, at the bottom of the well which has been observed at the resolution of the CP-FTMW experiment. The experimentally determined splitting of these states is approximately 1.33 cm^{-1}, well within the uncertainty of the calculations presented.

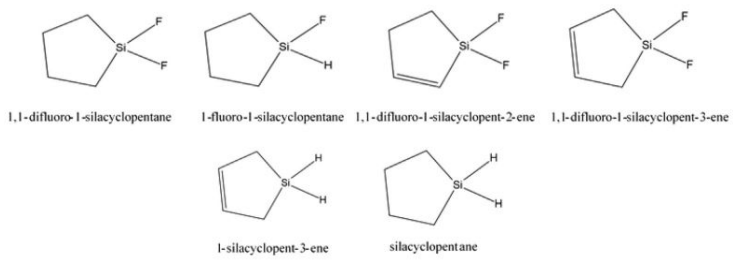

Figure 16. Molecular structures of molecules under comparison.

In order to understand more regarding the determined structure of *c*-$C_4H_8SiF_2$, it is ideal to compare it to other molecules within the silacyclopentane family. Because second moments measure the extension of a molecule's mass along a given axis (or outside a plane), it provides an efficient way to interpret a molecule's structure, especially when only parent isotopologue data are available [41, 42]. Within Table 7, the second moments for six molecules can be seen. In addition to *c*-$C_4H_8SiF_2$, this table includes 1,1-difluoro-1-silacyclopent-2-ene (*c*-$(CH)_2CH_2CH_2SiF_2$) [13], 1,1-difluoro-1-silacyclopent-3-ene (*c*-$CH_2(CH)_2CH_2SiF_2$) [43], 1-fluoro-1-silacyclopentane (*c*-C_4H_8SiHF) [11], silacyclopent-3-ene (*c*-$CH_2(CH)_2CH_2SiH_2$) [43], and finally *c*-$C_4H_8SiH_2$ [10]. The second moments reported in Table 7 were obtained using the PLANM program obtained from PROSPE [40] in conjunction with the rotational constants reported in the respective works. The structures of these molecules can be seen in Fig. 16.

Table 7. Second moment comparison between *c*-$C_4H_8SiF_2$ and related molecular species.

	P_{aa} (amu-Å^2)	P_{bb} (amu-Å^2)	P_{cc} (amu-Å^2)
***c*-$C_4H_8SiF_2$**	227.27110(12)	83.037692(12)	67.164670(12)
***c*-$(CH)_2CH_2CH_2SiF_2$ [13]**	224.058503(94)	77.698347(94)	62.708151(94)
***c*-$CH_2(CH)_2CH_2SiF_2$ [43]**	217.351320(13)	78.740452(13)	63.705230(13)
***c*-C_4H_8SiHF [11]**	185.68(01)	79.82(01)	27.70(01)
***c*-$CH_2(CH)_2CH_2SiH_2$) [43]**	105.135570(77)	78.740452(77)	6.224120(77)
***c*-$C_4H_8SiH_2$ [10]**	109.85388(1)	80.028848(1)	12.35876(1)

The second moment values presented in Table 7 may provide structural insight [41, 42], but care must be taken in order to make comparisons within a family. First of all, halogen substitution will cause a shift in the *a*-, *b*-, and *c*-axis system, so it is easiest to make comparisons among species with equal substitution above and below the ring (difluoro molecules, for example). Because ring-planarity in these molecules moves mass out of the *ab*-plane and into the *ac*-plane, we can monitor planarity by comparison of the P_{bb} (out-of-*ac*-plane mass) and P_{cc} (out-of-*ab*-plane mass) values. We will focus on P_{bb} here because the change in P_{cc} values due to halogenation make them also hard to follow. *c*-$(CH)_2CH_2CH_2SiF_2$, *c*-$CH_2(CH)_2CH_2SiF_2$, and *c*-$CH_2(CH)_2CH_2SiH_2$ are known to be planar [13, 43]. Their P_{bb} values all lie within 1.1 amu-Å^2 of one another. The nonplanar molecules, *c*-$C_4H_8SiF_2$ and *c*-$C_4H_8SiH_2$, have an increase in P_{bb} greater than 1.1 amu-Å^2 from any of the comparator planar molecules with an increase of > 4 amu-Å^2 for *c*-$C_4H_8SiF_2$. This can only be due to the carbons twisting out of the *ab*-plane and into the *ac*-plane as is shown in Fig. 15.

Another comparison that can be drawn between the six molecules listed in Table 7 is the presence of splitting within the spectra from non-degenerate energy levels present due to ring-twisting. For the work performed on *c*-$C_4H_8SiH_2$ [10], *c*-$(CH)_2CH_2CH_2SiF_2$ [13] and *c*-C_4H_8SiHF [11], no split transitions were reported. However, for *c*-$C_4H_8SiF_2$, *c*-$CH_2(CH)_2CH_2SiF_2$, and *c*-$CH_2(CH)_2CH_2SiH_2$ splitting was observed [43]. Though, it should be noted that the source of the splitting for *c*-$CH_2(CH)_2CH_2SiF_2$ was undetermined. Within the present work, fifteen split transitions were observed and assigned. What is interesting about the specific transitions that exhibited splitting was that they were not from the strongest transitions but from weaker transitions with higher *J* values. These transitions tended to be weaker in intensity in our spectrum, so their observation is due to the deep averaging and resolution capabilities of the CP-FTMW, the molecule's large dipole moment,

and smaller rotational constants due to the mass of the molecule. As a result, we hypothesize that the similar molecule *c*-$C_4H_8SiH_2$ should possess split transitions but were not observed because the higher *J* values were not accessible in the experiment.

The evolution of experiments performed on the members of the silacyclopentane family, therefore, is representative of the sensitivity improvements that have been made with the CP-FTMW. The observation of split transitions where there are none predicted within computational uncertainty provides a basis to improve current theoretical approaches so that models may be refined. Yet, the heavy-atom experimental (r_s) structure agrees well with the equilibrium geometry predicted by the theoretical approaches employed indicating that the optimized structures are correct.

6. SUMMARY

Within this work, the pure rotational spectrum of *c*-$C_4H_8SiF_2$ was studied using CP-FTMW. In addition to the parent species, the isotopologues of ^{13}C, ^{29}Si, and ^{30}Si were also measured and fit, resulting in the generation of a heavy atom structure. This structure exhibited ring-twisting that caused certain transitions to appear split. Potential energy surfaces for the ring-twisting motion were undertaken and the experimentally determined energy level difference observed in comparison to these surfaces is reasonable. The ring structure of *c*-$C_4H_8SiF_2$ has been determined to be nonplanar through Kraitchman analysis and comparison of the P_{bb} second moment amongst a family of similar molecules.

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II. THE MOLECULAR STRUCTURE AND CURIOUS MOTIONS IN 1,1-DIFLUOROSILACYCLOPENT-3-ENE AND SILACYCLOPENT-3-ENE AS DETERMINED BY MICROWAVE SPECTROSCOPY AND QUANTUM CHEMICAL CALCULATIONS

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ABSTRACT

The molecules 1,1-difluorosilacyclopent-3-ene ($3SiCPF_2$) and silacyclopent-3-ene (3SiCP) have been synthesized and studied using chirped pulse, Fourier transform microwave (CP-FTMW) spectroscopy. For 3SiCP this is the first ever microwave study of the molecule and, for $3SiCPF_2$, the spectra reported in this work have been combined with that of previous work in a global fit. The spectra of each contain splitting which has been fit using a Hamiltonian consisting of semirigid and Coriolis coupling parameters. A refit of the original $3SiCPF_2$ work was also carried out. All fits and approaches are reported. Analyses of the spectra provide evidence that the molecule is planar which is in agreement with the high-level calculations, but the source of the splitting in the spectra has not been determined.

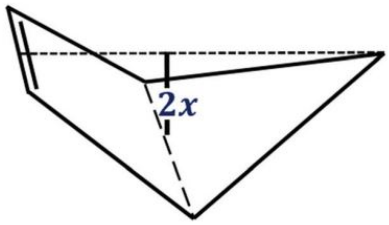

Figure 1. Definition of ring puckering coordinate, x, for cyclopentene and related molecules.

1. INTRODUCTION

The ring-puckering vibrations of four-membered ring and "pseudo-four-membered ring" molecules, such as cyclopentene, have been experimentally investigated by far-infrared, Raman, and microwave spectroscopy [1, 2, 3, 4, 5, 6, 7, 8, 9] for more than half a century. Interest in this vibration arose after R. P. Bell [10] predicted that the potential energy function (PEF) for this motion in a four-membered ring should be quartic in nature. This proved to be mostly true although Laane [9] in 1971 showed that the PEF would be of the form

$$V(x) = ax^4 + bx^2. \tag{1}$$

The constant a arises primarily from angle strain forces while b derives from both torsional and angle strain interaction. This is the case for both four-membered and pseudo-four-membered ring molecules. The ring-puckering coordinate for the latter type is shown in Fig. 1 for cyclopentene.

The great interest in determining the one-dimensional PEF shown in Eqn. 1 has not only been to demonstrate that the quantum mechanical solution works extremely well, but also to provide insight into the conformations and intramolecular forces of these molecules. Cyclopentene was the first pseudo-four-membered ring to be studied [11], and it was shown to be a puckered molecule with a negative b coefficient and a barrier to planarity of 232 cm^{-1}. The barrier was due to CH_2–CH_2 interactions.

In our present study we will report our microwave results for 1,1-difluorosilacyclopent-3-ene (3SiCPF$_2$) and silacyclopent-3-ene (3SiCP). These results are complemented by high level theoretical calculations. The far-infrared spectra of 3SiCP [12] were reported in 1969 and the Raman spectra [13] in 1975. Vibrational assignments [14] were reported in 1972, molecular mechanics calculations [15] in 1989, and theoretical calculations in 2014 [16]. Laane has performed a 2D ring puckering/twisting potential for 3SiCP [17], while Al-Saadi [18] has performed ring puckering calculations for both and 3SiCP and 3SiCPF$_2$. Microwave results have previously been reported for 3SiCPF$_2$ [19], but 3SiCP has not been previously studied. In addition, gas phase electron diffraction results have been previously reported for both 3SiCPF$_2$ and 3SiCP [20]. All work on 3SiCP and 3SiCPF$_2$ are consistent that the molecular ring is planar and the potential energy constant b in Eqn. 1 is small.

We have recently reported the microwave and theoretical work on 1,1-difluorosilacyclopent-2-ene [21] (2SiCPF$_2$). This molecule's experimental (ground state) and theoretical (equilibrium) structure was determined to be planar, with a small, but positive value for the potential energy constant, b.

2. EXPERIMENTAL

The two title compounds were synthesized at the College of Charleston. All reagent transfers and reactions were carried out under an atmosphere of argon or *in vacuo* using standard Schlenk techniques. Solvents were dried with lithium aluminum hydride, stored under argon, and were distilled immediately prior to use. Antimony trifluoride was purified via sublimation, and all other reagents were used as received. ^{1}H, ^{13}C, ^{19}F, and ^{29}Si NMR spectra were obtained using a Bruker 400 MHz NMR spectrometer. NMR chemical shifts were referenced to solvent peaks as internal standards and coupling constant errors were typically about 0.2 Hz.

2.1. SYNTHESIS OF 3SiCPF$_2$

A 20 cm Schlenk tube with a vacuum adapter was equipped with a stir bar, and 1,1-dichlorosilacyclopent-3-ene (4.00 g, 26.3 mmol) was added to the tube. The compound was frozen with liquid nitrogen and antimony trifluoride (4.68 g, 26.3 mmol) was added to the tube while purging with argon. The reaction mixture was frozen with liquid nitrogen, evacuated to 0.10 torr, and closed. The reaction mixture was heated to 55 °C for 1 h while stirring. The product was collected and purified by separating volatile components on a temperature gradient under reduced pressure (0.10 torr). The product was collected in a liquid nitrogen trap after passing through a trap at -65 °C. A total of 1.67 g, 13.9 mmol of purified 1,1-difluoro-1-silacyclopent-3-ene was collected. Yield: 53%. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 6.00 (tt, 4.6 and 1.2 Hz, 2H,=C-H) 1.43 (m, 3.6 and 1.2 Hz, 4H, CH_2). ^{13}C NMR (400 MHz, $CDCl_3$): δ (ppm) 129.38 (t, 4.0 Hz), 11.36 (t, 15.0 Hz).^{19}F NMR (400 MHz, $CDCl_3$): δ (ppm) -139.52 (m, 3.7). ^{29}Si NMR (400 MHz, $CDCl_3$): δ (ppm) 14.84 (t, 323.0 Hz).

2.2. SYNTHESIS OF 3SiCP

Into a 250 mL Schlenk flask equipped with a stir bar was added 1,1-dichloro-silacyclopent-3-ene (20.0 g, 13.2 mmol) in 100 mL of dibutyl ether. The solution was brought to -15 °C and lithium aluminum hydride (1.00 g, 26.4 mmol) was added directly to the flask while purging with argon. The mixture stirred for one hour and the cold bath was removed. After the reaction mixture warmed to rt and stirred for 1 h, the progression of the reaction was checked using ^{1}H NMR spectroscopy. Upon completion, volatile components were vacuum transferred to a second 250 mL Schlenk flask. The flask containing vacuum transferred solvent and product was purified by separating components based on vapor pressure through cold traps under reduced pressure (0.12 torr). The traps were kept at -55 °C, -70 °C, and the temperature of boiling liquid nitrogen (-196 °C). The purified product

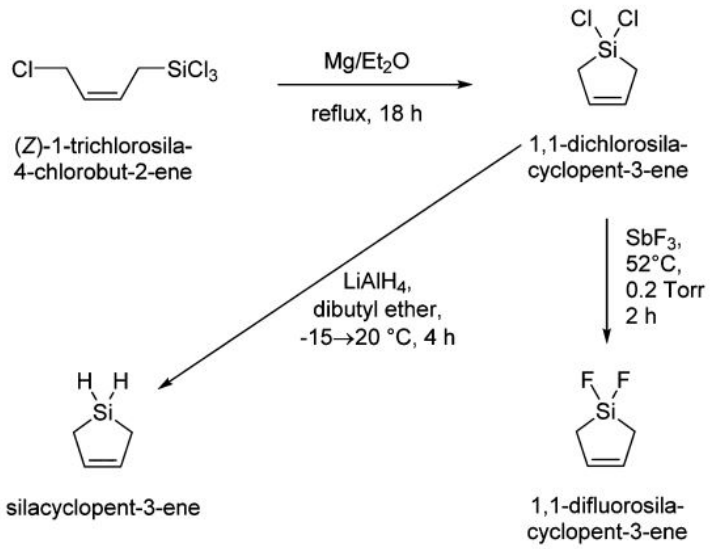

Figure 2. Synthesis processes for 3SiCP and $3SiCPF_2$.

was collected in the liquid nitrogen trap, and solvent and side products were collected in the other two traps. A total of 6.85 g, 81.6 mmol of purified product was isolated. Yield: 62% (Figure 2). ^{1}H NMR (400 MHz,$CDCl_3$): δ (ppm) 5.93 (s, 2H,=C–H), 3.97 (s, 2H, SiH_2), 1.54 (s, 4H, CH_2). ^{13}C NMR (400 MHz, $CDCl_3$): δ (ppm) 131.14, 11.74. ^{29}Si NMR (400 MHz, $CDCl_3$): δ (ppm) -27.69.

2.3. MICROWAVE SPECTROSCOPY

Microwave experiments were performed at Missouri S&T using a chirped-pulse, Fourier transform microwave (CP-FTMW) spectrometer. This spectrometer has been detailed in the literature elsewhere [22, 23, 24, 25, 26]. In the current work, the spectrometer was used in the traditional setup without using multi-antenna detection [26]. Spectra were obtained using 4 μs chirps in separate 6–12 and 12–18 GHz scans. Each scan consisted of the supersonic nozzle being pulsed at 5 Hz with 5, 20 μs free induction decays (FIDs) being collected with each gas pulse until the sample was consumed. For $3SiCPF_2$, 99,900 FIDs were collected and averaged in each scan while 70,000 and 60,000 FIDs were collected

for the 6–12 and 12–18 GHz scans of 3SiCP, respectively. The resultant scans for each molecule are presented in Fig. 3 and 4. The FIDs were averaged in the time domain and Fourier transformed using Kisiel's FFTS [27] software with the default Bartlett window. Using these parameters, typical linewidths have full-width, half maximum (FWHM) values of 60–80 kHz unless otherwise broadened (unresolved splitting, *etc.*) with an attributed 10 kHz uncertainty in the line centers.

Before spectra were acquired, individual tanks containing 3% $3SiCPF_2$ and 3% 3SiCP diluted in Ar were prepared. The resulting samples were introduced into the spectrometer's vacuum chamber (held at 10^{-6} torr) using an absolute pressure of 500 torr (-260 torr relative) through a standard Parker-Hannifins® Series 9 solenoid valve with 0.8 mm orifice.

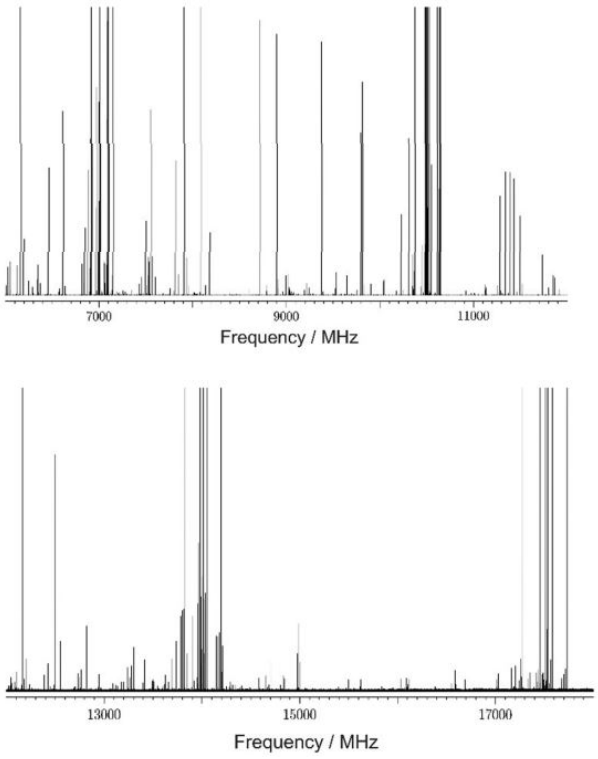

Figure 3. The 6–12 (top) and 12–18 (bottom) GHz spectrum of $3SiCPF_2$. The most intense transitions have been cut off in order to see less intense transitions.

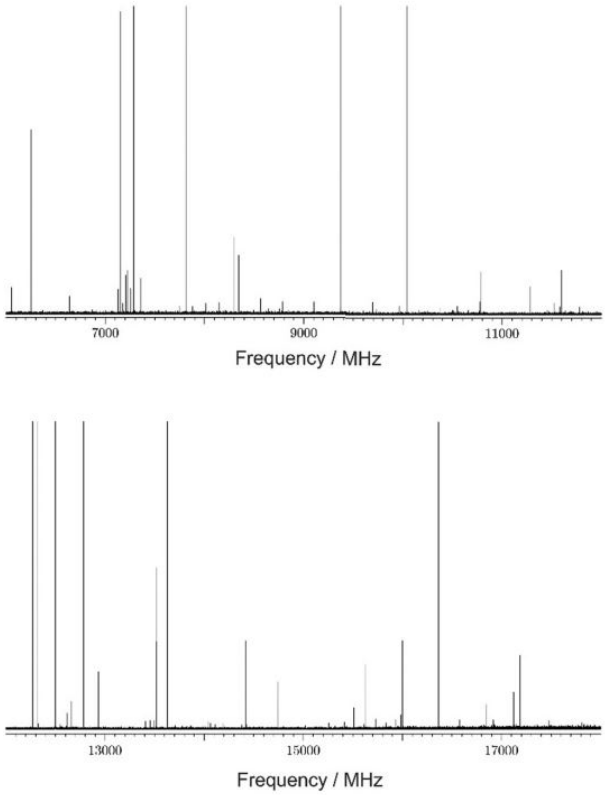

Figure 4. The 6–12 (top) and 12–18 (bottom) GHz spectrum of 3SiCP. The most intense transitions have been cut off in order to see less intense transitions.

3. QUANTUM CHEMICAL CALCULATIONS

3.1. STRUCTURE CALCULATIONS

The geometrical structures, rotational constants and potential energies of diverse conformations of $3SiCPF_2$ and 3SiCP were calculated using CCSD/cc-pVTZ *ab initio* computations at Texas A&M University. The Gaussian 16 program [28] was used for the computations, and the GaussView 6.1.1 graphical interface [29] was used to visualize the structures.

The calculated geometrical structures of $3SiCPF_2$ and 3SiCP are shown in Fig. 5 and the principal rotational constants and dipole moments for these structures are reported in Table 1. The labelling of the carbon atoms is also indicated in the figure. As can be seen,

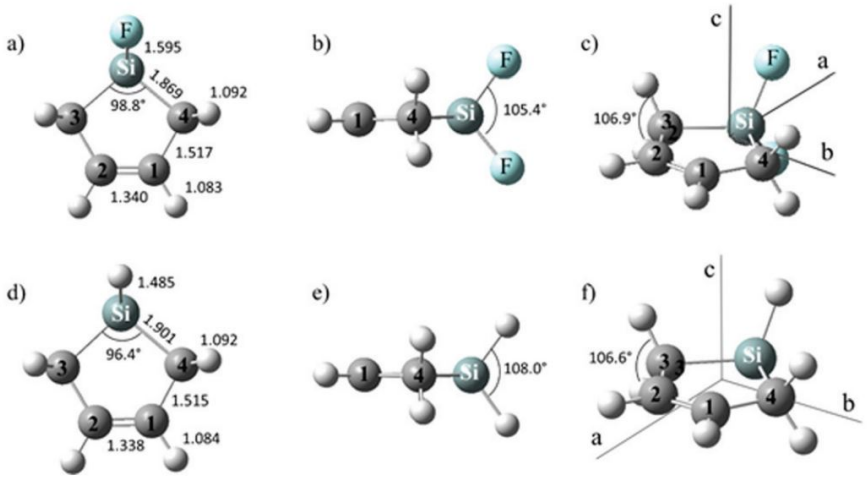

Figure 5. (a–c) Calculated structural parameters of $3SiCPF_2$ and (d–f) 3SiCP in their minimum energy conformations from CCSD/cc-pVTZ computations. The bond distances are in Ångströms (Å). The principal rotation axes *a*, *b* and *c* are shown in (c) and (f).

one effect of substituting the electronegative halide atoms is to shorten the Si–C bonds. The C–Si–C angles are increased by about 2.4 degrees in the dihalide. The F–Si–F angle is about 2.6 degrees smaller than the H–Si–H angle. The other bonds and bond angles are much less affected and have typical magnitudes for Si–C, C–C, and C=C bonds.

Table 1. Theoretically calculated rotational constants for $3SiCPF_2$ and 3SiCP at the CCSD/cc-pVTZ level.

	c-$C_4H_6{}^{28}SiF_2$	c-$C_4H_6{}^{28}SiH_2$
***A*/MHz**	3522.5	5937.3
***B*/MHz**	1780.3	4545.2
***C*/MHz**	1690.6	2731.0
$\lvert\mu_a\rvert$**/D**	2.19	0.31
$\lvert\mu_b\rvert$**/D**	0.00	0.00
$\lvert\mu_c\rvert$**/D**	0.00	0.00

3.2. KINETIC ENERGY AND POTENTIAL ENERGY CALCULATIONS

The quantum mechanical problem has the form

$$\frac{-\hbar^2}{2}\frac{\partial}{\partial x}g_{44}(x)\frac{\partial}{\partial x}\Phi(x) + V(x)\Phi(x) = E\Phi(x) \tag{2}$$

where V is given in Eqn. 1. The Laane ASYMNEW program [30] based on vector and numerical methods was used to calculate the coordinate dependent kinetic energy functions for both molecules. The geometrical parameters for the computed planar structures of these molecules provided the input for the program. The reciprocal reduced mass functions $g_{44}(x)$ were calculated with a dependence on the puckering coordinate x (subscripts 1 to 3 on g are reserved for the molecular rotations).

The conformational energies V *vs.* x were calculated for 10 and 12 values of the ring-puckering coordinate of $3SiCPF_2$ and 3SiCP, respectively. Using Maple software [31] this data was then used to determine the potential energy parameter a and b in Eqn. 1 in order to produce the theoretical PEF. The DA1OPTN Meinander–Laane potential energy program [32] was used to calculate the energy levels and the energy level spacings of $3SiCPF_2$.

The Hermite polynomial coefficients of the wavefunctions for the potential energy functions were calculated using the DA1OPTN Meinander–Laane potential energy program [32]. The wavefunctions were calculated using MAPLE 2015.1 computing environment [31].

A principal aim of this investigation was to understand the energetics of the ring-puckering vibration of $3SiCPF_2$. The one-dimensional quantum mechanical expression we utilized for this study is given in Eqn. 2 and the form of the PEF is given in Eqn. 1. Using the geometrical parameters from the CCSD/cc-pVTZ computations, the kinetic energy functions for $3SiCPF_2$ was calculated.

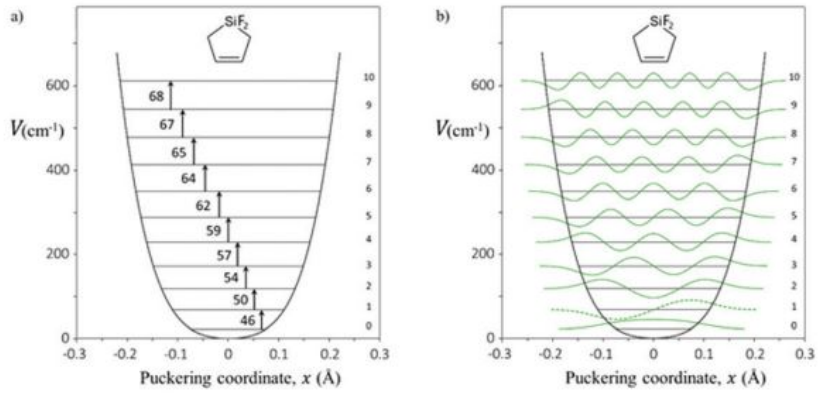

Figure 6. (a) Theoretical ring-puckering PEF for $3SiCPF_2$. The calculated transitions are also shown. (b) Calculated wavefunctions for the lower energy levels. The molecule is calculated to be planar.

This is given by

$$g_{44}(x) = 4.143 \times 10^{-3} - 1.750 \times 10^{-2}x^2 - 1.421 \times 10^{-2}x^4 - 1.281 \times 10^{-1}x^6. \quad (3)$$

The corresponding calculated reduced mass for the ring-puckering for $3SiCPF_2$ is 241.4 μ.

The calculated PES that fitted to the calculated potential energies for 10 different configurations of $3SiCPF_2$ is given by

$$V_{3SiCPF_2}(cm^{-1}) = 2.139 \times 10^5 x^4 + 5.865 \times 10^3 x^2. \quad (4)$$

Fig. 6 show the calculated PES, lowest ring-puckering transitions, energy levels and wavefunctions for $3SiCPF_2$. Fig. 7 shows the experimentally fit PES for 3SiCP previously determined by the Laane research group in 2014 [16]. Our calculated wavefunctions for this molecule are also shown. As mentioned previously, the FIR transitions were observed and reported by Laane in 1969 [12].

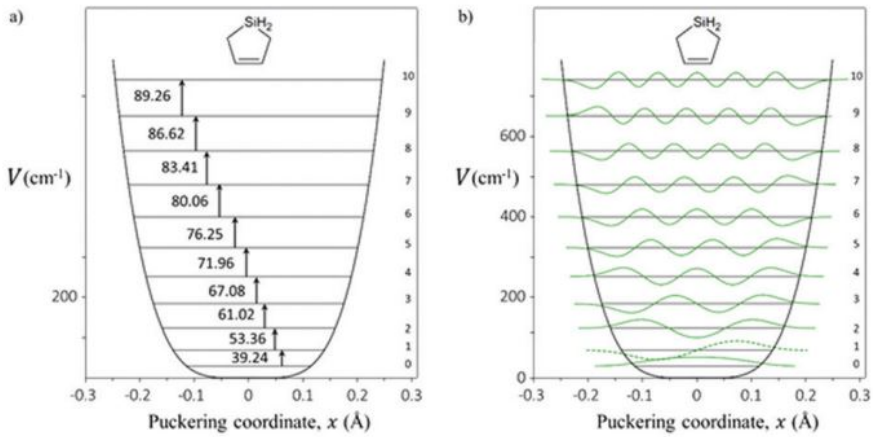

Figure 7. (a) Experimentally fit ring-puckering PEF for 3SiCP. The calculated transitions are also shown in the figure. (b) Calculated wavefunctions for the lower energy levels. The molecule is calculated to be planar.

Fig. 8 shows a comparison of the ring-puckering PEFs for $3SiCPF_2$ and the hydride 3SiCP. The potential energy constant for Eqn. 1 and the calculated reduced masses for each are given in Table 2. $3SiCPF_2$ is calculated to be slightly more rigid than 3SiCP.

Table 2. Potential energy parameters[a] for $3SiCPF_2$ and 3SiCP using $V = ax^4 + bx^2$.

Molecule	Reduced mass/μ	a	b	Barrier, cm^{-1}
$3SiCPF_2$[b]	241.40	2.139 x 10^5	5.865 x 10^3	0
3SiCP[b]	127.84	2.273 x 10^5	2.751 x 10^3	0
3SiCP[c]	128.64	2.130 x 10^5	-0.054 x 10^4	0.3
3SiCP[d]	158.44	2.089 x 10^5	2.810 x 10^2	0

[a] Units for a are cm^{-1} $Å^{-4}$; units for b are cm^{-1} $Å^{-2}$. The reduced mass is in atomic units.
[b] From CCSD/cc-pVTZ computations.
[c] From ref. [12]. The PEF was experimentally fit according to an estimated reduced mass reported in 1969.
[d] From ref. [16]. The PEF was experimentally fit according to the calculated reduced mass reported in ref. [17].

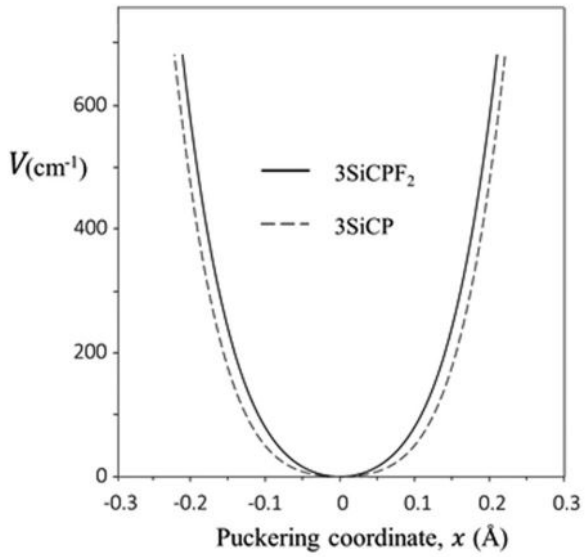

Figure 8. Comparison of calculated PEFs for $3SiCPF_2$ and 3SiCP from CCSD/cc-pVTZ computations.

4. RESULTS AND DISCUSSION

4.1. ASSIGNMENT

Assignments were performed on both $3SiCPF_2$ and 3SiCP using Pickett's SPFIT/SPCAT [33] program suite in conjunction with Kisiel's AABS [34] software front-end. Both molecules were fit using a Watson *S*-reduced Hamiltonian in the I^r representation [35]. Rotational constants and quartic centrifugal distortion constants D_J and D_{JK} were needed to adequately describe each data set. All assignments and fit files have been reproduced in a easily read format using PIFORM [36] and may be found in the Supplementary Information.

Assignments began with $3SiCPF_2$ because the previous work by Durig and Laane [19] provided rotational constants and dipole moments for the parent species in the ground vibrational state. The values reported were A = 3546.36 ± 1.40 MHz, B = 1798.07 ± 0.02 MHz, and C = 1706.25 ± 0.02 MHz and $|\mu_a|$= 2.02 ± 0.06 D, $|\mu_b|$ = 0 D, and $|\mu_c|$ = 0.00 ± 0.09 D. This agreed well with our calculated values presented in Table 1 providing additional confidence for their use. As expected, this greatly simplified assignment as

we were able to input these values directly into SPCAT and predict transitions accurately. From there the relative "correct intensity" feature of the spectrometer was utilized as the predicted intensities matched very well with prediction [37]. Once enough transitions were added, however, we were able to update the fit to utilize semirigid Watson *S*-reduced terms, not previously included because of this species being reported on prior to their complete development [35]. *R*- and *Q*-branch, *a*-type transitions, in accordance with dipole moment values, were assigned.

During the assignment of $3SiCPF_2$, some, but not all, transitions presented as doublets (see Fig. 9) or were broadened significantly from the typical 60–80 kHz FWHM transitions linewidth. In addition to this, centrifugal distortion constants began to grow unreasonably large for an otherwise large ring molecule. Both of these are strong indicators of a motion in the molecule leading to a splitting in vibrational ground state. In order to verify that this was the case, and these indicators were not being misinterpreted, two sets of fits were undertaken where split transitions were taken into account. One where the spectra were fit to two different sets of rotational constants and another where they were fit to singular set of rotational constants. In SPFIT/SPCAT, motions of the molecule resulting in splitting are fit using vibrational states as labels. Therefore, $v = 0$ and $v = 1$ correspond to concepts such as A and E of a methyl rotor or + and - of a ring-twisting/puckering motion.

The two fits are reported in Table 3. In each, one rotation-vibration parameters, F_{bc} was required. This correspond to Coriolis parameter F_a as described by Pickett [38]. Because we had trouble isolating the source of the splitting (see Curious Motions section), it isn't entirely clear as to where this term arises, but adequate fits cannot be obtained without the term being included in each of the fitting approach. ΔE_{01} is also necessary to account for the differences between the two states. Although fitting this type of spectra is described as a tunnelling motion in Pickett, it is fit using vibrational states as labels. Also, when these terms were added, centrifugal distortion parameters decreased to more reasonable values; being on the order of similar silicon-ring molecules. Due to the agreement between

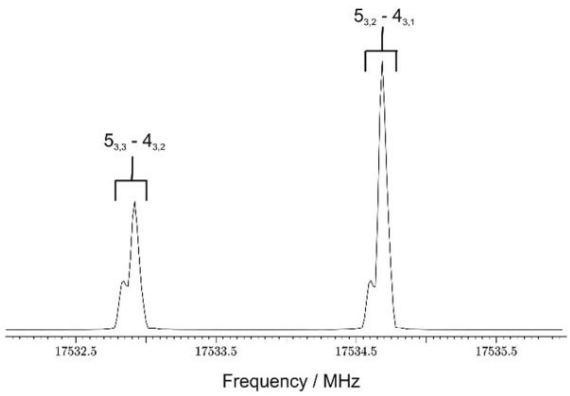

Figure 9. An example of splitting observed in the $3SiCPF_2$ spectrum during assignment. The spectra shown are for the $J'_{K_a,K_c} - J''_{K_a,K_c} = 5_{3,3} - 4_{3,2}$ and $5_{3,2} - 4_{3,1}$ transitions. Splitting appears as "shoulders" on the transitions at this resolution.

methods, the limited data set of transitions, and the fact that not all transitions presented as doublets, it was determined to proceed with a single set of rotational constants in all minor isotopologue fits.

All singly-substituted minor isotopologue spectra of $3SiCPF_2$ were observed and fit for the first time. These fits are presented in Table 4. Assignments were aided by using the rotational constants generated from the theoretical structure for the different isotopologues and adjusting these values based on the ratios between the parent experimental-to-theoretical *A*, *B*, and *C* values. Doubling was present again in the silicon isotopologues, but there was no doubling observed in the weaker ^{13}C species. In accordance with theory, only two sets of parameters were possible for all ^{13}C isotopologues as carbons 1 and 2 and 3 and 4 were spectroscopically equivalent. In total, 99 transitions were observed for the singly-substituted species in the spectral region.

The next molecule to be fit was 3SiCP. In accordance with $3SiCPF_2$, only *R*- and *Q*-branch, *a*-type transitions were observed. These spectra, as shown in Fig. 4, were considerably weaker and less dense than that of $3SiCPF_2$. Both of these observations agreed well with the dipole moments and rotational constants' magnitudes from theory. Due to the spectra being less intense, only the parent, ^{30}Si, and ^{29}Si species were observed before all

Table 3. Spectroscopic parameters of the parent isotopologue of $3SiCPF_2$. The fits are in excellent agreement when performed together and separately[a].

Fit separate			
Parameter	Fit together	$\nu = 0$	$\nu = 1$
A/MHz	3544.4280(35)[b]	3544.4239(30)	3545.87(56)
B/MHz	1798.1391(23)	1794.1419(23)	1798.1316(45)
C/MHz	1706.3013(25)	1706.2988(27)	1706.3085(29)
D_J/kHz	0.162(40)	0.201(36)	
D_{JK}/kHz	5.82(14)	5.87(13)	
F_{bc}/MHz	0.86(13)	0.68(16)	
ΔE_{01}/MHz	11,800(1410)	13,010(720)	
RMS[c]/kHz	16.6	11.8	
N[d]	38	26	12

[a] See text for details.
[b] Values in parentheses for the literature values are the reported uncertainties given in units of the least significant figure. Values in parentheses for the fitted rotational constants are the 1σ uncertainties (67% confidence interval) given in units of the least significant figure.
[c] Microwave RMS ($\sqrt{(\sum[(obs-calc)^2]/N)}$).
[d] Number of transitions.

sample was exhausted. Table 5 reports the fitted parameters for all observed isotopologues. The theoretical rotational constants provided excellent starting points for assignment as the prediction generated by SPCAT and output by AABS were closely matched. As mentioned previously, a Watson *S*-reduced Hamiltonian in the I^r representation was used. This time, however, all quartic centrifugal distortion constants were determined. As also was the case of $3SiCPF_2$, doubling was observed in the spectra. Again, only the F_{bc} Coriolis parameter and ΔE_{01} were needed for assignment. There were not enough intense transitions to observe the doubling on the minor isotopologues, however, so they were fit without the Coriolis terms and holding the centrifugal distortion terms to the parent values. A total of 27 transitions were observed for the parent while 4 were observed for the ^{30}Si and ^{29}Si isotopologues.

Table 4. Spectroscopic parameters of the minor isotopologues of $3SiCPF_2$. Split transitions were observed and assigned for the silicon-30 and silicon-29 species, but not for the carbon-13 species.

Parameter	^{30}Si	^{29}Si	^{13}C (3 & 4)	^{13}C (1 & 2)
A/MHz	3544.41(37)[a]	3543.45(47)	3494.65(29)	3533.34(33)
B/MHz	1794.5529(25)	1796.3240(36)	1795.3127(22)	1773.2146(22)
C/MHz	1703.0745(24)	1704.6780(36)	1692.4510(22)	1681.4202(20)
D_J/kHz	0.245(39)	0.223(58)	0.258(37)	0.181(36)
D_{JK}/kHz	5.42(15)	5.73(16)	5.32(17)	5.08(11)
F_{bc}/MHz	0.50(32)	0.86(19)	—	—
ΔE_{01}/MHz	8,390(1,460)	11,480(1,350)	—	—
RMS[b]/kHz	20.1	24.5	15.2	14.3
N[c]	27	28	22	22

[a] Values in parentheses for the literature values are the reported uncertainties given in units of the least significant figure. Values in parentheses for the fitted rotational constants are the 1σ uncertainties (67% confidence interval) given in units of the least significant figure.
[b] Microwave RMS ($\sqrt{(\sum[(obs-calc)^2]/N)}$).
[c] Number of transitions.

4.2. REFITS AND GLOBAL FITS

As mentioned prior, the previous work by Durig and Laane [19] provided a great starting point for the $SiCPF_2$ fits reported here. However, there were two aspects of our work that didn't agree well with the prior work or made comparisons inequivalent. Those were that the authors reported not observing any splitting of transitions and that this work happened prior to the development of Watson's semirigid Hamiltonians, so that there were no centrifugal distortion terms with which to compare while also directly affecting the reported rotational constants as they will adjust accordingly to best-fit the data set. Because it is important to understand our data in the context of all microwave data available, we embarked on working with the previously measured transitions in order to add our data and produce global fits for the entire data set. All fits have been reproduced in an easily read format using PIFORM [36] and may be found in the Supplementary Information.

Table 5. Spectroscopic parameters for all isotopologues of 3SiCP. Split transitions were observed and assigned for the parent only.

Parameter	Parent	^{29}Si	^{30}Si
A/MHz	5948.1093(47)[a]	5947.902(40)	5949.02(13)
B/MHz	4538.2601(39)	4509.5059(39)	4460.985(38)
C/MHz	2748.4793(41)	2717.0641(39)	264.090(18)
D_J/kHz	0.71(11)	[0.71][b]	[0.71]
D_K/kHz	1.18(25)	[1.18]	[1.18]
d_1/kHz	-0.340(38)	[-0.340]	[-0.340]
] d_2/kHz	-0.111(21)	[-0.111]	[-0.111]
F_{bc}/MHz	6.06(15)	—	—
ΔE_{01}/MHz	131,812(381)	—	—
RMS[c]/kHz	23.1	5.2	16.5
N[d]	27	4	4

[a] Values in parentheses for the literature values are the reported uncertainties given in units of the least significant figure. Values in parentheses for the fitted rotational constants are the 1σ uncertainties (67% confidence interval) given in units of the least significant figure.
[b] Values in brackets are held to the determined parent values.
[c] Microwave RMS ($\sqrt{(\sum[(obs-calc)^2]/N)}$).
[d] Number of transitions.

The first goal, then, was to reproduce the fits of Durig and Laane [19] to be sure that the transitions didn't have any obvious reporting (*i.e.* typographical) errors. Using SPFIT and only the assigned transition states, then, we reproduced fits of rotational constants only for all vibrational states reported. These are found in Table 6 as a comparison of the reported literature values (top portion of the table) with our fitted values from their reported transitions (bottom portion of the table). As expected, our values overall agree very well with those reported with the largest discrepancies coming from the A rotational constant which is the most difficult to determine using small data sets of only a-type transitions. This is especially true for the $\nu = 3$ state where only four (4) transitions were reported. This state also (unsurprisingly) had the largest discrepancies with our refit of the data. Due to this excellent agreement, particularly in the $\nu = 0$ state which would be used for our global fits, we proceeded forward.

Table 6. Refit of the $3SiCPF_2$ rotational constants from Durig and Laane[a].

Vibrational state	*A*/MHz	*B*/MHz	*C*/MHz
Literature Values			
$\nu = 0$	3546.36(140)[b]	1798.07(2)	1706.52(2)
$\nu = 1$	3543.54(200)	1801.89(4)	1714.02(2)
$\nu = 2$	3542.17(240)	1805.19(19)	1720.47(4)
$\nu = 3$	3539(3)	1808.01(20)	1726.22(4)
Rotational constants from literature transitions[c]			
$\nu = 0$	3546.1(14)	1798.070(14)	1706.247(13)
$\nu = 1$	3543.6(20)	1801.878(40)	1714.021(15)
$\nu = 2$	3542.2(23)	1805.19(18)	1720.470(39)
$\nu = 3$	3830(103)	1811.7(12)	1724.87(43)

[a] See text for details.
[b] Values in parentheses for the literature values are the reported uncertainties given in units of the least significant figure. Values in parentheses for the fitted rotational constants are the 1σ uncertainties (67% confidence interval) given in units of the least significant figure.
[c] Microwave RMS ($\sqrt{(\sum[(obs-calc)^2]/N)}$) and number of transitions for rotational constants fits: $\nu = 0$, RMS = 0.336 MHz, $N = 22$; $\nu = 1$, RMS = 0.204 MHz, $N = 9$; $\nu = 2$, RMS = 0.167 MHz, $N = 7$; $\nu = 3$, RMS = 0.018 MHz, $N = 4$.

In order to do our best not to bias any conclusions, we started the global fits by setting the transitions observed in the Durig and Laane [19] work $\nu = 0$ state to our $\nu = 0$ (lower state of a the splitting) and added the transitions to our parent transition listing holding the Coriolis terms to our originally determined values. This brought the new number of transitions to 60 and extended the frequency range of measured transitions to 39 GHz. 50 kHz uncertainty was given to these transitions as had been done in the previous work. The results are presented in Table 7 as "Holding Coriolis" alongside our other global fit approaches. A listing of the quantum number assignments and formatted fit files for all global fits using PIFORM on SPFIT .fit files may be found in the Supplementary Information. As was needed for our data set alone, D_J and D_{JK} were determinable and in good agreement with our determined values, but all other quartic centrifugal distortion were not determinable, even with the extended data set.

Table 7. Global fits of $3SiCPF_2$ transitions with those from Durig and Laane[a].

Parameter	Holding Coriolis	Adjusted Transitions	Fit Coriolis
A/MHz	3544.4281(60)[b]	3543.62(45)	3544.4249(38)
B/MHz	1798.1390(32)	1798.1370(19)	1798.1388(19)
C/MHz	1706.3031(31)	1706.3029(20)	1706.3012(19)
D_J/kHz	0.191(24)	0.186(19)	0.165(15)
D_{JK}/kHz	5.75(17)	5.61(11)	5.76(10)
D_K/kHz	—	-200(113)	—
F_{bc}/MHz	[0.86][c]	[0.86]	0.807(97)
ΔE_{01}/MHz	[11,800]	[11,800]	12,430(370)
RMS[d]/kHz	163	51.6	49.1
N[e]	60	60	60

[a] See texts for details.
[b] Values in parentheses for the literature values are the reported uncertainties given in units of the least significant figure. Values in parentheses for the fitted rotational constants are the 1σ uncertainties (67% confidence interval) given in units of the least significant figure.
[c] Values in brackets are held. For exact held values, see the Supplementary Information.
[d] Microwave RMS ($\sqrt{(\sum[(obs-calc)^2]/N)}$), where *N* is the number of transitions.
[e] Number of transitions.

As can be observed from Table 7, however, the Microwave RMS of this approach was 163 kHz, over 6×'s that of the average error attributed to the uncertainties. A quick scan of the obs - calc showed that a few transitions from the previous work were being assigned to states that were well away from where they were being predicted. However, when we produced predictions using SPCAT, they were much closer to other quantum number assignments; including those which corresponded to our $v = 1$ (splitting) state. These transitions were adjusted where applicable and a new fit was produced, still holding the fit to our original Coriolis values. This fit is labelled "Adjusted Transitions" in Table 7 to reflect the Coriolis being held and only the transitions were adjusted. This time D_K was determinable in addition to D_J and D_{JK} and the Microwave RMS was reduced from 163 to 51.6 kHz.

Although this was significant improvement from the "Holding Coriolis" global fit, as mentioned previously, such a large magnitude in the value for D_K (-200 kHz) could be an indicator that the Coriolis terms need refinement in the fit. As a complete analysis,

then, we let all parameters adjust in the final fit labelled "Fit Coriolis" in Table 7. This fit again lowered the Microwave RMS to 49.1 kHz, which is a true RMS of approximately 1.6, which agrees well with our data without Durig and Laane's transitions (true RMS of 2.15). Another notable aspect is that D_K was undeterminable, as it was with our previous data set, and the rotational constants, as well as the remaining D_J and D_{JK}, values agree very well with our data set's determined values. It should be noted that F_{bc} and ΔE_{01} are not significantly different (*i.e.* they are within error) from our previously determined values for these parameters and became better determined. Taking all of the information into account, we surmise that the "Fit Coriolis" best represents the data set but suggest that spectroscopic work on $3SiCPF_2$ at higher frequencies – for which we don't have access – would help to provide more information toward this conclusion.

4.3. STRUCTURE OF $3SiCPF_2$ AND 3SiCP

One very important aspect of the chemistry and spectroscopy of silicon-containing ring molecules concerns their structure. Especially with regards to their fully carbonated counterparts. Because there was a significant amount of isotopic data available, as well as a significant amount of data for comparison, we embarked on developing experimental ring-structure analysis for the $3SiCPF_2$. The first approach utilized Kraitchman substitution structures [39]. Given the small amount of data for 3SiCP molecules, however, a Kraitchman analysis might not be very meaningful. The Kraitchman analysis for $3SiCPF_2$ only, then, is presented in Table 8.

The first notable item from the Kraitchman analysis is that the *c*-coordinate has non-zero values for all atomic substitutions except for ^{30}Si, where it is effectively zero. This, however, does not agree well with our theoretical and previous theoretical work on the molecule [18]. To reconcile this inconsistency, then, it was important to compare the structural implications of these positions as well as understand the nature of the Kraitchman analysis and its pitfalls, especially when comparing to equilibrium structures. Due to

Table 8. Kraitchman [39] substitution coordinates for $3SiCPF_2$[a].

Atom	*a*/Å	*b*/Å	*c*/Å
^{29}Si	0.5153(97)[b]	0.137(36)[c]	0.145(25)[c]
^{30}Si	0.5345(45)	0.008(310)[d]	0.018(140)[d]
^{13}C (1/2)	-1.9874(19)	±0.6741(56)	-0.090(43)[c]
^{13}C (3/4)	-0.6431(52)	±1.4209(24)	0.168(22)[c]

[a] Kraitchman analyses only give magnitudes. Signs reported have been assigned in accordance with their theoretical values.
[b] Numbers in parentheses represent the Costain errors [40] in the least significant figure.
[c] Theoretical value is 0.00 Å for this coordinate. Therefore, sign has been assigned based on most reasonable value.
[d] Reported values of zero are where the Kraitchman substitution method returned an imaginary result.

the way the Kraitchman analysis is performed, substitution structures from this analysis method have been known to have problems with atomic positions close to a zero value for a coordinate. In other works [41], the authors have utilized the double substitution method of Rudolph [42] in order to arrive at more reasonable values for molecular geometries. In this work, this is noticeable from the large error in this coordinate for the ^{30}Si substituted species.

Because only singly substituted data were available, however, we had to take a different approach for $3SiCPF_2$. To investigate further, we input the Kraitchman coordinates into Kisiel's EVAL program on the PROSPE website [36]. This provided a unique set of r_S parameters for substituting the ^{29}Si and ^{30}Si independently. These parameters are compared to the r_e values from our equilibrium structure and the electron diffraction work of Rankin and coworkers [20] in Table 9. As we are both attempting to get the best experimental structure and determine the shape of the ring, the best comparator is to look at the Si–C bond lengths as they should be largely consistent across a number of molecules and geometries and match well with theory. There is an obvious outlier in the group with the ^{29}Si structure having vastly different Si–C_3 and Si–C_4 bond lengths both compared within itself and across the different methods. This was a good indicator that Kraitchman was probably not doing a good enough job with the structure derived from this isotopologue. The structure derived

from ^{30}Si, however, showed great consistency and agreement both with all Si–C bonds in the structure and with the calculated and electron diffraction structure, so we will use that structure as our best experimental r_S structure.

Table 9. Experimentally determined microwave r_s structure values compared to theoretical r_e and electron diffraction [20] for $3SiCPF_2$.

Bond of angle	r_e	r_s (^{29}Si)	r_s (^{30}Si)	Elec. diff.[20]
C_1=C_2/Å	1.340	1.3482(79)[a]	1.3482(79)	1.378(7)
C_2–C_3/Å	1.517	1.5593(97)	1.5593(97)	1.519[b]
Si–C_3/Å	1.869	1.942(30)	1.86(24)	1.847(3)
Si–C_4/Å	1.869	1.729(28)	1.85(24)	1.847(3)
C_1–C_4/Å	1.517	1.5593(97)	1.5593(97)	1.59[c]
C_1–C_4–Si/°	101.0	102.70(90)	99.8(60)	102.7(4)
C_3–Si–C_4/°	98.8	101.29(53)	100.24(89)	98.7(4)
C_2=C_1–C_4/°	119.6	118.62(65)	118.62(65)	117.9(3)
C_2–C_3–Si/°	101.0	97.35(74)	99.5(59)	102.7(4)
C_1=C_2–C_3/°	119.6	118.62(65)	118.62(65)	117.9(3)
C_4–C_1=C_2–C_3/°	0.00	0.0(54)	0.0(54)	—[d]
C_1=C_2–C_3–Si/°	0.00	-7.2(40)	-11.6(60)	13.9(8)

[a] Numbers in parentheses represent the 1σ uncertainties (67% confidence interval) from the Costain errors [40] in the least significant figure.
[b] Fixed in ref. [20].
[c] Reported as δ in ref. [20].
[d] Not reported in ref. [20].

Settling on the ^{30}Si Kraitchman coordinate as the basis for the r_S, the r_e, r_S, and electron diffraction ring structure parameters are in excellent agreement with one another with one exception, the dihedral angle formed from the double bond carbons, an adjacent carbon, and the silicon atom (listed as the C_1=C_2–C_3–Si angle in Table 9). In the electron diffraction work, this is defined as δ and determined to be 13.9(8)° [20]. This value is in excellent agreement (at least in magnitude) with our value of -11.6(60)°. In the electron diffraction work, this angle is attributed to a low amplitude ring-shrinkage deformation vibration. This seems to be plausible as explained in the Curious Motions subsection immediately following this structure discussion.

Because the Kraitchman substitution approach wasn't entirely conclusive and there has yet to be any discussion of the 3SiCP molecule, we decided to utilize Bohn's method of planar moment analysis to arrive at conclusions for the experimental structure [43]. This method takes advantage of similarities in functionalization to provide fundamental insights regarding structure. The advantage to using it here is that we are able to utilize the most determined set of parameters – those for the parent $3SiCPF_2$ and 3SiCP isotopologues – as our basis for comparison. Second moments for $3SiCPF_2$, 3SiCP and similar molecules 1,1-difluorosilacyclopent-2-ene ($2SiCPF_2$) [21], 1,1-difluorosilacyclopentane ($SiCPF_2$) [44], and silacyclopentane (SiCP) [45] are presented in Table 10.

Table 10. Second moment comparisons of similar molecules.

Molecule	P_{aa}/amu Å^2	P_{bb}/amu Å^2	P_{cc}/amu Å^2
$3SiCPF_2$[a]	217.32825(29)[b]	78.85566(29)	63.72848(29)
$2SiCPF_2$[c]	224.058503(94)	77.698347(94)	62.708151(94)
$SiCPF_2$[d]	227.27110(12)	83.037692(12)	67.164670(12)
3SiCP[a]	105.13543(15)	78.74044(15)	6.22421(15)
SiCP[e]	109.853881(11)	80.028848(11)	12.305876(11)

[a] This work. [b] Numbers in parentheses represent 1 σ uncertainties (67% confidence interval) given in units of the least significant figure. [c] Ref. [21]. [d] Ref. [44]. [e] Ref. [45].

In order to interpret structure using Table 10 care must be taken in order to make comparisons within a family. First of all, halogen substitution will cause shifts in the principal axis system, so it is easiest to make comparisons among species with the equal substitution above and below the ring (fluorination above and below the ring or completely halogenated). Table 10 has been organized in this way. Ring planarity in all of these molecules moves mass out of the *ab*-plane and into the *ac*-plane, therefore we can monitor ring planarity by a comparison of the P_{bb} (out-of-*ac*-plane mass) and P_{cc} (out-of-*ab*-plane mass) values. We will focus on P_{bb} here because the halogenation makes P_{cc} values change dramatically while P_{bb} is very consistent, allowing us to make comparisons amongst the entire family.

Inspection of P_{bb} in Table 10 shows that the values range from 77.69–83.04 amu Å^2 across the family. This may not seem like very much, but, investigating further, it is noticed that the species determined to be nonplanar – SiCP and $SiCPF_2$ – both have values above 80 amu Å^2. This is because whereas change in position of the double bond may slightly affect where the axis system lies, it will only do so by about 1 amu Å^2, the planar contribution of a hydrogen atom, whereas breaking planarity involves the larger contribution of out-of-plane carbon atoms [43, 44]. Albeit small, $3SiCPF_2$ and 3SiCP are both closer in their P_{bb} value to planar $2SiCPF_2$ than nonplanar SiCP and $SiCPF_2$, therefore bringing us to conclude the molecule is planar as the equilibrium structure would suggest.

4.4. CURIOUS MOTIONS

As discussed in previous subsections, splitting was observed in the spectra of both molecules. This splitting was fit using either one or two Coriolis coupling terms and an energy splitting for the two levels. Furthermore, in $3SiCPF_2$, for which there was previous microwave data, these additions improved the fit of the dataset in the global fit so much that it was concluded that this must be the correct approach to this molecule.

Although significant evidence exists for both molecules containing a motion of some sort, it is unclear as to the source of such a motion. From the calculations we presented earlier, it is obvious that this motion doesn't come from an inversion barrier in the puckering coordinate. Extensively high-level calculations presented here show that each 3SiCP and $3SiCPF_2$ may have very flat wells, but they do not actually increase in energy to form a barrier. Even when calculations are presented that result in a barrier, that barrier is not high enough to adequately represent the level separation determined by our spectroscopic analysis. This makes the source of this splitting very curious, but intriguing and, although we have a large amount of evidence pointing to a motion in 3SiCP and $3SiCPF_2$, we still do not know the source of the motion.

Because our work presented in this manuscript and verified by other previous literature shows that this motion is not due to the puckering coordinate, we will present a couple of hypotheses for the cause here. What we do know is that the Coriolis term F_{bc} is needed indicating a motion about the *a*-axis in the *bc*-plane. The first is a steering wheel wagging motion of the fluorine atoms. Calculations performed by the authors on this motion show there is no discernible barrier that would lead to a splitting of the energy levels. The other, more plausible, source is the shrinkage deformation vibration mentioned in the electron diffraction work in the prior subsection. Being a large amplitude motion, this motion could account for both the observed splitting and the substitution structure differences from the equilibrium structure. However, it isn't clear what is entailed in this motion as there are many possibilities along the ring and, furthermore, what exactly to calculate to begin to test this hypothesis.

5. CONCLUSIONS

The molecules $3SiCPF_2$ and 3SiCP have been synthesized and studied using microwave spectroscopic techniques with accompanying high-level computational approaches. The microwave data collected previously on $3SiCPF_2$ by Durig and Laan [19] has been combined with the new data collected here into a global fit that better describes both sets of experimental transitions. The molecules have both been determined to be planar experimentally using a combination of substitution and planar moment structure approaches. Splitting of spectra observed in both molecules cannot be isolated to a specific source, but the evidence presented here leads the authors to believe that the splitting is not due to an inversion motion from the puckering coordinate. It is speculated that a more comprehensive investigation on all possible large amplitude motions in the molecules needs to be undertaken to determine the source of the motions.

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III. THE ROTATIONAL SPECTRUM AND RING STRUCTURES OF SILACYCLOHEX-2-ENE AND 1,1,-DIFLUOROSILACYCLOHEX-2-ENE

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ABSTRACT

Silacyclohex-2-ene and 1,1-difluorosilacyclohex-2-ene have been synthesized and the chirped pulse, Fourier transform microwave spectra of each have been observed and analyzed in the 5.5-18.75 GHz region of the electromagnetic spectrum with some intense transitions being observed outside the region. Quantum chemical calculations have been performed at the B3LYP-D3BJ/Def2TZVP level of theory and predict μ_a to be the largest dipole moment component with a significantly larger value in this component for 1,1-difluorosilacyclohex-2-ene. In accordance with this prediction, the spectra were predominantly *a*-type with the observation of a few *b*- and *c*-type transitions. Signal-to-noise was adequate in both spectra to observe ^{29}Si, ^{30}Si, and all singly-substituted ^{13}C isotopologues in natural abundance. All spectra have been fit to a semirigid rotational Hamiltonian and are presented. Analysis of the experimental structures of both molecules indicate that the quantum chemical calculated structures for the atoms in the ring are a very close depiction of the experimentally determined structures. The structures of each molecule are compared to similar molecules for context where it is shown that both molecules possess a similar "half-chair" conformation to that of the carbon analogue, cyclohexene.

1. INTRODUCTION

Cyclohexene has long been known to have a predominate conformer structure of "half-chair" with C_2 symmetry [1, 2]. This structure is where four carbons, including the carbons of the double bond, are planar and the two furthest sp^3 hybridized carbons from the double bond have one carbon slightly above the plane and one slightly below the plane. This structure plays a role in the cyclohexene chemistry.

In recent years, the authors have undertaken rotational spectroscopy studies that investigate the structural differences in substituting a carbon with a silicon atom [3, 4, 5, 6, 7, 8]. These systems have led to interesting physiochemical results like ring puckering motions, planar vs. nonplanar ring structures, or C_2 symmetry in straight-chain alkane species where one may expect C_{2v}. In some of these systems, the potential energy surfaces of the ring puckering motion may be flatter at the base through the puckering coordinate than the carbon analogs or may result in a double well. The results are often different than what is expected because it is common to think that silicon would have very similar structure and chemistry to carbon.

This work, then, replaces a silicon with a carbon in cyclohexene and a similar derivative to investigate the structure. In this work, then, we present the first known report on the microwave rotational spectra of silacyclohex-2-ene and 1,1-difluorosilacyclohex-2-ene using chirped pulse, Fourier transform microwave (CP-FTMW) spectroscopy. Analyses of the resulting spectra and structures are aided and compared to quantum chemical calculations while also being discussed in terms of other similar molecules, including cyclohexene.

2. QUANTUM CHEMICAL CALCULATIONS

Silacyclohex-2-ene and 1,1-difluorosilacyclohex-2-ene structures were optimized utilizing the Gaussian16 program suite [9] at the B3LYP-D3BJ/Def2TZVP level. The minimum energy structures for each are presented in Figures 1 and 2 in three sets of principle axis system planes (*ab*, *ac*, and *bc*). Both molecules have bends in the six-member ring resulting in the ring not being planar.

Dipole moment components and rotational spectroscopic parameters for each molecule were also calculated. These are presented in Table 1. Besides the expected difference in the rotational constants due to the significant addition of mass from the fluorines, one obvious distinction that arises between the two molecules is the significant increase in the mu_a dipole moment component. This component almost triples in magnitude upon the addition of the fluorines from 1.19 D to -3.17 D. Because both were expected to be a predominantly *a*-type spectra, this was viewed as a significantly favorable increase for observing isotopologues of the 1,1-difluorosilacyclohex-2-ene molecule in natural abundance in order to compare structural parameters such as both lengths and angles directly with quantum chemical calculations.

3. EXPERIMENTAL METHODS

The experiment is broken into two parts: synthesis of the molecules and microwave rotational experiments.

The synthetic work was carried out in three steps. First, 1,1-dichlorosilacyclohex-2-ene was prepared as a precursor for 1,1-difluorosilacyclohex-2-ene and 1-silacyclohex-2-ene as previously reported [7] with the exception of using trichlorosila-5-chloropent-2-ene. The product 1,1-dichloro-1-silacyclohex-2-ene was obtained and purified by trap-to-trap distillation under vacuum (0.1 Torr) and the product was collected in a trap at -38°C with a

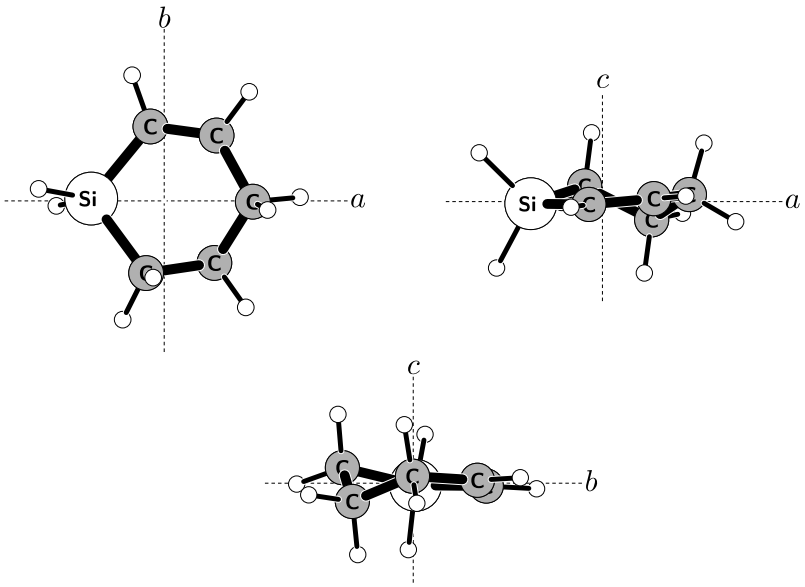

Figure 1. The quantum chemical structure of silacyclohex-2-ene presented in the *ab*-, *ac*-, and *bc*-planes. The structure has been optimized at the B3LYP-D3BJ/Def2TZVP level of theory.

yield of 68%. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 6.95 (4.19 and 3.85 Hz ^{1}H, =C-H), 5.87 (dt, 2.0 and 2.41 Hz 1H, =CH), 2.27 (m, CH_2, 2.29-2.25), 1.99 (m, CH_2, 2.02-1.96), 1.32 (m, CH_2, 2.02-1.96). ^{13}C NMR (400 MHz, $CDCl_3$): δ (ppm), 154.70, 123.37, 29.97, 20.26, 17.66. ^{29}Si NMR (400 MHz, $CDCl_3$): δ (ppm) 10.13.

In the second step, an equimolar amount of 1,1-dichlorosilacyclohex-2-ene and freshly sublimed antimony trifluoride were added to a Schlenk tube and degassed after being frozen with liquid nitrogen. The tube was allowed to come to room temperature and then was heated in an oil bath to 55°C for two hours with stirring. The product 1,1-difluorosilacyclohex-2-ene was collected using trap-to-trap distillation with a yield of 50%. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 7.17 (dt, 4.44 - 4.24 Hz, 1H, =C-H), 5.70 (dt, 1.97 – 1.99 Hz, ^{1}H, =C-H), 2.25 (m, 2.27 – 2.22, 2H, CH_2), 1.98 (m, 2.01 – 1.94, 2H, CH_2), 0.96 (m, 1.00 – 0.95, 2H, CH_2). ^{13}C NMR (400 MHz, $CDCl_3$): δ (ppm), (159.68), (t, 5.50 Hz), t 118.79, (t, 19.04 Hz), 30.40 s, 21.55 t, 9.89 (t, 1.59 Hz). ^{19}F NMR (400 MHz, $CDCl_3$): δ (ppm), -141.83. ^{29}Si NMR (400, MHz, $CDCl_3$): δ (ppm) -16.19 (t, 294.42 Hz).

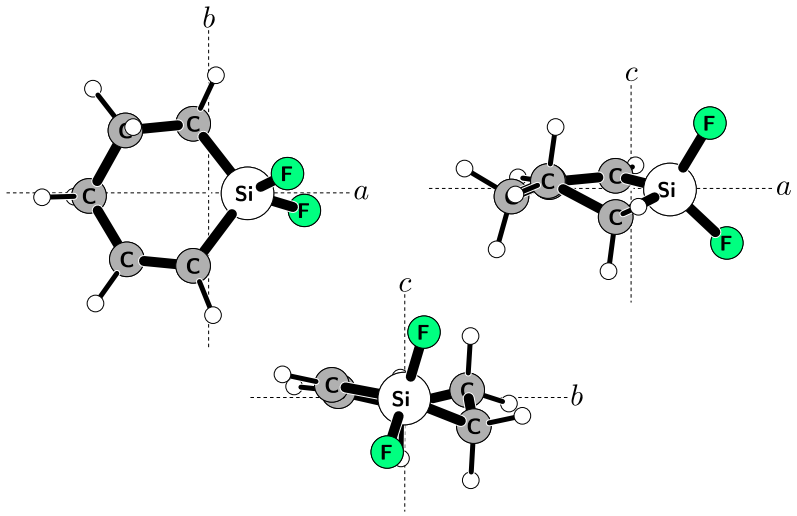

Figure 2. The quantum chemical structure of 1,1-difluorosilacyclohex-2-ene presented in the *ab*-, *ac*-, and *bc*-planes. The structure has been optimized at the B3LYP-D3BJ/Def2TZVP level of theory.

The third step, the silacyclohex-2-ene is prepared by the reduction of the 1,1-dichlorosilacyclohex-2-ene using lithium aluminum hydride in diethyl ether for two hours at 40°C. ^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) 6.88 (dt, 4.03 Hz, 2.08Hz 1H,=C-H), 3.91 (5, 2H, CH_2), 2.15 (m, 2.18-2.14, 2H, CH_2), 1.82 (m, 1.85-1.79, 2H, CH_2) m, 0.89-0.87, 2H, CH_2). ^{13}C NMR (400 MHz, two hr $CDCl_3$): δ ppm, 152.05 (s), 118.64 (s), 30.37 (s), 4.47 (s). ^{29}Si NMR (400, MHz, $CDCl_3$): δ (ppm) -52.52 (s).

The microwave experiments were carried out at Missouri University of Science and Technology (Missouri S&T) using a multi-antenna detection, chirped pulse, Fourier transform microwave (MAD-CP-FTMW) spectrometer in the standard CP-FTMW orientation. The details of this spectrometer are reported elsewhere [10, 11, 12]. Both samples — liquids under typical laboratory conditions — were introduced into the system via a heated nozzle reservoir with a backing gas of argon at 25 psig [13]. Since the sample was volatile, no heat was applied to the reservoir as vaporization was sufficient at room temperature.

Table 1. Quantum chemical calculation parameters for silacyclohex-2-ene and 1,1-difluorosilacyclohex-2-ene.[a]

Parameter	Silacyclohex-2-ene	1,1-Difluorosilacyclohex-2-ene
A / MHz	3980.7	2728.7
B / MHz	3041.9	1368.4
C / MHz	1875.5	1202.0
D_J / kHz	0.697	0.099
D_{JK} / kHz	-0.970	0.350
D_K / kHz	0.391	-0.046
d_1 / kHz	-0.098	-0.011
d_2 / kHz	-0.048	0.008
mu_a / D	1.19	-3.17
mu_b / D	-0.34	0.18
mu_c / D	0.20	-0.41

[a] See text for details.

Spectra of both molecules were then acquired in 5.5-10.25 GHz, 9.75-14.5 GHz, and 14-18.75 GHz regions of the electromagnetic spectrum using 4 μs chirp widths. A Parker-Hannifin® Series 9 supersonic nozzle pulsed sample into the chamber at a rate of 3 Hz with 3 free induction decays (FIDs) per gas pulse. Approximately 100,000 20 μs FIDs were collected and averaged in each range for the samples except for 1,1-difluorosilacyclohex-2-ene where only 34,000 FIDs were collected before the sample was completely depleted. Fourier transformation of the FIDs were performed with Kisiel's FFTS program [14] using a Bartlett windowing function. A zoom-in on portions of the spectra collected for both molecules is presented in Figures 3 and 4. Typical linewidths for the spectra were 70-80 kHz with an attributed 10 kHz uncertainty for the line centers.

4. RESULTS AND DISCUSSION

Spectra for both molecules were assigned using Kisiel's AABS package [15] used in conjunction with Pickett's SPFIT/SPCAT program suite [16] in the I^r representation. A semirigid, Watson S-reduced [17] Hamiltonian was employed for fitting of both molecular

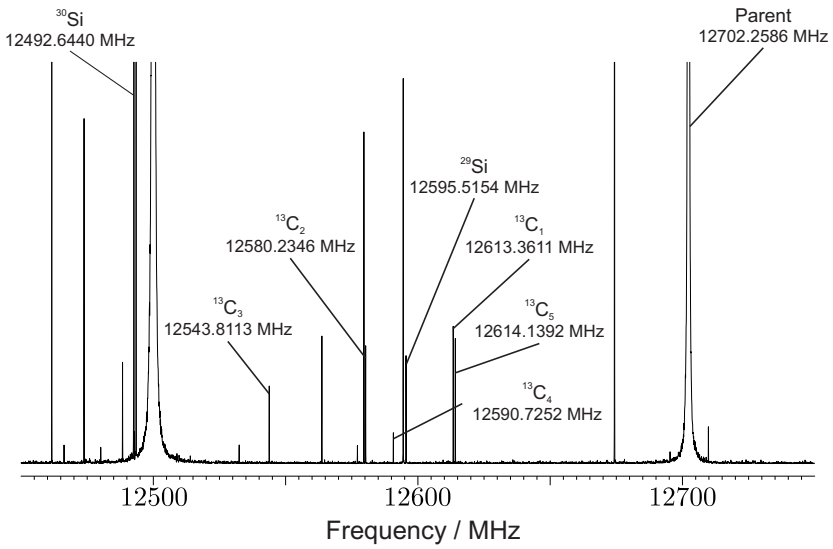

Figure 3. The $J', K_a', K_c' \leftarrow J$", K_a", K_c" = $3_{13} - 2_{12}$ transition for all assigned isotopologue species of silacyclohex-2-ene. There is significant S:N on all singly-substituted species for unambiguous assignment.

spectra. All rotational constants and quartic centrifugal distortion constants were determined for both molecules while the sextic centrifugal distortion term H_J was determined for 1,1-difluorosilacyclohex-2-ene. As expected from quantum chemical calculations, the spectra were predominantly *a*-type for both species with observation of a few *b*- and *c*-type transitions. Although 1,1-difluorosilacyclohex-2-ene was significantly stronger in intensity, Figures 3 and 4 show that the signal-to-noise was sufficient on both species to observe all singly-substituted ^{29}Si, ^{30}Si, and ^{13}C isotopologues in natural abundance. Determined parameters for each isotopologue of both species are presented in Tables 2 and 3 with quality of fit details and assigned transition quantum numbers being reported in the Supporting Information.

The ability to observe and fit isotopologue spectra in natural abundance allowed for comparisons of the experimental structures of the molecules to each other, to similar molecules, and with theory. To start, comparisons are made with theory. It should be noted, though, that comparisons between calculated equilibrium structures and isotopic

Table 2. Determined spectroscopic parameters for silacyclohex-2-ene.

Parameter	$SiH_2CH{=}CHCH_2CH_2CH_2$	$^{29}SiH_2CH{=}CHCH_2CH_2CH_2$	$^{30}SiH_2CH{=}CHCH_2CH_2CH_2$	$SiH_2{}^{13}CH{=}CHCH_2CH_2CH_2$
A / MHz	3978.8253(6)[a]	3978.706(1)	3978.604(1)	3911.49(1)
B / MHz	3040.3460(5)	3002.687(1)	2966.756(1)	3038.967(1)
C / MHz	1879.6657(4)	1865.199(1)	1851.272(1)	1864.023(1)
D_J / kHz	0.326(6)	0.29(4)	0.39(4)	[0.326]
D_{JK} / kHz	0.058(6)	[0.058][d]	[0.058]	[0.058]
D_K / kHz	0.644(9)	0.60(2)	0.65(3)	[0.644]
d_1 / kHz	-0.122(1)	-0.128(5)	-0.125(9)	[-0.122]
d_2 / kHz	-0.0256(7)	-0.018(2)	-0.022(4)	[-0.0256]
N[b]	167	52	31	7
Microwave RMS[c] / kHz	14.2	11.6	12.0	4.7

Parameter	$SiH_2CH{=}{}^{13}CHCH_2CH_2CH_2$	$SiH_2CH{=}CH{}^{13}CH_2CH_2CH_2$	$SiH_2CH{=}CHCH_2{}^{13}CH_2CH_2$	$SiH_2CH{=}CHCH_2CH_2{}^{13}CH_2$
A / MHz	3928.49(1)	3978.37(1)	3928.50(1)	3913.31(2)
B / MHz	3019.279(1)	2984.286(1)	3019.728(1)	3035.890(2)
C / MHz	1860.440(1)	1858.260(1)	1862.492(1)	1864.698(2)
D_J / kHz	[0.326]	[0.326]	[0.326]	[0.326]
D_{JK} / kHz	[0.058]	[0.058]	[0.058]	[0.058]
D_K / kHz	[0.644]	[0.644]	[0.644]	[0.644]
d_1 / kHz	[-0.122]	[-0.122]	[-0.122]	[-0.122]
d_2 / kHz	[-0.0256]	[-0.0256]	[-0.0256]	[-0.0256]
N[b]	8	8	8	9
Microwave RMS[c] / kHz	7.9	7.3	4.7	12.5

[a] Numbers in parentheses give standard errors (1σ, 67% confidence level) in units of the least significant figure.
[b] Number of observed transitions used in the fit. [c] Microwave RMS is defined as $(\sqrt{(\sum[(obs-calc)^2]/N)})$.
[d] Value in brackets held to the parent determined value.

Table 3. Determined spectroscopic parameters for 1,1-difluorosilacyclohex-2-ene.

Parameter	$SiF_2CH{=}CHCH_2CH_2CH_2$	$^{29}SiF_2CH{=}CHCH_2CH_2CH_2$	$^{30}SiF_2CH{=}CHCH_2CH_2CH_2$	$SiF_2{}^{13}CH{=}CHCH_2CH_2CH_2$
A / MHz	2742.0553(4)[a]	2742.041(2)	2742.079(2)	2709.92(5)
B / MHz	1379.1798(2)	1376.931(1)	1374.7185(4)	1378.627(1)
C / MHz	1209.0375(3)	1207.3059(9)	1205.6110(5)	1202.692(1)
D_J / kHz	0.084(3)	0.084(8)	0.080(4)	0.08(1)
D_{JK} / kHz	0.341(2)	0.61(2)	0.37(3)	0.39(3)
D_K / kHz	-0.10(1)	[-0.10][d]	[-0.10]	[-0.10]
d_1 / kHz	-0.01195(9)	-0.024(6)	[-0.01195]	[-0.01195]
d_2 / kHz	0.00725(4)	[0.00725]	[0.00725]	[0.00725]
H_J / Hz	-0.14(1)	[-0.14]	[-0.14]	[-0.14]
N[b]	300	49	35	34
Microwave RMS[c] / kHz	15.0	11.6	6.7	14.3

Parameter	$SiF_2CH{=}{}^{13}CHCH_2CH_2CH_2$	$SiF_2CH{=}CH{}^{13}CH_2CH_2CH_2$	$SiF_2CH{=}CHCH_2{}^{13}CH_2CH_2$	$SiF_2CH{=}CHCH_2CH_2{}^{13}CH_2$
A / MHz	2716.36(3)	2741.71(4)	2719.12(3)	2709.44(2)
B / MHz	1369.0360(7)	1357.9809(9)	1368.8934(7)	1377.6553(5)
C / MHz	1196.3364(8)	1192.800(1)	1196.8417(8)	1203.3727(5)
D_J / kHz	0.095(7)	0.074(9)	0.083(6)	0.085(5)
D_{JK} / kHz	0.32(3)	0.33(4)	0.33(2)	0.36(3)
D_K / kHz	[-0.10]	[-0.10]	[-0.10]	[-0.10]
d_1 / kHz	[-0.01195]	[-0.01195]	[-0.01195]	[-0.01195]
d_2 / kHz	[0.00725]	[0.00725]	[0.00725]	[0.00725]
H_J / Hz	[-0.14]	[-0.14]	[-0.14]	[-0.14]
N[b]	33	35	33	31
Microwave RMS[c] / kHz	9.1	11.8	8.6	5.9

[a] Numbers in parentheses give standard errors (1σ, 67% confidence level) in units of the least significant figure.
[b] Number of observed transitions used in the fit. [c] Microwave RMS is defined as $(\sqrt{(\sum[(obs-calc)^2]/N)})$.
[d] Value in brackets held to the parent determined value.

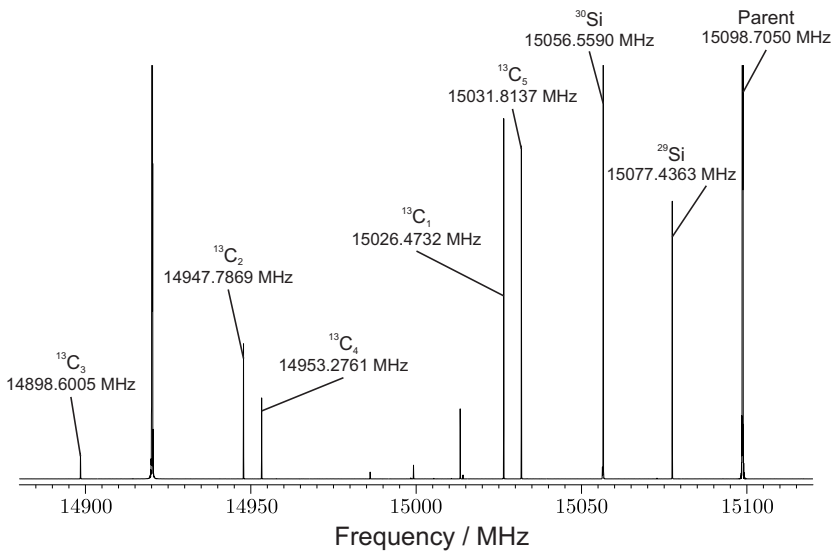

Figure 4. The $J', K_a', K_c' \leftarrow J$", K_a", K_c" = $6_{06} - 5_{05}$ transition for all assigned isotopologue species of 1,1-difluorosilacyclohex-2-ene. There is significant S:N on all singly-substituted species for unambiguous assignment.

substitution structures are not direct and should only be used as a guide for determinating how close visual representations of theory are to the determined experimental structures. For experimental strucure parameters, Kraitchman coordinates [18] were determined for all singly substituted atoms using Kisiel's KRA program from the PROSPE website [19, 20]. These coordinates with Costain errors [21] are reported for both molecules and compared to theoretical coordinates in Table 4. Signs for the coordinates are not determined by Kraitchman analyses and have been assigned based on the coordinate values from theory. All determined coordinates for both molecules are in good agreement with the theoretical structures.

Atomic coordinate positions aren't always easy to understand structurally in the context of the entire molecule. To clarify this, bond lengths, angles, and dihedral angles have been analyzed for every atom determined using Kraitchman coordinates and Kisiel's EVAL program [19, 20]. Structural parameters for both molecules have been reported and compared to the corresponding theoretical values in Table 5. Inspection of Table 5

reveals some interesting insights into the two systems. The first is the C_1SiC_5 bond angle. In 1,1-difluorosilacyclohex-2-ene, the angle is measured to be 108.1(16)° or 108.0(11)° depending on if ^{29}Si or ^{30}Si is used, respectively. This is in good agreement with the theoretical value of 106.885° and is close to that of the common tetrahedral bond angle of 109.5°. However, the C_1SiC_5 bond angle is significantly reduced for silacyclohex-2-ene to a value of 103.80(37)° for both substitution species (^{29}Si and ^{30}Si); further away from the common tetrahedral angle of 109.5° and closer to that of the ∠HOH in water of 104.5°. This is particularly interesting given that there are not significant differences in the Si-C_1 and Si-C_5 bond lengths amongst the molecules.

An explanation for this widening of the bond angle may be found from the assigned Mulliken charges given in the theoretical calculations. For silacyclohex-2-ene, the silicon atom is assigned a charge of +0.319 while C_1 and C_5 have values of -0.220 and -0.306, respectively. In 1,1-difluorosilacyclohex-2-ene, the value for silicon has increased dramatically to +0.833 in response to the electron withdrawing nature of the fluorine atoms. However, C_1 and C_5 have barely changed to -0.258 and -0.325, respectively, showing that much of the adjustment to the electron withdrawing fluorines is happening directly on the silicon.

Further inspection of Table 4 provides more interesting insights. The first is that there is a significantly different value in the C_1=C_2 bond length of the experimentally determined structures for silacyclohex-2-ene and 1,1-difluorosilacyclohex-2-ene versus that of theory. Silacyclohex-2-ene is determined to be 1.3374(66) Å while 1,1-difluorosilacyclohex-2-ene is determined to be 1.3674(63) Å. Theory has this parameter to be essentially the same between the molecules at 1.33663 Å and 1.33853 Å, respectively. While that may not be drastically different, it is interesting that the molecule with the heavily electron withdrawing groups has the slight elongation of this bond despite not having significantly different values in the Si-C bonds.

The final measurements of interest involve the planarity of the ring itself. These are addressed by evaluating the dihedral angles formed from atoms as one navigates around the ring. Theoretical calculations for both structures have $SiC_1C_2C_3$ very close to planar with C_4 and C_5 having positions above or below this plane (depending on ring orientation). This is confirmed from the experimental structure with the exception that some atoms, particularly the silicon, are very near the *b* and *c* axis, both complicating the accuracy of the Kraitchman coordinate position and giving larger errors in those coordinates. This proximity and large uncertainty in the dihedral angle is very similar to that observed in 1,1-difluorosilacyclopent-3-ene [6], which had doubling in some transitions possibly due to an unidentified motion. No such doubling was observed in these spectra, however, which lead the authors to conclude that the large uncertainty in any dihedral angle is just due to the uncertainty in the coordinate positions as the determined values, ignoring the errors, are very close to the theoretical structures. From this evidence, it can be concluded that the theoretical structure of the silicon and carbon atoms is a close approximation to the theoretical structures presented.

It is important to put the structure of silacyclohex-2-ene and 1,1-difluorosilacyclohex-2-ene into context with similar molecules. The most direct comparison will be that with a previous Raman study of silacyclohex-2-ene [22]. This work found that the "ring twisting angle", most comparable to dihedral $\angle C_4C_5SiC_1$, was 38.5° or 38.6° depending on the analytical approach in the work. This is in excellent agreement with the dihedral $\angle C_4C_5{}^{29}SiC_1$ value of -37.0(20)° and dihedral $\angle C_4C_5{}^{30}SiC_1$ value of -37.1(19)° determined in this work, providing additional evidence to support the results presented here.

Finally, it is useful to look at how these structures compare to similar carbon and silicon-containing molecules, including cyclohexene. To aid with this, Table 6 presents the planar moments of a few similar molecules. These are quantifications of the mass distributions out of a plane. P_{aa} will quantify the mass distribution out of the *bc*-plane, P_{bb} will quantify the mass distribution out of the *ac*-plane, and P_{cc} quantifies the mass

Table 4. Comparisons of Kraitchman coordinates with Costain errors [18, 21] for silacyclohex-2-ene and 1,1-difluorosilacyclohex-2-ene to that of theory.

	a-coordinate / Å		b-coordinate / Å		c-coordinate / Å	
Silacyclohex-2-ene atom	Experiment	Theory	Experiment	Theory	Experiment	Theory
Si-29	-1.4509(10)[a,b]	-1.4552150	0.049(31)	0.046568	-0.040(37)	-0.042831
Si-30	-1.4509(10)	-1.4552150	0.046(32)	0.046568	-0.041(36)	-0.042831
C(1)	-0.2627(57)	-0.275216	1.4842(10)	1.483828	-0.054(28)	-0.057514
C(2)	1.0560(14)	1.044040	1.2970(12)	1.303757	0.067(22)	0.059657
C(3)	1.76743(85)	1.766300	0.000(20)[c]	-0.015381	0.143(10)	0.142865
C(4)	0.9805(15)	1.000027	-1.2376(12)	-1.237183	-0.3814(39)	-0.370994
C(5)	-0.3627(42)	-0.360926	-1.4280(11)	-1.439114	0.3303(46)	0.316283
	a-coordinate / Å		b-coordinate / Å		c-coordinate / Å	
1,1-Difluorosilacyclohex-2-ene atom	Experiment	Theory	Experiment	Theory	Experiment	Theory
Si-29	0.7767(19)	0.778765	-0.032(47)	-0.009808	0.00(21)	-0.021147
Si-30	0.7775(19)	0.778765	0.000(57)	-0.009808	0.00(14)	-0.021147
C(1)	-0.2876(60)	-0.310744	-1.4592(12)	-1.460007	0.2578(68)	0.253210
C(2)	-1.64009(97)	-1.636961	-1.3288(12)	-1.330299	0.104(15)	0.126726
C(3)	-2.39093(69)	-2.394123	0.000(28)	-0.061126	-0.165(10)	-0.161449
C(4)	-1.64837(96)	-1.664891	1.2485(13)	1.249370	0.160(10)	0.148129
C(5)	-0.2769(56)	-0.308506	1.3737(11)	1.382704	-0.5846(26)	-0.572674

[a] Numbers in parentheses give Costain errors [21] in units of the least significant figure.
[b] Kraitchman analyses give absolute value coordinates. Signs have been assigned based on the corresponding theoretical coordinate positions.
[c] Imaginary values from the Kraitchman analysis are assigned a coordinate value of 0 Å for reporting.

distribution out of the *ab*-plane. Comparisons in these values are not always direct as the inertial frame shifts, but they can give some qualitative insights between similar molecules. The first interesting comparison is in the P_{cc} values of silacyclohex-2-ene (12.18744(3) uÅ^2) and cyclohexene (10.3098(8) uÅ^2 [1] or 10.310(1) uÅ^2 [2]). Figure 1 shows that C_4 and C_5 atoms are the only heavy atoms outside the *ab*-plane, very similar to the "half-chair" structure of cyclohexene [1, 2] and the similarity in the values supports this. The addition of the fluorines in 1,1-difluorosilacyclohex-2-ene complicate this direct comparison but because the theoretical structures have been determined to be an accurate depiction of the experimental structure, we take the theoretical c-coordinate positions and subtract the fluorines' contribution to P_{cc} resulting in an approximate value of 11.19 uÅ^2 for the remaining atoms, very similar to silacyclohex-2-ene and cyclohexene. Figure 5 shows the "half-chair" structure as determined for the molecules in this work.

Table 5. Comparisons of determinable r_S parameters for silacyclohex-2-ene and 1,1-difluorosilacyclohex-2-ene to that of theory.

	Silacyclohex-2-ene		1,1-Difluorosilacyclohex-2-ene	
r_S Parameter	Experiment	Theory	Experiment	Theory
^{29}Si-C_1 / Å	1.863(24)[a]	1.85962	1.799(48)	1.83450
^{30}Si-C_1 / Å	1.866(25)	1.85962	1.825(50)	1.83450
^{29}Si-C_5 / Å	1.872(25)	1.87977	1.851(75)	1.85079
^{30}Si-C_5 / Å	1.869(26)	1.87977	1.828(62)	1.85079
C_1=C_2 / Å	1.3374(66)	1.33663	1.3674(63)	1.33853
C_2-C_3 / Å	1.481(18)	1.50622	1.550(24)	1.50570
C_3-C_4 / Å	1.557(16)	1.53102	1.489(24)	1.53135
C_4-C_5 / Å	1.5320(48)	1.53796	1.5656(70)	1.54179
$\angle C_1{}^{29}SiC_5$ /°	103.80(37)	104.064	108.1(16)	106.885
$\angle C_1{}^{30}SiC_5$ / °	103.80(37)	104.064	108.0(11)	106.885
$\angle{}^{29}SiC_1C_2$ / °	121.35(66)	121.429	119.6(17)	119.848
$\angle{}^{30}SiC_1C_2$ / °	121.30(67)	121.429	119.0(14)	119.848
$\angle C_1C_2C_3$ / °	126.93(40)	126.592	125.48(53)	126.727
$\angle C_2C_3C_4$ / °	115.84(43)	116.128	116.08(33)	116.308
$\angle C_3C_4C_5$ / °	112.66(35)	113.434	113.59(56)	113.480
$\angle C_4C_5{}^{29}Si$ / °	108.65(75)	109.024	106.7(39)	108.206
$\angle C_4C_5{}^{30}Si$ / °	108.67(75)	109.024	107.0(27)	108.206
Dihedral $\angle{}^{29}SiC_1C_2C_3$ / °	3.9(38)	3.402	-5.6(76)	-3.428
Dihedral $\angle{}^{30}SiC_1C_2C_3$ / °	3.9(38)	3.402	-5.3(52)	-3.428
Dihedral $\angle C_1C_2C_3C_4$ / °	19.3(28)	19.760	-18.6(17)	-20.490
Dihedral $\angle C_2C_3C_4C_5$ / °	-56.7(12)	-56.072	56.9(11)	56.266
Dihedral $\angle C_3C_4C_5{}^{29}Si$ / °	63.5(12)	62.174	-63.0(52)	-60.551
Dihedral $\angle C_3C_4C_5{}^{30}Si$ / °	63.6(12)	62.174	-63.6(36)	-60.551
Dihedral $\angle C_4C_5{}^{29}SiC_1$ / °	-37.0(20)	-35.595	36.(10)	34.233
Dihedral $\angle C_4C_5{}^{30}SiC_1$ / °	-37.1(19)	-35.595	36.3(68)	34.233
Dihedral $\angle C_5{}^{29}SiC_1C_2$ / °	5.3(32)	5.068	-4(12)	-4.248
Dihedral $\angle C_5{}^{30}SiC_1C_2$ / °	5.4(32)	5.068	-5(8)	-4.248

[a] Numbers in parentheses give the errors derived using the Costain errors [21] in units of the least significant figure.

The next interesting comparison is that of the P_{bb} values of multiple six-membered rings with a silicon. All values are near 120 uÅ^2 for the molecules presented, but the first molecules known to be studied with a double bond in the ring from this work are significantly lower in this value. This is because the molecules without a double bond exist in traditional chair conformations with slightly more contribution originating from one of the carbons being further along the *b*-axis, outside the *ac*-plane. However, it should

Table 6. Comparisons of second moments for multiple parent isotopologues of similar molecules to silacyclohex-2-ene and 1,1-difluorosilacyclohex-2-ene.

Molecule	P_{aa} / uÅ^2	P_{bb} / uÅ^2	P_{cc} / uÅ^2	Reference
silacyclohex-2-ene	154.03673(3)[a]	114.82970(3)	12.18744(3)	This Work
1,1-difluorosilacyclohex-2-ene	300.06446(6)	117.93664(6)	66.37000(6)	This Work
silacyclohexane	154.4244(7)	122.3362(7)	17.1515(7)	[23]
cyclohexene	100.8992(8)	96.3294(8)	10.3098(8)	[1]
cyclohexene	100.899(1)	96.329(1)	10.310(1)	[2]
1-fluoro-1-silacyclohexane (axial)	214.20745(6)	122.21878(6)	46.91095(6)	[24]
1-fluoro-1-silacyclohexane (equatorial)	274.8381(1)	121.9286(1)	21.2112(1)	[24]
cyclohexane-d_2	110.95119(5)	102.57538(5)	16.54449(5)	[25]
1-methyl-1-silacyclohexane (axial)	219.09864(6)	123.53275(6)	53.31346(6)	[26]
1-methyl-1-silacyclohexane (equatorial)	282.96261(7)	123.49348(7)	23.27675(7)	[26]
1,1-difluorosilacyclopent-2-ene	227.27110(12)	83.037692(12)	67.164670(12)	[7]
1,1-difluorosilacyclo-pentane	227.27110(12)	83.037692(12)	67.164670(12)	[4]

[a] Numbers in parentheses give standard errors (1σ, 67% confidence level) in units of the least significant figure.

be noted that the value being near 120 uÅ^2 does separate it from five-membered rings because these are all much different in value from 1,1-difluorosilacyclopent-2-ene [7] and 1,1-difluorosilacyclopentane [7].

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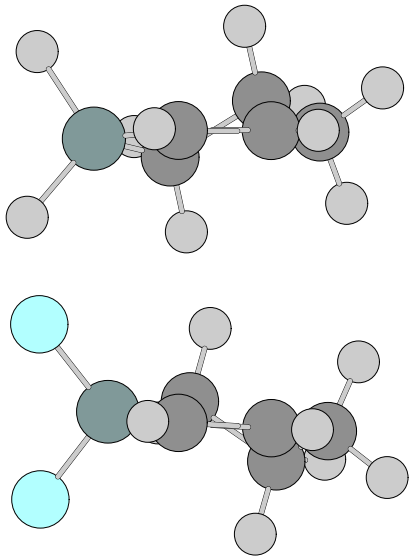

Figure 5. Silacyclohex-2-ene (top) and 1,1-difluorosilacyclohex-2-ene (bottom) looking directly into the double bond. Both molecules have a half-chair configuration like cyclohexene, but with the C_4 atom exaggerated.

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IV. A CHIRPED PULSE FOURIER TRANSFORM MICROWAVE SPECTROMETER WITH MULTI-ANTENNA DETECTION

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ABSTRACT

The construction of a new chirped pulse Fourier transform microwave (CP-FTMW) spectrometer with multiple-antenna detection (MAD) is reported. The instrument design and execution represent a completely new approach to possibly increasing sensitivity in CP-FTMW spectroscopy as it does not involve increased sampling, power, or passes of microwaves with the molecular sample. This is particularly advantageous for experiments where only one sampling point is available. The MAD-CP-FTMW or "MAD Chirp" is demonstrated on both linear molecule carbonyl sulfide (OCS) and asymmetric-top molecule 1,3-difluorobenzene (DFBZ) with detection points at the broadcast antenna as well as in the quadrature to the traditional receiving antenna. Signal-to-noise comparisons with each sample at each detection point have been made and are reported. Experiments demonstrating the signals detected in these new positions are molecular and not an artifact of a reflection are reported. Although this represents a first step to a possible new approach to addressing CP-FTMW sensitivity, no sensitivity increase based on this method is currently reported.

1. INTRODUCTION

Chirped pulse, Fourier transform microwave (CP-FTMW) spectroscopy is a broadband rotational spectroscopic technique realized by Pate in the mid-2000s [1, 2]. The technique is modeled after the advancements made by Flygare in the 1970s [3, 4, 5] and Khodos et al. in the early 2000s [6] known as fast passage microwave spectroscopy. More than 10 years after its inception, the CP-FTMW technique has seen its operational range extended from near-radio wave bands to the mm-wave and sub-THz regions of the electromagnetic spectrum, as well as its applicability expanded to areas of chemical dynamics, analytical chemistry, and chirality determination [7]. Researchers continue to unlock potential uses for the technique and implement enhancements or adaptations to the original design. These include minimizing power requirements by capitalizing on the chirp ranges (decreasing chirp width effectively increases deliverable power) and using solid-state amplifier technology [8, 9, 10, 11], decreasing acquisition time by utilizing multiple sampling sources [2], and collecting multiple free induction decay (FID) acquisitions per gas pulse [2, 10, 12]. Using CP-FTMW techniques as foundational principles, waveguide [13] and chemical sensing spectrometer designs [14] have also been developed.

Introduction of molecular sample into the original CP-FTMW is accomplished by a supersonic jet expansion method. However sampling techniques have extended to designs inclusive of Laval flow [15, 16], static [14] and buffer gas cells [17], skimming techniques, and heated reservoir supersonic beam techniques (for liquid sampling) [18]. Regarding sampling, the canonical CP-FTMW paper by Pate notes a signal-to-noise improvement of N^2 when, instead of utilizing a singular pulsed valve nozzle introduction, multiple nozzles are used (where N is the number of nozzles) [2]. This gain is a huge advantage especially in the limit of averaging millions of free induction decays as adding a singular nozzle can increase signal-to-noise by a factor of four, decreasing sample time and consumption (increasing signal quadratically while increasing sample linearly actually reduces the consumption by a factor of N nozzles).

This multi-sampling sensitivity increase, however, cannot be realized in many new implementations of the CP-FTMW spectrometer for various reasons. The most common two reasons being chamber size constraints and exotic sampling methods (like laser ablation [19] or electric discharge). In the case of exotic sampling, the systems being studied are usually the very types of systems that would benefit the most from a sensitivity boost as their number densities are low ($\approx$ ppm levels of total sample in most cases) compared to many stable monomer species.

Due to the interest of using CP-FTMW in many different chemical physics, physical chemistry, and analytical chemistry problems, different approaches to increase the sensitivity of these spectrometers (without having to increase input power) has become a very important topic. As mentioned previously, research into this field has included high fidelity solid state amplifiers, narrowing the chirp regions through mixing with predetermined oscillators (either with a standard oscillator or frequency combs), and providing more passes through the sample using reflector techniques [20]. One approach to sensitivity has been to work in the 2-8 GHz region (and lower) where higher power availability is much more affordable [21]. Another approach is to study larger molecular systems which provide favorable state populations in the more traditional CP-FTMW spectrometer ranges (2-18 GHz) [11]. Each of these approaches have proven to be a uniquely successful pathway to increasing sensitivity while preserving the overarching advantage of the technique; broadband capability.

Although there has been much work done with signals in the excitation and interaction stages of the experiment, excluding enhancements due to circuit components or design (cable length, etc.), to the authors' knowledge, little-to-no work has been done to fundamentally increase sensitivity at the point of molecular signal detection. In this work, we report, for the first time, a completely different approach to potential signal gain in CP-FTMW. Although no true sensitivity increase is reported, this new approach focuses on the detection scheme where multiple antennae in a CP-FTMW setup are used to simultaneously collect the signal. It is shown that these signals are detectable on the broadcast antenna as well as

in quadrature to excitation and typical detection. As is detailed in this work, this approach provides a new avenue by which to increase sensitivity. For laboratories already possessing a traditional CP-FTMW and/or a multi-antennae microwave three-wave mixing (M3WM) experiment, the setup can typically be implemented via minimal component purchases and free data post-processing tools. In situations where space is limited, quadrature detection can be easily accommodated by the inclusion of a Teflon window with no effective difference in transition line centers. The implementation of such a scheme on the broadcast antenna is accompanied by a minor reduction in incident power due to the inclusion of a circulator, but, in some cases, the potential signal gain will outweigh this cost.

2. EXPERIMENTAL SETUP

The instrument circuit design is based on our prior CP-FTMW designs and won't be discussed except to note deviations [10, 12]. A diagram of the instrument setup is presented in Fig. 1. The four-antennae orthogonal design was inspired by the CP-FTMW/ microwave three-wave mixing (M3WM) instrument of Pate and coworkers as this was the original purpose of the instrument [22]. One difference from this design, however, is that in the current work two antennae reside outside the chamber and are set up on a bracketing system which allow for the antennae to rotate clockwise up to 270 degrees with hard stops at 90 degrees. This idea was inspired by the M3WM experiment of Schnell and coworkers where one antenna is rotated approximately 45 degrees in comparison to the other, but this deviation was enough to produce the chiral signal effect [23]. The original intent of this design was to study the angular effect on the chiral signal in depth and allow flexibility for studying antennae orientation in M3WM. The other antennae may be rotated to the hard stop (or another setting) and set up with a second power amplifier and switch and low noise amplifier combination for M3WM. The antennae outside the vacuum chamber detect signals through a 0.32 cm Teflon window that resides in a flange specifically designed for the aperture of the antennae.

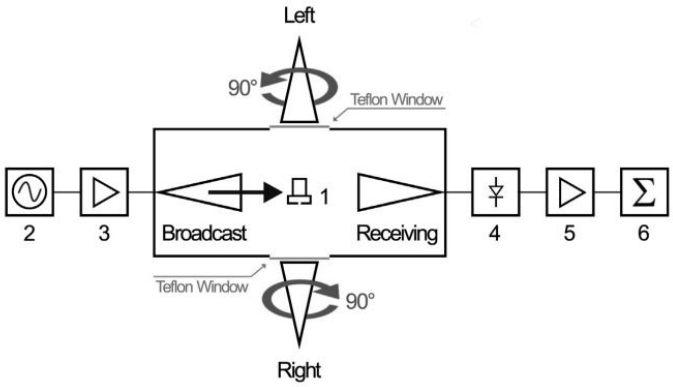


Figure 1. The standard CP-FTMW setup with multi-antenna detection capability at Missouri S&T. The direction of polarization is indicated with an arrow. The design is inspired by the M3WM instruments of Pate and Schnell [22, 23]. As shown, only one antenna is detecting but the other antennae may be rotated (see text) and set up with a second power amplifier and switch and low noise amplifier combination for M3WM or may be outfitted with switch and low noise amplifiers to enable multi-antenna detection (MAD) capability.

The instrument setup in this work consists of the antennae positioned in-plane (at 0 degrees) with respect to each other. Each reception antenna was individually outfitted with a switch and low noise amplifier for multi-antenna detection (MAD) testing. In the case of the broadcast antenna, a circulator is required before the switch and low noise amplifier for excitation and signal collection. Experiments were performed with and without a circulator in order to monitor the effect of power loss on the detected signal and assess the advantage (or disadvantage) of using the broadcast antenna as an additional receiver. In addition, microwave foam experiments (MAST Technologies MF22-0009-00) with the foam inserted in front of the traditional receiving antenna were performed with and without a circulator in order to determine the source of detected signals for the non-traditional detection antennae. In order to perform all MAD experiments equivalently, the common operational setup would not suffice due to chamber geometry and nozzle placement. Instead, tests were performed utilizing the windowed antenna as the source of excitation as shown in Fig. 2. Careful comparison of the data showed that the measured transition line centers were unaffected by the use of the external antennae with the Teflon windows with respect to the internal

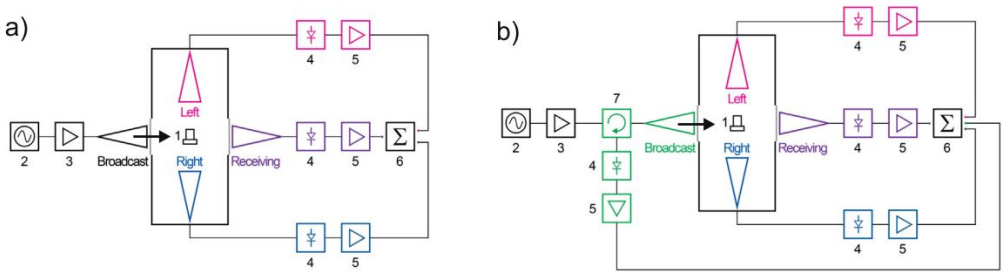


Figure 2. The test setups for MAD-CP-FTMW. The setup in a) is without a circulator to collect on the broadcast antenna and the setup in b) shows the insertion of a circulator for detection on the broadcast antenna. The direction of polarization in both experiments is indicated with an arrow. The components (other than antennae) are 1. Solenoid Valve, 2. Arbitrary Waveform Generator, 3. 40 W Power Amplifier, 4. SPST Switch, 5. Low Noise Amplifier, 6. Oscilloscope, and 7. Circulator. Signals were collected individually on a singular oscilloscope channel for each antenna tested. Cable lengths and all components were kept exactly the same across all tests in order to minimize test variance.

antennae. The foam test setup is depicted in Fig. 3 with a picture of the complete foam coverage of the receiving antenna. As is shown, the foam does not interfere with the rest of the experiment. The foam has < -40 dB insertion loss across the spectrometer's bandwidth which equates to a 99.99% loss in microwave signal, effectively eliminating signal reflections from the traditional receiving antenna. Finally, cable lengths and all components were kept exactly the same across all tests in order to minimize test variance by testing each detection point individually, but signals may be detected simultaneously with additional components.

In order to ensure results were repeatable on different types of molecular tops, experiments were performed with 3% carbonyl sulfide (OCS) in argon (Ar) and 1,3-difluorobenzene (DFBZ) residing in a modified heated liquid reservoir nozzle cap [18], picked up with an Ar carrier. The DFBZ sample was not heated. OCS and DFBZ were introduced into the chamber at optimized absolute pressures of 210 mmHg and 1800 mmHg, respectively. 4.75 GHz chirp lengths of 4 μs were used. 10 k and 35 k FIDs of 20 μs at 100 GSa/s were coadded for DFBZ and OCS, respectively. Collected FIDs were subsequently

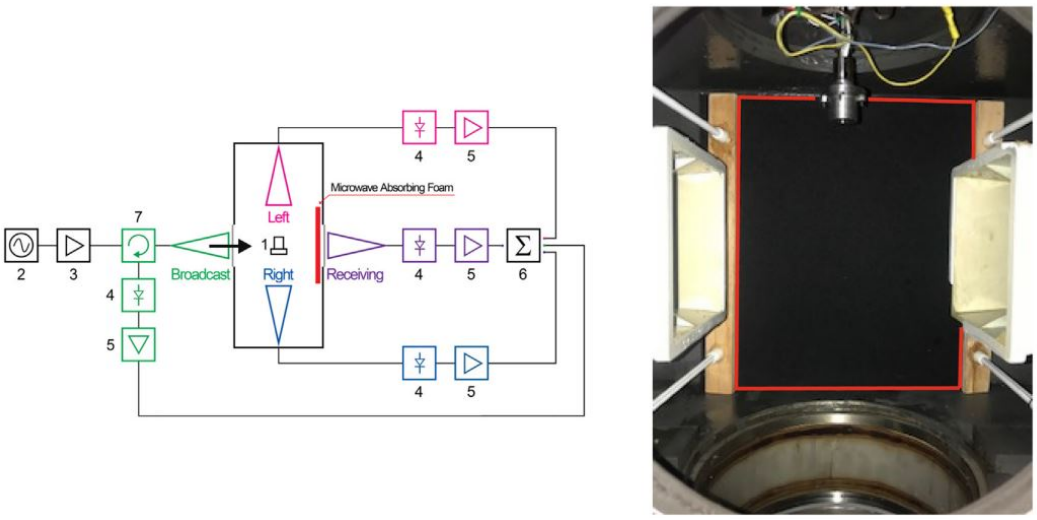


Figure 3. The MAD-CP-FTMW absorbing foam test setup. The direction of polarization is indicated with an arrow. Signals were collected individually on a singular oscilloscope channel for each antenna tested. The foam (MAST Technologies MF22-0009-00) is 2.54 cm (1 inch) thick with < -40 dB insertion loss across the spectrometer's bandwidth. The foam covers the traditional receiving antenna in order to eliminate any possibility of any detected molecular signal or reflections. In addition, the interior of the chamber is coated with microwave absorbing paint to minimize ringing effects. The photo (right) of this experimental setup has been edited to have the foam outlined in red in order to visibly distinguish it from the surrounding apparatus.

fast Fourier transformed using the Bartlett windowing type with Kisiel's FFTS software [24]. All molecular signals were confirmed by running the experiment with and without pulsing the nozzle.

3. RESULTS AND DISCUSSION

The results of the DFBZ tests are found in Table 1. Two transitions, 13623.7 and 12727.3 MHz, were selected in order to mitigate possible saturation effects as DFBZ does possess very strong monomer spectra on the spectrometer. Neither transition apparently exhibited these effects, but the results for both are still reported. As is presented in Table 1, molecular signal is detected at every antenna position, even in quadrature. The signal persists, at the same level for all non-traditional antenna, even after foam insertion. There is,

however, a complete blanking of the original signal for the traditional receiving antenna with the foam installed. As can be determined by inspection of Table 1, there is no appreciable loss or gain (< factor of 10 in most cases) from the insertion of the circulator and/or the foam across any singular detection point, but there is a considerable difference in signal strength (factor of 10 - 100) from the quadrature detectors (left and right) with respect to the in-line detectors (receiving and broadcast).

After the DFBZ experiments were performed, OCS monomer tests were performed to evaluate the observed effect on a linear top. The results of these tests after 35 k FID averages (circulator only) are presented in Table 2. Once again, signal was observed on every antenna even for weakly abundant species. The two most abundant transitions, $^{16}O^{12}C^{32}S$ and $^{16}O^{12}C^{34}S$, possessed such strong signals on the receiving and broadcast antennae that the spectra were saturated and considered unreliable for comparison. However, the weaker $^{16}O^{13}C^{32}S$ and $^{18}O^{12}C^{32}S$ exhibited very similar results to those observed in DFBZ, where the signal-to-noise detected on the receiving and broadcast antennae were within a factor of 10 of one another while the measured signal-to-noise on the orthogonal antennae were weaker by an approximate factor of 10–100.

These results clearly show that there is a detectable electric field at all points tested, inclusive of quadrature. Furthermore, the foam tests and quadrature detection of signal effectively eliminate the source of these signals being the result of a reflection, meaning that their source must be molecular. Although there is a considerable difference in signal strength, it is remarkable that signal can be collected in quadrature for a CP-FTMW experiment as, to our knowledge, this has never been attempted nor reported. Although the tests performed here maintained exactly the same circuit components for consistency amongst signal testing, the authors were also able to detect these signals simultaneously. Detection in this way is oscilloscope limited and the digitization rate had to be reduced in order to collect signal data. It is cautioned, therefore, that any potential implementation of MAD-CPFTMW verify oscilloscope hardware capabilities first before making investments

toward implementation. It should be noted FID phase alignment with respect to antenna position is also important for coaddition purposes in order to preserve/enhance signal-to-noise ratios, but this will be the focus of future work and only the MAD capability is presented here. The authors are currently constructing a spectrometer with a greater variety of detection point positions in order to test the phase dependence of angular positioning (if any). It was also observed during these experiments that each antenna was individually parameterizable for gas settings, so it is possible to increase non-traditional antennae signal-to-noise with respect to each other with gas settings, but this was not done. Instead, signals were parameterized such that the traditional antenna signal was maximized in order to best recreate the typical operating procedure of a CP-FTMW instrument in order to minimize variations in experimental setups.

From the previous theoretical literature reported by Dicke [26, 27] which is the basis of the pulsed microwave technique, it is theorized that signal should only copropagate with the direction of excitation. To our findings, however, this conclusion is somewhat of a void in the literature and has not been examined or challenged, particularly since the development of CP-FTMW spectroscopy. This is interesting because much of the fundamental literature on pulsed microwave techniques involves $\frac{\pi}{2}$ pulsing schemes, but it is well known that CP-FTMW experiments can range from the weak-field limit to a rapid adiabatic passage limit due to the wide range of available power amplifier options and pulsing capabilities of current arbitrary waveform generators [2, 7, 28]. Furthermore, it is rare in CP-FTMW practice to precisely adjust chirp bandwidth and pulse duration to completely satisfy the $\frac{\pi}{2}$ condition for all transitions in the spectra. Typically, only the strongest transitions are parameterized to maximize signal response for an already standardized frequency region for the spectrometer in question. This was the method of parameterization utilized here which resulted in the observation at nontraditional detection points. This could be one explanation for the observation of such spectra in both quadrature and on the broadcast antenna. Furthermore, it is shown that the in-line detectors possessed a much greater

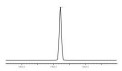
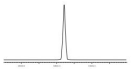
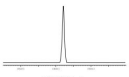
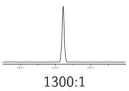
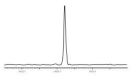
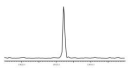
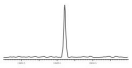
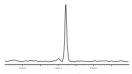
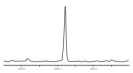
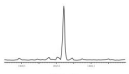
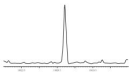
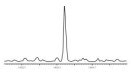
S:N ratio in practically all experiments performed. Although the broadcast antenna is not what is traditionally considered the copropagation direction, it does lie on the same axis of detection, so this may be a rationale for this result.

Another explanation could be that it is not an entirely remarkable discovery that detection is possible in all directions inclusive of quadrature for a microwave experiment, as this is the basis for M3WM. The major difference between CP-FTMW and M3WM is that there is one excitation pulse as opposed to two orthogonal excitation pulses followed by an orthogonal detection. The authors do realize that these microwave pulses are tailored for specific dipole moment components and $\frac{\pi}{2}$ and π conditions, but it has been shown that the chiral signal of a M3WM experiment can be detected at angles other than fully orthogonal (45 degrees) which was one of the original thrust of these experiments [23]. The 45 degree orientation of Schnell's experiment "was chosen so that the recording horn could record a portion of the three-wave mixing signal produced, but also could still record conventional broadband rotational spectra for diagnostic purposes." This may have been a similar experiment to what is being perform here, just in a different plane of detection. An extension of this rationale could be due to the polarization field itself not being unidirectional. We have performed these tests and have found that approximately 0.1% of the polarization field reaches the orthogonal antenna which is in accordance with the observed orthogonal signal, but it is difficult to know if this is causation or coincidence without more extensive study. The aforementioned spectrometer currently being constructed will also be helpful in performing these tests.

Lastly, this effect has been shown to be applicable to asymmetric and linear tops, but both test molecules only possess one dipole moment component in order to avoid complications that could arise with the excitation pulse and dipole moment alignment with the field. These signals are observed regardless of the direction of the dipole moment and the incident electric field. Because of these results, it is hypothesized that this effect is applicable to all molecules, but this was not tested due to these possible complications and

comparing results. These possible complications include transition intensity fluctuation across transition types as a function of detection position, etc. This will also be the focus of our future experiments into this technique.

Table 1. Directionality S:N tests on DFBZ with and without a circulator and with and without foam at 13623.7 MHz (J'_{K_a,K_c} - J''_{K_a,K_c} = $5_{1,5}$ - $4_{0,4}$) and 12727.3 MHz (J'_{K_a,K_c} - J''_{K_a,K_c} = $5_{0,5}$ - $4_{1,4}$) [25] using 10 k FID averages. Actual spectra for each test is shown. The intensity (y-axis) has been adjusted so that the top of the peak fills the available window.

13623.7 MHz	No Foam S:N		Foam S:N	
Antenna	Circulator	No Circulator	Circulator	No Circulator
Recieving[a]	 8200:1	 4500:1	 No Signal	No Signal
Broadcast	 2300:1	N/A N/A	 1300:1	N/A N/A
Left[b]	 15:1	 80:1	 71:1	 55:1
Right[b]	 45:1	 26:1	 33:1	 38:1
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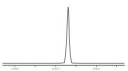
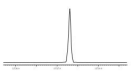
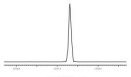
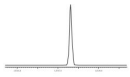
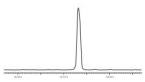
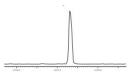
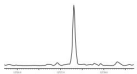
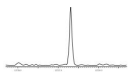
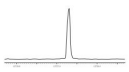
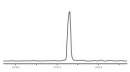
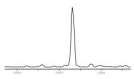
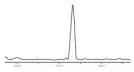
Recieving[a]	 10,200:1	 4500:1	No Signal	 No Signal
Broadcast	 3200:1	N/A N/A	 6300:1	N/A N/A
Left[b]	 17:1	 120:1	 29:1	 32:1
Right[b]	 180:1	 140:1	 40:1	 46:1

[a] Receiving refers to the antenna in the traditional receiving position.[b] Left and right antenna are positioned in quadrature to broadcast and receiving antennae.

Table 2. Directionality S:N tests on four OCS *J'* - *J''* = 1 - 0 isotopologue transitions with insertion of a circulator recorded after 35 k FID averages.

Isotopologue	Frequency/MHz	Abundance/%	Receiving[a]	Broadcast	Left[b]	Right[b]
$^{16}O^{12}C^{32}S$	12162.979	93.60	8,300,000:1[c]	2,000,000:1[c]	60,000:1	46,000:1
$^{16}O^{12}C^{34}S$	11865.662	4.22	6,200:1	140:1	230:1	110:1
$^{16}O^{13}C^{32}S$	12123.842	0.38	750:1	340:1	28:1	9:1
$^{18}O^{12}C^{32}S$	11409.7	0.20	510:1	380:1	5:1	8:1

[a] Receiving refers to the antenna in the traditional receiving position.
[b] Left and right antenna are positioned in quadrature to broadcast and receiving antennae.
[c] Signal strength saturated, so measurement possibly inaccurate.

4. CONCLUSIONS

A CP-FTMW experiment has been demonstrated to be able to detect signal from a molecular source at multiple points of detection. These multiple detection points may be utilized simultaneously in order to enhance S:N without increasing sample consumption or power. This multi-antenna detection (MAD) system has been demonstrated, by use of microwave absorbing foam, to be molecular in nature and not the result of a reflection. Further exemplifying this, there is detectable signal completely orthogonal to the point of excitation, much like that shown in M3WM. The only major difference between the two techniques being that M3WM utilizes excitation in two orthogonal directions with detection in the third orthogonal axis. Unlike M3WM, this effect does not require dipole moment components in every direction of the principal axis system (PAS), but has been demonstrated on molecules (DFBZ and OCS) which have only one dipole moment component in the PAS and are both asymmetric (DFBZ) and linear (OCS) tops. This detection capability is not fully understood, but could be the result of CP-FTMW spectroscopy typically working in a powering regime that can vary from the weak power limit to rapid adiabatic passage, even though much of the theory is established for the ideal $\frac{\pi}{2}$ condition. It is hypothesized that signal can be detected in any direction with any type of molecular top and dipole moment

component composition, but it is unknown if detection in multiple directions will affect the intensity information ascertained from transition types associated with multiple dipole moment components.

ACKNOWLEDGEMENTS

This material is based upon work supported by the National Science Foundation under Grant Nos. CHE-1841346 and CHE2019072. The authors would like to thank the membership of the Midwest Microwave Consortium and, in particular, Steve Cooke for many thought-provoking discussions related to the subject of the MAD-CP-FTMW design and testing. The authors would also like to thank and acknowledge Fred Eickelmann of the Missouri S&T Materials Research Center machine shop for his immense help with machining the parts needed to assemble the MAD-CPFTMW spectrometer.

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V. CONSTRUCTION AND DEMONSTRATION OF A 6-18 GHZ MICROWAVE THREE-WAVE MIXING EXPERIMENT USING MULTIPLE SYNCHRONIZED ARBITRARY WAVEFORM GENERATORS

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ABSTRACT

This manuscript details the construction and demonstration of the first known microwave three-wave mixing (M3WM) experiment utilizing multiple arbitrary waveform generators (AWGs) completely operable in the 6–18 GHz frequency range for use in chirality determination and quantification. Many M3WM techniques, which involve two orthogonal, subsequent Rabi $\frac{\pi}{2}$ and π microwave pulses, suffer from flexibility in pulse types and timings as well as frequency due to most instruments only using one, one-channel AWG and the M3WM probability decreasing with an increasing quantum number, J. In this work, we presented an M3WM instrument that allows that flexibility by introducing multiple, synchronized AWGs and adheres to the high probability transition loop pathways in carvone. The functionality and reliability of the instrument were demonstrated using a series of experiments and mixtures of the R and S enantiomers and determined to be of similar accuracy to other reported M3WM setups with the additional benefit of flexibility in pulsing schemes.

1. INTRODUCTION

Chirality determination in science and technology is one of the largest fundamental molecular challenges in existence today [1]. This is because the enantiomers that arise from chiral centers have almost identical physical and chemical properties, but biological

processes often produce, need, or use one enantiomer in large preference to another. Synthetic processes, though, often end in a mixture of enantiomeric products, even when the chemistry utilized is selectively targeted to result in specific stereochemistry. Therefore, it is of large importance to be able to detect and quantify these mixtures quickly and accurately, especially when trying to produce these chemicals on a large scale, as is often the case in the pharmaceuticals industry.

In 2013, it was demonstrated that chiral gas molecules could be distinguished via a microwave three-wave mixing (M3WM) experiment [2]. Later, this experiment was extended to a modified CP-FTMW-type experiment [3]. No matter the setup, M3WM involves exciting, in succession, a pair of linked rotational transitions of different types (*a*-, *b*-, or *c*-type) and then listening to/collecting the free induction decay (FID) from a third type of transition, completing a transition loop [4]. Transitions in microwave rotational spectroscopy occur through a coupling of a molecule's electric dipole moment to an imposed electric field. Transition types arise from a specific component of that electric dipole moment with a nonzero magnitude. M3WM loops are allowed, then, because chiral species, by definition, possess electric dipole moments where all three components are nonzero in magnitude. Moreover, by definition, each enantiomer possesses one dipole moment component that is the same in magnitude but completely opposite in sign. It is this difference that is leveraged in the M3WM experiment and results in FIDs of each enantiomer being exactly 180° out-of-phase with one another, allowing absolute geometry determination and providing a pathway for the quantitative analysis of mixtures.

For this to be achieved, the experimental setup must contain two crucial components. The first is that the experimental setup consists of antennae optimally oriented to propagate/detect electric fields in each of the three dimensions. The second is that two of those antennae deliver a specialized pulsing scheme consisting of a $\frac{\pi}{2}$ pulse followed by a π pulse, where $\frac{\pi}{2}$ and π are the Rabi flip angles. However, in practice, not all rotational transitions can achieve the full $\frac{\pi}{2}$ condition because the transition moments for the various

angular momentum projections on a space-fixed axis are dependent on the projection quantum number, M_J [3, 5]. Therefore, $\frac{\pi}{2}$ and π have become terminology for the microwave pulse duration needed for maximum coherence and double maximum coherence (resulting in no traditional rotational signal), respectively. In previous works, it was also shown that in order to maximize the probability of enantiomeric separation signal with M3WM and minimize spatial degeneracy influences, it is best to follow an *RQP*-branch (i.e., ΔJ = 1, 0, -1) loop rather than *QQQ* or *PQR* cycle and to minimize loop *J*-states [6, 7]. Lastly, because the chiral signal is proportional to the population difference and the transition dipole moment, but there is generally sufficient microwave power available, it is best to follow a scheme that starts with the largest frequency difference on the weakest dipole moment component and ends with monitoring a transition corresponding to the strongest dipole moment component also at a high-frequency difference [3].

Since the discovery of M3WM, there have been many subsequent experimental and theoretical works showing how such approaches can be utilized to distinguish between enantiomers [8, 9, 10, 11, 12, 13, 14], provide enantiomeric excess (*ee*) information inclusive of mixtures [15], and demonstrate or suggest methodologies which may be carried out in order to selectively choose or build up the population in one chiral species over another (chiral quantum coherent control) [16, 17, 18, 19, 20]. In all known M3WM experimental setups using arbitrary waveform generators (AWGs), however, no setup has utilized multiple AWG sources. Multiple AWGs or very fast digital-to-analog converted channels on a single AWG will most likely be needed to pursue chiral quantum coherent control techniques as the microwave pulse schemes are generally complex or involve synchronous pulses. Furthermore, due to the spatial degeneracy influences, microwave powering costs, and required pulse schemes mentioned above, M3WM experiments typically consist of at least one excitation/listening component in the radiofrequency region (i.e., <~3 GHz). In this

work, therefore, we present the construction and demonstration of the first known M3WM experiment utilizing multiple, synchronized AWG sources entirely operable in the 6-18 GHz region of the electromagnetic spectrum.

2. MATERIALS AND METHODS

M3WM experiments were carried out using a modified chirped pulse, Fourier transform microwave (CP-FTMW) spectrometer with multi-antenna detection, which was described elsewhere [21]. A diagram of the instrument setup is presented in Figure 1, with pertinent differences between that and the MAD-CP-FTMW experiment being described here. As described in reference [21], the MAD-CP-FTMW instrument consists of four antennae arranged in a cross pattern exactly facing each other with the supersonic expansion source centered above, pointing at the throat of a diffusion pump. Two of these antennae are located inside the vacuum chamber, and two are located outside. The two external antennae have Teflon windows allowing the microwaves to pass into the chamber where they are broadcast onto the molecular sample. Using the inside or the outside antennae in traditional CP-FTMW experiments showed no observable difference in line centers. For M3WM instruments, three orthogonal microwave fields are required to maximize enantioseparation efficiency. With our single polarized antennae (Steatite® QWH-SL-2-18-S-HG-R), this can be achieved by rotating one of the exterior antennae by 90°. The exterior antennae are mounted in such a fashion that they may be rotated up to 270°. The resulting arrangement is similar to that of Lobsinger et al. [3], where three antennae (colored blue, green, and red in Figure 1) are used for the M3WM experiments, and the fourth antennae may be accessed to quickly shift back to traditional CP-FTMW spectroscopy if desired.

As shown in Figure 1, two antennae (blue and green) are used for excitation, and one antenna (red) is used for detecting the resultant free induction decay (FID) of the molecular response to the excitation. This is different from traditional CP-FTMW spectroscopy, where only one excitation source is generally utilized. In order to provide the experiment with

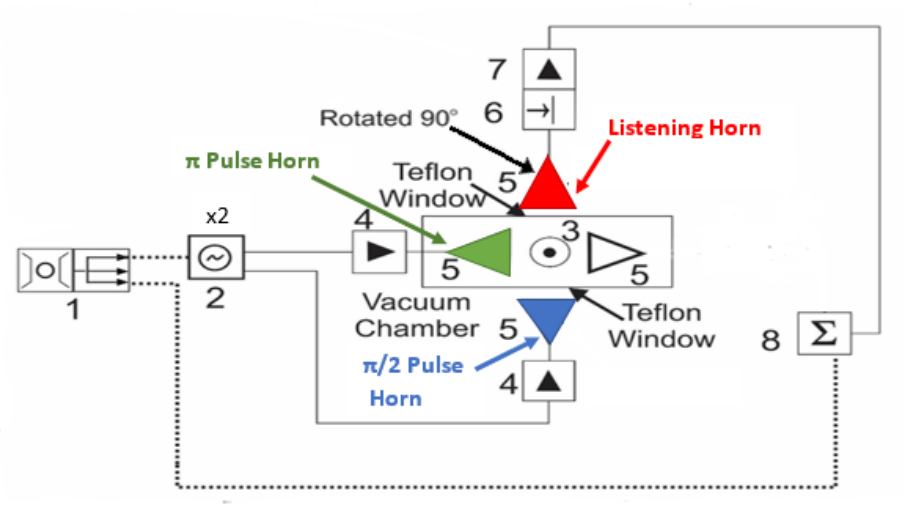

Figure 1. The standard MAD-CP-FTMW setup for M3WM experiments at Missouri S&T. The setup consists of (1) rubidium clock oscillator (Stanford Research Systems® Model FS725 Rubidium Frequency Standard), (2) two synchronized arbitrary waveform generators (Tektronix®AWG 70000 Arbitrary Waveform Generator with Tektronix® AWGSYNC01 synchronization hub), (3) pulsed nozzle source (Parker Hannifin® Series 9 supersonic nozzle), (4) one 40 W power amplifier (Microsemi® model L0618-46-T680) and one 1 W amplifier (Avantek® APT-18649), (5) three broadband horn antennae (Steatite® QWH-SL-2-18-S-HG-R), (6) a pin diode switch (ATM® PNR S1517D), (7) a low noise amplifier (RF-Lambda® RLNA06G18G45), and (8) an oscilloscope (Tekronix® DPO 72304DX Digital Phosphor Oscilloscope). The colors of the three horns indicated what part of the pulse sequence they correspond to, as described in the manuscript. The red horn is rotated 90° in relation to the others.

adequate microwave power, a 1 W microwave power amplifier (Avantek® APT-18649) and a 40 W microwave power amplifier (Microsemi® model L0618-46-T680) were employed for excitation. On the detection antenna, an SPST switch (ATM® PNR S1517D) and a low noise amplifier (RF-Lambda® RLNA06G18G45) are used to block out all signals except for those resulting from the FID, which requires amplification in order to be interpreted by the oscilloscope (Tekronix® DPO 72304DX Digital Phosphor Oscilloscope.)

As mentioned previously, M3WM experiments require microwave pulses occurring in a $\frac{\pi}{2}$-π coherence scheme. In previous M3WM designs, this was achieved multiple ways, from using a switch on a singular AWG [3], using multi-channel AWGs [14, 22], invoking a dual-polarized antenna [19], and switching electric fields [2, 11, 13, 15]. The difference

Figure 2. Picture of the Tektronix® AWG 70000 AWGs (bottom) with the Tektronix® AWGSYNC01 synchronization hub (top). The synchronization hub works on up to four AWGs at one time.

between these designs to the design presented in this work is the implementation of two synchronized AWGs to generate the microwave coherence pulses needed for the experiment simultaneously. This provides a specific advantage not possessed by the other approaches in that now the user may have control over the type of pulse (or pulse profile) while also not being limited to one pulse having to finish before another pulse begins. This arrangement allows for future experiments involving the excitation pulse schemes with greater flexibility as the waveforms are written with code instead of manipulated via hardware. The AWGs are synchronized using a synchronization hub (AWGSYNC01) with one AWG acting as the primary unit and the others acting as secondary units. Up to four units may be controlled by the synchronization hub at any given time (see Figure 2 for a picture of the setup), but the M3WM experiments performed here only consist of two synchronized AWGs.

Another unique aspect of the experimental setup is that the entire instrument operates in the 6-18 GHz region of the electromagnetic spectrum. This is not because of the AWGs, but because this is the optimal region for the antennae and power amplifiers.

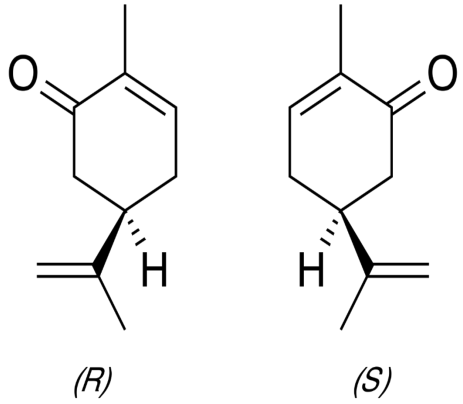

Figure 3. Enantiomers of carvone.

In total, four M3WM experiments on enantiomeric mixtures of carvone were carried out. These included (A) 5 mL of pure R-carvone, (B) 5 mL of pure S-carvone, (C) 1:1 mixture of R-Carvone (2.5 mL) and S-carvone (2.5 mL), and finally (D) 3:1 mixture of R-carvone (3 mL) and S-carvone (1 mL). The enantiomers of carvone are presented in Figure 3. The R-carvone (Product No.: A13900, Purity: 98%) and S-carvone (Product No.: L07130, Purity 96%) samples were manufactured by Alfa Aesar® and obtained through ThermoFisher Scientific®. No further purification was performed on the samples after purchase. Quality documentation for the two enantiomers can be found in the Supplemental Material.

Each of the four liquid carvone samples were placed into a heated nozzle reservoir and warmed to 95° C to promote vaporization [23]. Argon was used as a backing gas and sample was introduced at 50 psig. A Parker Hannifin® Series 9 supersonic nozzle pulsed sample into the chamber at a rate of 3 Hz with 3 FIDS per gas pulse. In total, 500,000 FIDS, each FID being 20 μs in length, were averaged together for each experimental run.

The mixing scheme chosen for all four mixtures is presented in Figure 4. Transitions were selected based on the previous rotational study of carvone by Moreno and colleagues [24]. This study started by determining, theoretically, the three most stable structures of carvone. These structures are labelled EQ1, EQ2, and EQ3. For another to be submitted

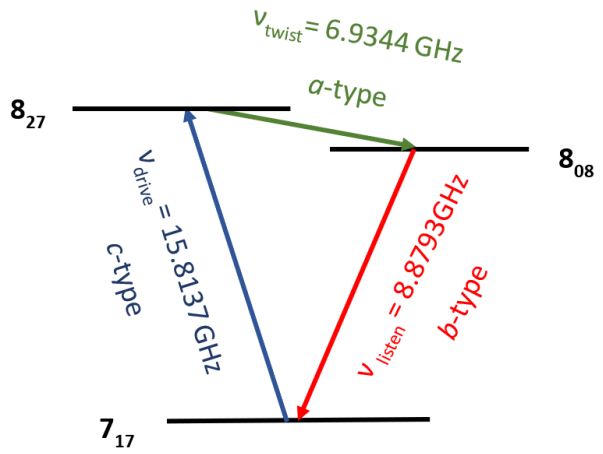

Figure 4. Energy level diagram for the microwave three-wave-mixing transitions of the carvone EQ2 conformation. The ν_{drive}, ν_{twist}, and ν_{listen} are the *c*-, *a*-, and *b*-type transition frequencies respectively.

work on this molecule, we performed optimization calculations of these conformers at the B3LYP/6-311G++(d,p) level using Gaussian09 [25] and these structures are presented in Figure 5. Of these conformers, EQ2 was determined to be the most stable conformer with the strongest of these transitions being *b*-type as the dipole moment component ordering is $\mu_b > \mu_a > \mu_c$. As a result, it was decided that the optimal mixing scheme would consist of *c*-type $\frac{\pi}{2}$ "drive" transition, an *a*-type π "twist" transition, and a *b*-type "listen" transition with antennae colored blue, green, and red corresponding to the transition color scheme in Figure 4. Candidate transition loops fitting this scheme were then determined by utilizing the fitted spectral constants in the Moreno work in SPCAT to predict transition frequencies and quantum numbers.

The best transition loop for these experiments consisted of a drive pulse centered at 15.8137 GHz, a twist pulse centered at 6.9344 GHz, and a listen transition at 8.8793 GHz. The drive pulse was amplified by a 1 W amplifier for a duration of 7.45 μs and broadcast into the chamber via the external horn (again, colored blue) seen in Figure 1. Secondly, the twisting pulse at 6.9344 GHz was amplified with a 40 W power amplifier and broadcast from the antenna labelled green in Figure 1 for a duration of 300 ns. The

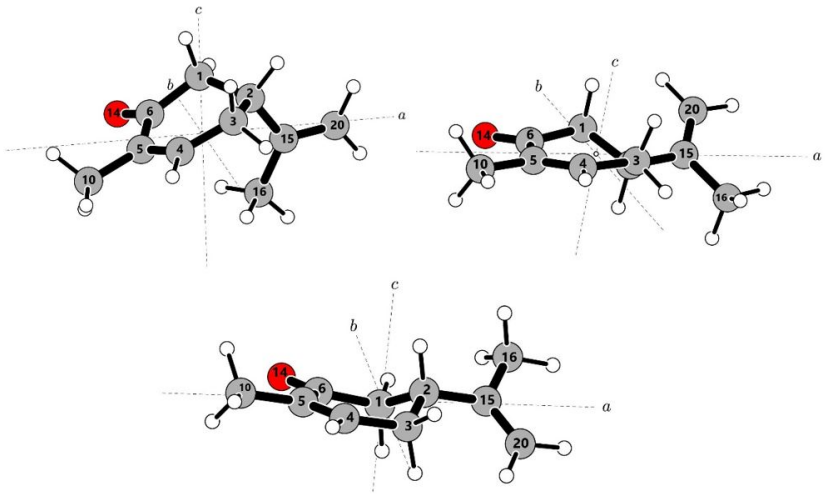

Figure 5. EQ1, EQ2, and EQ3 conformations of carvone, respectively, as reported by Reference [24]. The conformations are each presented in the principal axis system. EQ2 is the most stable conformer and the one from which the transition cycle of Figure 4 was derived.

resultant listening frequency of 8.8793 GHz was received by the red colored antenna in the schematic in Figure 1, low noise amplified and the subsequential FID was recorded. Timings for the drive and twist pulse were achieved by maximizing the coherence signal in a traditional CP-FTMW experiment utilizing the power amplifiers that would be employed in the M3WM experiment. Since maximizing the coherence pulse is assumed to be the $\frac{\pi}{2}$ condition, this timing was used directly for the drive pulse and doubled for the twist pulse.

3. RESULTS

The results found at the listening frequency of each of the four experiments are presented in Figure 6. For experiments A and B, the "pure" R- (98%) and S-carvone (96%), respectively, the signal-to-noise ratio (SNR) was determined to be almost equal: 21:1 and 20:1, respectively. For experiment C, the 1:1 sample mixture, no transition was observed. Lastly, in experiment D, the 3:1 R:S sample mixture resulted in a SNR of 7.8:1.

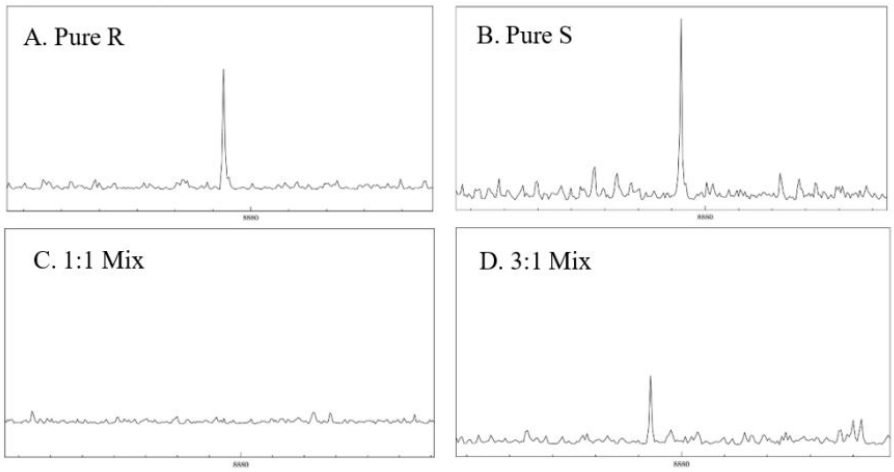

Figure 6. Spectra of the four samples of the enantiomers of carvone obtained at the listening frequency of 8.8793 GHz. A.) 98% R-carvone produced a signal-to-noise ratio (SNR) of 21:1. B.) 96% S-carvone produced a SNR of 20:1. C.) 1:1 mixture of the R- and S-carvone samples. No transition observed. D.) 3:1 mixture of R- to S-carvone samples produced a SNR of 7.8:1.

4. DISCUSSION

The results of experiments A, B, and C follow precisely what have been observed in previous M3WM experiments as the "pure" R- and S-carvone are almost identical in SNR and no signal is observed in the racemic mixture after 500,000 averages. The only difference between the two values may be attributed to fact that the 98% and 96% are minimum purities. To validate this further, we obtained a Certificate of Analysis of the samples from the supplier (found in the Suppemental Material). The R-carvone sample was determined to be 99.3% pure while the S-carvone sample was 98.9% pure. This slight difference in purity can easily explain the small difference in SNR (21:1 vs. 20:1) between the two samples.

To explain the results of Experiment D, we must first try to understand the specific SNR expected in a 3:1 mixture and then check if these results match with what would be expected. In order to achieve this, we will first present some well understood principles regarding enantiomeric excess (*ee*) of a mixture. The *ee* of a mixture is defined by the

following:

$$\%ee = \frac{|R - S|}{R + S} \times 100\%, \tag{1}$$

where R and S are masses (or volumes) of the R and S enantiomers. Defined for optical rotation, this value is given as:

$$\%ee = \frac{|\alpha_{observed}|}{\alpha_{pure}} \times 100\%. \tag{2}$$

Equation 2 comes from the observation that when an absolute racemic mixture is present, the optical rotation of the light is 0°. Similarly, it has been shown that M3WM experiments exhibit no signal for a racemic mixture because the FID signals deconstructivity interfere due to being 180° out-of-phase with one another. Taking this similarity into account, then, the same equation may be used to determine the *ee* of a mixture using SNR:

$$\%ee = \frac{|SNR_{observed}|}{SNR_{pure}} \times 100\%. \tag{3}$$

However, we should note that our "pure" samples are not pure but 99.3% and 98.9% for R- and S-carvone, respectively, resulting in slight differences in our observed pure SNR's. A 3:1 mixture of R-to-S taking the purities into account, then, should give a 50.2% *ee* of R-carvone (50% just assuming absolutely pure). Using Equation 3 for the 3:1 mixture and using the results of Experiments A and B disregarding the small discrepancies in purities give % *ee* of 39% and 37%, respectively.

At first this result would seem very concerning as the values are almost 25% off from the accepted certificate of analysis. However, the results of experiments A, B, and C along with some literature results provide the basis of the conclusion that the instrument, as constructed, is fully operational. The first is that the uncertainty in *ee* in previous studies was shown to be approximately ± 5% across 10 experiments [22]. Our experiment falls easily within the 3σ 95% confidence interval of this work being 11% and 13% off, respectively.

Furthermore, the SNR signals of 7.8:1 and 21:1 or 20:1 are lower to begin with and it has also been shown that chirality determination is greatly increased when signals are above 50:1 in SNR.

However, this result on its own is not satisfactory, so we investigated the FID and FFT information more to understand these results.The first item undertaken was to look at the real and imaginary FFT portions of the pure R- and S-carvone species. They are presented in Figure 7. If the FID signals are more than 90° out-of-phase, they will be opposite in sign in the imaginary part of the FFT. This is exactly the case, however, there are dispersion signals in the real part of the FIDs indicating that the signals may not be 180° out-of-phase with one another. The raw FID data, however, contains many manmade signals that overwhelm the traditional microwave signals, even in common CP-FTMW arrangement. In order to understand the signal we are interested in at 8.8793 GHz, then, we put the signal through a math bandpass filtering process of only allowing ± 0.5 MHz around the real and imaginary 8.8793 GHz signal and while blanking out the rest of the FT signal. From there, an inverse FFT was employed to reconstruct the time domain FID signal for which we were interested. Those FIDs are presented in Figure 8.

The full FIDs of Figure 8, however, do not provide the resolution to see the oscillations of the 8.8793 GHz signal. Therefore, a representative "zoom-in" of each FID has been presented in Figure 9 along with an overlay of the two signals. From the overlay, it is apparent that the signals are not, in fact, 180° out-of-phase as our Real and Imaginary FT data implied. To show that this spectrometer is fundamentally equivalent to previous M3WM experiments, we need to show that this signal can be shown to give more accurate *ee* measurements than those from the magnitude spectrum alone.

The first determination, then, is to understand how the *ee* measurement depends on phase in a M3WM experiment. For this, Shubert et al. provide the proportionality [10]:

$$s \propto ee \cdot \cos(2\pi\nu t + \Phi_{MW} + \Phi_{RF} \pm \frac{\pi}{2}(1 + \frac{\mu_X\mu_Y\mu_Z}{|\mu_X\mu_Y\mu_Z|})), \tag{4}$$

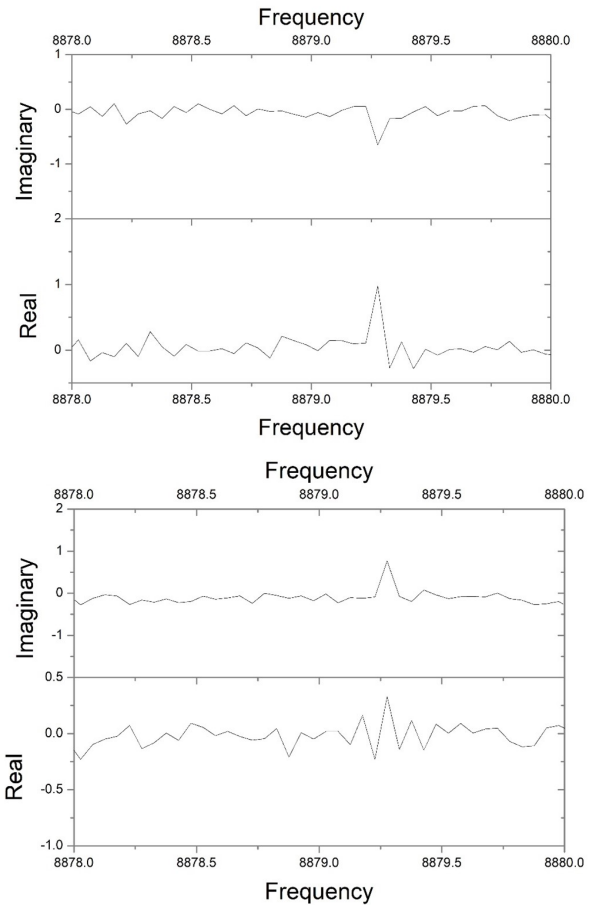

Figure 7. Real and Imaginary parts of the "pure" (top) R-carvone and (bottom) S-carvone FFT's at the listening frequency. Notice that the real signal has some dispersion in both samples, but the imaginary part is exactly opposite in sign showing that the signals are uniquely out-of-phase with one another.

where Φ_{MW} and Φ_{RF} are the phases of the microwave and radiofrequency pulses typically used for the drive and twist pulses, respectively. This leads to an observed phase of the enantiomers, Φ_{obs}, at the start of the FID, t_r, as [10]:

$$\Phi_{obs} = -2\pi\nu t_r + \Phi_{MW} + \Phi_{RF} \quad \text{if} \quad \mu_X\mu_Y\mu_Z < 0 \tag{5}$$

$$\Phi_{obs} = -2\pi\nu t_r + \Phi_{MW} + \Phi_{RF} \pm \pi \quad \text{if} \quad \mu_X\mu_Y\mu_Z > 0 \tag{6}$$

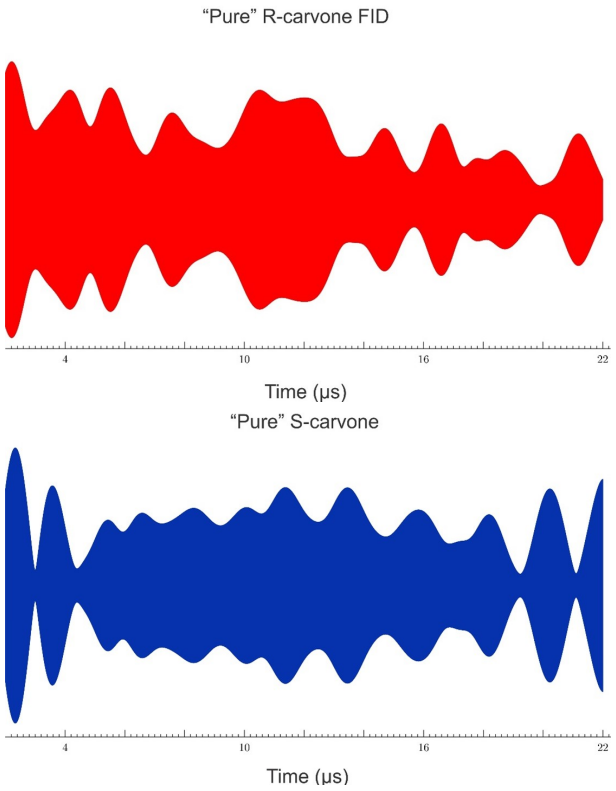

Figure 8. The full R-carvone (top) and S-carvone (bottom) FID signal after math filtering (see text). There is not much phase information that can be gathered from the signal at this level.

However, if the drive and twist phases are out-of-phase, then the $\pm\pi$ of Equation 6 will readjust to the observed phase of the enantiomers. Using Equations 5 and 6 into Equation 4, we can arrive at a new proportionality:

$$s \propto ee \cdot |\cos(\Phi_{OBS1} - \Phi_{OBS2})|, \tag{7}$$

where $\Phi_{OBS1} - \Phi_{OBS2}$ is the phase difference between the enantiomers.

Using sine function math fitting tools on the pure R- and S-carvone FIDs, we determined the $\Phi_{OBS1} - \Phi_{OBS2}$ to be 136.6° out-of-phase. The sine fitting tool utilizes a specific number of points (128 in our experiments) of the Fourier-filtered FID $f(t) = a\sin(bt + c)$, and fits them to the function where a is the amplitude of the FID, b is the

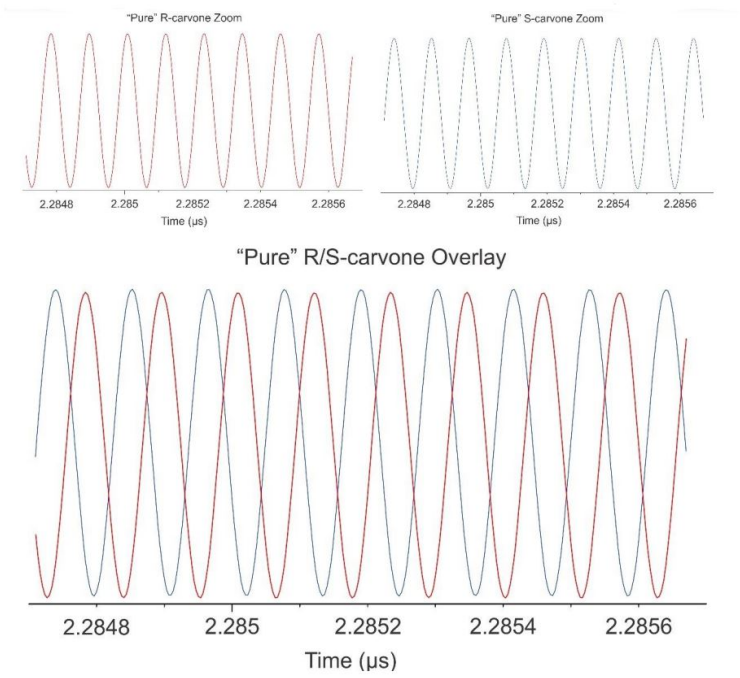

Figure 9. The full R-carvone (top-left) and S-carvone (top-right) zoomed-in FID signal after math filtering (see text) and an overlay (bottom) of the two zoomed-in FIDs. The FIDs are out-of-phase, but not 180° like traditional M3WM experiments.

frequency of the signal, and c is the phase. The fitting tool utilizes a Marquart-Levenberg algorithm using the sum of the least-squares deviations as the maximum-likelihood criterion. It should be noted here that all fits had an R^2 value > 0.99999. The mathematically derived 136.6° was in excellent agreement with a much less rigorous Lissajous plot method employed (135.1°). Previous experience with FID averaging in the CP-FTMW experiment shows that there is an uncertainty of ±0.5 ps in the time domain. Using this we can now establish a calibration phase discrepancy of 136.6 ± 0.3° for the determination of any resultant SNR mixtures. This means we need to adjust Equation 3 to:

$$\%ee = \frac{|SNR_{observed}|}{|SNR_{pure}||\cos(\Phi_{OBS1} - \Phi_{OBS2})|} \times 100\%. \quad (8)$$

Using Equation 8, then, for the 3:1 mixture and using the results of Experiments A and B give % *ee* of 53.7 ± 0.3 % and 50.9 ± 0.2 %, respectively. These values are in much better agreement with the exact value of 50.2 % *ee* given earlier using the certified values and certainly agree with the reported 5% *ee* uncertainty in a M3WM experiment (using S-carvone SNR values, we are < 1 % off the accepted) [22].

The last question that requires addressing is how is the relatively large twist frequency possible? Patterson and Doyle explain that the twist frequency, $\nu_{twist} \leq c/4L$ where c is the speed of light and L is the characteristic length of the sample [26]. The solenoid valve employed for the supersonic beam is 0.8 mm in diameter. Also, it has been shown that multiple nozzle beams will interact when placed within 20.5 cm of each other. This gives 0.08 cm ≤ L ≤ 20.5 cm for a scenario with one beam. This beam is not skimmed or columnated in any way. Using c = 3.0 x 10^{10} cm/s, 0.366 GHz ≤ ν_{twist} ≤ 93.75 GHz. However, it has been shown that the 180° signal persists up to 4 GHz as has been shown by both Schnell and Pate, but starts to become considerably out-of-phase with our value of 6.9344 GHz, perhaps starting to show that the characteristic length of the sample with one supersonic nozzle in the interaction zone is on the order of 10 cm or less. This, along with the tracking of the explicit phase of the pure signals using a calibrant, really allows for any twist frequency to be used as long as the phase discrepancies are tracked as it is well documented that $\Phi_{listen} = \Phi_{drive} + \Phi_{twist}$ [27].

We conclude, therefore, that this instrument, although different in multiple ways from previous M3WM experiments, has been fully developed and demonstrated to be comparable or better than other known M3WM techniques when Fourier-filtering techniques are leveraged.

ACKNOWLEDGEMENTS

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VI. INTERNAL ROTATION ANALYSIS AND STRUCTURE DETERMINATION OF R-CARVONE

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ABSTRACT

When the spectrum of R-carvone was collected at Missouri S&T in preparation for a microwave three-wave mixing experiment, splittings within the rotational transitions indicative of large amplitude motion were observed that were unassigned in both the original study of S-carvone by Moreno et al. [1] and the monoterpenoid study by Loru et al. [2]. It was discovered that these splittings were due to the internal rotation of carvone's two non-equivalent methyl rotors. This prompted a reinvestigation into the ground state, pure rotational spectrum of R-carvone using chirped pulse, Fourier transform microwave (CP-FTMW) spectroscopy within the 5-18 GHz region of the electromagnetic spectrum. The parent species of all six conformers as well as the ^{13}C and ^{18}O singly substituted isotopologues of select conformers were observed in natural abundance and analyzed using XIAM. This marks the first time the AX1 parent conformer and ^{18}O singly substituted isotopologues are reported within a rotational study on carvone. The r_s experimentally determined structures of EQ1, EQ2, EQ3, and AX3 were obtained via Kraitchman analysis and are reported, along with the experimentally determined barrier heights to internal rotation.

1. INTRODUCTION

Carvone ($C_{10}H_{14}O$, 5-isopropenyl-2-methylcyclohex-2-ene-1-one) is a member of the terpene family—a group of secondary metabolites whose members are often recognized by their unique fragrances and diverse activities. As such, terpenes can often be found within natural flora, oils, synthetic flavorings, solvents, and perfumes. The two enantiomers of carvone are no exception. S-(+)-carvone is the main component in caraway oil while R-(-)-carvone is the molecule that gives spearmint its distinct aroma. The drastic difference in the two enantiomers' odor demonstrates the unique biological roles that enantiomers of chiral molecules can possess. In addition, the two enantiomers have important characteristics related to biological and pharmacological activities including being antioxidants, antimicrobials, anticarcinogenic, antimutagenics, and antidiabetics, among others [3, 4]. As a result, the study of the enantiomers of carvone has been of great interest for many years.

The molecule of carvone can exist within two structural conformations, referred to as the equatorial (EQ) and axial (AX) conformers, depending on the orientation of the isopropenyl group. In addition, each conformer processes three possible rotamers, whose structures can be seen within Figure 1. These six structures will be referred to as EQ1, EQ2, EQ3, AX1, AX2, and AX3 for the remainder of this work, following the nomenclature used by Egawa et al. [5] (see Figure 1). The natural abundance of the six conformers has been calculated as 28%, 44%, 26%, 0.12%, 0.13%, and 0.17%, respectively [6]. It has been reported previously that there is an enthalpy difference of 2.0 kcal/mol between the axial and lower energy equatorial structures [7].

Over the past few decades, carvone has been the center of numerous studies. Theoretically, carvone's geometry, electron structure, chemical reactivity [8] and magnetic-field-induced axial birefringence [9] have been investigated and reported. Experimentally, carvone has been studied via optical absorption [10], electron spin spectroscopy [10], photoionization spectroscopy [11], IR [5, 10, 12], Raman [12], circular dichroism [6, 12], optical rotatory dispersion [6], gas electron diffraction [5], REMPI spectroscopy [13], vi-

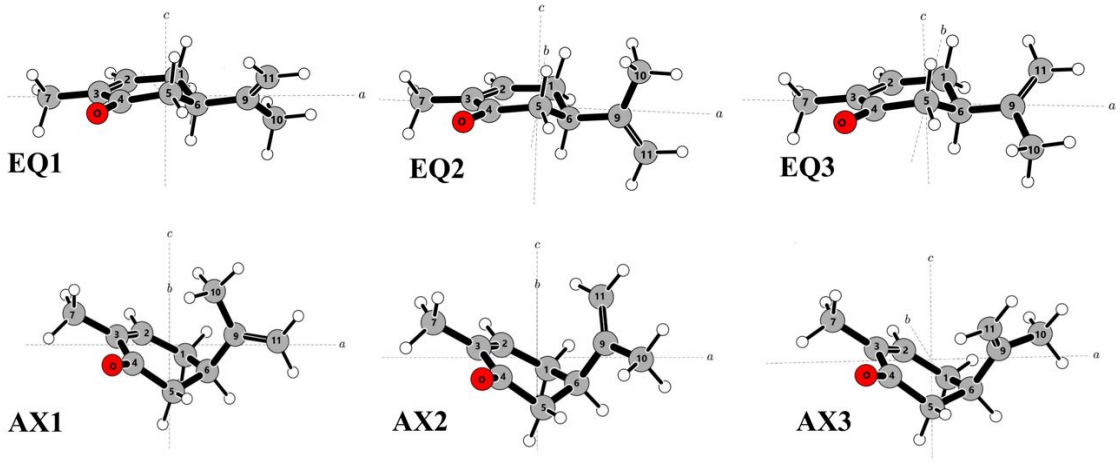

Figure 1. Theoretical structures for the six conformers of carvone calculated using the DFT method and B3LYP/6-31++G(d,p) level of theory.

brational spectroscopy [14], NMR [15], multidimensional gas chromatography [15], X-ray powder diffraction [16], and X-ray absorption [17]. Rotationally, carvone was first studied in 2013 by Moreno et al. using a molecular beam, Fourier transform microwave (MB-FTMW) spectrometer within the 4-20 GHz region of the electromagnetic spectrum [1]. They were able to identify the parent conformers of EQ1 and EQ2 within the experimental data but did not observe EQ3, due to relaxation processes in their supersonic jet, or any axial conformers [1]. Six years later, however, the rotational spectrum of EQ3, along with two axial conformers (AX2 and AX3) and isotopologues of EQ1 and EQ2, would be identified and reported by Loru et al. within their study on monoterpenoids [2].

In addition, a year after the original rotational study, the enantiomers of carvone were utilized by Schnell et al. to perform chirality-sensitive microwave spectroscopy, also known as microwave three-wave mixing (M3WM). This was done to demonstrate their capability to discriminate between enantiomers and measure enantiomeric excess via broadband rotational spectroscopy [18]. Since then, carvone has also been utilized to demonstrate the success of M3WM with chiral mixtures [19], within the 6-18 GHz region

of the electromagnetic spectrum [20], and within coherent enantiomer-selective enrichment [21]. As a result, carvone has become known within the rotational community as an excellent calibrant for M3WM.

It was carvone's use as a M3WM calibrant that first drew our group's attention to the molecule. While performing preliminary work in preparation for the demonstration of our M3WM spectrometer [20], a traditional microwave spectrum was collected for R-carvone within the 5-18 GHz region. Within this spectrum, it was noticed that line splittings characteristic of large amplitude motion were present throughout and had been unassigned within the two previous traditional rotational studies [1, 2]. Upon further investigation, it was determined that these splittings were produced by the two non-equivalent methyl rotors present within carvone's structure.

It has been well documented that thermal population in the excited states and *M*-degeneracies greatly limit the success of certain M3WM schemes for chirality discernment due to a decrease in population transfer efficiency [22]. However, no studies have been performed to deduce the effects of internal rotation on the success of M3WM. Yet, internal rotation breaks the symmetry of the molecule and causes degeneracies to form within the rotational states. With two non-equivalent methyl rotors, for example, each rotational state is split into five symmetry states as shown in Figure 2 [23]. As a result, M3WM schemes, which traditionally consist of three interconnected rotational states, would now possess fifteen rotation states. Thus – in similar fashion to *M*-degenericies – the cyclic excitation would now involve a number of coupled, partially incomplete, three-level systems, limiting the efficiency of the population transfer and scheme. If carvone is to continue to be a standard calibrant for M3WM, it is imperative that its internal rotation is well understood.

Within this work, therefore, an in-depth analysis of the rotational spectrum of R-carvone, accounting for internal rotation, is undertaken. The microwave spectrum of all six conformer parents have been observed, marking the first experimentally reported spectrum for AX1. In addition, the ^{13}C isotopologues for EQ1, EQ2, EQ3, and AX3 as

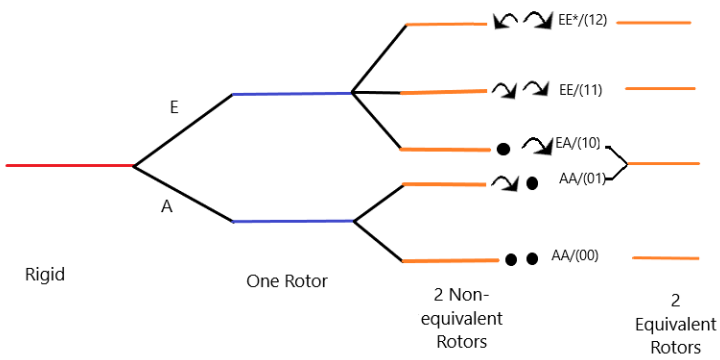

Figure 2. Schematic splittings in the rotational energy states of molecules due to the internal rotation of one rotor, two non-equivalent rotors, and two equivalent rotors. The dots represent the rotors standing still, while the arrows represent the individual rotors rotating in a given direction. Carvone possesses two non-equivalent methyl rotors.

well as the ^{18}O isotopologues for EQ1, EQ2, and EQ3 in natural abundance have been observed and reported, resulting in the experimentally determined structures (r_s) for these four conformers. Splittings due to two non-equivalent methyl rotors have been observed, analyzed, and reported, including the experimentally determined barrier heights to internal rotation as well as the delta and epsilon angles descriptive of each methyl rotor.

2. EXPERIMENTAL

The microwave experiments were carried out at Missouri University of Science and Technology (Missouri S&T) using a multi-antenna detection, chirped pulse Fourier transform microwave (MAD-CP-FTMW) spectrometer, which has been introduced previously [24]. For these experiments, the instrument was operated in its traditional configuration, in which the broadcasting and receiving horns are both in-plane and separated by 180°. No data was collected using multi-antenna detection.

The R-carvone used within this study was manufactured by Alfa Aesar® (Product Number: L07130) and obtained through ThermoFisher Scientific®. The sample had a purity of 98%. Quality documentation can be found in the Supporting Information. No

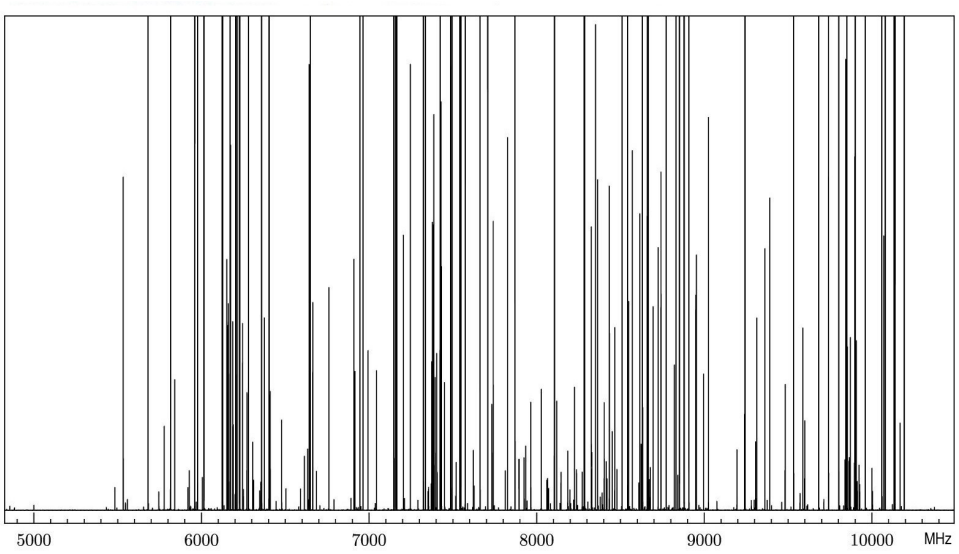

Figure 3. The 5.5 to 10.25 GHz experimental spectrum for R-carvone. Intensities of the strongest transitions are cut off so that less intense transitions are visible.

further purification or analysis was performed on the sample after purchase. For the experiment to be carried out, the sample of R-carvone was placed into a heated nozzle reservoir and warmed to 95 °C to promote vaporization as the sample was initially liquid at room temperature [25]. Industrial grade argon was used as a backing gas and sample was introduced at a pressure of 50 psig. A Parker Hannifin® Series 9 supersonic nozzle pulsed sample into the chamber at a rate of 3 Hz with 3 free induction decays (FIDs) collected per gas pulse.

Spectra of R-carvone was then acquired in the 5.5-10.25 GHz, 9.75-14.5 GHz, and 14-18.75 GHz regions of the electromagnetic spectrum using 4 μs chirp widths. In total, 280,000 FIDs, each FID being 20 μs in length, were averaged together in each region. This equates to roughly 12 hours of collection time per frequency range. The experimental spectrum for each frequency range can be seen in Figures 3, 4, and 5. Typical linewidths for the spectra were 70-85 kHz with an attributed 10 kHz uncertainty in the line centers. However, there were several observed transitions with increased linewidths between 90-200 kHz for which higher uncertainties were attributed to their line centers.

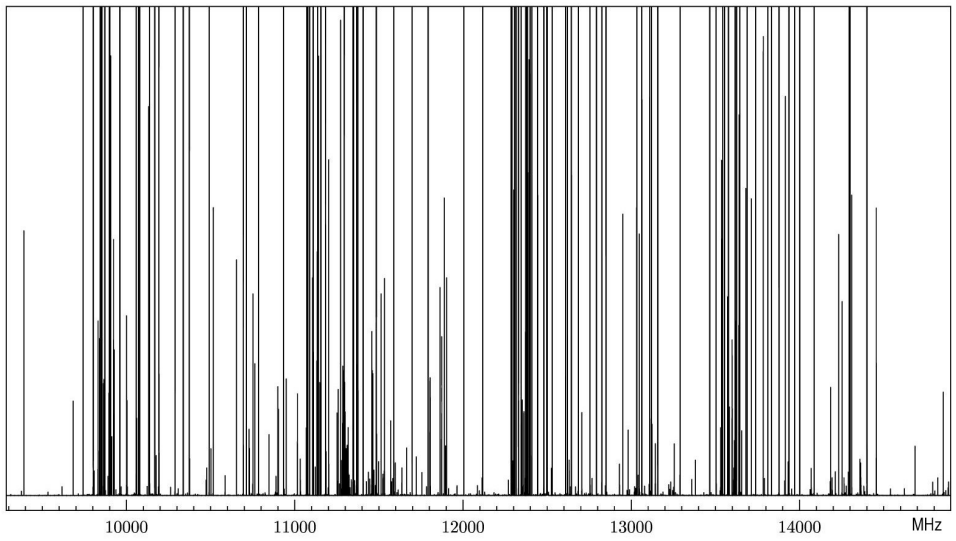

Figure 4. The 9.75 to 14.5 GHz experimental spectrum for R-carvone. Intensities of the strongest transitions are cut off so that less intense transitions are visible.

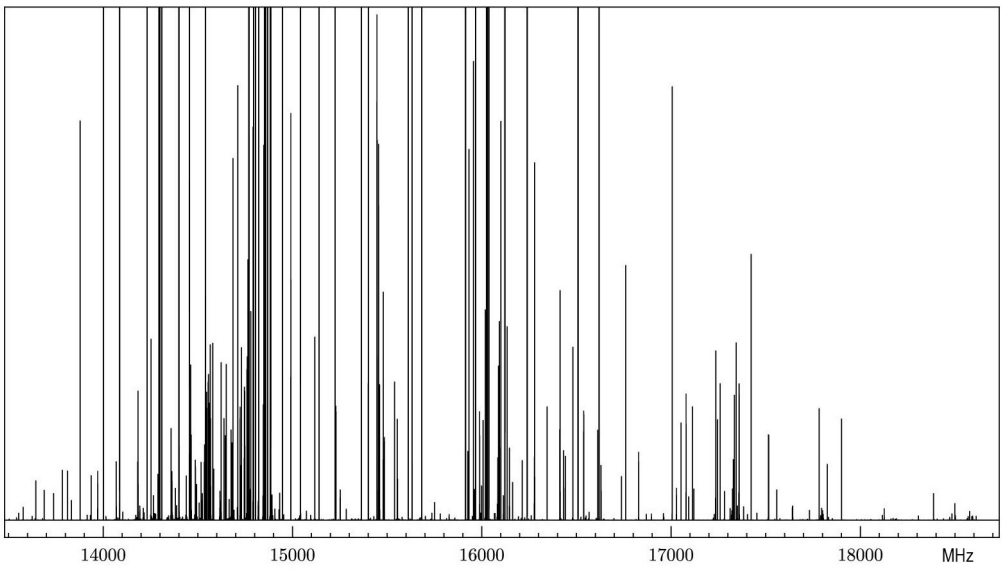

Figure 5. The 14.0 to 18.75 GHz experimental spectrum for R-carvone. Intensities of the strongest transitions are cut off so that less intense transitions are visible.

3. QUANTUM CHEMICAL CALCULATIONS

3.1. STRUCTURE CALCULATIONS

The geometric structures of all six theoretical conformers of R-carvone were optimized using the DFT method and B3LYP/6-31++G(d,p) level of theory at Missouri S&T. The optimized structures provided the rotational constants utilized as starting values in the initial experimental analysis. The equilibrium structures were then utilized in the barrier height calculations mentioned within the following section. In order to carry out the calculations, Gaussian09 [26] was used in conjunction with GaussView 5.0 [27] for visualizing structures. The calculated geometrical structures of the molecules are shown in Figure 1.

3.2. BARRIER HEIGHTS TO INTERNAL ROTATION CALCULATIONS

In addition, the barrier heights to internal rotation were also calculated for each theoretical conformer and methyl rotor pair. These calculations were undertaken after splittings indicative of large amplitude motion were observed within the recorded spectrum. In similar fashion to the optimization of the geometric structures, these calculations were performed at the DFT method and B3LYP/6-31++G(d,p) level of theory. In order to carry out the calculations, Gaussian09 [26] was used in conjunction with GaussView 5.0 [27]. The calculated barrier heights for each conformer and methyl rotor pair are presented in Table 1 and were utilized as starting values in the initial experimental analysis. Figure 6 depicts the three-fold energy potentials from which the barrier heights were calculated.

Barrier heights to internal rotation can range from 0 cm^{-1} – which is equivalent to free rotation of the methyl rotor – to theoretically ∞ cm $^{-1}$ – which is equivalent to a rigid rotor. However, the closer the value is to 1,000 cm^{-1}, the more likely it is that the individual splittings will be unable to be resolved due to the resolution of the instrumentation utilized. It should be noted that the two methyl rotors present within carvone's structure are non-equivalent rotors and, as a result, there is a potential for quintuplet splitting to occur

Table 1. Theoretical barrier heights to internal rotation for the twelve conformer and methyl rotor pairs of carvone as calculated by the DFT method and B3LYP/6-31++G(d,p) level of theory.

	Methyl Rotor 1 (C_{10})	**Methyl Rotor 2 (C_7)**
EQ1	571.5 cm^{-1}	487.6 cm^{-1}
EQ2	570.6 cm^{-1}	489.6 cm^{-1}
EQ3	543.4 cm^{-1}	487.4 cm^{-1}
AX1	984.7 cm^{-1}	484.5 cm^{-1}
AX2	549.7 cm^{-1}	500.2 cm^{-1}
AX3	500.2 cm^{-1}	493.7 cm^{-1}

within the spectrum based on the calculations. These splittings would correspond to AA, AE, EA, EE, and EE^* symmetries as shown in Figure 2 [23]. Since 11 of the 12 methyl rotor-conformer pairs have a theoretical value between 400-600 cm^{-1}, it is anticipated that many of quintuplet splittings produced by the two non-equivalent methyl rotors will be present, but some may not be fully resolved.

4. RESULTS AND ANALYSIS

Analysis of the spectrum was performed using XIAM [28] which was obtained from the PROSPE website [29]. A Watson *S*-reduced Hamiltonian in the I^r representation was employed while fitting the spectrum. For internal rotation purposes, two internal rotors with three-fold potential energy barriers were specified. In total, 49 individual fits were undertaken, and 5,362 transitions were assigned. This includes the 6 parent fits, which can be found in Table 2, and 43 signally substituted isotopologue fits, which can be found in the Supporting Information. All ^{13}C isotopologues were observed and reported for EQ1, EQ2, EQ3, and AX3. In addition, ^{18}O isotopologues were observed and reported for EQ1, EQ2, and EQ3. No isotopologues were able to be observed for AX1 and AX2 due to their

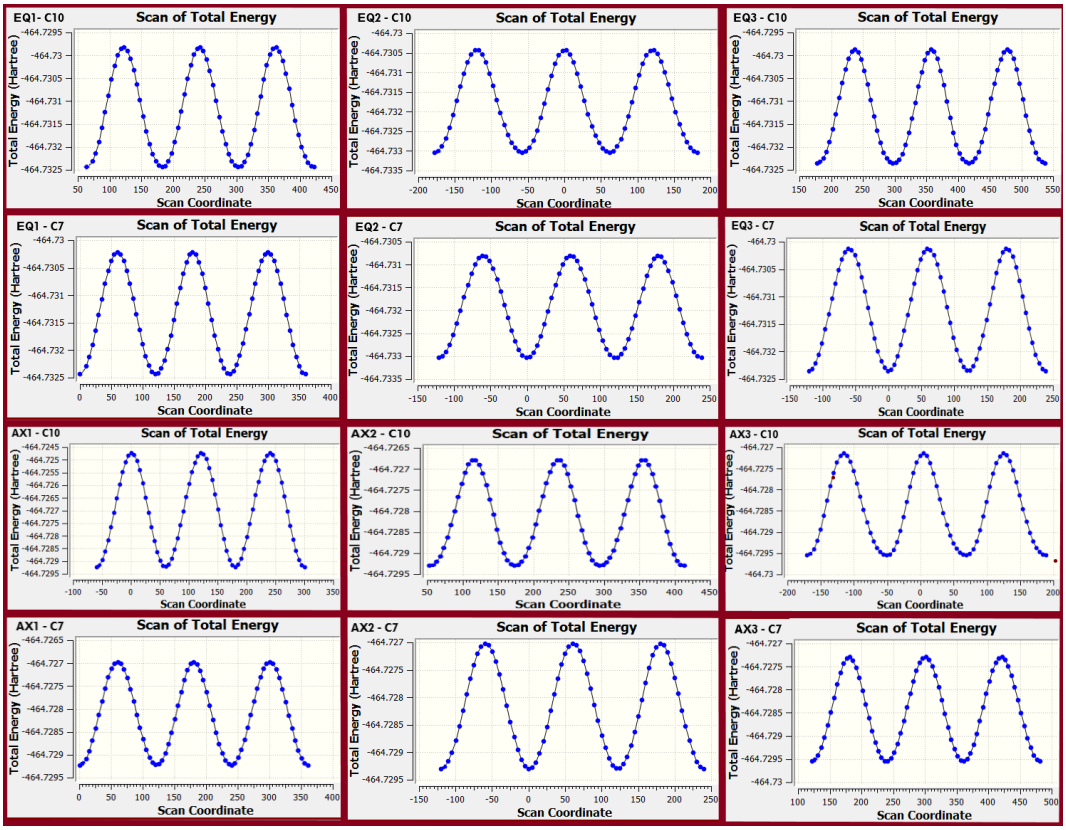

Figure 6. Three-fold energy potentials for each conformer/methyl rotor pair calculated at the B3LYP/6-31++G(d,p) level for the internal rotation of the two non-equivalent methyl rotors of carvone. The top two rows are the equatorial conformers with methyl rotor 1 (C_{10}) and methyl rotor 2 (C_7), respectively. The bottom two rows are the axial conformers with methyl rotor 1 (C_{10}) and methyl rotor 2 (C_7), respectively.

low intensities. Overall, the theoretical calculations appear to be in good agreement with the experimental data as the rotational constants differ by roughly 1%. Quantum number assignments and fits can be found in the Supporting Information.

Within the spectrum, *a*-type, *b*-type, and *c*-type transitions were observed. The order of intensity and prevalence of the transitions were *b*-types > *a*-types > *c*-types. These observations are in accordance with the predicted dipole moment component values, which can be found in Table 2. In addition, the majority of transitions were *R*-branch transitions with the second most abundant transitions being *Q*-branch transitions. Very few *P*-branch transitions were observed.

Table 2. Carvone experimental parameters for parent conformers as compared to theory (DFT).

Ground Vibrational State	**EQ2**		**EQ1**		**EQ3**	
	Exp.	Theory	Exp.	Theory	Exp.	Theory
A (MHz)	2,237.17545 (38)[a]	2,228.5	2,256.91156 (63)	2,250.6	2,212.79171 (59)	2,205.3
B (MHz)	656.28007 (13)	648.4	672.904561 (88)	664.9	684.52048 (21)	673.7
C (MHz)	579.63785 (13)	572.7	554.501886 (89)	549.1	554.73059 (21)	550.1
D_J (kHz)	0.02367 (33)		0.01121 (27)		—	
D_{JK} (kHz)	0.0597 (11)		0.02291 (85)		—	
D_K (kHz)	0.0225 (56)		-0.157 (28)		—	
d_J (kHz)	-0.002778 (89)		—		—	
d_K (kHz)	0.001892 (5)		—		—	
$V_{3,1}$ (cm^{-1})	599 (4)	571.0	524.62 (93)	518.3	533 (5)	543.3
δ_1 (radian)	0.546 (62)	0.93	1.2260 (43)	1.2	1.960 (21)	2.0
ε_1 (raidan)	3.91 (19)	3.7	[1.476][b]	1.5	0.488 (40)	0.48
$V_{3,2}$ (cm^{-1})	485.67 (80)	489.6	492.70 (75)	487.6	484.92 (24)	487.4
δ_2 (radian)	2.838 (26)	3.0	2.880 (27)	3.0	0.153 (15)	0.14
ε_2 (raidan)	3.03 (13)	3.7	3.836 (91)	3.9	[1.897]	1.9
$\lvert\mu_a\rvert$ (D)[c]		2.0		2.1		1.8
$\lvert\mu_b\rvert$ (D)[c]		3.0		3.2		2.7
$\lvert\mu_c\rvert$ (D)[c]		0.7		0.6		0.4
ν_{RMS} (kHz)[d]	23.9		18.7		23.7	
Number of Transitions[e]	952		849		84	
	AX3		**AX2**		**AX1**	
	Exp.	Theory	Exp.	Theory	Exp.	Theory
A (MHz)	1,687.81523 (45)	1,729.4	1,621.82901 (44)	1,661.1	1,8412.69484 (89)	1,814.9
B (MHz)	878.274 (19)	838.8	904.92504 (17)	857.5	804.41478 (38)	804.8
C (MHz)	771.30598 (16)	732.6	780.45575 (17)	741.2	738.98350 (38)	738.6
D_J (kHz)	0.18359 (42)		0.17883 (50)		0.01774 (71)	
D_{JK} (kHz)	0.1583 (18)		0.1089 (15)		0.0307 (32)	
D_K (kHz)	—		—		—	
d_J (kHz)	-0.00211 (18)		—		0.00257 (32)	
d_K (kHz)	—		—		—	
$V_{3,1}$ (cm^{-1})	510(1)	500.2	562 (4)	549.7	[985]	984.7
δ_1 (radian)	0.542 (23)	0.58	1.061 (26)	0.84	[2.014]	2.0
ε_1 (raidan)	0.392 (21)	0.36	6.2766 (63)	6.3	[1.668]	1.7
$V_{3,2}$ (cm^{-1})	499.74 (31)	493.7	482.22 (90)	500.2	489 (1)	494.5
δ_2 (radian)	2.5406 (31)	2.5	2.528 (14)	2.6	2.555 (24)	2.7
ε_2 (raidan)	[1.398]	1.4	4.131 (47)	4.7	1.34 (18)	1.5
$\lvert\mu_a\rvert$ (D)[c]		2.4		1.5		1.3
$\lvert\mu_b\rvert$ (D)[c]		3.2		2.8		3.2
$\lvert\mu_c\rvert$ (D)[c]		0.6		1.4		0.5
ν_{RMS} (kHz)[d]	23.2		22.3		19.7	
Number of Transitions[e]	325		198		60	

[a] Numbers in parentheses give standard errors at 1σ (67% confidence) level to the least significant figure.
[b] Held to theoretical value.
[c] Determined at the B3LYP/6-31++G level of theory.
[d] MW RMS is defined as $\sqrt{(\sum[(obs-calc)^2]/n)}$.
[e] Number of transitions include frequencies counted for multiple symmetries. See text for more details.

As mentioned previously, splittings in the spectra due to internal rotation from two non-equivalent methyl rotors were observed. An example of one such transition exhibiting the characteristic quintuplet splitting is the $7_{35} \leftarrow 6_{34}$ transition for the EQ1 conformer is

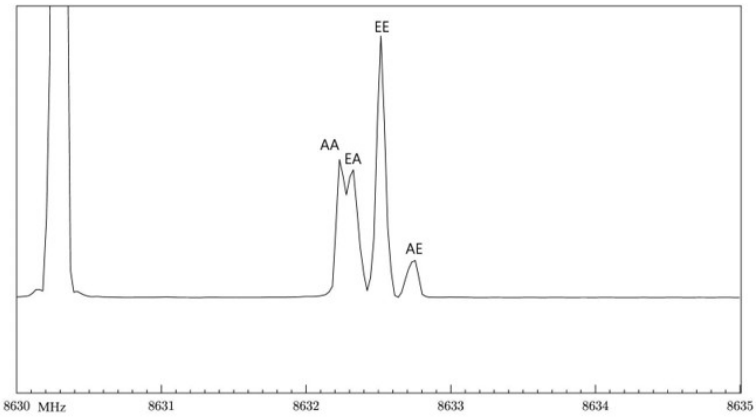

Figure 7. Example of internal rotation splitting seen in spectra for the $7_{35} \leftarrow 6_{34}$ transition of the EQ1 conformer.

shown in Figure 7. For this particular transition, the EE$*$ splitting is below the assigned noise floor and was not included. Within the fit, line centers with full-width half maximums (FWHM) around 70 kHz or less were assigned to a single symmetry state and given the standard measurement uncertainty of 10 kHz. However, if the FWHM for an observed line was greater than 70 kHz and multiple symmetries were predicted underneath the same FWHM, all predicted symmetries were assigned to the line center. The measurement uncertainty was increased to account for this and assigned a value equal to the FWHM divided by 7. Increasing the measurement uncertainty for the assigned transitions resulted in a higher ν_{RMS} value for the overall fit, as shown in Table 2, though these values are still within accepted limits for fits with internal rotation. It should be noted that all symmetry assignments were included in the number of transitions reported in Table 2. Thus, the number of individual lines centers assigned in the fit is lower than the number of transitions reported as some line centers were assigned to multiple symmetries of the same transition.

In order to properly fit the internal rotation symmetries using XIAM, the starting values for barrier heights to internal rotation, as well as the delta and epsilon angles had to first be specified for each rotor. Delta (δ) angles are defined as the angle between the internal rotation axis and the a-axis, while epsilon (ε) angles are defined as the angle between the

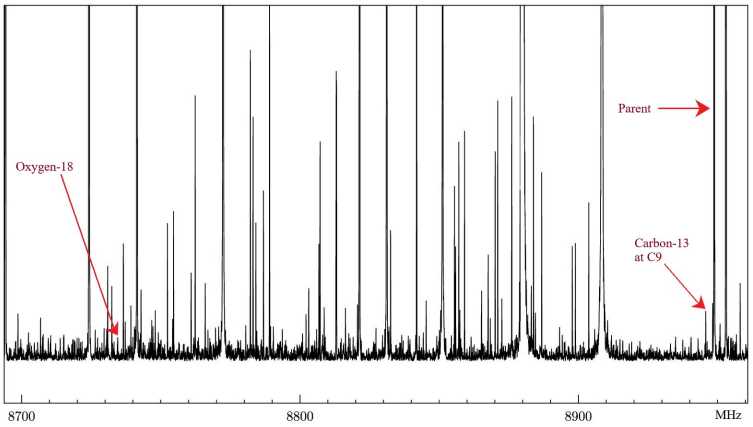

Figure 8. Example of the relative intensity profile for isotopic species observed for the $13_{3,11} \leftarrow 13_{2,12}$ transition of the EQ2 conformer. All species are labeled within the figure.

b-axis and the projection of the internal rotation axis onto the *bc*-plane [28]. In essence, the delta and epsilon angles are the polar coordinate of the internal rotation axis in the principal axis system [28]. The barrier heights, delta, and epsilon angles were initially held to their theoretical values obtained through the quantum chemical calculations to obtain preliminary fits, then were opened once a more accurate description of the rotational constants and centrifugal distortion constants were obtained.

The identification of the ^{13}C and ^{18}O isotopologues was accomplished by obtaining the ratio of the calculated rotational constants of the parent to the experimentally determined ones and using this ratio to adjust the "calculated" isotopologue rotational constants acquired by simply changing the atomic masses of the specific nuclei in question. This yielded isotopologue rotational constant predictions with great accuracy and ease, making traditional assignment for these species much simpler. Then, the correct relative intensity aspect of the CP-FTMW technique was utilized in order to accurately identify each singly substituted species in natural abundance. An example of this relative intensity profile can be found in Figure 8 for the $13_{3,11} \leftarrow 13_{2,12}$ transition of the EQ2 conformer.

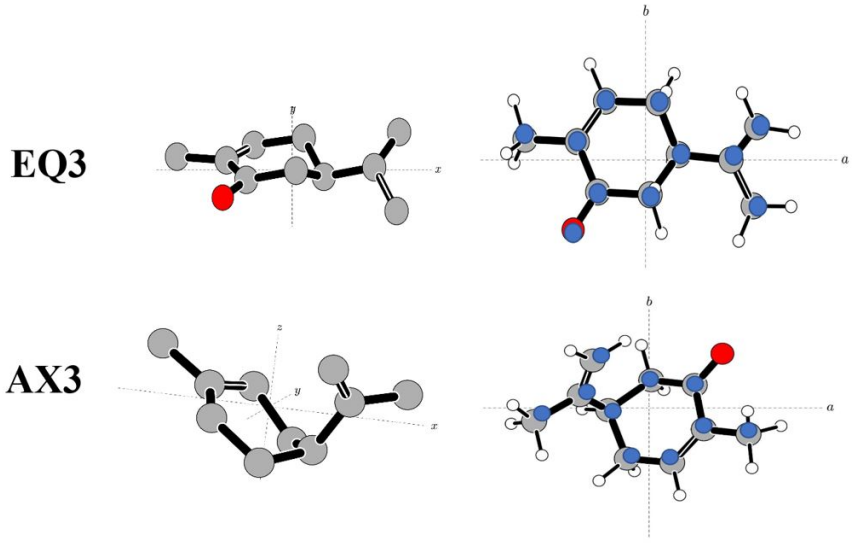

Figure 9. Experimentally determined (r_s) structures for EQ3 and AX3. The leftmost figures are the experimentally determined structures from Kraitchman analysis. The rightmost figures show the experimentally determined coordinates (in blue) overlapped with the theoretical structures determined from quantum chemical calculations (full structure).

After successfully assigning the spectra associated with each isotopologue, Kraitchman [30] substitution structures for the EQ1, EQ2, EQ3, and AX3 conformers were determined. This process was carried out using Kisiel's KRA program [29]. The results from the Kraitchman analysis are presented in the Supporting Information. The Kisiel's EVAL program [31] was then utilized to calculate the corresponding bond angles, bond lengths, and dihedral angles for the experimentally determined structures. Both the KRA and EVAL programs were obtained from the PROSPE website [29]. Because magnitudes and not absolute atom positions are given in the Kraitchman analysis, experimental structure determinations were aided by substitution of the computational sign values for the experimentally determined positions. From this analysis, the experimental substation structures for EQ3 and AX3 were determined and are shown in Figure 9. During the Kraitchman analysis, discrepancies in the EQ2 and EQ1 fits were discovered and are in the process of being reworked. More information is provided in the Discussion section.

5. DISCUSSION

For the molecule of carvone, Moreno et al. [1] and Loru et al. [2] have previously reported the rotational constants and centrifugal distortion constants for the conformers of EQ1, EQ2, EQ3, AX2, and AX3. In addition, Loru et al. also presented the r_o structures for EQ1 and EQ2 [2]. The rotational constants and r_s structures presented here are in good agreement with both theory and the previously reported values. One interesting thing of note is that our reported centrifugal distortion values are lower than those presented by Moreno et al. [1] and Loru et al. [2]. It is believed that our values differ due to the inclusion of internal rotation within this work. Thus, some of the line shifts attributed to centrifugal distortion in the two previous works belong instead to internal rotation.

Overall, the experimental data presented in Table 2 appears to be in good agreement with theoretical values as the two differ by roughly 1% for the rotational constants and barrier heights, and less than 10% for the delta and epsilon values. It should be noted that the ν_{RMS} values are slightly higher than would normally be expected. Typically, since our instrument's experimental uncertainty is 10 kHz, the ν_{RMS} would be expected to be lower than 20 kHz for parent conformers. However, as mentioned in the results section, some line centers were attributed to multiple symmetries. As a result, the measurement uncertainty for these transition assignments was increased to account for this and assigned a value equal to the FWHM divided by 7 instead of the standard 10 kHz. Increasing the measurement uncertainty for the assigned transitions resulted in a higher ν_{RMS} value for the overall fit.

This work also marks the first time experimentally determined barrier heights to internal rotation are reported for the conformers of carvone. All experimentally determined barrier heights fell around 500-600 cm^{-1}. Due to this, it was observed that many low- to mid- intensity transitions possessed quintuplet splittings as shown in Figure 7. However, many of the larger, more intense transitions were presented as a single peak with a larger

FWHM. This indicates that the internal rotation of the methyl rotors was still affecting these transitions, but the quintuplet splittings were unresolvable due to the intensity and frequency overlap of the symmetry splittings.

The only barrier height that was unable to be experimentally determined was the barrier height for methyl rotor 1 in AX1 (C_{10}), which was predicted to be around 985 cm^{-1}. This is due to the fact the XIAM has a hard time fitting high barrier heights and, as a result, the value had to be held to facilitate the fit. It is believed that this particular barrier height is nearly double that of the others due to non-covalent interactions between the methyl rotor and the oxygen present within carvone's structure as AX1 brings these two components into the closest proximity of all six conformers. This theory is supported by the NCI plots presented by Loru et al. [2], but has yet to be investigated at Missouri S&T.

The number of transitions reported for each conformer match almost perfectly to the natural abundances of the conformers as the number of transitions reported from greatest to least are EQ2 > EQ1 > AX3 > AX2 > EQ3 > AX1. The only outlier is EQ3, which has the second lowest number of transitions, but is the third most abundant conformer naturally. There are two explanations as to why this might be. First, the abundance of lines present for a particular conformer is directly influenced by the conformer's dipole moment. The total dipole moments for the conformers of carvone are 3.9 D, 3.6 D, 3.3 D, 3.5 D, 3.5 D, and 4.0 D for EQ1, EQ2, EQ3, AX1, AX2, and AX3, respectively, as determined at the B3LYP/6-31++G(d,p) level of theory. Since EQ3 has the lowest total dipole moment of the six conformers, it is reasonable that it would also have one of the lowest amount of transitions present. Secondly, as shown in Figure 10, there is a low conformational barrier height between the conformers of EQ1 and EQ3. This could also explain why EQ3 was not as abundant within the spectrum as some EQ3 conformers may have relaxed into EQ1 conformers during the supersonic expansion of the sample as described by Moreno et al. [1]. This would result in its abundance within the experimental sample being lower than

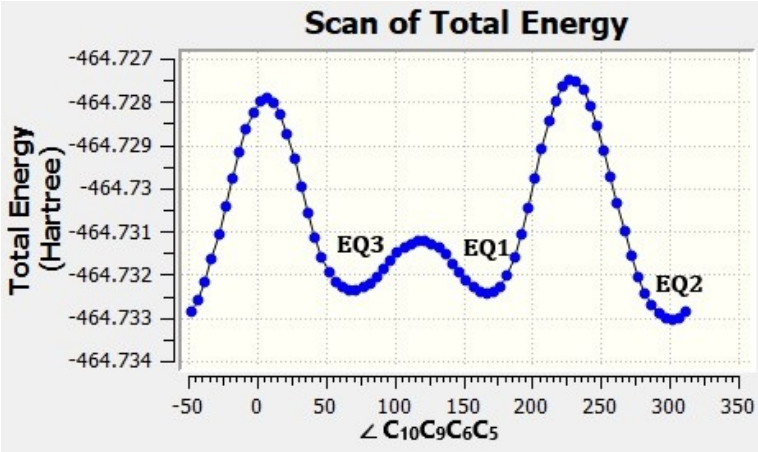

Figure 10. Interconversion barriers between the EQ conformers of carvone calculated at the B3LYP/6-31++G(d,p) level of theory.

its natural abundance. No further experiments were performed to verify this. However, a detailed discussion of conformational stability and relaxation in the supersonic expansion can be found in reference [32].

Within Figure 9, only the experimentally determined structures for EQ3 and AX3 are presented even though isotopologues and Kraitchman analysis were also reported for EQ1 and EQ2 in the Supporting Information. This is due to discrepancies found within the EVAL outputs for EQ1 and EQ2. As shown within the Supporting Information, the C_4–C_5 bond length is calculated to be 1.45 Å and 1.42 Å for EQ1 and EQ2, respectively. However, this value should be closer to 1.54 Å as that is the average bond length for a carbon-carbon single bond. Similarly, the C_9–C_{11} bond length is calculated to be 1.61 Å for EQ2. Yet, this value should be closer to 1.33 Å as that is the average bond length for a carbon-carbon double bond. This is an excellent example as to why Kraitchman analysis is so essential to rotational studies as it helps verify results to a higher degree than theory comparisons can do individually. Going off of the theoretical values alone, our fits are in excellent agreement. However, if they were truly excellent, discrepancies would not have appeared during the Kraithcman analysis. These discrepancies caused us to take a step back to analyze if something may have gone astray, such as a misassignment

of coordinate signs in EVAL, an improper fit, or error in the starting values generated by quantum chemical calculations. It was ultimately determined that the delta and epsilon values originally obtained via quantum chemical calculations were inaccurate. In running the quantum chemical calculations again, the delta and epsilon values shown in Table 3 were obtained, which match the information provided by Dr. Maria Sanz that was initially reported in reference [2]. Since these inaccurate values were used as starting values – and were even held constant for the first part of the fit – the error carried through our analysis. As can be seen in Table 3, these values are drastically different from the fit values.

It has yet to be determined how or why the first set of quantum chemical calculations produced different delta and epsilon values. Our best guess is that the convergence requirements were not tight enough and a local minimum instead of a global minimum was settled on. However, the two structures were still close enough to have similar rotational constants and nearly indistinguishable visual outputs. While the changes in delta and epsilon values would not drastically change the predicted frequencies of the transitions, it would change the spacing between the quintuplet splittings. It is believed, therefore, that larger, more intense transitions were not affected by this mistake as all symmetry splittings were predicted under the same FWHM. However, low- to mid-intensity transitions within dense regions of the spectrum may have been misassigned either in terms of the symmetry or overall transition, leading to the incorrect delta/epsilon values and the discrepancies in the EVAL output. Therefore, the 24 fits associated with EQ1 and EQ2 will need to be evaluated for any misassignments before their experimentally determined structures can be reported and before this information can be formally published. However, due to external factors, this was unable to be completed prior to this dissertation's submission. It is our hope that these fits can be evaluated quickly and that a formal publication can be submitted by the fall of 2023.

Table 3. Comparison of the EQ2 and EQ1 delta/epsilon values obtained from quantum chemical calculation and experimentation.

	Original Calculations	New Calculations	Loru et al. [2]	Current Fits
EQ2				
δ_1 (radian)	0.93	2.20	2.20	0.55
ε_1 (radian)	3.74	2.54	2.57	3.91
δ_2 (radian)	2.97	0.18	0.18	2.84
ε_2 (radian)	3.32	2.56	2.56	3.03
EQ1				
δ_1 (radian)	1.24	1.94	1.93	1.23
ε_1 (radian)	1.48	4.80	4.83	—
δ_2 (radian)	3.01	0.13	0.13	2.88
ε_2 (radian)	3.87	2.41	2.39	3.84

6. SUMMARY

Within this work, the pure rotational spectrum of R-carvone was studied using CP-FTMW with a focus on the internal rotation of the two non-equivalent methyl rotors. The presense of these rotors caused many transitions to exhibit quintuplet splitting. This study marked the first rotational study to observe and fit the experimental spectrum of AX1. In addition to the parent species of the six conformers, the isotopologues of ^{13}C for EQ1, EQ2, EQ3 and AX3 as well as the isotopologues of ^{18}O for EQ1, EQ2, and EQ3 were also measured and fit. This allowed for the generation of the heavy atom structures for the EQ1, EQ2, EQ3, and AX3 conformers. However, only the EQ3 and AX3 experimental structures have been confirmed to date as more work is needed on EQ1 and EQ2 to confirm their structures. It is our hope that this is completed by fall of 2023 so that an updated manuscript can be submitted for publication.

ACKNOWLEDGEMENTS

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SECTION

4. CONCLUSIONS AND FUTURE WORK

In conclusion, the works presented in this dissertation demonstrate the versatility of rotational spectroscopy—not only in terms of the types of molecules that can be study, but its ability to branch out into the study of other physical chemistry properties beyond structure determination, such as chirality determination and quadrature detection. In terms of structure, the ability for rotational spectroscopy to correctly determine the structure of molecules exhibiting large amplitude motion was successfully demonstrated within this work. This was represented by the ring-twisting of 1,1-difluoro-1-silacyclopentane, the curious motions of 1,1-difluorosilacyclopent-3-ene, and the internal rotation of carvone. These studies were made possible due to leveraging the deep averaging capability of CP-FTMW.

In addition, rotation spectroscopy's capability to distinguish between enantiomers using a M3WM scheme within the 6-18 GHz region of the electromagnetic spectrum was exhibited within this work—and was also graciously represented on the cover of *Symmetry*. This was done by utilizing the brand-new multi-antenna detection, chirped pulse Fourier transform microwave spectrometer equipped with synchronized arbitrary waveform generators at Missouri S&T. Before this experiment, many in the microwave community did not believe it was possible to successfully perform a M3WM experiment above 3 GHz. However, our stubbornness and frugality proved them wrong. Thus, the success of M3WM to work within the 6-18 GHz region has opened up a realm of possibilities for the community in terms of scheme selection and molecule eligibility. Most importantly, it makes M3WM

more achievable for groups who may not have the funds to perform radio frequencies measurements, allowing another group of scientists an opportunity to potentially change the field.

Though these works were a success overall, there is still so much more that can be done. First and foremost, the final analysis of the internal rotation of carvone needs to be completed. This includes re-evaluating the EQ1 and EQ2 fits for any possible misassignments and re-performing the Kraitchman analysis for structure determinations. It is this author's hope that this work will be completed shortly after submission of this dissertation and will be published by the end of 2023. In addition, the collaboration with Dr. Gamil Guirgis at the College of Charleston is as strong as ever. Therefore, it is expected that analysis of silcone containing molecules that exhibit large amplitude motion will continue for the Grubbs Group well into the future. Currently, experiments are underway involving 1-ethylsilacyclopentane, 1-ethyl-1-fluorosilacyclopentane, cyclopropylchloromethlydifluorosilane and 1,1-dichlorosilacyclohex-2-ene.

More excitingly, by the end of 2023, the construction of the new MAD-CPFTMW supported by National Science Foundation MRI grant should be completed. With the installation of this instrument, a new era of rotational spectroscopy will be available at Missouri S&T. In addition to expanding the capability of sourcing techniques, increasing measurement sensitivity, and offering remote accessibility to the wider community, this instrument will also allow for a diverse array of experiments to be performed that were previously not possible. Firstly, it will allow for the testing of multi-antenna detection up to 360°, which will hopefully provide insight into molecular excitation and emission.

Secondly, this instrument will allow for further experimentation on Chiral Coherent Quantum Control, also known as Enantiomer-Selective Population Enrichment. This technique allows for the selective excitation of one enantiomer over another by sending each enantiomer into a separate quantum state. While a large portion of this author's graduate

career was spent on preliminary work regarding this technique, no concrete experimental data was able to be obtained. Therefore, it is our hope that with this new instrument, further experimentation is able to be performed which leads to a successful selective excitation.

Lastly, future work is currently planned to utilize the microwave three-wave mixing technique to study dipole forbidden transitions. The reason we want to study dipole forbidden transitions via M3WM is because forbidden transitions pathways are made through off-diagonal nuclear electric quadrupole containing tensor components. Since M3WM schemes also contain off-diagonal components, it seems appropriate to use this type of technique to study these transitions and see if they have any association to chirality. Preliminary work has been performed during this author's graduate career using 2-bromo-1,1,1,2-tetrafluoroethane, but much work is still left to be done.

While much work has already been done, there are still a plethora of research opportunities to push the boundary of rotational spectroscopy. It is this author's hope that the new MAD-CPFTMW "Octo" will help aid these discoveries.

APPENDIX A.

SUPPORTING INFORMATION FOR PURE ROTAITONAL SPECTRUM AND STRUCTURE DETERMINATION OF 1,1-DIFLUOROR-1-SILACYCLOPENTANE

PURE ROTATIONAL SPECTRUM AND STRUCTURAL DETERMINATION OF 1,1-DIFLUORO-1-SILACYCLOPENTANE

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SUPPORTING INFORMATION

S1 – S6 are the microwave transition assignments and fits for all reported isotopologues of 1,1-difluoro-1-silacyclopentane. Transition assignments are given in $J\ K_a\ K_c' \leftarrow J\ K_a\ K_c''$. The experimental frequencies are given in MHz.

Table of Contents:

and Dihedral Angles (units are given in Å, degrees, and degrees, respectively) in 1,1-difluoro-1-silacyclopentane.

S8. Output of Kraitchman Analysis Program (atom positions are absolute and given in Å) in 1,1-difluoro-1-silacylopentane.

S9. List of Split Transitions

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S1. Parent MW Transition Assignments – Fit Together

	obs	o-c	error o-c	blends wt	Notes
/ instead of : below denotes (o-c)>3*err					
1: 12 1 11 0 12 1 12 0	6465.9554	-0.0071	0.010		
2: 2 1 2 0 1 1 1 0	6602.3211	0.0011	0.010		
3: 2 0 2 0 1 0 1 0	6686.7109	0.0025	0.010		
4: 2 1 1 0 1 1 0 0	6777.9245	0.0054	0.010		
5: 3 2 2 0 3 0 3 0	6785.4410	-0.0291	0.010		
6: 4 2 3 1 4 0 4 1	6816.6147	-0.0098	0.010		
7: 5 2 4 0 5 0 5 0	6875.7880	0.0040	0.010		
8: 6 2 5 0 6 0 6 0	6974.5913	0.0004	0.010		
9: 7 2 6 0 7 0 7 0	7124.3846	0.0081	0.010		
10: 8 2 7 0 8 0 8 0	7334.4675	0.0133	0.010		
11: 9 2 8 0 9 0 9 0	7610.7506	0.0196	0.010		
12: 10 2 9 0 10 0 10 0	7955.1533	0.0141	0.010		

13:	12 2 11 0	12 0 12 0	8838.8193	0.0062	0.010	
14:	13 2 12 0	13 0 13 0	9367.5925	0.0090	0.010	
15:	5 0 5 0	4 2 2 0	9790.9324	0.0021	0.010	
16:	3 1 3 0	2 1 2 0	9901.3727	-0.0018	0.010	
17:	14 2 13 0	14 0 14 0	9945.4351	-0.0212	0.010	
18:	3 0 3 0	2 0 2 0	10021.5193	-0.0289	0.010	
19:	3 2 2 0	2 2 1 0	10035.1567	0.0068	0.010	
20:	3 2 1 0	2 2 0 0	10048.7732	-0.0036	0.010	
21:	3 1 2 0	2 1 1 0	10164.6875	-0.0024	0.010	
22:	8 3 6 0	8 1 7 0	12230.5287	-0.0035	0.010	
23:	7 3 5 0	7 1 6 0	12471.7478	0.0039	0.010	
24:	6 0 6 0	5 2 3 0	12962.5734	0.0092	0.010	
25:	4 1 4 0	3 1 3 0	13198.0062	-0.0108	0.010	
26:	4 0 4 0	3 0 3 0	13346.3759	0.0077	0.010	
27:	4 2 3 0	3 2 2 0	13377.5284	0.0071	0.010	
28:	4 3 2 0	3 3 1 0	13386.7282	0.0007	0.010	
29/	4 3 1 0	3 3 0 0	13387.1954	-0.0303	0.010	
30:	4 2 2 0	3 2 1 0	13411.3706	0.0050	0.010	
31:	4 1 3 0	3 1 2 0	13548.7229	0.0059	0.010	
32/	5 1 5 0	4 1 4 0	16491.6651	0.0353	0.010	
33:	5 0 5 0	4 0 4 0	16658.4186	-0.0214	0.010	
34:	5 2 4 1	4 2 3 1	16717.5840	-0.0292	0.010	
35/	5 2 4 0	4 2 3 0	16717.6441	0.0433	0.010	
36/	5 4 2 1	4 4 1 1	16732.5942	-0.0695	0.010	-0.0762 0.50
37:	5 4 1 1	4 4 0 1	16732.5942	-0.0829	0.010	-0.0762 0.50
38:	5 4 2 0	4 4 1 0	16732.6822	0.0222	0.010	0.0155 0.50
39:	5 4 1 0	4 4 0 0	16732.6822	0.0088	0.010	0.0155 0.50
40/	5 3 3 1	4 3 2 1	16735.9755	-0.0625	0.010	

41/ 5 3 3 0 4 3 2 0 16736.0747 0.0441 0.010

42/ 5 3 2 0 4 3 1 0 16737.8168 0.0459 0.010

43: 5 2 3 0 4 2 2 0 16784.3859 0.0021 0.010

44/ 5 1 4 0 4 1 3 0 16928.9422 0.0552 0.010

45: 6 1 6 0 5 1 5 0 19781.7507 0.0081 0.010

46/ 6 0 6 1 5 0 5 1 19955.9758 -0.0567 0.010

47: 6 0 6 0 5 0 5 0 19956.0405 0.0226 0.010

48: 6 2 4 0 5 2 3 0 20168.9774 -0.0071 0.010

49: 6 1 5 0 5 1 4 0 20303.9517 0.0358 0.010 0.0000 0.50

50: 6 1 5 1 5 1 4 1 20303.9517 -0.0358 0.010 0.0000 0.50

PARAMETERS IN FIT (values truncated):

10099	A /MHz	3364.654176(18)	1
20099	B /MHz	1716.4320797(29)	2
30099	C /MHz	1628.6325533(27)	3
299	DJ /kHz	0.17637(11)	4
1199	DJK /kHz	1.00210(21)	5
2099	DK /kHz	0.6147(24)	6
210001	Fbc /MHz	0.83594(27)	7
11	E1 /MHz	39756.547(28)	8

MICROWAVE AVG = 0.000073 MHz, IR AVG = 0.00000

MICROWAVE RMS = 0.025291 MHz, IR RMS = 0.00000

END OF ITERATION 1 OLD, NEW RMS ERROR= 2.52909 2.52909

distinct frequency lines in fit: 47

distinct parameters of fit: 8

MICROWAVE lines fitted lines lines RMS RMS ERROR J range Ka range freq. range

total dv=0 dv.ne.0 UNFITTD e>900

v"= 0 42 42 0 0 0 0.019590 1.95902 1 14 0 4 6466 20304

v"= 1 5 5 0 0 0 0.052686 5.26864 4 6 0 4 6817 19956

---

total: 47 47 0 0 0 0.025264 2.52637

Standard errors are obtained by multiplying the previous errors by: 2.776393.

PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:

(values rounded)

10099	A /MHz	3364.654176(50)	1
20099	B /MHz	1716.4320798(82)	2
30099	C /MHz	1628.6325533(77)	3
299	DJ /kHz	0.17637(31)	4
1199	DJK /kHz	1.00210(59)	5
2099	DK /kHz	0.6148(68)	6
210001	Fbc /MHz	0.83595(75)	7
11	E1 /MHz	39756.547(79)	8

CORRELATION COEFFICIENTS, C.ij:

A B C -DJ -DJK -DK Fbc E1

A	1.0000						
B	-0.0002	1.0000					
C	0.0004	0.0009	1.0000				
-DJ	0.0001	-0.0002	-0.0003	1.0000			
-DJK	-0.0008	-0.0006	0.0006	-0.0001	1.0000		
-DK	-0.0009	-0.0001	0.0002	0.0000	-0.0008	1.0000	
Fbc	0.0004	0.0008	-0.0008	0.0000	0.0008	0.0003	1.0000
E1	0.0000	0.0001	0.0000	0.0003	0.0000	0.0001	0.0001	1.0000

Mean value of |C.ij|, i.ne.j = 0.0003

Mean value of C.ij, i.ne.j = 0.0000

No correlations with absolute value greater than 0.9950

Worst fitted lines (obs-calc/error):

36: -7.6	40: -6.2	46: -5.7	44: 5.5
42: 4.6	41: 4.4	35: 4.3	32: 3.5
29: -3.0	34: -2.9	5: -2.9	18: -2.9
47: 2.3	33: -2.1	17: -2.1	11: 2.0
38: 1.6	12: 1.4	10: 1.3	25: -1.1
6: -1.0	24: 0.9	14: 0.9	9: 0.8
45: 0.8	26: 0.8	27: 0.7	1: -0.7
48: -0.7	19: 0.7	13: 0.6	31: 0.6
4: 0.5	30: 0.5	7: 0.4	23: 0.4
20: -0.4	22: -0.3	3: 0.2	21: -0.2

43: 0.2 15: 0.2 16: -0.2 2: 0.1

28: 0.1 8: 0.0 49: 0.0 50: 0.0

39: 0.0 37: 0.0

36/ 5 4 2 1 4 4 1 1	16732.5942	-0.0695	0.010	-0.0762 0.50
40/ 5 3 3 1 4 3 2 1	16735.9755	-0.0625	0.010	
46/ 6 0 6 1 5 0 5 1	19955.9758	-0.0567	0.010	
44/ 5 1 4 0 4 1 3 0	16928.9422	0.0552	0.010	
42/ 5 3 2 0 4 3 1 0	16737.8168	0.0459	0.010	
41/ 5 3 3 0 4 3 2 0	16736.0747	0.0441	0.010	
35/ 5 2 4 0 4 2 3 0	16717.6441	0.0433	0.010	
32/ 5 1 5 0 4 1 4 0	16491.6651	0.0353	0.010	
29/ 4 3 1 0 3 3 0 0	13387.1954	-0.0303	0.010	
34: 5 2 4 1 4 2 3 1	16717.5840	-0.0292	0.010	

_____

_____/ SPFIT output reformatted with PIFORM

S2. Parent MW Transition Assignments – Fit Separately

---

	obs	o-c	error o-c	blends wt	Notes
/ instead of : below denotes (o-c)>3*err					
1: 12 1 11 0 12 1 12 0	6465.9554	-0.0049	0.010		
2: 2 1 2 0 1 1 1 0	6602.3211	0.0026	0.010		
3: 2 0 2 0 1 0 1 0	6686.7109	0.0041	0.010		
4: 2 1 1 0 1 1 0 0	6777.9245	0.0063	0.010		

5:	3	2	2	0	3	0	3	0	6785.4410	-0.0230	0.010
6:	4	2	3	1	4	0	4	1	6816.6147	0.0000	0.010
7:	5	2	4	0	5	0	5	0	6875.7880	0.0038	0.010
8:	6	2	5	0	6	0	6	0	6974.5913	-0.0035	0.010
9:	7	2	6	0	7	0	7	0	7124.3846	0.0003	0.010
10:	8	2	7	0	8	0	8	0	7334.4675	0.0023	0.010
11:	9	2	8	0	9	0	9	0	7610.7506	0.0064	0.010
12:	10	2	9	0	10	0	10	0	7955.1533	0.0002	0.010
13:	12	2	11	0	12	0	12	0	8838.8193	-0.0009	0.010
14:	13	2	12	0	13	0	13	0	9367.5925	0.0104	0.010
15:	5	0	5	0	4	2	2	0	9790.9324	-0.0077	0.010
16:	3	1	3	0	2	1	2	0	9901.3727	-0.0012	0.010
17:	14	2	13	0	14	0	14	0	9945.4351	-0.0068	0.010
18:	3	0	3	0	2	0	2	0	10021.5193	-0.0282	0.010
19:	3	2	2	0	2	2	1	0	10035.1567	0.0053	0.010
20:	3	2	1	0	2	2	0	0	10048.7732	-0.0055	0.010
21:	3	1	2	0	2	1	1	0	10164.6875	-0.0029	0.010
22:	8	3	6	0	8	1	7	0	12230.5287	-0.0091	0.010
23:	7	3	5	0	7	1	6	0	12471.7478	0.0089	0.010
24:	6	0	6	0	5	2	3	0	12962.5734	-0.0048	0.010
25:	4	1	4	0	3	1	3	0	13198.0062	-0.0134	0.010
26:	4	0	4	0	3	0	3	0	13346.3759	0.0054	0.010
27:	4	2	3	0	3	2	2	0	13377.5284	0.0020	0.010
28:	4	3	2	0	3	3	1	0	13386.7282	-0.0085	0.010
29/	4	3	1	0	3	3	0	0	13387.1954	-0.0396	0.010
30:	4	2	2	0	3	2	1	0	13411.3706	-0.0009	0.010
31:	4	1	3	0	3	1	2	0	13548.7229	0.0021	0.010
32:	5	1	5	0	4	1	4	0	16491.6651	0.0269	0.010

33:	5 0 5 0	4 0 4 0	16658.4186	-0.0294	0.010	
34/	5 2 4 1	4 2 3 1	16717.5840	0.0312	0.010	
35/	5 2 4 0	4 2 3 0	16717.6441	0.0319	0.010	
36:	5 4 2 1	4 4 1 1	16732.5942	-0.0163	0.010	-0.0231 0.50
37:	5 4 1 1	4 4 0 1	16732.5942	-0.0297	0.010	-0.0231 0.50
38:	5 4 2 0	4 4 1 0	16732.6822	-0.0010	0.010	-0.0078 0.50
39:	5 4 1 0	4 4 0 0	16732.6822	-0.0145	0.010	-0.0078 0.50
40:	5 3 3 1	4 3 2 1	16735.9755	-0.0032	0.010	
41:	5 3 3 0	4 3 2 0	16736.0747	0.0274	0.010	
42:	5 3 2 0	4 3 1 0	16737.8168	0.0290	0.010	
43:	5 2 3 0	4 2 2 0	16784.3859	-0.0109	0.010	
44/	5 1 4 0	4 1 3 0	16928.9422	0.0452	0.010	
45:	6 1 6 0	5 1 5 0	19781.7507	-0.0097	0.010	
46:	6 0 6 1	5 0 5 1	19955.9758	-0.0040	0.010	
47:	6 0 6 0	5 0 5 0	19956.0405	0.0054	0.010	
48/	6 2 4 0	5 2 3 0	20168.9774	-0.0308	0.010	
49:	6 1 5 0	5 1 4 0	20303.9517	0.0162	0.010	0.0000 0.50
50:	6 1 5 1	5 1 4 1	20303.9517	-0.0162	0.010	0.0000 0.50

PARAMETERS IN FIT (values truncated):

10000	A /MHz	3364.6527(21)	1
20000	B /MHz	1716.43162(64)	2
30000	C /MHz	1628.63176(66)	3
10011	A /MHz	3364.6453(30)	4
20011	B /MHz	1716.4204(28)	5
30011	C /MHz	1628.6277(24)	6
299	DJ /kHz	0.145(12)	7
1199	DJK /kHz	0.910(29)	8

2099 DK /kHz 1.06(24) 9

210001 Fbc /MHz 0.930(27) 10

11 E1 /MHz 39755.59(34) 11

MICROWAVE AVG = -0.000484 MHz, IR AVG = 0.00000

MICROWAVE RMS = 0.016551 MHz, IR RMS = 0.00000

END OF ITERATION 1 OLD, NEW RMS ERROR= 1.65511 1.65511

distinct frequency lines in fit: 47

distinct parameters of fit: 11

MICROWAVE lines fitted lines lines RMS RMS ERROR J range Ka range freq. range

total dv=0 dv.ne.0 UNFITTD e>900

v"= 0 42 42 0 0 0 0.016404 1.64044 1 14 0 4 6466 20304

v"= 1 5 5 0 0 0 0.017506 1.75064 4 6 0 4 6817 19956

---

total: 47 47 0 0 0 0.016525 1.65252

Standard errors are obtained by multiplying the previous errors by: 1.891144

PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:

(values rounded)

10000 A /MHz 3364.6527(41) 1

20000 B /MHz 1716.4316(12) 2

30000 C /MHz 1628.6318(12) 3

10011	A /MHz	3364.6453(57)	4
20011	B /MHz	1716.4204(53)	5
30011	C /MHz	1628.6278(45)	6
299	DJ /kHz	0.145(23)	7
1199	DJK /kHz	0.911(56)	8
2099	DK /kHz	1.07(45)	9
210001	Fbc /MHz	0.930(52)	10
11	E1 /MHz	39755.59(64)	11

Worst fitted constants, with greater than 20% uncertainty: %

2099	DK /kHz	1.07(45)	9	42.9

CORRELATION COEFFICIENTS, C.ij:

	A	B	C	A	B	C	-DJ	-DJK
A	1.0000							
B	0.2968	1.0000						
C	0.4064	0.9470	1.0000					
A	0.3335	0.2732	0.3156	1.0000				
B	0.1817	0.0620	0.0857	-0.2331	1.0000			
C	0.0375	0.4344	0.4316	0.4314	-0.7733	1.0000		
-DJ	-0.2194	-0.9112	-0.9144	-0.3010	-0.0230	-0.4994	1.0000	
-DJK	-0.5338	-0.1656	-0.2418	-0.0899	-0.3397	0.1133	0.0539	1.0000
-DK	-0.5209	0.1332	0.0576	-0.2385	0.1153	-0.0116	-0.0785	-0.3338
Fbc	-0.4696	-0.0764	-0.3000	-0.1326	-0.2666	0.0455	0.1043	0.7978

E1 -0.1974 -0.1859 -0.2608 -0.2848 0.4084 -0.4599 0.3172 -0.1236

-DK Fbc E1

-DK 1.0000

Fbc -0.1601 1.0000

E1 0.3317 0.0726 1.0000

Mean value of |C.ij|, i.ne.j = 0.2933

Mean value of C.ij, i.ne.j = -0.0465

No correlations with absolute value greater than 0.9950

Worst fitted lines (obs-calc/error):

44: 4.5	29: -4.0	35: 3.2	34: 3.1
48: -3.1	33: -2.9	42: 2.9	18: -2.8
41: 2.7	32: 2.7	36: -2.3	5: -2.3
25: -1.3	43: -1.1	14: 1.0	45: -1.0
22: -0.9	23: 0.9	28: -0.9	38: -0.8
15: -0.8	17: -0.7	11: 0.6	4: 0.6
20: -0.5	47: 0.5	26: 0.5	19: 0.5
1: -0.5	24: -0.5	3: 0.4	46: -0.4
7: 0.4	8: -0.3	40: -0.3	21: -0.3
2: 0.3	10: 0.2	31: 0.2	27: 0.2
16: -0.1	30: -0.1	13: -0.1	9: 0.0
12: 0.0	50: 0.0	49: 0.0	39: 0.0
37: 0.0	6: 0.0		

44/ 5 1 4 0 4 1 3 0 16928.9422 0.0452 0.010

29/ 4 3 1 0 3 3 0 0	13387.1954	-0.0396	0.010
35/ 5 2 4 0 4 2 3 0	16717.6441	0.0319	0.010
34/ 5 2 4 1 4 2 3 1	16717.5840	0.0312	0.010
48/ 6 2 4 0 5 2 3 0	20168.9774	-0.0308	0.010
33: 5 0 5 0 4 0 4 0	16658.4186	-0.0294	0.010
42: 5 3 2 0 4 3 1 0	16737.8168	0.0290	0.010
18: 3 0 3 0 2 0 2 0	10021.5193	-0.0282	0.010
41: 5 3 3 0 4 3 2 0	16736.0747	0.0274	0.010
32: 5 1 5 0 4 1 4 0	16491.6651	0.0269	0.010

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_____/ SPFIT output reformatted with **PIFORM**

S3. ^{29}Si MW Transition Assignments

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	obs	o-c	error o-c	blends wt	Notes
/ instead of : below denotes (o-c)>3*err					
1: 2 1 2 0 1 1 1 0	6595.3619	-0.0006	0.010		
2: 2 0 2 0 1 0 1 0	6679.5821	-0.0064	0.010		
3: 2 1 1 0 1 1 0 0	6770.5945	-0.0062	0.010		
4: 3 1 3 0 2 1 2 0	9890.9531	0.0038	0.010		
5: 3 0 3 0 2 0 2 0	10010.9070	-0.0059	0.010		
6: 3 2 2 0 2 2 1 0	10024.4430	0.0000	0.010		
7: 3 2 1 0 2 2 0 0	10037.9967	-0.0017	0.010		
8: 3 1 2 0 2 1 1 0	10153.7254	0.0012	0.010		
9: 4 1 4 0 3 1 3 0	13184.1400	0.0038	0.010		

```
 10:  4  0  4  0    3  0  3  0          13332.2665  -0.0024  0.010
 11:  4  2  3  0    3  2  2  0          13363.2392  -0.0203  0.010
 12/  4  3  2  0    3  3  1  0          13372.3748  -0.0429  0.010
 13/  4  3  2  1    3  3  1  1          13372.4730   0.0532  0.010
 14/  4  3  1  0    3  3  0  0          13372.7938  -0.1179  0.010
 15:  4  3  1  1    3  3  0  1          13372.9307   0.0171  0.010
 16:  4  2  2  0    3  2  1  0          13396.9314   0.0040  0.010
 17:  4  1  3  0    3  1  2  0          13534.1346   0.0160  0.010
 18:  5  1  5  0    4  1  4  0          16474.3230   0.0152  0.010
 19:  5  0  5  0    4  0  4  0          16640.9334  -0.0047  0.010
 20:  5  2  4  0    4  2  3  0          16699.8215   0.0253  0.010
 21:  5  3  3  0    4  3  2  0          16718.1460   0.0148  0.010
 22:  5  3  2  0    4  3  1  0          16719.8680   0.0112  0.010
 23:  5  2  3  0    4  2  2  0          16766.2441   0.0076  0.010
 24:  5  1  4  0    4  1  3  0          16910.6866   0.0089  0.010
-------------------------------------------------------------------------------
PARAMETERS IN FIT (values truncated):
      10099          A  /MHz       3364.85(18)                  1
      20099          B  /MHz       1714.55740(99)               2
      30099          C  /MHz       1626.93831(99)               3
        299         DJ  /kHz       [ 0.176369586]               4
       1199        DJK  /kHz       [ 1.00210376]                5
       2099         DK  /kHz       [ 0.61478149]                6
     210001        Fbc  /MHz       [ 0.835945002]               7
         11         E1  /MHz      [39756.547178064]             8
 MICROWAVE AVG =       -0.001121 MHz, IR AVG =       0.00000
 MICROWAVE RMS =        0.029664 MHz, IR RMS =       0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=       2.96639       2.96639
```

distinct frequency lines in fit: 24

distinct parameters of fit: 3

MICROWAVE lines fitted lines lines RMS RMS ERROR J range Ka range freq. range

total dv=0 dv.ne.0 UNFITTD e>900

v''= 0	22	22	0	0	0	0.028567	2.85666	1	5	0	3	6595	16911
v''= 1	2	2	0	0	0	0.039514	3.95136	3	4	3	3	13372	13373

---

total:	24	24	0	0	0	0.029634	2.96337

Standard errors are obtained by multiplying the previous errors by: 3.171204

PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:

(values rounded)

10099	A /MHz	3364.86(57)	1
20099	B /MHz	1714.5574(31)	2
30099	C /MHz	1626.9383(31)	3
299	DJ /kHz	[0.176369586]	4
1199	DJK /kHz	[1.00210376]	5
2099	DK /kHz	[0.61478149]	6
210001	Fbc /MHz	[0.835945002]	7
11	E1 /MHz	[39756.547178064]	8

CORRELATION COEFFICIENTS, C.ij:

	A	B	C
A	1.0000		
B	0.3778	1.0000	
C	-0.3994	-0.8652	1.0000

Mean value of |C.ij|, i.ne.j = 0.5475

Mean value of C.ij, i.ne.j = -0.2956

No correlations with absolute value greater than 0.9950

Worst fitted lines (obs-calc/error):

14: -11.8	13: 5.3	12: -4.3	20: 2.5
11: -2.0	15: 1.7	17: 1.6	18: 1.5
21: 1.5	22: 1.1	24: 0.9	23: 0.8
2: -0.6	3: -0.6	5: -0.6	19: -0.5
16: 0.4	4: 0.4	9: 0.4	10: -0.2
7: -0.2	8: 0.1	1: -0.1	6: 0.0

14/ 4 3 1 0	3 3 0 0	13372.7938	-0.1179 0.010
13/ 4 3 2 1	3 3 1 1	13372.4730	0.0532 0.010
12/ 4 3 2 0	3 3 1 0	13372.3748	-0.0429 0.010
20: 5 2 4 0	4 2 3 0	16699.8215	0.0253 0.010
11: 4 2 3 0	3 2 2 0	13363.2392	-0.0203 0.010
15: 4 3 1 1	3 3 0 1	13372.9307	0.0171 0.010
17: 4 1 3 0	3 1 2 0	13534.1346	0.0160 0.010

18: 5 1 5 0 4 1 4 0 16474.3230 0.0152 0.010

21: 5 3 3 0 4 3 2 0 16718.1460 0.0148 0.010

22: 5 3 2 0 4 3 1 0 16719.8680 0.0112 0.010

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_____/ SPFIT output reformatted with PIFORM

S4. ^{30}Si MW Transition Assignments

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	obs	o-c	error o-c	blends wt	Notes

/ instead of : below denotes (o-c)>3*err

1: 2 1 2 0 1 1 1 0	6588.5476	0.0001	0.010		
2: 2 0 2 0 1 0 1 0	6672.6100	0.0047	0.010		
3: 2 1 1 0 1 1 0 0	6763.4118	-0.0009	0.010		
4: 3 1 3 0 2 1 2 0	9880.7396	-0.0011	0.010		
5: 3 0 3 0 2 0 2 0	10000.4905	0.0051	0.010		
6: 3 2 2 0 2 2 1 0	10013.9175	-0.0246	0.010		
7: 3 2 1 0 2 2 0 0	10027.4281	0.0014	0.010		
8: 3 1 2 0 2 1 1 0	10142.9618	0.0048	0.010		
9: 4 1 4 0 3 1 3 0	13170.5467	-0.0034	0.010		
10: 4 0 4 0 3 0 3 0	13318.4678	0.0160	0.010		
11: 4 2 3 0 3 2 2 0	13349.2892	0.0108	0.010		
12/ 4 3 2 0 3 3 1 0	13358.3461	-0.0388	0.010		
13/ 4 3 2 1 3 3 1 1	13358.4508	0.0638	0.010		
14/ 4 3 1 0 3 3 0 0	13358.8272	-0.0476	0.010		
15: 4 2 2 0 3 2 1 0	13382.7770	0.0053	0.010		

16: 4 1 3 0 3 1 2 0 13519.7993 0.0084 0.010

17: 5 1 5 0 4 1 4 0 16457.3515 -0.0125 0.010

18: 5 0 5 0 4 0 4 0 16623.8147 0.0173 0.010

19: 5 2 4 0 4 2 3 0 16682.3316 -0.0199 0.010

20: 5 4 2 0 4 4 1 0 16697.2502 0.0110 0.010 0.0044 0.50

21: 5 4 1 0 4 4 0 0 16697.2502 -0.0021 0.010 0.0044 0.50

22: 5 3 3 0 4 3 2 0 16700.5906 0.0028 0.010

23: 5 3 2 0 4 3 1 0 16702.3126 0.0136 0.010

24: 5 2 3 0 4 2 2 0 16748.4678 0.0146 0.010

25: 5 1 4 0 4 1 3 0 16892.7908 -0.0251 0.010

PARAMETERS IN FIT (values truncated):

10099	A /MHz	3364.79(20)	1
20099	B /MHz	1712.7134(12)	2
30099	C /MHz	1625.2808(12)	3
299	DJ /kHz	0.121(21)	4
1199	DJK /kHz	1.107(67)	5
2099	DK /kHz	[0.61478149]	6
210001	Fbc /MHz	[0.835945002]	7
11	E1 /MHz	[39756.547178064]	8

MICROWAVE AVG = -0.000020 MHz, IR AVG = 0.00000

MICROWAVE RMS = 0.021354 MHz, IR RMS = 0.00000

END OF ITERATION 1 OLD, NEW RMS ERROR= 2.13538 2.13538

distinct frequency lines in fit: 24

distinct parameters of fit: 5

MICROWAVE lines fitted lines lines RMS RMS ERROR J range Ka range freq. range

	total	dv=0	dv.ne.0	UNFITTD	e>900							
v"= 0	23	23	0	0	0	0.017247	1.72470	1	5	0	4	6589 16893
v"= 1	1	1	0	0	0	0.063800	6.38000	3	4	3	3	13358 13358
total:	24	24	0	0	0	0.021323	2.13229					

Standard errors are obtained by multiplying the previous errors by: 2.399960

---------- PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:

(values rounded)

10099	A /MHz	3364.80(47)	1
20099	B /MHz	1712.7135(30)	2
30099	C /MHz	1625.2808(30)	3
299	DJ /kHz	0.122(50)	4
1199	DJK /kHz	1.11(16)	5
2099	DK /kHz	[0.61478149]	6
210001	Fbc /MHz	[0.835945002]	7
11	E1 /MHz	[39756.547178064]	8

Worst fitted constants, with greater than 20% uncertainty: %

299	DJ /kHz	0.122(50)	4	41.5

CORRELATION COEFFICIENTS, C.ij:

	A	B	C	-DJ	-DJK
A	1.0000				
B	0.2517	1.0000			
C	-0.2914	-0.1490	1.0000		
-DJ	-0.1471	-0.5703	-0.5749	1.0000	
-DJK	0.4329	-0.0569	-0.0440	-0.3086	1.0000

Mean value of |C.ij|, i.ne.j = 0.2827

Mean value of C.ij, i.ne.j = -0.1458

No correlations with absolute value greater than 0.9950

Worst fitted lines (obs-calc/error):

13: 6.4	14: -4.8	12: -3.9	25: -2.5
6: -2.5	19: -2.0	18: 1.7	10: 1.6
24: 1.5	23: 1.4	17: -1.2	11: 1.1
16: 0.8	15: 0.5	5: 0.5	8: 0.5
2: 0.5	20: 0.4	9: -0.3	22: 0.3
7: 0.1	4: -0.1	3: -0.1	1: 0.0
21: 0.0			

13/ 4 3 2 1 3 3 1 1	13358.4508	0.0638	0.010
14/ 4 3 1 0 3 3 0 0	13358.8272	-0.0476	0.010
12/ 4 3 2 0 3 3 1 0	13358.3461	-0.0388	0.010
25: 5 1 4 0 4 1 3 0	16892.7908	-0.0251	0.010

6: 3 2 2 0 2 2 1 0	10013.9175	-0.0246	0.010
19: 5 2 4 0 4 2 3 0	16682.3316	-0.0199	0.010
18: 5 0 5 0 4 0 4 0	16623.8147	0.0173	0.010
10: 4 0 4 0 3 0 3 0	13318.4678	0.0160	0.010
24: 5 2 3 0 4 2 2 0	16748.4678	0.0146	0.010
23: 5 3 2 0 4 3 1 0	16702.3126	0.0136	0.010

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_____/ SPFIT output reformatted with PIFORM

S5. $^{13}C_1$ / $^{13}C_4$ MW Transition Assignments

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	obs	o-c	error o-c	blends wt	Notes
/ instead of : below denotes (o-c)>3*err					
1: 2 1 2 0 1 1 1 0	6566.6039	0.0026	0.010		
2: 2 0 2 0 1 0 1 0	6656.4294	0.0050	0.010		
3: 2 1 1 0 1 1 0 0	6754.2074	0.0011	0.010		
4: 3 1 3 0 2 1 2 0	9847.4475	-0.0065	0.010		
5: 3 0 3 0 2 0 2 0	9974.7194	0.0031	0.010		
6: 3 2 2 0 2 2 1 0	9990.5772	0.0000	0.010		
7: 3 2 1 0 2 2 0 0	10006.4634	-0.0016	0.010		
8: 3 1 2 0 2 1 1 0	10128.7630	0.0074	0.010		
9: 4 1 4 0 3 1 3 0	13125.5172	0.0020	0.010		
10: 4 0 4 0 3 0 3 0	13281.3476	-0.0295	0.010		

11/ 4 0 4 1 3 0 3 1	13281.4293	0.0478	0.010
12: 4 2 3 0 3 2 2 0	13317.6688	0.0163	0.010
13/ 4 3 1 0 3 3 0 0	13328.9471	-0.0574	0.010
14: 4 2 2 0 3 2 1 0	13357.0598	-0.0033	0.010
15: 4 1 3 0 3 1 2 0	13500.1010	0.0105	0.010
16/ 5 1 5 0 4 1 4 0	16400.0484	-0.0413	0.010
17/ 5 1 5 1 4 1 4 1	16400.1325	0.0347	0.010
18: 5 0 5 0 4 0 4 0	16573.3730	0.0026	0.010
19: 5 2 4 0 4 2 3 0	16642.0488	-0.0125	0.010
20: 5 4 1 0 4 4 0 0	16659.6741	0.0168	0.010
21: 5 3 3 0 4 3 2 0	16663.4463	-0.0291	0.010
22/ 5 3 3 1 4 3 2 1	16663.5414	0.0585	0.010
23/ 5 3 2 0 4 3 1 0	16665.6351	-0.0558	0.010
24/ 5 3 2 1 4 3 1 1	16665.7370	0.0395	0.010
25: 5 2 3 0 4 2 2 0	16719.6493	0.0139	0.010
26: 5 1 4 0 4 1 3 0	16866.8650	-0.0215	0.010

PARAMETERS IN FIT (values truncated):

10099	A /MHz	3320.68(16)	1
20099	B /MHz	1712.0044(11)	2
30099	C /MHz	1618.2019(12)	3
299	DJ /kHz	0.140(21)	4
1199	DJK /kHz	1.072(68)	5
2099	DK /kHz	[0.61478149]	6
210001	Fbc /MHz	[0.835945002]	7
11	E1 /MHz	[39756.547178064]	8

MICROWAVE AVG = 0.000137 MHz, IR AVG = 0.00000

MICROWAVE RMS = 0.027729 MHz, IR RMS = 0.00000

END OF ITERATION 1 OLD, NEW RMS ERROR= 2.77287 2.77287

distinct frequency lines in fit: 26

distinct parameters of fit: 5

MICROWAVE lines fitted lines lines RMS RMS ERROR J range Ka range freq. range

total dv=0 dv.ne.0 UNFITTD e>900

v''= 0	22	22	0	0	0	0.022828	2.28283	1	5	0	4	6567	16867
v''= 1	4	4	0	0	0	0.046020	4.60202	3	5	0	3	13281	16666

---

total:	26	26	0	0	0	0.027691	2.76908

Standard errors are obtained by muliplying the previous errors by: 3.085365

PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:

(values rounded)

10099	A /MHz	3320.69(50)	1
20099	B /MHz	1712.0044(36)	2
30099	C /MHz	1618.2019(37)	3
299	DJ /kHz	0.140(64)	4
1199	DJK /kHz	1.07(20)	5
2099	DK /kHz	[0.61478149]	6
210001	Fbc /MHz	[0.835945002]	7
11	E1 /MHz	[39756.547178064]	8

Worst fitted constants, with greater than 20% uncertainty: %

299 DJ /kHz 0.140(64) 4 46.2

CORRELATION COEFFICIENTS, C.ij:

A B C -DJ -DJK

A 1.0000

B 0.2109 1.0000

C -0.3049 -0.0608 1.0000

-DJ -0.0974 -0.5375 -0.6774 1.0000

-DJK 0.4379 -0.0689 0.0985 -0.3950 1.0000

Mean value of |C.ij|, i.ne.j = 0.2889

Mean value of C.ij, i.ne.j = -0.1395

No correlations with absolute value greater than 0.9950

Worst fitted lines (obs-calc/error):

22: 5.9	13: -5.7	23: -5.6	11: 4.8
16: -4.1	24: 4.0	17: 3.5	10: -2.9
21: -2.9	26: -2.1	20: 1.7	12: 1.6
25: 1.4	19: -1.2	15: 1.1	8: 0.7
4: -0.6	2: 0.5	14: -0.3	5: 0.3
18: 0.3	1: 0.3	9: 0.2	7: -0.2
3: 0.1	6: 0.0		

22/ 5 3 3 1 4 3 2 1	16663.5414	0.0585	0.010
13/ 4 3 1 0 3 3 0 0	13328.9471	-0.0574	0.010
23/ 5 3 2 0 4 3 1 0	16665.6351	-0.0558	0.010
11/ 4 0 4 1 3 0 3 1	13281.4293	0.0478	0.010
16/ 5 1 5 0 4 1 4 0	16400.0484	-0.0413	0.010
24/ 5 3 2 1 4 3 1 1	16665.7370	0.0395	0.010
17/ 5 1 5 1 4 1 4 1	16400.1325	0.0347	0.010
10: 4 0 4 0 3 0 3 0	13281.3476	-0.0295	0.010
21: 5 3 3 0 4 3 2 0	16663.4463	-0.0291	0.010
26: 5 1 4 0 4 1 3 0	16866.8650	-0.0215	0.010

_____

_____/ SPFIT output reformatted with PIFORM

S6. $^{13}C_2$ / $^{13}C_3$ MW Transition Assignments

---

	obs	o-c	error o-c	blends wt	Notes

/ instead of : below denotes (o-c)>3*err

1: 2 1 2 0 1 1 1 0	6511.2455	0.0004	0.010
2: 2 0 2 0 1 0 1 0	6596.3207	-0.0038	0.010
3: 2 1 1 0 1 1 0 0	6688.2973	0.0017	0.010
4: 3 1 3 0 2 1 2 0	9764.7465	0.0014	0.010
5: 3 0 3 0 2 0 2 0	9885.8836	-0.0026	0.010
6: 3 2 2 0 2 2 1 0	9899.6310	0.0093	0.010
7: 3 2 1 0 2 2 0 0	9913.3916	-0.0035	0.010
8: 3 1 2 0 2 1 1 0	10030.2430	0.0066	0.010

```
 9:  4  1  4  0    3  1  3  0          13015.8056  -0.0080  0.010
10:  4  0  4  0    3  0  3  0          13165.3227  -0.0051  0.010
11:  4  2  3  0    3  2  2  0          13196.8019   0.0037  0.010
12:  4  2  2  0    3  2  1  0          13231.0104   0.0051  0.010
13:  4  1  3  0    3  1  2  0          13369.4009  -0.0087  0.010
14:  5  1  5  0    4  1  4  0          16263.8329   0.0035  0.010
15:  5  0  5  0    4  0  4  0          16431.8968   0.0001  0.010
16:  5  2  4  0    4  2  3  0          16491.6689   0.0024  0.010
17:  5  4  2  0    4  4  1  0          16506.8160  -0.0089  0.010
18:  5  3  3  0    4  3  2  0          16510.2850   0.0184  0.010
19:  5  3  2  0    4  3  1  0          16512.0249  -0.0049  0.010
20/  5  2  3  0    4  2  2  0          16559.1208  -0.0407  0.010
21/  5  2  3  1    4  2  2  1          16559.1994   0.0338  0.010
22:  5  1  4  0    4  1  3  0          16704.6923   0.0004  0.010
--------------------------------------------------------------------------------
PARAMETERS IN FIT (values truncated):
      10099          A  /MHz       3351.83(17)                 1
      20099          B  /MHz       1694.2074(12)               2
      30099          C  /MHz       1605.6822(12)               3
        299         DJ  /kHz        0.089(21)                  4
       1199        DJK  /kHz        1.537(71)                  5
       2099         DK  /kHz       [ 0.61478149]               6
     210001        Fbc  /MHz       [ 0.835945002]              7
         11         E1  /MHz      [39756.547178064]            8
 MICROWAVE AVG =       0.000040 MHz, IR AVG =       0.00000
 MICROWAVE RMS =       0.012881 MHz, IR RMS =       0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=       1.28808       1.28808
  distinct frequency lines in fit:    22
```

distinct parameters of fit: 5

MICROWAVE lines fitted lines lines RMS RMS ERROR J range Ka range freq. range

total dv=0 dv.ne.0 UNFITTD e>900

v"= 0	21	21	0	0	0	0.010890	1.08898	1	5	0	4	6511	16705	
v"= 1	1	1	0	0	0	0.033800	3.38000	4	5	2	2	16559	16559	

---

total:	22	22	0	0	0	0.012850	1.28502

Standard errors are obtained by multiplying the previous errors by: 1.465311

PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:

(values rounded)

10099	A /MHz	3351.84(25)	1
20099	B /MHz	1694.2075(18)	2
30099	C /MHz	1605.6823(18)	3
299	DJ /kHz	0.090(31)	4
1199	DJK /kHz	1.54(10)	5
2099	DK /kHz	[0.61478149]	6
210001	Fbc /MHz	[0.835945002]	7
11	E1 /MHz	[39756.547178064]	8

Worst fitted constants, with greater than 20% uncertainty: %

299 DJ /kHz 0.090(31) 4 35.3

CORRELATION COEFFICIENTS, C.ij:

A B C -DJ -DJK

A 1.0000

B 0.2784 1.0000

C -0.3513 -0.1043 1.0000

-DJ -0.0366 -0.6045 -0.6048 1.0000

-DJK 0.3244 0.0254 0.0323 -0.3595 1.0000

Mean value of |C.ij|, i.ne.j = 0.2721

Mean value of C.ij, i.ne.j = -0.1400

No correlations with absolute value greater than 0.9950

Worst fitted lines (obs-calc/error):

20: -4.1 21: 3.4 18: 1.8 6: 0.9

17: -0.9 13: -0.9 9: -0.8 8: 0.7

10: -0.5 12: 0.5 19: -0.5 2: -0.4

11: 0.4 7: -0.3 14: 0.3 5: -0.3

16: 0.2 3: 0.2 4: 0.1 22: 0.0

1: 0.0 15: 0.0

20/ 5 2 3 0 4 2 2 0 16559.1208 -0.0407 0.010

21/ 5 2 3 1 4 2 2 1 16559.1994 0.0338 0.010

18: 5 3 3 0 4 3 2 0 16510.2850 0.0184 0.010

6: 3 2 2 0 2 2 1 0 9899.6310 0.0093 0.010

17: 5 4 2 0 4 4 1 0 16506.8160 -0.0089 0.010

13: 4 1 3 0 3 1 2 0 13369.4009 -0.0087 0.010

9: 4 1 4 0 3 1 3 0 13015.8056 -0.0080 0.010

8: 3 1 2 0 2 1 1 0 10030.2430 0.0066 0.010

10: 4 0 4 0 3 0 3 0 13165.3227 -0.0051 0.010

12: 4 2 2 0 3 2 1 0 13231.0104 0.0051 0.010

_____

_____/ SPFIT output reformatted with PIFORM

S7. Output of Structure Evaluation Program for Ring Bond Lengths, Angles, and Dihedral Angles (units are given in Å, degrees, and degrees, respectively) in 1,1-difluoro-1-silacyclopentane.

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| E V A L - Internals and their errors from Cartesians

|

|_____

_____|

version 19.VI.2017 Zbigniew KISIEL

WARNING:

The EVAL uncertainties are evaluated by assuming that
the correlation matrix is a unit matrix.
The EVAL uncertainties may thus differ significantly
(but typically by not more than 30% either way)
from uncertainties in explicitly fitted internals
corresponding to the input Cartesians.

```
!    11dfscpentane
!
INPUT CARTESIANS:
Si      -0.57203  0.00536    0.00000  0.07957    0.00000  0.07175
C(1)     0.61901  0.00950   -1.25993  0.00466    0.64503  0.01014
C(2)     1.96596  0.00162   -0.76925  0.00425    0.02674  0.12546
C(3)     1.96596  0.00162    0.76925  0.00425   -0.02674  0.12546
C(4)     0.61901  0.00950    1.25993  0.00466   -0.64503  0.01014

CALCULATED INTERNALS:
!
! Bond Lengths
!
        Si   C(1)   =   1.84988 +- 0.06029
        C(1) C(2)   =   1.56119 +- 0.05054
        Si   C(4)   =   1.84988 +- 0.06029
        C(2) C(3)   =   1.53943 +- 0.00861
        C(3) C(4)   =   1.56119 +- 0.05061
!
!  Bond Angles
!
```

C(1) Si C(4) = 99.84152 +- 0.44335

C(2) C(1) Si = 101.73199 +- 2.58199

C(3) C(2) C(1) = 109.13935 +- 3.04329

C(4) C(3) C(2) = 109.13935 +- 3.04801

C(4) Si C(1) = 99.84152 +- 0.44335

!

! Dihedral Angles

!

Si C(1) C(2) C(3) = 34.81062 +- 8.45254

C(1) C(2) C(3) C(4) = -48.08302 +-10.48885

C(2) C(3) C(4) Si = 34.81062 +- 8.44819

C(3) C(4) Si C(1) = -12.34288 +- 4.97238

C(4) Si C(1) C(2) = -12.34288 +- 4.97426

S8. Output of Kraitchman Analysis Program (atom positions are absolute and given in Å) in 1,1-difluoro-1-silacylopentane.

```
_____
|
|
|   KRA  -  SINGLE ISOTOPIC SUBSTITUTION - Various permutations
|
|           of Kraitchman's equations for symmetric/asymmetric tops
|

|_____
____ |
 version 27.XI.2013                                Zbigniew KISIEL
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11dfscpentane

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parent species

Planar calculation will be made from I.a and I.b

Si-29

The parent species:

X, Y, Z =	3364.65417600	1716.43207980	1628.63255330
eX, eY, eZ =	0.00005000	0.00000820	0.00000770
IX, IY, IZ =	150.20236213	294.43577229	310.30879493
eIX,eIY,eIZ =	0.00000223	0.00000141	0.00000147
PX, PY, PZ =	227.27110254	83.03769239	67.16466975

Mass = 122.03633380

The isotopic species:

X, Y, Z =	3364.86000000	1714.55740000	1626.93830000
eX, eY, eZ =	0.57000000	0.00310000	0.00310000
IX, IY, IZ =	150.19317446	294.75770540	310.63194283
eIX,eIY,eIZ =	0.02544240	0.00053294	0.00059188
PX, PY, PZ =	227.59823689	83.03370595	67.15946851

Mass change = 0.99956780

Total mass = 123.03590160

M DM/(M+DM) = 0.99144712

KRAITCHMAN RESULTS:

	a	b	
PLANAR:	0.56985 +- 0.00047	0.09637*i+- 0.13344	
+Costain err.	0.56985 +- 0.00267	0.09637*i+- 0.13434	

	a	b	c
NONPLANAR:	0.57444 +- 0.01117	0.06349*i+- 0.10136	0.07249*i+- 0.08870
+Costain err.	0.57444 +- 0.01148	0.06349*i+- 0.10407	0.07249*i+- 0.09108

R= 0.56629 +- 0.02019

DIX,DIY,DIZ =	-0.00918768	0.32193311	0.32314790
DPX,DPY,DPZ =	0.32713435	-0.00398644	-0.00520124
IXY,IXZ,IYZ =	-144.23341016	-160.10643280	-15.87302264

Si-30

The parent species:

X, Y, Z =	3364.65417600	1716.43207980	1628.63255330
eX, eY, eZ =	0.00005000	0.00000820	0.00000770
IX, IY, IZ =	150.20236213	294.43577229	310.30879493
eIX,eIY,eIZ =	0.00000223	0.00000141	0.00000147
PX, PY, PZ =	227.27110254	83.03769239	67.16466975

Mass = 122.03633380

The isotopic species:

X, Y, Z =	3364.80000000	1712.71350000	1625.28080000
eX, eY, eZ =	0.47000000	0.00300000	0.00300000
IX, IY, IZ =	150.19585265	295.07504028	310.94873267
eIX,eIY,eIZ =	0.02097957	0.00051686	0.00057396
PX, PY, PZ =	227.91396015	83.03477252	67.16108013

Mass change = 1.99684360

Total mass = 124.03317740

M DM/(M+DM) = 1.96469588

KRAITCHMAN RESULTS:

	a	b	
PLANAR:	0.57043 +- 0.00023	0.05769*i+- 0.09296	
+Costain err.	0.57043 +- 0.00264	0.05769*i+- 0.09653	

	a	b	c
NONPLANAR:	0.57203 +- 0.00467	0.03864*i+- 0.06946	0.04283*i+- 0.06262
+Costain err.	0.57203 +- 0.00536	0.03864*i+- 0.07957	0.04283*i+- 0.07175

R= 0.56911 +- 0.00934

DIX,DIY,DIZ =	-0.00650948	0.63926799	0.63993774
DPX,DPY,DPZ =	0.64285761	-0.00291986	-0.00358962
IXY,IXZ,IYZ =	-144.23341016	-160.10643280	-15.87302264

C-13 1/4

The parent species:

X, Y, Z =	3364.65417600	1716.43207980	1628.63255330
eX, eY, eZ =	0.00005000	0.00000820	0.00000770
IX, IY, IZ =	150.20236213	294.43577229	310.30879493
eIX,eIY,eIZ =	0.00000223	0.00000141	0.00000147
PX, PY, PZ =	227.27110254	83.03769239	67.16466975

Mass = 122.03633380

The isotopic species:

X, Y, Z =	3320.69000000	1712.00440000	1618.20190000
eX, eY, eZ =	0.50000000	0.00360000	0.00370000
IX, IY, IZ =	152.19096182	295.19725825	312.30899247
eIX,eIY,eIZ =	0.02291556	0.00062074	0.00071409
PX, PY, PZ =	227.65764445	84.65134802	67.53961380

Mass change = 1.00335484

Total mass = 123.03968863

M DM/(M+DM) = 0.99517275

KRAITCHMAN RESULTS:

	a	b
PLANAR:	0.86869 +- 0.00036	1.41732 +- 0.00817

+Costain err. 0.86869 +- 0.00176 1.41732 +- 0.00823

	a	b	c
NONPLANAR:	0.61901 +- 0.00918	1.25993 +- 0.00450	0.64503 +- 0.00987
+Costain err.	0.61901 +- 0.00950	1.25993 +- 0.00466	0.64503 +- 0.01014

R= 1.54488 +- 0.00684

DIX,DIY,DIZ =	1.98859968	0.76148596	2.00019754
DPX,DPY,DPZ =	0.38654191	1.61365563	0.37494406
IXY,IXZ,IYZ =	-144.23341016	-160.10643280	-15.87302264

C-13 2/3

The parent species:

X, Y, Z =	3364.65417600	1716.43207980	1628.63255330
eX, eY, eZ =	0.00005000	0.00000820	0.00000770
IX, IY, IZ =	150.20236213	294.43577229	310.30879493
eIX,eIY,eIZ =	0.00000223	0.00000141	0.00000147
PX, PY, PZ =	227.27110254	83.03769239	67.16466975

Mass = 122.03633380

The isotopic species:

X, Y, Z =	3351.84000000	1694.20750000	1605.68230000
eX, eY, eZ =	0.25000000	0.00180000	0.00180000
IX, IY, IZ =	150.77658987	298.29817481	314.74408418
eIX,eIY,eIZ =	0.01124581	0.00031693	0.00035283
PX, PY, PZ =	231.13283456	83.61124962	67.16534025

Mass change = 1.00335484

Total mass = 123.03968863

M DM/(M+DM) = 0.99517275

KRAITCHMAN RESULTS:

	a	b	
PLANAR:	1.96613 +- 0.00011	0.76972 +- 0.00754	
+Costain err.	1.96613 +- 0.00077	0.76972 +- 0.00779	

	a	b	c
NONPLANAR:	1.96596 +- 0.00143	0.76925 +- 0.00378	0.02674 +- 0.11221
+Costain err.	1.96596 +- 0.00162	0.76925 +- 0.00425	0.02674 +- 0.12546

R= 2.11127 +- 0.00268

DIX,DIY,DIZ =	0.57422774	3.86240252	4.43528925
DPX,DPY,DPZ =	3.86173202	0.57355723	0.00067050
IXY,IXZ,IYZ =	-144.23341016	-160.10643280	-15.87302264

S9. List of Split Transitions

	EXP.FREQ.	CALC.FREQ.	DIFF.	EXP.ERR.-EST.ERR.	AVG. CALC.FREQ.	DIFF.	WT.
4 2 3 1 4 0 4 1	6816.61474	6816.61474	-0.00000	0.01000	0.00000		
4 0 4 1 3 0 3 1	13281.42931	13281.38148	0.04783	0.01000	0.00000		
4 3 2 1 3 3 1 1	13358.45081	13358.38695	0.06385	0.01000	0.00000		
4 3 2 1 3 3 1 1	13372.47301	13372.41981	0.05320	0.01000	0.00000		
4 3 1 1 3 3 0 1	13372.93068	13372.91358	0.01710	0.01000	0.00000		
5 1 5 1 4 1 4 1	16400.13250	16400.09779	0.03471	0.01000	0.00000		
5 2 3 1 4 2 2 1	16559.19939	16559.16551	0.03388	0.01000	0.00000		
5 3 3 1 4 3 2 1	16663.54144	16663.48290	0.05854	0.01000	0.00000		
5 3 2 1 4 3 1 1	16665.73700	16665.69741	0.03959	0.01000	0.00000		
5 2 4 1 4 2 3 1	16717.58400	16717.55272	0.03128	0.01000	0.00000		
5 4 2 1 4 4 1 1	16732.59423	16732.61061	-0.01638	0.01000	0.00000		
5 4 1 1 4 4 0 1	16732.59423	16732.62401	-0.02977	0.01000	0.00000		
5 3 3 1 4 3 2 1	16735.97550	16735.97879	-0.00329	0.01000	0.00000		
6 0 6 1 5 0 5 1	19955.97580	19955.97989	-0.00409	0.01000	0.00000		
6 1 5 1 5 1 4 1	20303.95166	20303.96793	-0.01627	0.01000	0.00000		

APPENDIX B.

SUPPLIMENTARY INFORMATION FOR THE MOLECULAR STRUCTURE AND CURIOUS MOTIONS IN 1,1-DIFLUOROSILACYCLOPENT-3-ENE AND SILACYCLOPENT-3-ENE AS DETERMINED BY MICROWAVE SPECTROSCOPY AND QUANTUM CHEMICAL CALCULATIONS

Supplemental Data Fits and Analyses

11dfscp3ene Separate

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		obs	o-c	error	blends	o-c	wt
Notes							
/ instead of : below denotes (o-c)>3*err							
1:	2 1 2 0 1 1 1 0	6917.0167	0.0086	0.010			
2:	2 1 2 1 1 1 1 1	6917.0190	-0.0174	0.010			
3:	2 0 2 0 1 0 1 0	7005.3453	-0.0010	0.010			
4:	2 0 2 1 1 0 1 1	7005.3468	-0.0140	0.010			
5:	2 1 1 0 1 1 0 0	7100.6875	-0.0067	0.010			
6:	3 2 2 0 3 0 3 0	7186.1321	-0.0037	0.010			
7:	4 2 3 0 4 0 4 0	7218.1642	-0.0057	0.010			
8:	5 2 4 0 5 0 5 0	7279.1347	0.0066	0.010			
9:	2 1 2 0 1 1 1 0	6917.0151	0.0070	0.010	-0.0072	0.50	
10:	2 1 2 1 1 1 1 1	6917.0151	-0.0214	0.010	-0.0072	0.50	
11:	2 0 2 0 1 0 1 0	7005.3482	0.0018	0.010	-0.0054	0.50	
12:	2 0 2 1 1 0 1 1	7005.3482	-0.0126	0.010	-0.0054	0.50	
13:	2 1 1 0 1 1 0 0	7100.6825	-0.0117	0.010			
14:	3 2 2 0 3 0 3 0	7186.1321	-0.0037	0.010			
15:	4 2 3 0 4 0 4 0	7218.1618	-0.0082	0.010			
16:	5 2 4 0 5 0 5 0	7279.1432	0.0151	0.010			
17:	3 1 3 0 2 1 2 0	10373.3425	0.0075	0.010			
18:	3 0 3 0 2 0 2 0	10499.2285	0.0081	0.010			
19:	3 2 2 0 2 2 1 0	10513.1606	0.0051	0.010			

```
 20:  3  2  1  0    2  2  0  0          10527.2463   0.0080  0.010
 21:  3  1  2  0    2  1  1  0          10648.7744  -0.0049  0.010
 22:  4  1  4  0    3  1  3  0          13827.1864   0.0204  0.010  -0.0073 0.50
 23:  4  1  4  1    3  1  3  1          13827.1864  -0.0351  0.010  -0.0073 0.50
 24:  4  0  4  0    3  0  3  0             13982.7281   -0.0056  0.010
25: 4  2  3  0    3  2  2  0           14014.7855   0.0175  0.010
 26:  4  3  2  0    3  3  1  0          14024.1248  -0.0011  0.010
 27:  4  3  1  0    3  3  0  0          14024.6266   0.0096  0.010
 28:  4  2  2  0    3  2  1  0          14049.7693   0.0187  0.010   0.0221 0.50
 29:  4  2  2  1    3  2  1  1          14049.7693   0.0256  0.010   0.0221 0.50
 30:  4  1  3  1    3  1  2  1          14194.0110   0.0127  0.010  -0.0029 0.50
 31:  4  1  3  0    3  1  2  0          14194.0110  -0.0184  0.010  -0.0029 0.50
 32:  5  1  5  0    4  1  4  0          17277.9158   0.0568  0.010   0.0204 0.50
 33:  5  1  5  1    4  1  4  1          17277.9158  -0.0160  0.010   0.0204 0.50
 34:  5  0  5  0    4  0  4  0             17453.0393   -0.0097  0.010
35:  5  0  5  1    4  0  4  1           17453.1552   0.0004  0.010
 36:  5  2  4  0    4  2  3  0             17513.9781   -0.0290  0.010
37:  5  2  4  1    4  2  3  1           17514.0783   0.0173  0.010
 38:  5  4  2  1    4  4  1  1           17529.0060  -0.0176  0.010
--------------------------------------------------------------------------------

PARAMETERS IN FIT (values truncated and Nlines statistics):

      10000          A  /MHz       3544.4238(21)                 1
      20000          B  /MHz       1798.1419(16)                 2
      30000          C  /MHz       1706.2987(19)                 3

        299         DJ  /kHz          0.201(25)                   4
```

1199	DJK /kHz	5.873(92)	5
10011	A /MHz	3545.23(46)	6
20011	B /MHz	1798.1357(38)	7
30011	C /MHz	1706.3101(26)	8
210001	Fbc /MHz	0.68(11)	9
11	E1 /MHz	13006.(510)	10

MICROWAVE AVG = -0.000519 MHz, IR AVG = 0.00000

MICROWAVE RMS = 0.011774 MHz, IR RMS = 0.00000

END OF ITERATION 1 OLD, NEW RMS ERROR= 1.17742 1.17742

distinct frequency lines in fit: 32

distinct parameters of fit: 10

MICROWAVE	lines fitted	lines	lines	RMS	RMS ERROR	J range	Ka range	freq. range
total	dv=0	dv.ne.0	UNFITTD	e>900	v"= 0	26	26	0 0 0
0.011266	1.12664	1	5	0	3	6917	17514	v"= 1
6	6	0 0 0	0.013639	1.36387	1	5	0	4
6917	17529							

-----total:	32	32	0	0	0	0.011748	1.17478

NOTE: the RMS values above are for Nlines statistics, but the 'total' values may differ slightly from those in the .FIT file since the o-c values for this evaluation are as rounded in the .FIT.

PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:
(values rounded and degrees of freedom, Ndegf=Nlines-Nconst, statistics)

10000	A /MHz	3544.4239(30)	1
20000	B /MHz	1798.1419(23)	2
30000	C /MHz	1706.2988(27)	3
299	DJ /kHz	0.201(36)	4
1199	DJK /kHz	5.87(13)	5
10011	A /MHz	3545.23(65)	6
20011	B /MHz	1798.1357(53)	7
30011	C /MHz	1706.3102(37)	8
210001	Fbc /MHz	0.68(16)	9
11	E1 /MHz	13006.(724)	10

--- Worst fitted constants, with greater than 20% uncertainty:
%

210001 Fbc /MHz 0.68(16) 9 23.7 ----------

CORRELATION COEFFICIENTS, C.ij:

A B C -DJ -DJK A B C

1.0000

0.1035 1.0000

0.1674 -0.6544 1.0000

-DJ -0.0519 0.1311 -0.7375 1.0000

-DJK -0.5554 -0.2623 0.2744 -0.2528 1.0000

-0.2469 -0.3943 0.5300 -0.4740 0.3138 1.0000

0.2506 -0.3141 0.5264 -0.4625 -0.2849 0.4727 1.0000

-0.0181 0.4082 -0.2389 -0.0829 0.0232 -0.4992 -0.6754 1.0000

Fbc 0.2616 0.3453 -0.3940 0.4112 0.1576 -0.5005 -0.4920 0.1760

E1 0.0261 -0.2312 0.2273 -0.2420 -0.4966 0.2740 0.5636 -0.1893

Fbc E1

Fbc 1.0000

E1 -0.7338 1.0000

Mean value of |C.ij|, i.ne.j = 0.3362

Mean value of C.ij, i.ne.j = -0.0854

No correlations with absolute value greater than 0.9950

Worst fitted lines (obs-calc/error):

36: -2.9 28: 2.2 32: 2.0 38: -1.8

25: 1.8 2: -1.7 37: 1.7 16: 1.5

4: -1.4 13: -1.2 34: -1.0 27: 1.0

1: 0.9 15: -0.8 18: 0.8 20: 0.8

17: 0.8 22: -0.7 9: -0.7 5: -0.7

8: 0.7 7: -0.6 24: -0.6 11: -0.5

19: 0.5 21: -0.5 6: -0.4 14: -0.4

30: -0.3 26: -0.1 3: -0.1 35: 0.0

33: 0.0 31: 0.0 29: 0.0 23: 0.0

12: 0.0 10: 0.0

36: 5 2 4 0 4 2 3 0 17513.9781 -0.0290 0.010

28: 4 2 2 0 3 2 1 0 14049.7693 0.0187 0.010 0.0221

0.50 32: 5 1 5 0 4 1 4 0 17277.9158 0.0568 0.010

0.0204 0.50

38: 5 4 2 1 4 4 1 1 17529.0060 -0.0176 0.010

25: 4 2 3 0 3 2 2 0 14014.7855 0.0175 0.010

2: 2 1 2 1 1 1 1 1 6917.0190 -0.0174 0.010

37: 5 2 4 1 4 2 3 1 17514.0783 0.0173 0.010

16: 5 2 4 0 5 0 5 0 7279.1432 0.0151 0.010

4: 2 0 2 1 1 0 1 1 7005.3468 -0.0140 0.010

13: 2 1 1 0 1 1 0 0 7100.6825 -0.0117 0.010

_____

_____/ SPFIT output reformatted with PIFORM

11dfscp3ene Together

	obs	o-c	error	blends	Notes	o-c	wt
/ instead of : below denotes (o-c)>3*err							
1: 2 1 2 0 1 1 1 0	6917.0167	0.0025	0.010				
2: 2 1 2 1 1 1 1 1	6917.0190	0.0039	0.010				
3: 2 0 2 0 1 0 1 0	7005.3453	-0.0020	0.010				
4: 2 0 2 1 1 0 1 1	7005.3468	-0.0029	0.010				
5: 2 1 1 0 1 1 0 0	7100.6875	-0.0022	0.010				
6: 3 2 2 0 3 0 3 0	7186.1321	-0.0176	0.010				
7: 4 2 3 0 4 0 4 0	7218.1642	-0.0095	0.010				
8: 5 2 4 0 5 0 5 0	7279.1347	0.0244	0.010				
9: 2 1 2 0 1 1 1 0	6917.0151	0.0009	0.010	0.0004	0.50		
10: 2 1 2 1 1 1 1 1	6917.0151	0.0000	0.010	0.0004	0.50		
11: 2 0 2 0 1 0 1 0	7005.3482	0.0008	0.010	-0.0004	0.50		
12: 2 0 2 1 1 0 1 1	7005.3482	-0.0015	0.010	-0.0004	0.50		
13: 2 1 1 0 1 1 0 0	7100.6825	-0.0071	0.010				
14: 3 2 2 0 3 0 3 0	7186.1321	-0.0176	0.010				
15: 4 2 3 0 4 0 4 0	7218.1618	-0.0120	0.010				
16/ 5 2 4 0 5 0 5 0	7279.1432	0.0330	0.010				
17: 3 1 3 0 2 1 2 0	10373.3425	-0.0036	0.010				
18: 3 0 3 0 2 0 2 0	10499.2285	0.0037	0.010				
19: 3 2 2 0 2 2 1 0	10513.1606	0.0041	0.010				
20: 3 2 1 0 2 2 0 0	10527.2463	0.0049	0.010				
21: 3 1 2 0 2 1 1 0	10648.7744	0.0000	0.010				

22: 4 1 4 0 3 1 3 0 13827.1864 0.0015 0.010 0.0022 0.50

23: 4 1 4 1 3 1 3 1 13827.1864 0.0028 0.010 0.0022 0.50

24: 4 0 4 0 3 0 3 0 13982.7281 -0.0169 0.010

25: 4 2 3 0 3 2 2 0 14014.7855 0.0163 0.010

26: 4 3 2 0 3 3 1 0 14024.1248 -0.0038 0.010

27: 4 3 1 0 3 3 0 0 14024.6266 -0.0022 0.010

28: 4 2 2 0 3 2 1 0 14049.7693 0.0119 0.010 0.0126 0.50

29: 4 2 2 1 3 2 1 1 14049.7693 0.0133 0.010 0.0126 0.50

30: 4 1 3 1 3 1 2 1 14194.0110 -0.0066 0.010 -0.0112 0.50

31: 4 1 3 0 3 1 2 0 14194.0110 -0.0156 0.010 -0.0112 0.50

32: 5 1 5 0 4 1 4 0 17277.9158 0.0267 0.010 0.0273 0.50

33: 5 1 5 1 4 1 4 1 17277.9158 0.0279 0.010 0.0273 0.50

34/ 5 0 5 0 4 0 4 0 17453.0393 -0.0325 0.010

35/ 5 0 5 1 4 0 4 1 17453.1552 0.0354 0.010

36/ 5 2 4 0 4 2 3 0 17513.9781 -0.0301 0.010

37: 5 2 4 1 4 2 3 1 17514.0783 0.0256 0.010

38: 5 4 2 1 4 4 1 1 17529.0060 -0.0255 0.010 --

PARAMETERS IN FIT (values truncated and Nlines statistics):

10099	A /MHz	3544.4280(19)	1
20099	B /MHz	1798.1391(12)	2
30099	C /MHz	1706.3013(13)	3
299	DJ /kHz	0.161(21)	4
1199	DJK /kHz	5.818(79)	5

210001 Fbc /MHz 0.861(72) 6

11 E1 /MHz 11799.(749) 7

MICROWAVE AVG = -0.000031 MHz, IR AVG = 0.00000

MICROWAVE RMS = 0.016637 MHz, IR RMS = 0.00000

END OF ITERATION 1 OLD, NEW RMS ERROR= 1.66374 1.66374

distinct frequency lines in fit: 32

distinct parameters of fit: 7

MICROWAVE lines fitted lines lines RMS RMS ERROR J range Ka range freq. range total dv=0 dv.ne.0 UNFITTD e>900 v"= 0 26 26 0 0 0 0.015337 1.53370 1 5 0 3 6917 17514 v"= 1 6 6 0 0 0 0.021240 2.12396 1 5 0 4 6917 17529

-----total: 32 32 0 0 0 0.016604 1.66043

NOTE: the RMS values above are for Nlines statistics, but the 'total' values may differ slightly from those in the .FIT file since the o-c values for this evaluation are as rounded in the .FIT.

PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:

(values rounded and degrees of freedom, Ndegf=Nlines-Nconst, statistics)

10099 A /MHz 3544.4280(35) 1

20099	B /MHz	1798.1391(23)	2
30099	C /MHz	1706.3013(25)	3
299	DJ /kHz	0.162(40)	4
1199	DJK /kHz	5.82(14)	5
210001	Fbc /MHz	0.86(13)	6
11	E1 /MHz	11799.(1409)	7

--- Worst fitted constants, with greater than 20% uncertainty: %

299	DJ /kHz	0.162(40)	4	24.9

CORRELATION COEFFICIENTS, C.ij:

	A	B	C	-DJ	-DJK	Fbc	E1
1.0000							
0.2881	1.0000						
0.1957	-0.3504	1.0000					
-DJ	-0.1510	-0.2017	-0.7392	1.0000			
-DJK	-0.5044	-0.3132	0.3200	-0.4272	1.0000		
Fbc	0.3335	0.1211	-0.1794	0.2246	-0.3261	1.0000	
E1	0.0971	-0.0409	-0.0668	0.2832	-0.5499	0.6489	1.0000

Mean value of |C.ij|, i.ne.j = 0.3030

Mean value of C.ij, i.ne.j = -0.0637

No correlations with absolute value greater than 0.9950

Worst fitted lines (obs-calc/error):

35: 3.5	16: 3.3	34: -3.2	36: -3.0
32: 2.7	37: 2.6	38: -2.5	8: 2.4
6: -1.8	14: -1.8	24: -1.7	25: 1.6
28: 1.3	15: -1.2	30: -1.1	7: -0.9
13: -0.7	20: 0.5	19: 0.4	2: 0.4
26: -0.4	18: 0.4	17: -0.4	4: -0.3
1: 0.2	27: -0.2	5: -0.2	22: 0.2
3: -0.2	9: 0.0	11: 0.0	33: 0.0
31: 0.0	29: 0.0	23: 0.0	21: 0.0
12: 0.0	10: 0.0		

35/ 5 0 5 1 4 0 4 1	17453.1552	0.0354	0.010	
16/ 5 2 4 0 5 0 5 0	7279.1432	0.0330	0.010	
34/ 5 0 5 0 4 0 4 0	17453.0393	-0.0325	0.010	
36/ 5 2 4 0 4 2 3 0	17513.9781	-0.0301	0.010	
32: 5 1 5 0 4 1 4 0	17277.9158	0.0267	0.010	0.0273 0.50
37: 5 2 4 1 4 2 3 1	17514.0783	0.0256	0.010	
38: 5 4 2 1 4 4 1 1	17529.0060	-0.0255	0.010	
8: 5 2 4 0 5 0 5 0	7279.1347	0.0244	0.010	

6: 3 2 2 0 3 0 3 0 7186.1321 -0.0176 0.010

14: 3 2 2 0 3 0 3 0 7186.1321 -0.0176 0.010

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Silicon 30 11dfscp3ene

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obs o-c error blends

Notes o-c wt

/ instead of : below denotes (o-c)>3*err

1: 2 1 2 0 1 1 1 0 6903.7342 -0.0125 0.010

2: 2 0 2 0 1 0 1 0 6991.7507 -0.0024 0.010

3: 2 1 1 0 1 1 0 0 7086.6956 -0.0079 0.010

4: 3 1 3 0 2 1 2 0 10353.4645 0.0031 0.010

5: 3 0 3 0 2 0 2 0 10478.9132 -0.0005 0.010

6: 3 2 2 0 2 2 1 0 10492.7269 0.0110 0.010

7: 3 2 1 0 2 2 0 0 10506.6646 -0.0024 0.010

8: 3 1 2 0 2 1 1 0 10627.7917 -0.0212 0.010

9: 4 1 4 0 3 1 3 0 13800.7090 0.0081 0.010

10: 4 0 4 0 3 0 3 0 13955.8093 -0.0004 0.010

11: 4 2 3 0 3 2 2 0 13987.5399 0.0103 0.010

```
 12:  4  3  2  0    3  3  1  0          13996.8145   0.0113  0.010
 13:  4  3  1  0    3  3  0  0          13997.3130   0.0101  0.010
 14:  4  2  2  0    3  2  1  0          14022.1986   0.0098  0.010
 15:  4  1  3  0    3  1  2  0          14166.1041  -0.0092  0.010
 16:  5  1  5  0    4  1  4  0          17244.8050  -0.0215  0.010
 17:  5  0  5  0    4  0  4  0          17419.6070  -0.0157  0.010
 18:  5  0  5  1    4  0  4  1          17419.6936   0.0128  0.010
 19:  5  2  4  0    4  2  3  0          17479.9890   0.0095  0.010
 20/  5  2  4  1    4  2  3  1          17480.0751   0.0381  0.010
 21:  5  4  1  0    4  4  1  0          17494.9301   0.0023  0.010
 22:  5  3  3  0    4  3  2  0          17498.6608  -0.0277  0.010
 23:  5  3  2  0    4  3  1  0          17500.4135  -0.0207  0.010
 24/  5  2  3  0    4  2  2  0          17548.3730  -0.0358  0.010
25/  5  2  3  1    4  2  2  1          17548.4450   0.0366  0.010
 26/  5  1  4  0    4  1  3  0          17700.4308  -0.0378  0.010
 27/  5  1  4  1    4  1  3  1          17700.5151   0.0429  0.010
-------------------------------------------------------------------------------

PARAMETERS IN FIT (values truncated and Nlines statistics):

      10099         A  /MHz       3544.41(16)                 1
      20099         B  /MHz       1794.5529(11)               2
      30099         C  /MHz       1703.0745(10)               3
        299        DJ  /kHz          0.244(16)                4
       1199       DJK  /kHz          5.417(68)                5

     210001       Fbc  /MHz          0.49(14)                 6
```

11 E1 /MHz 8391.(624) 7

MICROWAVE AVG = -0.000358 MHz, IR AVG = 0.00000 MICROWAVE RMS = 0.020135 MHz, IR RMS = 0.00000 END OF ITERATION 1 OLD, NEW RMS ERROR= 2.01347 2.01347

distinct frequency lines in fit: 27
distinct parameters of fit: 7

MICROWAVE lines fitted lines lines RMS RMS ERROR J range Ka range freq. range total dv=0 dv.ne.0 UNFITTD e>900 v"= 0 23 23 0 0 0 0.016290 1.62898 1 5 0 4 6904 17700 v"= 1 4 4 0 0 0 0.034624 3.46245 4 5 0 2 17420 17701

-----total: 27 27 0 0 0 0.020091 2.00912

NOTE: the RMS values above are for Nlines statistics, but the 'total' values may differ slightly from those in the .FIT file since the o-c values for this evaluation are as rounded in the .FIT.

PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:
(values rounded and degrees of freedom, Ndegf=Nlines-Nconst, statistics)

10099	A /MHz	3544.41(37)	1
20099	B /MHz	1794.5529(25)	2
30099	C /MHz	1703.0745(25)	3
299	DJ /kHz	0.245(39)	4

1199 DJK /kHz 5.42(15) 5

210001 Fbc /MHz 0.50(32) 6

11 E1 /MHz 8391.(1459) 7 ----------

---------- Worst

fitted constants, with greater than 20% uncertainty: %

210001 Fbc /MHz 0.50(32) 6 65.5

CORRELATION COEFFICIENTS, C.ij:

A B C -DJ -DJK Fbc E1

1.0000

0.2455 1.0000

-0.3277 -0.1203 1.0000

-DJ -0.1266 -0.6108 -0.5330 1.0000

-DJK 0.3571 -0.1005 -0.1342 -0.2341 1.0000

Fbc 0.0363 0.1487 0.0256 0.0616 -0.4057 1.0000

E1 0.0821 0.1323 0.0155 0.0739 -0.4053 0.9757 1.0000

Mean value of |C.ij|, i.ne.j = 0.2454

Mean value of C.ij, i.ne.j = -0.0402

No correlations with absolute value greater than 0.9950

Worst fitted lines (obs-calc/error):

27: 4.3 20: 3.8 26: -3.8 25: 3.7
24: -3.6 22: -2.8 16: -2.1 8: -2.1
23: -2.1 17: -1.6 18: 1.3 1: -1.2
12: 1.1 6: 1.1 11: 1.0 13: 1.0
14: 1.0 19: 0.9 15: -0.9 9: 0.8
3: -0.8 4: 0.3 7: -0.2 2: -0.2
21: 0.2 5: -0.1 10: 0.0

27/ 5 1 4 1 4 1 3 1 17700.5151 0.0429 0.010
20/ 5 2 4 1 4 2 3 1 17480.0751 0.0381 0.010
26/ 5 1 4 0 4 1 3 0 17700.4308 -0.0378
0.010 25/ 5 2 3 1 4 2 2 1 17548.4450
0.0366 0.010
24/ 5 2 3 0 4 2 2 0 17548.3730 -0.0358 0.010
22: 5 3 3 0 4 3 2 0 17498.6608 -0.0277 0.010
16: 5 1 5 0 4 1 4 0 17244.8050 -0.0215 0.010
8: 3 1 2 0 2 1 1 0 10627.7917 -0.0212 0.010
23: 5 3 2 0 4 3 1 0 17500.4135 -0.0207 0.010
17: 5 0 5 0 4 0 4 0 17419.6070 -0.0157 0.010

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_____/ SPFIT output reformatted with PIFORM

11dfscp3ene Silicon 29

		obs	o-c	error	blends	Notes	o-c	wt
/ instead of : below denotes (o-c)>3*err								
1:	2 1 2 0	1 1 1 0	6910.3172	-0.0100	0.010			
2:	2 0 2 0	1 0 1 0	6998.4765	-0.0080	0.010			
3:	2 1 1 0	1 1 0 0	7093.6164	-0.0028	0.010			
4/	3 1 3 0	2 1 2 0	10363.2869	-0.0349	0.010			
5:	3 0 3 0	2 0 2 0	10488.9676	0.0007	0.010			
6:	3 2 2 0	2 2 1 0	10502.8531	0.0172	0.010			
7:	3 2 1 1	2 2 0 1	10516.8477	-0.0093	0.010			
8:	3 1 2 0	2 1 1 0	10638.1811	0.0055	0.010			
9:	4 1 4 0	3 1 3 0	13813.8359	0.0060	0.010			
10:	4 0 4 0	3 0 3 0	13969.1522	0.0183	0.010			
11:	4 2 3 0	3 2 2 0	14001.0318	0.0185	0.010			
12:	4 3 2 0	3 3 1 0	14010.3395	0.0073	0.010			
13:	4 3 1 0	3 3 0 0	14010.8423	0.0118	0.010			
14:	4 2 2 0	3 2 1 0	14035.8366	-0.0078	0.010			
15:	4 1 3 0	3 1 2 0	14179.9058	-0.0023	0.010			
16:	5 1 5 0	4 1 4 0	17261.2242	0.0137	0.010			
17:	5 0 5 0	4 0 4 0	17436.1286	-0.0288	0.010			
18:	5 0 5 1	4 0 4 1	17436.2094	0.0006	0.010			
19/	5 2 4 1	4 2 3 1	17496.9020	0.0328	0.010			
20/	5 4 2 1	4 4 1 1	17511.7384	-0.0484	0.010			
21/	5 4 1 0	4 4 0 0	17511.8382	0.0339	0.010	0.0406	0.50	

22: 5 4 2 0 4 4 1 0 17511.8382 0.0472 0.010 0.0406 0.50

23: 5 3 3 0 4 3 2 0 17515.6155 -0.0182 0.010

24/ 5 3 2 1 4 3 1 1 17517.3184 -0.0384 0.010

25/ 5 3 2 0 4 3 1 0 17517.4132 0.0395 0.010

26/ 5 2 3 0 4 2 2 0 17565.5338 -0.0474 0.010

27/ 5 2 3 1 4 2 2 1 17565.6178 0.0399 0.010

28: 5 1 4 0 4 1 3 0 17717.6676 -0.0067 0.010

PARAMETERS IN FIT (values truncated and Nlines statistics):

10099 A /MHz 3543.44(16) 1

20099 B /MHz 1796.3239(12) 2

30099 C /MHz 1704.6779(12) 3

299 DJ /kHz 0.223(20) 4

1199 DJK /kHz 5.728(58) 5

210001 Fbc /MHz 0.863(68) 6

11 E1 /MHz 11476.(475) 7

MICROWAVE AVG = -0.000387 MHz, IR AVG = 0.00000

MICROWAVE RMS = 0.024462 MHz, IR RMS = 0.00000

END OF ITERATION 1 OLD, NEW RMS ERROR= 2.44624 2.44624

distinct frequency lines in fit: 27

distinct parameters of fit: 7

MICROWAVE lines fitted lines lines RMS RMS ERROR J range Ka range freq. range total dv=0 dv.ne.0 UNFITTD e>900 v"= 0 21 21 0 0 0 0.021309 2.13087 1 5 0 4 6910 17718 v"= 1 6 6 0 0 0 0.033095 3.30954 2 5 0 4 10517 17566

-----total: 27 27 0 0 0 0.024425 2.44245

NOTE: the RMS values above are for Nlines statistics, but the 'total' values may differ slightly from those in the .FIT file since the o-c values for this evaluation are as rounded in the .FIT.

PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:
(values rounded and degrees of freedom, Ndegf=Nlines-Nconst, statistics)

10099	A /MHz	3543.45(47)	1
20099	B /MHz	1796.3240(36)	2
30099	C /MHz	1704.6780(36)	3
299	DJ /kHz	0.223(58)	4
1199	DJK /kHz	5.73(16)	5
210001	Fbc /MHz	0.86(19)	6
11	E1 /MHz	11476.(1350)	7

--- Worst fitted constants, with greater than 20% uncertainty: %

299	DJ /kHz	0.223(58)	4	26.1
210001	Fbc /MHz	0.86(19)	6	22.4

CORRELATION COEFFICIENTS, C.ij:

	A	B	C	-DJ	-DJK	Fbc	E1
1.0000							
0.2727	1.0000						
-0.3813	-0.1257	1.0000					
-DJ	-0.0516	-0.6035	-0.5985	1.0000			
-DJK	0.3591	-0.0279	-0.0131	-0.2852	1.0000		
Fbc	-0.2197	0.1838	0.1218	-0.1778	-0.2508	1.0000	
E1	0.1701	-0.1232	-0.0865	0.1506	-0.2006	-0.1997	1.0000

Mean value of |C.ij|, i.ne.j = 0.2192

Mean value of C.ij, i.ne.j = -0.0994

No correlations with absolute value greater than 0.9950

Worst fitted lines (obs-calc/error):

20: -4.8 26: -4.7 21: 4.1 27: 4.0

25: 4.0 24: -3.8 4: -3.5 19: 3.3

17: -2.9 11: 1.8 10: 1.8 23: -1.8

6: 1.7 16: 1.4 13: 1.2 1: -1.0

7: -0.9 2: -0.8 14: -0.8 12: 0.7

28: -0.7 9: 0.6 8: 0.5 3: -0.3

15: -0.2 5: 0.1 18: 0.1 22: 0.0

20/ 5 4 2 1 4 4 1 1 17511.7384 -0.0484 0.010

26/ 5 2 3 0 4 2 2 0 17565.5338 -0.0474 0.010

21/ 5 4 1 0 4 4 0 0 17511.8382 0.0339 0.010 0.0406 0.50

27/ 5 2 3 1 4 2 2 1 17565.6178 0.0399 0.010

25/ 5 3 2 0 4 3 1 0 17517.4132 0.0395 0.010

24/ 5 3 2 1 4 3 1 1 17517.3184 -0.0384 0.010

4/ 3 1 3 0 2 1 2 0 10363.2869 -0.0349 0.010

19/ 5 2 4 1 4 2 3 1 17496.9020 0.0328 0.010

17: 5 0 5 0 4 0 4 0 17436.1286 -0.0288 0.010

11: 4 2 3 0 3 2 2 0 14001.0318 0.0185 0.010

_____

_____/ SPFIT output reformatted with PIFORM 11dfscp3ene 3&4 Carbon-13

---

obs o-c error blends

Notes o-c wt

/ instead of : below denotes (o-c)>3*err

1: 2 1 2 1 1 1 6872.6291 -0.0069 0.010

2: 2 0 2 1 0 1 6970.9813 -0.0081 0.010

```
  3:  2  1  1    1  1  0              7078.3533  -0.0062  0.010
  4:  3  1  3    2  1  2             10306.1667  -0.0005  0.010
5:  3  0  3    2  0  2             10445.2035   0.0011  0.010
  6:  3  2  2    2  2  1             10463.1129  -0.0225  0.010
  7:  3  2  1    2  2  0             10481.1953  -0.0010  0.010
  8:  3  1  2    2  1  1             10614.6259  -0.0018  0.010
  9:  4  1  4    3  1  3             13736.5388   0.0130  0.010
 10/  4  0  4    3  0  3             13906.2416   0.0316  0.010
 11:  4  2  3    3  2  2             13947.2820  -0.0114  0.010
 12:  4  3  2    3  3  1             13959.3061   0.0039  0.010
 13:  4  3  1    3  3  0             13960.0713   0.0210  0.010
 14:  4  2  2    3  2  1             13992.0602  -0.0090  0.010
15:  4  1  3    3  1  2             14147.2335   0.0086  0.010
 16:  5  1  5    4  1  4             17162.9131  -0.0180  0.010
17:  5  0  5    4  0  4             17350.6456   0.0150  0.010
 18/  5  2  4    4  2  3             17428.3805  -0.0308  0.010
19:  5  3  3    4  3  2             17452.5122   0.0019  0.010
 20:  5  3  2    4  3  1             17455.1171  -0.0044  0.010
21:  5  2  3    4  2  2             17516.4748   0.0275  0.010
 22:  5  1  4    4  1  3             17674.6145  -0.0141  0.010
-------------------------------------------------------------------------------
PARAMETERS IN FIT (values truncated and Nlines statistics):

      10000         A  /MHz       3494.65(16)                1
      20000         B  /MHz       1795.3127(12)              2
      30000         C  /MHz       1692.4509(12)              3
        200        DJ  /kHz        0.258(21)                 4
       1100        DJK /kHz         5.32(10)                 5
```

MICROWAVE AVG = -0.000504 MHz, IR AVG = 0.00000

MICROWAVE RMS = 0.015180 MHz, IR RMS = 0.00000

END OF ITERATION 1 OLD, NEW RMS ERROR= 1.51802 1.51802

distinct frequency lines in fit: 22

distinct parameters of fit: 5

upper state lower state

overall limits of quantum number 1: 2 5 1 4 1 5 limits of quantum number 2: 0 3 0 3 0 3 limits of quantum number 3: 1 5 0 4 0 5

frequency range: 6872 17674

PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:

(values rounded and degrees of freedom, Ndegf=Nlines-Nconst, statistics)

10000	A /MHz	3494.65(29)	1
20000	B /MHz	1795.3127(22)	2
30000	C /MHz	1692.4510(22)	3
200	DJ /kHz	0.258(37)	4
1100	DJK /kHz	5.32(17)	5

CORRELATION COEFFICIENTS, C.ij:

	A	B	C	-DJ	-DJK
1.0000					
0.2196	1.0000				
-0.3381	-0.1109	1.0000			
-DJ	-0.1561	-0.5635	-0.5699	1.0000	
-DJK	0.5035	-0.1318	-0.1142	-0.2625	1.0000

Mean value of |C.ij|, i.ne.j = 0.2970

Mean value of C.ij, i.ne.j = -0.1524

No correlations with absolute value greater than 0.9950

Worst fitted lines (obs-calc/error):

10: 3.2	18: -3.1	21: 2.8	6: -2.2
13: 2.1	16: -1.8	17: 1.5	22: -1.4
9: 1.3	11: -1.1	14: -0.9	15: 0.9
2: -0.8	1: -0.7	3: -0.6	20: -0.4
12: 0.4	19: 0.2	8: -0.2	5: 0.1
7: -0.1	4: -0.1		

10/ 4 0 4	3 0 3	13906.2416	0.0316 0.010
18/ 5 2 4	4 2 3	17428.3805	-0.0308 0.010
21: 5 2 3	4 2 2	17516.4748	0.0275 0.010
6: 3 2 2	2 2 1	10463.1129	-0.0225 0.010

13: 4 3 1 3 3 0 13960.0713 0.0210 0.010

16: 5 1 5 4 1 4 17162.9131 -0.0180

0.010 17: 5 0 5 4 0 4 17350.6456

0.0150 0.010

22: 5 1 4 4 1 3 17674.6145 -0.0141 0.010

9: 4 1 4 3 1 3 13736.5388 0.0130 0.010

11: 4 2 3 3 2 2 13947.2820 -0.0114 0.010

_____

_____/ SPFIT output reformatted with PIFORM

11dfscp3ene 1&2 Carbon-13

---

		obs	o-c	error	blends	Notes	o-c	wt
	/ instead of : below denotes (o-c)>3*err							
1:	2 1 2 1 1 1	6817.4411	-0.0080	0.010				
2:	2 0 2 1 0 1	6905.7642	-0.0020	0.010				
3:	2 1 1 1 1 0	7001.0493	0.0115	0.010				
4:	3 1 3 2 1 2	10224.0152	-0.0017	0.010				
5:	3 0 3 2 0 2	10349.9358	0.0078	0.010				
6:	3 2 2 2 2 1	10363.7596	-0.0032	0.010				
7:	3 2 1 2 2 0	10377.7232	0.0034	0.010				
8:	4 1 4 3 1 3	13628.0931	-0.0184	0.010				
9:	4 0 4 3 0 3	13783.8285	0.0108	0.010				
10:	4 2 3 3 2 2	13815.5901	-0.0186	0.010				
11:	4 3 2 3 3 1	13824.8574	-0.0214	0.010				
12:	4 3 1 3 3 0	13825.3949	0.0163	0.010				
13:	4 2 2 3 2 1	13850.2917	0.0095	0.010				
14:	4 1 3 3 1 2	13994.8006	0.0115	0.010				
15:	5 1 5 4 1 4	17029.1166	0.0217	0.010				
16:	5 0 5 4 0 4	17204.6058	-0.0070	0.010				
17:	5 2 4 4 2 3	17265.0912	-0.0168	0.010				
18:	5 4 1 4 4 0	17280.0412	-0.0142	0.010				
19:	5 3 3 4 3 2	17283.8167	0.0203	0.010				
20:	5 3 2 4 3 1	17285.5681	0.0258	0.010				
21:	5 2 3 4 2 2	17333.5501	-0.0152	0.010				

22: 5 1 4 4 1 3 17486.3099 -0.0108 0.010

PARAMETERS IN FIT (values truncated and Nlines statistics):

10000	A /MHz	3533.34(20)	1
20000	B /MHz	1773.2145(14)	2
30000	C /MHz	1681.4202(12)	3
200	DJ /kHz	0.181(22)	4
1100	DJK /kHz	5.082(69)	5

MICROWAVE AVG = 0.000063 MHz, IR AVG = 0.00000

MICROWAVE RMS = 0.014271 MHz, IR RMS = 0.00000

END OF ITERATION 1 OLD, NEW RMS ERROR= 1.42713 1.42713

distinct frequency lines in fit: 22

distinct parameters of fit: 5

upper state lower state

overall limits of quantum number 1: 2 5 1 4 1 5 limits of quantum number 2: 0 4 0 4 0 4 limits of quantum number 3: 1 5 0 4 0 5

frequency range: 6817 17486

PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:
(values rounded and degrees of freedom, Ndegf=Nlines-Nconst, statistics)

10000		A /MHz	3533.34(33)	1
20000		B /MHz	1773.2146(22)	2
30000		C /MHz	1681.4202(20)	3
	200	DJ /kHz	0.181(36)	
4	1100	DJK /kHz	5.08(11)	
		5		

CORRELATION COEFFICIENTS, C.ij:

	A	B	C	-DJ	-DJK
1.0000					
0.2714	1.0000				
-0.2826	-0.1350	1.0000			
-DJ	-0.1734	-0.6098	-0.5574	1.0000	
-DJK	0.4238	-0.0484	-0.0161	-0.3158	1.0000

Mean value of |C.ij|, i.ne.j = 0.2834
Mean value of C.ij, i.ne.j = -0.1443

No correlations with absolute value greater than 0.9950

Worst fitted lines (obs-calc/error):

20: 2.6 15: 2.2 11: -2.1 19: 2.0

10: -1.9 8: -1.8 17: -1.7 12: 1.6

21: -1.5 18: -1.4 14: 1.1 3: 1.1

22: -1.1 9: 1.1 13: 0.9 1: -0.8

5: 0.8 16: -0.7 7: 0.3 6: -0.3

2: -0.2 4: -0.2

20: 5 3 2 4 3 1 17285.5681 0.0258 0.010 15: 5 1 5 4 1 4 17029.1166 0.0217 0.010

11: 4 3 2 3 3 1 13824.8574 -0.0214 0.010 19: 5 3 3 4 3 2 17283.8167 0.0203 0.010

10: 4 2 3 3 2 2 13815.5901 -0.0186 0.010

8: 4 1 4 3 1 3 13628.0931 -0.0184 0.010

17: 5 2 4 4 2 3 17265.0912 -0.0168 0.010 12: 4 3 1 3 3 0 13825.3949 0.0163 0.010

21: 5 2 3 4 2 2 17333.5501 -0.0152 0.010

18: 5 4 1 4 4 0 17280.0412 -0.0142 0.010

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_____/ SPFIT output reformatted with PIFORM

3SiCP Parent

```
-------------------------------------------------------------------------------=========
                                  obs          o-c      error      blends
Notes                                                      o-c      wt
   / instead of : below denotes (o-c)>3*err
-------------------------------------------------------------------------------=========
  1:  1  0  1  0    0  0  0  0          7286.7327  -0.0038  0.010
  2:  7  4  3  0    7  4  4  0          8010.9727   0.0095  0.010
  3:  4  2  2  0    4  2  3  0          8294.1383   0.0047  0.010
  4:  2  2  1  0    2  0  2  0         10164.4008   0.0147  0.010
  5/  3  1  2  0    3  1  3  0           10370.5351  -0.0781  0.010
6:  3  1  2  1    3  1  3  1          10370.6312   0.0090  0.010
  7:  6  3  3  1    6  3  4  1         11284.8654  -0.0026  0.010
  8:  6  3  3  0    6  3  4  0         11285.1515   0.0250  0.010
  9:  2  1  2  0    1  1  1  0         12783.6925   0.0086  0.010
 10:  3  2  2  0    3  0  3  0          12933.9109   0.0049  0.010
 11: 11  6  5  1   11  6  6  1           12958.0310   0.0000  0.010
 12: 11  6  5  0   11  6  6  0           12960.3195   0.0038  0.010
 13:  2  0  2  0    1  0  1  0          13627.9828  -0.0257  0.010
 14:  2  0  2  1    1  0  1  1          13628.0354   0.0206  0.010
 15:  5  2  3  0    5  2  4  0          14043.8868   0.0272  0.010
 16:  8  4  4  1    8  4  5  1          14370.0898   0.0013  0.010
 17/  8  4  4  0    8  4  5  0          14370.7425  -0.0334  0.010
 18:  3  3  1  0    3  1  2  0          14425.1058  -0.0089  0.010
 19:  4  3  2  0    4  1  3  0          15018.8384   0.0035  0.010
 20:  4  1  3  0    4  1  4  0          15832.9268   0.0204  0.010
 21/  2  1  1  0    1  1  0  0          16363.1866  -0.0370  0.010
```

22/ 2 1 1 1 1 1 0 1 16363.2638 0.0356 0.010

23: 4 2 3 0 4 0 4 0 16842.6227 0.0050 0.010 -0.0177 0.50

24: 4 2 3 1 4 0 4 1 16842.6227 -0.0404 0.010 -0.0177 0.50

25: 5 3 3 0 5 1 4 0 17475.7920 0.0097 0.010

26: 7 3 4 0 7 3 5 0 17703.8579 0.0031 0.010

27: 5 1 4 0 4 3 1 0 17981.2284 -0.0001 0.010

PARAMETERS IN FIT (values truncated and Nlines statistics):

10099	A / /MHz	5948.1093(16)	1
20099	B / /MHz	4538.2601(14)	2
30099	C / /MHz	2748.4792(14)	3
299	DJ / /kHz	0.712(39)	4
2099	DK / /kHz	1.182(90)	5
40199	d1 / /kHz	-0.340(13)	6
50099	d2 / /kHz	-0.1114(77)	7
11	E1 / /MHz	131812.(134)	8
210001	Fbc / /MHz	6.060(53)	9

MICROWAVE AVG = -0.000206 MHz, IR AVG = 0.00000

MICROWAVE RMS = 0.023051 MHz, IR RMS = 0.00000

END OF ITERATION 1 OLD, NEW RMS ERROR= 2.30512 2.30512

distinct frequency lines in fit: 26

distinct parameters of fit: 9

MICROWAVE lines fitted lines lines RMS RMS ERROR J range Ka range freq. range total dv=0 dv.ne.0 UNFITTD e>900

v"= 0 20 20 0 0 0 0.024484 2.44841 0 11 0 6 7287 17981 v"= 1 6 6 0 0 0 0.017230 1.72297 1 11 0 6 10371 16363

-----total: 26 26 0 0 0 0.023014 2.30139

NOTE: the RMS values above are for Nlines statistics, but the 'total' values may differ slightly from those in the .FIT file since the o-c values for this evaluation are as rounded in the .FIT.

PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:
(values rounded and degrees of freedom, Ndegf=Nlines-Nconst, statistics)

10099	A / /MHz	5948.1093(47)	1
20099	B / /MHz	4538.2601(39)	2
30099	C / /MHz	2748.4793(41)	3
299	DJ / /kHz	0.71(11)	4
2099	DK / /kHz	1.18(25)	5
40199	d1 / /kHz	-0.340(38)	6
50099	d2 / /kHz	-0.111(21)	7
11	E1 / /MHz	131812.(381)	8

210001 Fbc / /MHz 6.06(15) 9

--- Worst fitted constants, with greater than 20% uncertainty: %

2099 DK / /kHz 1.18(25) 5 21.7

CORRELATION COEFFICIENTS, C.ij:

A / B / C / -DJ / -DK / d1 / d2 / E1 /

1.0000
0.8145 1.0000
0.5750 0.6865 1.0000
-DJ / -0.4719 -0.5909 -0.8317 1.0000 -DK / -0.4090
-0.1983 0.1696 0.0120 1.0000 d1 / -0.1765 -0.2867
0.3925 -0.3586 0.1613 1.0000 d2 / 0.1028 0.2035 -
0.3216 0.3508 0.1276 -0.9395 1.0000
E1 / -0.2297 0.0075 -0.0447 0.1271 0.3824 -0.0880 0.0557 1.0000
Fbc / -0.2090 0.0017 -0.0414 0.1295 0.3358 -0.0765 0.0401 0.9420

Fbc /

Fbc / 1.0000

Mean value of |C.ij|, i.ne.j = 0.3025
Mean value of C.ij, i.ne.j = 0.0095

No correlations with absolute value greater than 0.9950

Worst fitted lines (obs-calc/error):

5: -7.8	21: -3.7	22: 3.6	17: -3.3
15: 2.7	13: -2.6	8: 2.5	14: 2.1
20: 2.0	23: -1.8	4: 1.5	25: 1.0
2: 0.9	6: 0.9	18: -0.9	9: 0.9
10: 0.5	3: 0.5	1: -0.4	12: 0.4
19: 0.3	26: 0.3	7: -0.3	16: 0.1
27: 0.0	24: 0.0	11: 0.0	

5/ 3 1 2 0 3 1 3 0 10370.5351 -0.0781 0.010

21/ 2 1 1 0 1 1 0 0 16363.1866 -0.0370 0.010

22/ 2 1 1 1 1 1 0 1 16363.2638 0.0356 0.010

17/ 8 4 4 0 8 4 5 0 14370.7425 -0.0334 0.010

15: 5 2 3 0 5 2 4 0 14043.8868 0.0272 0.010

13: 2 0 2 0 1 0 1 0 13627.9828 -0.0257 0.010

8: 6 3 3 0 6 3 4 0 11285.1515 0.0250 0.010

14: 2 0 2 1 1 0 1 1 13628.0354 0.0206 0.010

20: 4 1 3 0 4 1 4 0 15832.9268 0.0204 0.010

23: 4 2 3 0 4 0 4 0 16842.6227 0.0050 0.010 -0.0177 0.50

_____

_____/ SPFIT output reformatted with PIFORM 3SiCP 29Si

```
-------------------------------------------------------------------------------=========
                                  obs          o-c       error      blends
Notes                                                      o-c      wt
   / instead of : below denotes (o-c)>3*err
-------------------------------------------------------------------------------=========
  1:  1  0  1    0  0  0              7226.5573  -0.0098  0.010
  2:  2  1  2    1  1  1             12660.6888   0.0024  0.010
  3:  2  0  2    1  0  1             13515.1930   0.0000  0.010
  4:  2  1  1    1  1  0             16245.5505   0.0024  0.010
-------------------------------------------------------------------------

PARAMETERS IN FIT (values truncated and Nlines statistics):

      10000        A  /  /MHz        5947.901(40)                  1
      20000        B  /  /MHz        4509.5060(39)                 2
      30000        C  /  /MHz        2717.0640(39)                 3
        200       DJ /  /kHz         [ 0.707924819]                4
       2000       DK /  /kHz         [ 1.136789663]                5
      40100       d1 /  /kHz         [-0.348099707]                6
      50000       d2 /  /kHz         [-0.105283752]                7

 MICROWAVE AVG =       -0.001225 MHz, IR AVG =        0.00000
 MICROWAVE RMS =          0.005198 MHz, IR RMS =          0.00000
END OF ITERATION   1 OLD, NEW RMS ERROR=          0.51975
0.51975

  distinct frequency lines in fit:     4
distinct parameters of fit:     3
```

upper state lower state overall

limits of quantum number 1: 1

2 0 1 0 2 limits of

quantum number 2: 0 1 0

1 0 1 limits of quantum

number 3: 1 2 0 1

0 2

frequency range: 7226 16245

PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:

(values rounded and degrees of freedom, Ndegf=Nlines-Nconst, statistics)

10000	A / /MHz	5947.901(41)	1
20000	B / /MHz	4509.5060(40)	2
30000	C / /MHz	2717.0640(40)	3
200	DJ / /kHz	[0.707924819]	4
2000	DK / /kHz	[1.136789663]	5
40100	d1 / /kHz	[-0.348099707]	6
50000	d2 / /kHz	[-0.105283752]	7

CORRELATION COEFFICIENTS, C.ij:

A / B / C /

1.0000

0.2606 1.0000

-0.6454 -0.6364 1.0000

Mean value of |C.ij|, i.ne.j = 0.5142

Mean value of C.ij, i.ne.j = -0.3404

No correlations with absolute value greater than 0.9950

Worst fitted lines (obs-calc/error):

1: -1.0 4: 0.2 2: 0.2 3: 0.0

1:	1 0 1 0 0 0	7226.5573	-0.0098	0.010
4:	2 1 1 1 1 0	16245.5505	0.0024	0.010
2:	2 1 2 1 1 1	12660.6888	0.0024	0.010
3:	2 0 2 1 0 1	13515.1930	0.0000	0.010

_____

_____/ SPFIT output reformatted with PIFORM

3SiCP 30Si

---

	obs	o-c	error	blends
Notes			o-c	wt

/ instead of : below denotes (o-c)>3*err

1:	1 0 1 0 0 0	7155.0931	0.0206	0.010
2:	2 1 2 1 1 1	12543.2359	-0.0079	0.010
3:	2 0 2 1 0 1	13408.4800	-0.0206	0.010

4: 3 0 3 2 0 2 18783.6626 0.0122 0.010

PARAMETERS IN FIT (values truncated and Nlines statistics):

10000 A / /MHz 5949.015(41) 1

20000 B / /MHz 4460.985(11) 2
30000 C / /MHz 2694.0901(55) 3
200 DJ / /kHz [0.707924819] 4
2000 DK / /kHz [1.136789663] 5
40100 d1 / /kHz [-0.348099707] 6
50000 d2 / /kHz [-0.105283752] 7

MICROWAVE AVG = 0.001061 MHz, IR AVG = 0.00000
MICROWAVE RMS = 0.016347 MHz, IR RMS = 0.00000
END OF ITERATION 1 OLD, NEW RMS ERROR= 1.63472 1.63472

distinct frequency lines in fit: 4
distinct parameters of fit: 3

upper state lower state
overall limits of quantum number 1: 1 3 0 2 0 3 limits of quantum number 2: 0 1 0 1 0 1 limits of quantum number 3: 1 3 0 2 0 3

frequency range: 7155 18783

PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:
(values rounded and degrees of freedom, Ndegf=Nlines-Nconst, statistics)

10000	A / /MHz	5949.02(13)	1
20000	B / /MHz	4460.985(37)	2
30000	C / /MHz	2694.090(17)	3
200	DJ / /kHz	[0.707924819]	4
2000	DK / /kHz	[1.136789663]	5
40100	d1 / /kHz	[-0.348099707]	6
50000	d2 / /kHz	[-0.105283752]	7

CORRELATION COEFFICIENTS, C.ij:

A /	B /	C /
1.0000		
0.6085	1.0000	
-0.8952	-0.8220	1.0000

Mean value of |C.ij|, i.ne.j = 0.7752
Mean value of C.ij, i.ne.j = -0.3696

No correlations with absolute value greater than 0.9950

Worst fitted lines (obs-calc/error):

1: 2.1 3: -2.1 4: 1.2 2: -0.8

1: 1 0 1 0 0 0 7155.0931 0.0206 0.010
3: 2 0 2 1 0 1 13408.4800 -0.0206
0.010 4: 3 0 3 2 0 2 18783.6626
0.0122 0.010
2: 2 1 2 1 1 1 12543.2359 -0.0079 0.010

_____

_____/ SPFIT output reformatted with PIFORM 3SiCPF2 Durig and Laane v0

---

obs o-c error blends
Notes o-c wt
/ instead of : below denotes (o-c)>3*err

1/ 8 0 8 7 0 7 27774.3400 0.2597 0.050
2/ 8 1 8 7 1 7 27607.1200 0.3499 0.050
3: 8 2 7 7 2 6 27991.7800 0.1023 0.050
4/ 8 2 6 7 2 5 28252.1000 0.5245 0.050
5/ 8 1 7 7 1 6 28320.8900 0.3860 0.050
6/ 9 1 9 8 1 8 31042.2200 0.3534 0.050
7/ 9 0 9 8 0 8 31189.5700 0.2126 0.050
8: 9 2 8 8 2 7 31475.9300 -0.0194 0.050
9/ 9 3 7 8 3 6 31579.2200 -0.4290 0.050
10/ 9 3 6 8 3 5 31617.1400 -0.1922 0.050
11/ 9 2 7 8 2 6 31824.8200 0.7012 0.050

12/ 9 1 8 8 1 7 31830.9600 0.3897 0.050

13: 10 1 10 9 1 9 34473.2900 0.1354 0.050

14: 10 0 10 9 0 9 34597.3700 -0.0332 0.050

15/ 10 2 9 9 2 8 34954.9600 -0.2884 0.050

16/ 10 3 8 9 3 7 35091.9200 -0.4296 0.050

17/ 10 3 7 9 3 6 35155.3700 -0.2941 0.050

18: 11 1 11 10 1 10 37900.9800 0.0311 0.050

19/ 11 0 11 10 0 10 38001.4400 -0.2007 0.050

20/ 11 2 10 10 2 9 38428.6800 -0.5193 0.050

21/ 11 3 8 10 3 7 38703.8600 -0.3313 0.050

22/ 11 1 10 10 1 9 38810.6400 -0.1632 0.050

PARAMETERS IN FIT (values truncated):

10000	A /MHz	3546.08(19)	1
20000	B /MHz	1798.0697(20)	2
30000	C /MHz	1706.2465(18)	3

MICROWAVE AVG = 0.024792 MHz, IR AVG = 0.00000

MICROWAVE RMS = 0.335823 MHz, IR RMS = 0.00000

END OF ITERATION 1 OLD, NEW RMS ERROR= 6.71645 6.71645

distinct frequency lines in fit: 22

distinct parameters of fit: 3

upper state lower state overall

limits of quantum number 1: 8 11 7 10 7 11 limits of quantum number 2: 0 3 0 3 0 3 limits of quantum number 3: 6 11 5 10 5 11

frequency range: 27607 38810

Standard errors are obtained by muliplying the previous errors by: 7.227271

PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED: (values rounded)

10000	A /MHz	3546.1(14)	1
20000	B /MHz	1798.070(14)	2
30000	C /MHz	1706.247(13)	3

CORRELATION COEFFICIENTS, C.ij:

A B C

1.0000

0.6185 1.0000

-0.7793 -0.7991 1.0000

Mean value of |C.ij|, i.ne.j = 0.7323

Mean value of C.ij, i.ne.j = -0.3199

No correlations with absolute value greater than 0.9950 Worst fitted lines (obs-calc/error):

11: 14.0 4: 10.5 20: -10.4 16: -8.6

9: -8.6 12: 7.8 5: 7.7 6: 7.1

2: 7.0 21: -6.6 17: -5.9 15: -5.8

1: 5.2 7: 4.3 19: -4.0 10: -3.8

22: -3.3 13: 2.7 3: 2.0 14: -0.7

18: 0.6 8: -0.4

11/ 9 2 7 8 2 6 31824.8200 0.7012 0.050

4/ 8 2 6 7 2 5 28252.1000 0.5245 0.050

20/ 11 2 10 10 2 9 38428.6800 -0.5193 0.050

16/ 10 3 8 9 3 7 35091.9200 -0.4296 0.050

9/ 9 3 7 8 3 6 31579.2200 -0.4290 0.050

12/ 9 1 8 8 1 7 31830.9600 0.3897 0.050

5/ 8 1 7 7 1 6 28320.8900 0.3860 0.050

6/ 9 1 9 8 1 8 31042.2200 0.3534 0.050

2/ 8 1 8 7 1 7 27607.1200 0.3499 0.050

21/ 11 3 8 10 3 7 38703.8600 -0.3313 0.050

_____

_____/ SPFIT output reformatted with PIFORM

3SiCPF2 Durig and Laane v1

---

obs o-c error blends

Notes o-c wt

/ instead of : below denotes (o-c)>3*err

1/ 8 0 8 7 0 7 27885.8900 0.3057 0.050

2/ 8 1 8 7 1 7 27720.1000 0.2804 0.050

3: 9 1 9 8 1 8 31170.2400 0.1346 0.050

4/ 9 0 9 8 0 8 31317.9600 0.1927 0.050

5: 10 0 10 9 0 9 34742.4700 -0.0914 0.050

6: 10 1 10 9 1 9 34616.7900 0.0113 0.050

7/ 10 2 9 9 2 8 35077.9000 -0.1539 0.050

8/ 11 0 11 10 0 10 38162.9600 -0.2503 0.050

9/ 11 1 11 10 1 10 38059.8800 -0.2310 0.050

PARAMETERS IN FIT (values truncated):

10000	A /MHz	3543.57(40)	1
20000	B /MHz	1801.8784(81)	2
30000	C /MHz	1714.0210(30)	3

MICROWAVE AVG = 0.022026 MHz, IR AVG = 0.00000

MICROWAVE RMS = 0.204300 MHz, IR RMS = 0.00000

END OF ITERATION 1 OLD, NEW RMS ERROR= 4.08599 4.08599

distinct frequency lines in fit: 9

distinct parameters of fit: 3

upper state lower state overall

limits of quantum number 1: 8

11 7 10 7 11 limits

of quantum number 2: 0 2

0 2 0 2 limits of

quantum number 3: 8 11 7

10 7 11

frequency range: 27720 38162

Standard errors are obtained by muliplying the previous errors by: 5.004295

PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:
(values rounded)

10000 A /MHz 3543.6(20) 1
20000 B /MHz 1801.878(40) 2
30000 C /MHz 1714.021(15) 3

CORRELATION COEFFICIENTS, C.ij:

A B C

1.0000
0.2360 1.0000
-0.7995 -0.6690 1.0000

Mean value of |C.ij|, i.ne.j = 0.5682
Mean value of C.ij, i.ne.j = -0.4108
No correlations with absolute value greater than 0.9950
Worst fitted lines (obs-calc/error):
1: 6.1 2: 5.6 8: -5.0 9:
-4.6 4: 3.9 7: -3.1 3: 2.7
5: -1.8
6: 0.2

1/ 8 0 8 7 0 7 27885.8900 0.3057 0.050

2/ 8 1 8 7 1 7 27720.1000 0.2804 0.050

8/ 11 0 11 10 0 10 38162.9600 -0.2503 0.050

9/ 11 1 11 10 1 10 38059.8800 -0.2310 0.050

4/ 9 0 9 8 0 8 31317.9600 0.1927 0.050

7/ 10 2 9 9 2 8 35077.9000 -0.1539 0.050

3: 9 1 9 8 1 8 31170.2400 0.1346 0.050

5: 10 0 10 9 0 9 34742.4700 -0.0914 0.050

6: 10 1 10 9 1 9 34616.7900 0.0113 0.050

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_____/ SPFIT output reformatted with PIFORM

3SiCPF2 Durig and Laane v2

---

obs o-c error blends

Notes o-c wt

/ instead of : below denotes (o-c)>3*err

1/ 8 1 8 7 1 7 27814.1100 0.1774 0.050

2: 9 1 9 8 1 8 31276.9100 0.1004 0.050

3/ 9 0 9 8 0 8 31424.2100 -0.2435 0.050

4/ 10 0 10 9 0 9 34863.3500 0.2116 0.050

5: 10 1 10 9 1 9 34736.2100 -0.0216 0.050

6: 11 0 11 10 0 10 38297.4600 0.0332 0.050

7/ 11 1 11 10 1 10 38192.2200 -0.2179 0.050 ----------

PARAMETERS IN FIT (values truncated):

10000	A /MHz	3542.20(54)	1
20000	B /MHz	1805.187(43)	2
30000	C /MHz	1720.4696(89)	3

MICROWAVE AVG = 0.005666 MHz, IR AVG = 0.00000

MICROWAVE RMS = 0.166795 MHz, IR RMS = 0.00000

END OF ITERATION 1 OLD, NEW RMS ERROR= 3.33590 3.33590

distinct frequency lines in fit: 7

distinct parameters of fit: 3

	upper state	lower state	overall
limits of quantum number 1:	8 11	7 10	7 11
limits of quantum number 2:	0 1	0 1	0 1
limits of quantum number 3:	8 11	7 10	7 11

frequency range: 27814 38297

Standard errors are obtained by muliplying the previous errors by: 4.412981

PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED: (values rounded)

10000	A /MHz	3542.2(23)	1

20000 B /MHz 1805.19(18) 2

30000 C /MHz 1720.470(39) 3

CORRELATION COEFFICIENTS, C.ij:

A B C

1.0000

0.6421 1.0000

-0.7967 -0.9646 1.0000

Mean value of |C.ij|, i.ne.j = 0.8011

Mean value of C.ij, i.ne.j = -0.3731

No correlations with absolute value greater than 0.9950 Worst fitted lines (obs-calc/error):

3: -4.9 7: -4.4 4: 4.2 1: 3.5

2: 2.0 6: 0.7 5: -0.4

3/ 9 0 9 8 0 8 31424.2100 -0.2435 0.050

7/ 11 1 11 10 1 10 38192.2200 -0.2179 0.050

4/ 10 0 10 9 0 9 34863.3500 0.2116 0.050

1/ 8 1 8 7 1 7 27814.1100 0.1774 0.050

2: 9 1 9 8 1 8 31276.9100 0.1004 0.050

6: 11 0 11 10 0 10 38297.4600 0.0332 0.050

5: 10 1 10 9 1 9 34736.2100 -0.0216 0.050

_____

_____/ SPFIT output reformatted with PIFORM 3SiCPF2 Durig and Laane v3

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obs o-c error blends

Notes o-c wt

/ instead of : below denotes (o-c)>3*err

1: 8 1 8 7 1 7 27896.8500 -0.0098 0.050

2: 9 1 9 8 1 8 31370.9200 0.0250 0.050

3: 10 1 10 9 1 9 34841.5000 -0.0215 0.050

4: 11 1 11 10 1 10 38308.9100 0.0063 0.050

PARAMETERS IN FIT (values truncated):

10000	A /MHz	3830.(147)	1
20000	B /MHz	1811.7(17)	2
30000	C /MHz	1724.87(62)	3

MICROWAVE AVG = -0.000012 MHz, IR AVG = 0.00000

MICROWAVE RMS = 0.017535 MHz, IR RMS = 0.00000

END OF ITERATION 1 OLD, NEW RMS ERROR= 0.35071 0.35071

distinct frequency lines in fit: 4

distinct parameters of fit: 3

upper state lower state overall

limits of quantum number 1: 8 11 7 10 7 11 limits of quantum number 2: 1 1 1 1

1 1 limits of quantum number 3: 8 11 7 10

7 11 frequency range: 27896 38308

Standard errors are obtained by muliplying the previous errors by: 0.701420

PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:
(values rounded)

10000	A /MHz	3830.(103)	1
20000	B /MHz	1811.7(12)	2
30000	C /MHz	1724.87(43)	3

CORRELATION COEFFICIENTS, C.ij:

A	B	C
1.0000		
0.9991	1.0000	
-0.9998	-0.9998	1.0000

Mean value of |C.ij|, i.ne.j = 0.9996

Mean value of C.ij, i.ne.j = -0.3335

Worst correlations, with absolute value greater than 0.9950:

20000	B	<->	10000 A	0.999124
30000	C	<->	10000 A	-0.999756
30000	C	<->	20000 B	-0.999799

Worst fitted lines (obs-calc/error):

2: 0.5 3: -0.4 1: -0.2 4: 0.1

2: 9 1 9 8 1 8 31370.9200 0.0250 0.050

3: 10 1 10 9 1 9 34841.5000 -0.0215 0.050

1: 8 1 8 7 1 7 27896.8500 -0.0098 0.050

4: 11 1 11 10 1 10 38308.9100 0.0063 0.050

_____

_____/ SPFIT output reformatted with PIFORM

Holding Coriolis 3SiCPF2

---

obs o-c error blends

Notes o-c wt

/ instead of : below denotes (o-c)>3*err

1: 2 1 2 0 1 1 1 0 6917.0167 -0.0021 0.010

2: 2 1 2 1 1 1 1 1 6917.0190 -0.0007 0.010

3: 2 0 2 0 1 0 1 0 7005.3453 -0.0046 0.010

4: 2 0 2 1 1 0 1 1 7005.3468 -0.0055 0.010

5: 2 1 1 0 1 1 0 0 7100.6875 -0.0030 0.010

6: 3 2 2 0 3 0 3 0 7186.1321 -0.0171 0.010

7: 4 2 3 0 4 0 4 0 7218.1642 -0.0099 0.010

8: 5 2 4 0 5 0 5 0 7279.1347 0.0239 0.010

9: 2 1 2 0 1 1 1 0 6917.0151 -0.0037 0.010 -0.0042 0.50

10: 2 1 2 1 1 1 1 1 6917.0151 -0.0047 0.010 -0.0042 0.50

11: 2 0 2 0 1 0 1 0 7005.3482 -0.0017 0.010 -0.0030 0.50

12: 2 0 2 1 1 0 1 1 7005.3482 -0.0041 0.010 -0.0030 0.50

13: 2 1 1 0 1 1 0 0 7100.6825 -0.0080 0.010

14: 3 2 2 0 3 0 3 0 7186.1321 -0.0171 0.010

15: 4 2 3 0 4 0 4 0 7218.1618 -0.0123 0.010

16/ 5 2 4 0 5 0 5 0 7279.1432 0.0325 0.010

17: 3 1 3 0 2 1 2 0 10373.3425 -0.0089 0.010

18: 3 0 3 0 2 0 2 0 10499.2285 0.0011 0.010

19: 3 2 2 0 2 2 1 0 10513.1606 0.0005 0.010

20: 3 2 1 0 2 2 0 0 10527.2463 0.0019 0.010

21: 3 1 2 0 2 1 1 0 10648.7744 0.0003 0.010

22: 4 1 4 0 3 1 3 0 13827.1864 -0.0025 0.010 -0.0018 0.50

23: 4 1 4 1 3 1 3 1 13827.1864 -0.0011 0.010 -0.0018 0.50

24: 4 0 4 0 3 0 3 0 13982.7281 -0.0178 0.010

25: 4 2 3 0 3 2 2 0 14014.7855 0.0146 0.010

26: 4 3 2 0 3 3 1 0 14024.1248 -0.0077 0.010

27: 4 3 1 0 3 3 0 0 14024.6266 -0.0061 0.010

28: 4 2 2 0 3 2 1 0 14049.7693 0.0117 0.010 0.0124 0.50

29: 4 2 2 1 3 2 1 1 14049.7693 0.0131 0.010 0.0124 0.50

30: 4 1 3 1 3 1 2 1 14194.0110 -0.0030 0.010 -0.0076 0.50

31: 4 1 3 0 3 1 2 0 14194.0110 -0.0120 0.010 -0.0076 0.50

32: 5 1 5 0 4 1 4 0 17277.9158 0.0266 0.010 0.0273 0.50

33: 5 1 5 1 4 1 4 1 17277.9158 0.0279 0.010 0.0273 0.50

34: 5 0 5 0 4 0 4 0 17453.0393 -0.0294 0.010

35/ 5 0 5 1 4 0 4 1 17453.1552 0.0385 0.010

36: 5 2 4 0 4 2 3 0 17513.9781 -0.0272 0.010

37: 5 2 4 1 4 2 3 1 17514.0783 0.0286 0.010

38/ 5 4 2 1 4 4 1 1 17529.0060 -0.0301 0.010

39/ 5 4 2 0 4 4 1 0 17529.1118 0.0712 0.010

40/ 5 3 3 1 4 3 2 1 17532.8218 -0.0374 0.010

41: 5 3 3 0 4 3 2 0 17532.9140 0.0086 0.010

42/ 5 3 2 1 4 3 1 1 17534.5832 -0.0503 0.010

43: 5 3 2 0 4 3 1 0 17534.6821 0.0300 0.010

44: 5 2 3 0 4 2 2 0 17583.0556 -0.0125 0.010

45: 5 1 4 1 4 1 3 1 17735.2402 -0.0208 0.010

46/ 5 1 4 0 4 1 3 0 17735.3261 0.0361 0.010

47: 8 0 8 0 7 0 7 0 27774.3400 0.0013 0.050

48: 8 1 8 0 7 1 7 0 27607.1200 -0.0104 0.050

49: 8 2 7 0 7 2 6 0 27991.7800 0.1116 0.050

50: 8 2 6 0 7 2 5 0 28252.1000 0.0368 0.050

51: 8 1 7 0 7 1 6 0 28320.8900 0.0204 0.050

52: 9 1 9 0 8 1 8 0 31042.2200 0.0934 0.050

53: 9 0 9 0 8 0 8 0 31189.5700 0.0957 0.050

54/ 9 2 8 0 8 2 7 0 31475.9300 0.2142 0.050

55/ 9 3 7 0 8 3 6 0 31579.2200 -1.1108 0.050

56: 9 3 6 0 8 3 5 0 31617.1400 -0.0262 0.050

57/ 9 2 7 0 8 2 6 0 31824.8200 0.2603 0.050

58/ 9 1 8 0 8 1 7 0 31830.9600 0.1968 0.050

59: 10 1 10 0 9 1 9 0 34473.2900 0.0237 0.050

60: 10 0 10 0 9 0 9 0 34597.3700 0.0269 0.050

PARAMETERS IN FIT (values truncated):

10099	A /MHz	3544.4281(15)	1
20099	B /MHz	1798.13899(81)	2
30099	C /MHz	1706.30313(80)	3
299	DJ /kHz	0.1905(62)	4
1199	DJK /kHz	5.750(43)	5
210001	Fbc /MHz	[0.861530104]	6
11	E1 /MHz	[11805.724020849]	7

MICROWAVE AVG = -0.001555 MHz, IR AVG = 0.00000

MICROWAVE RMS = 0.163393 MHz, IR RMS = 0.00000

END OF ITERATION 1 OLD, NEW RMS ERROR= 3.79668 3.79668

distinct frequency lines in fit: 54

distinct parameters of fit: 5

MICROWAVE	lines fitted	lines	lines	RMS	RMS ERROR	J range	Ka range	freq. range
	total	dv=0	dv.ne.0	UNFITTD	e>900			
v"= 0	45	45	0	0	0	0.178496	3.94752	1 10 0 4 6917 34597
v"= 1	9	9	0	0	0	0.029165	2.91654	1 5 0 4 6917 17735
-----total:	54	54	0	0	0	0.163378	3.79519	

Standard errors are obtained by muliplying the previous errors by: 3.985684

PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED: (values rounded)

10099	A /MHz	3544.4281(60)	1
20099	B /MHz	1798.1390(32)	2
30099	C /MHz	1706.3031(31)	3
299	DJ /kHz	0.191(24)	4
1199	DJK /kHz	5.75(17)	5
210001	Fbc /MHz	[0.861530104]	6
11	E1 /MHz	[11805.724020849]	7

CORRELATION COEFFICIENTS, C.ij:

	A	B	C	-DJ	-DJK
1.0000					
0.1589	1.0000				
0.3843	-0.4718	1.0000			
-DJ	-0.2038	-0.2016	-0.5254	1.0000	
-DJK	-0.6255	-0.4547	-0.0023	-0.0729	1.0000

Mean value of |C.ij|, i.ne.j = 0.3101

Mean value of C.ij, i.ne.j = -0.2015

No correlations with absolute value greater than 0.9950

Worst fitted lines (obs-calc/error):

55: -22.2 39: 7.1 57: 5.2 42: -5.0

54: 4.3 58: 3.9 35: 3.9 40: -3.7

46: 3.6 16: 3.2 38: -3.0 43: 3.0

34: -2.9 37: 2.9 32: 2.7 36: -2.7

8: 2.4 49: 2.2 45: -2.1 53: 1.9

52: 1.9 24: -1.8 6: -1.7 14: -1.7

25: 1.5 44: -1.2 28: 1.2 15: -1.2

7: -1.0 17: -0.9 41: 0.9 13: -0.8

26: -0.8 30: -0.8 50: 0.7 27: -0.6

4: -0.5 60: 0.5 56: -0.5 59: 0.5

3: -0.5 9: -0.4 51: 0.4 5: -0.3

11: -0.3 1: -0.2 48: -0.2 20: 0.2

22: -0.2 18: 0.1

55/ 9 3 7 0 8 3 6 0 31579.2200 -1.1108 0.050

39/ 5 4 2 0 4 4 1 0 17529.1118 0.0712 0.010

57/ 9 2 7 0 8 2 6 0 31824.8200 0.2603 0.050

42/ 5 3 2 1 4 3 1 1 17534.5832 -0.0503 0.010

54/ 9 2 8 0 8 2 7 0 31475.9300 0.2142 0.050

58/ 9 1 8 0 8 1 7 0 31830.9600 0.1968 0.050

35/ 5 0 5 1 4 0 4 1 17453.1552 0.0385 0.010

40/ 5 3 3 1 4 3 2 1 17532.8218 -0.0374 0.010

46/ 5 1 4 0 4 1 3 0 17735.3261 0.0361 0.010

16/ 5 2 4 0 5 0 5 0 7279.1432 0.0325 0.010

---/ SPFIT output reformatted with PIFORM Adjusted Transitions

```
-------------------------------------------------------------------------------=========
                                  obs          o-c       error       blends
Notes                                                          o-c      wt
   / instead of : below denotes (o-c)>3*err
-------------------------------------------------------------------------------=========
  1:  2  1  2  0    1  1  1  0           6917.0167   0.0000  0.010
  2:  2  1  2  1    1  1  1  1           6917.0190   0.0012  0.010
  3:  2  0  2  0    1  0  1  0           7005.3453  -0.0003  0.010
  4:  2  0  2  1    1  0  1  1           7005.3468  -0.0013  0.010
5:  2  1  1  0    1  1  0  0           7100.6875   0.0025  0.010
  6:  3  2  2  0    3  0  3  0           7186.1321  -0.0059  0.010
  7:  4  2  3  0    4  0  4  0           7218.1642  -0.0069  0.010
  8:  5  2  4  0    5  0  5  0           7279.1347   0.0097  0.010
  9:  2  1  2  0    1  1  1  0           6917.0151  -0.0017  0.010  -0.0022 0.50
 10:  2  1  2  1    1  1  1  1           6917.0151  -0.0027  0.010  -0.0022 0.50
 11:  2  0  2  0    1  0  1  0           7005.3482   0.0024  0.010   0.0013 0.50
 12:  2  0  2  1    1  0  1  1           7005.3482   0.0000  0.010   0.0013 0.50
 13:  2  1  1  0    1  1  0  0           7100.6825  -0.0024  0.010
 14:  3  2  2  0    3  0  3  0           7186.1321  -0.0059  0.010
 15:  4  2  3  0    4  0  4  0           7218.1618  -0.0093  0.010
 16:  5  2  4  0    5  0  5  0           7279.1432   0.0182  0.010
 17:  3  1  3  0    2  1  2  0          10373.3425  -0.0077  0.010
 18:  3  0  3  0    2  0  2  0          10499.2285   0.0069  0.010
 19:  3  2  2  0    2  2  1  0          10513.1606   0.0034  0.010
 20:  3  2  1  0    2  2  0  0          10527.2463   0.0053  0.010
 21:  3  1  2  0    2  1  1  0          10648.7744   0.0068  0.010
 22:  4  1  4  0    3  1  3  0          13827.1864  -0.0040  0.010  -0.0034 0.50
 23:  4  1  4  1    3  1  3  1          13827.1864  -0.0027  0.010  -0.0034 0.50
```

24: 4 0 4 0 3 0 3 0 13982.7281 -0.0113 0.010

25: 4 2 3 0 3 2 2 0 14014.7855 0.0129 0.010

26: 4 3 2 0 3 3 1 0 14024.1248 -0.0055 0.010

27: 4 3 1 0 3 3 0 0 14024.6266 -0.0032 0.010

28: 4 2 2 0 3 2 1 0 14049.7693 0.0113 0.010 0.0120 0.50

29: 4 2 2 1 3 2 1 1 14049.7693 0.0126 0.010 0.0120 0.50

30: 4 1 3 1 3 1 2 1 14194.0110 0.0017 0.010 -0.0027 0.50

31: 4 1 3 0 3 1 2 0 14194.0110 -0.0071 0.010 -0.0027 0.50

32: 5 1 5 0 4 1 4 0 17277.9158 0.0199 0.010 0.0205 0.50

33: 5 1 5 1 4 1 4 1 17277.9158 0.0211 0.010 0.0205 0.50

34: 5 0 5 0 4 0 4 0 17453.0393 -0.0233 0.010

35/ 5 0 5 1 4 0 4 1 17453.1552 0.0446 0.010

36/ 5 2 4 0 4 2 3 0 17513.9781 -0.0383 0.010

37: 5 2 4 1 4 2 3 1 17514.0783 0.0175 0.010

38: 5 4 2 1 4 4 1 1 17529.0060 -0.0298 0.010

39/ 5 4 2 0 4 4 1 0 17529.1118 0.0715 0.010

40/ 5 3 3 1 4 3 2 1 17532.8218 -0.0428 0.010

41: 5 3 3 0 4 3 2 0 17532.9140 0.0034 0.010

42/ 5 3 2 1 4 3 1 1 17534.5832 -0.0533 0.010

43: 5 3 2 0 4 3 1 0 17534.6821 0.0271 0.010

44: 5 2 3 0 4 2 2 0 17583.0556 -0.0208 0.010

45: 5 1 4 1 4 1 3 1 17735.2402 -0.0213 0.010

46/ 5 1 4 0 4 1 3 0 17735.3261 0.0358 0.010

47: 8 0 8 0 7 0 7 0 27774.3400 -0.0052 0.050

48: 8 1 8 0 7 1 7 0 27607.1200 -0.0488 0.050

49: 8 2 7 0 7 2 6 0 27991.7800 0.0329 0.050

50: 8 2 6 0 7 2 5 0 28252.1000 -0.0296 0.050

```
 51:  8  1  7  0    7  1  6  0          28320.8900  -0.0327  0.050
 52:  9  1  9  0    8  1  8  0          31042.2200   0.0394  0.050
 53:  9  0  9  0    8  0  8  0          31189.5700   0.0790  0.050
 54:  9  2  8  0    8  2  7  0          31475.9300   0.0965  0.050
 55/  9  3  7  1    8  3  6  1          31579.2200  -0.2349  0.050
 56:  9  3  6  0    8  3  5  0          31617.1400  -0.0868  0.050
 57/  9  2  7  0    8  2  6  0          31824.8200   0.1590  0.050
 58:  9  1  8  0    8  1  7  0          31830.9600   0.1063  0.050
 59: 10  1 10  0    9  1  9  0           34473.2900  -0.0481  0.050
 60: 10  0 10  0    9  0  9  0           34597.3700  -0.0034  0.050
-------------------------------------------------------------------------------

PARAMETERS IN FIT (values truncated):

      10099          A  /MHz       3543.62(20)                1
      20099          B  /MHz       1798.13696(88)               2
      30099          C  /MHz       1706.30289(92)               3
        299         DJ  /kHz        0.1857(88)                4
       1199        DJK  /kHz          5.607(51)                5
       2099         DK  /kHz        -200.(50)                 6

     210001        Fbc  /MHz        [ 0.861530104]               7

         11         E1  /MHz      [11805.724020849]              8

 MICROWAVE AVG =        0.000486 MHz, IR AVG =        0.00000
```

MICROWAVE RMS = 0.051632 MHz, IR RMS = 0.00000

END OF ITERATION 1 OLD, NEW RMS ERROR= 2.13760 2.13760

distinct frequency lines in fit: 54

distinct parameters of fit: 6

MICROWAVE lines fitted

lines lines RMS RMS

ERROR J range Ka range freq.

range total dv=0 dv.ne.0

UNFITTD e>900 v"= 0 44

44 0 0 0 0.042724

1.78971 1 10 0 4 6917

34597 v"= 1 10 10 0

0 0 0.079686 3.24460 1

9 0 4 6917 31579

-----total: 54 54 0 0 0 0.051607 2.13528

Standard errors are obtained by muliplying the previous errors by: 2.267267

PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:

(values rounded)

10099	A /MHz	3543.62(45)	1
20099	B /MHz	1798.1370(19)	2
30099	C /MHz	1706.3029(20)	3
299	DJ /kHz	0.186(19)	4

1199	DJK /kHz	5.61(11)	5
2099	DK /kHz	-200.(113)	6
210001	Fbc /MHz	[0.861530104]	7
11	E1 /MHz	[11805.724020849]	8

--- Worst fitted constants, with greater than 20% uncertainty: %

2099	DK /kHz	-200.(113)	6	56.7

CORRELATION COEFFICIENTS, C.ij:

	A	B	C	-DJ	-DJK	-DK
1.0000						
0.3951	1.0000					
-0.4945	-0.5722	1.0000				
-DJ	0.7150	0.1528	-0.6742	1.0000		
-DJK	-0.5391	-0.5638	0.2643	-0.4262	1.0000	
-DK	-1.0000	-0.3940	0.4970	-0.7161	0.5351	1.0000

Mean value of |C.ij|, i.ne.j = 0.5293

Mean value of C.ij, i.ne.j = -0.1880

Worst correlations, with absolute value greater than 0.9950:

2099 -DK <-> 10099 A -0.999971

Worst fitted lines (obs-calc/error):

39: 7.1	42: -5.3	55: -4.7	35: 4.5
40: -4.3	36: -3.8	46: 3.6	57: 3.2
38: -3.0	43: 2.7	34: -2.3	45: -2.1
58: 2.1	44: -2.1	32: 2.1	54: 1.9
16: 1.8	37: 1.8	56: -1.7	53: 1.6
25: 1.3	28: 1.2	24: -1.1	48: -1.0
8: 1.0	59: -1.0	15: -0.9	52: 0.8
17: -0.8	7: -0.7	18: 0.7	21: 0.7
49: 0.7	51: -0.7	50: -0.6	6: -0.6
14: -0.6	26: -0.5	20: 0.5	41: 0.3
19: 0.3	22: -0.3	27: -0.3	30: -0.3
5: 0.2	13: -0.2	9: -0.2	4: -0.1
11: 0.1	2: 0.1		

39/ 5 4 2 0 4 4 1 0 17529.1118 0.0715 0.010

42/ 5 3 2 1 4 3 1 1 17534.5832 -0.0533 0.010

55/ 9 3 7 1 8 3 6 1 31579.2200 -0.2349 0.050

35/ 5 0 5 1 4 0 4 1 17453.1552 0.0446 0.010

40/ 5 3 3 1 4 3 2 1 17532.8218 -0.0428 0.010

36/ 5 2 4 0 4 2 3 0 17513.9781 -0.0383 0.010

46/ 5 1 4 0 4 1 3 0 17735.3261 0.0358 0.010

57/ 9 2 7 0 8 2 6 0 31824.8200 0.1590 0.050

38: 5 4 2 1 4 4 1 1 17529.0060 -0.0298 0.010

43: 5 3 2 0 4 3 1 0 17534.6821 0.0271 0.010

_____

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Fit Coriolis

---

obs o-c error blends

Notes o-c wt

/ instead of : below denotes (o-c)>3*err

1: 2 1 2 0 1 1 1 0 6917.0167 0.0029 0.010

2: 2 1 2 1 1 1 1 1 6917.0190 0.0044 0.010

3: 2 0 2 0 1 0 1 0 7005.3453 -0.0012 0.010

4: 2 0 2 1 1 0 1 1 7005.3468 -0.0017 0.010

5: 2 1 1 0 1 1 0 0 7100.6875 -0.0014 0.010

6: 3 2 2 0 3 0 3 0 7186.1321 -0.0106 0.010

7: 4 2 3 0 4 0 4 0 7218.1642 -0.0082 0.010

8: 5 2 4 0 5 0 5 0 7279.1347 0.0158 0.010

9: 2 1 2 0 1 1 1 0 6917.0151 0.0012 0.010 0.0008 0.50

10: 2 1 2 1 1 1 1 1 6917.0151 0.0004 0.010 0.0008 0.50

11: 2 0 2 0 1 0 1 0 7005.3482 0.0016 0.010 0.0007 0.50

12: 2 0 2 1 1 0 1 1 7005.3482 -0.0002 0.010 0.0007 0.50

13: 2 1 1 0 1 1 0 0 7100.6825 -0.0064 0.010

14: 3 2 2 0 3 0 3 0 7186.1321 -0.0106 0.010

15: 4 2 3 0 4 0 4 0 7218.1618 -0.0106 0.010

16: 5 2 4 0 5 0 5 0 7279.1432 0.0244 0.010

17: 3 1 3 0 2 1 2 0 10373.3425 -0.0031 0.010

18: 3 0 3 0 2 0 2 0 10499.2285 0.0048 0.010

19: 3 2 2 0 2 2 1 0 10513.1606 0.0024 0.010

20: 3 2 1 0 2 2 0 0 10527.2463 0.0050 0.010

21: 3 1 2 0 2 1 1 0 10648.7744 0.0009 0.010

22: 4 1 4 0 3 1 3 0 13827.1864 0.0021 0.010 0.0041 0.50

23: 4 1 4 1 3 1 3 1 13827.1864 0.0061 0.010 0.0041 0.50

24: 4 0 4 0 3 0 3 0 13982.7281 -0.0155 0.010

25: 4 2 3 0 3 2 2 0 14014.7855 0.0122 0.010

26: 4 3 2 0 3 3 1 0 14024.1248 -0.0106 0.010

27: 4 3 1 0 3 3 0 0 14024.6266 -0.0052 0.010

28: 4 2 2 0 3 2 1 0 14049.7693 0.0123 0.010 0.0130 0.50

29: 4 2 2 1 3 2 1 1 14049.7693 0.0136 0.010 0.0130 0.50

30: 4 1 3 1 3 1 2 1 14194.0110 0.0010 0.010 -0.0067 0.50

31: 4 1 3 0 3 1 2 0 14194.0110 -0.0145 0.010 -0.0067 0.50

32/ 5 1 5 0 4 1 4 0 17277.9158 0.0274 0.010 0.0303 0.50

33: 5 1 5 1 4 1 4 1 17277.9158 0.0331 0.010 0.0303 0.50

34/ 5 0 5 0 4 0 4 0 17453.0393 -0.0308 0.010 35/ 5 0 5 1 4 0 4 1 17453.1552 0.0474 0.010

36/ 5 2 4 0 4 2 3 0 17513.9781 -0.0384 0.010

37: 5 2 4 1 4 2 3 1 17514.0783 0.0277 0.010

38/ 5 4 2 1 4 4 1 1 17529.0060 -0.0313 0.010

39/ 5 4 2 0 4 4 1 0 17529.1118 0.0702 0.010

40/ 5 3 3 1 4 3 2 1 17532.8218 -0.0393 0.010

41: 5 3 3 0 4 3 2 0 17532.9140 -0.0102 0.010

42/ 5 3 2 1 4 3 1 1 17534.5832 -0.0524 0.010

43: 5 3 2 0 4 3 1 0 17534.6821 0.0262 0.010

44: 5 2 3 0 4 2 2 0 17583.0556 -0.0174 0.010

45: 5 1 4 1 4 1 3 1 17735.2402 -0.0094 0.010

46: 5 1 4 0 4 1 3 0 17735.3261 0.0278 0.010

47: 8 0 8 0 7 0 7 0 27774.3400 -0.0313 0.050

48: 8 1 8 0 7 1 7 0 27607.1200 -0.0429 0.050

49: 8 2 7 0 7 2 6 0 27991.7800 0.0311 0.050

50: 8 2 6 0 7 2 5 0 28252.1000 -0.0094 0.050

51: 8 1 7 0 7 1 6 0 28320.8900 -0.0319 0.050

52: 9 1 9 0 8 1 8 0 31042.2200 0.0405 0.050

53: 9 0 9 0 8 0 8 0 31189.5700 0.0433 0.050

54: 9 2 8 0 8 2 7 0 31475.9300 0.0860 0.050

55/ 9 3 7 1 8 3 6 1 31579.2200 -0.1770 0.050

56: 9 3 6 0 8 3 5 0 31617.1400 -0.0843 0.050

57/ 9 2 7 0 8 2 6 0 31824.8200 0.1897 0.050

58: 9 1 8 0 8 1 7 0 31830.9600 0.1162 0.050

59: 10 1 10 0 9 1 9 0 34473.2900 -0.0552 0.050

60: 10 0 10 0 9 0 9 0 34597.3700 -0.0509 0.050

PARAMETERS IN FIT (values truncated):

10099	A /MHz	3544.4249(16)	1
20099	B /MHz	1798.13881(85)	2
30099	C /MHz	1706.30123(83)	3
299	DJ /kHz	0.1645(67)	4
1199	DJK /kHz	5.760(47)	5

210001 Fbc /MHz 0.807(42) 6

11 E1 /MHz 12431.(159) 7

MICROWAVE AVG = 0.000437 MHz, IR AVG = 0.00000

MICROWAVE RMS = 0.049092 MHz, IR RMS = 0.00000

END OF ITERATION 1 OLD, NEW RMS ERROR= 2.15515 2.15515

distinct frequency lines in fit: 54

distinct parameters of fit: 7

MICROWAVE lines fitted lines lines RMS RMS ERROR J range Ka range freq. range total dv=0 dv.ne.0 UNFITTD e>900 v"= 0 44 44 0 0 0 0.045291 1.86718 1 10 0 4 6917 34597 v"= 1 10 10 0 0 0 0.063063 3.11339 1 9 0 4 6917 31579

-----total: 54 54 0 0 0 0.049070 2.15309

Standard errors are obtained by muliplying the previous errors by: 2.310072

PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED: (values rounded)

10099 A /MHz 3544.4249(38) 1

20099 B /MHz 1798.1388(19) 2

30099 C /MHz 1706.3012(19) 3

299 DJ /kHz 0.165(15) 4

1199 DJK /kHz 5.76(10) 5

210001 Fbc /MHz 0.807(97) 6

11 E1 /MHz 12431.(367) 7

CORRELATION COEFFICIENTS, C.ij:

A B C -DJ -DJK Fbc E1

1.0000
0.2086 1.0000
0.2316 -0.4895 1.0000
-DJ -0.0268 -0.1370 -0.5632 1.0000
-DJK -0.6158 -0.5149 0.0703 -0.1141 1.0000
Fbc 0.3874 0.1073 -0.2497 0.3759 -0.1335 1.0000
E1 -0.1294 0.1653 0.0525 -0.2046 -0.2388 -0.5549 1.0000

Mean value of |C.ij|, i.ne.j = 0.2653
Mean value of C.ij, i.ne.j = -0.1130

No correlations with absolute value greater than 0.9950
Worst fitted lines (obs-calc/error):

39: 7.0	42: -5.2	35: 4.7	40: -3.9
36: -3.8	57: 3.8	55: -3.5	38: -3.1
34: -3.1	32: 3.0	46: 2.8	37: 2.8
43: 2.6	16: 2.4	58: 2.3	44: -1.7
54: 1.7	56: -1.7	8: 1.6	24: -1.6

28: 1.3 25: 1.2 59: -1.1 6: -1.1

15: -1.1 14: -1.1 26: -1.1 41: -1.0

60: -1.0 45: -0.9 53: 0.9 48: -0.9

7: -0.8 52: 0.8 30: -0.7 13: -0.6

51: -0.6 47: -0.6 49: 0.6 27: -0.5

20: 0.5 18: 0.5 2: 0.4 22: 0.4

17: -0.3 1: 0.3 19: 0.2 50: -0.2

4: -0.2 5: -0.1

39/ 5 4 2 0 4 4 1 0 17529.1118 0.0702 0.010

42/ 5 3 2 1 4 3 1 1 17534.5832 -0.0524
0.010 35/ 5 0 5 1 4 0 4 1 17453.1552
0.0474 0.010

40/ 5 3 3 1 4 3 2 1 17532.8218 -0.0393 0.010

36/ 5 2 4 0 4 2 3 0 17513.9781 -0.0384
0.010 57/ 9 2 7 0 8 2 6 0 31824.8200
0.1897 0.050

55/ 9 3 7 1 8 3 6 1 31579.2200 -0.1770 0.050

38/ 5 4 2 1 4 4 1 1 17529.0060 -0.0313 0.010

34/ 5 0 5 0 4 0 4 0 17453.0393 -0.0308 0.010

32/ 5 1 5 0 4 1 4 0 17277.9158 0.0274 0.010 0.0303 0.50

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|                                                                      |
|   KRA  -  SINGLE ISOTOPIC SUBSTITUTION - Various permutations        |
|          of Kraitchman's equations for symmetric/asymmetric tops     |
|______________________________________________________________________|
```

version 27.XI.2013 Zbigniew KISIEL

11dfscp3ene

---

parent species

Planar calculation will be made from I.a and I.b

Si-29

----- The parent species:

X, Y, Z = 3544.42800000 1798.13910000
1706.30130000 eX, eY, eZ = 0.00350000 0.00230000
0.00250000 IX, IY, IZ = 142.58407986 281.05667965
296.18391840 eIX,eIY,eIZ = 0.00014080 0.00035950
0.00043396
PX, PY, PZ = 217.32825910 78.85565930 63.72842056

Mass = 120.02068630

The isotopic species:

X, Y, Z = 3543.45000000 1796.32400000 1704.67800000 eX, eY, eZ = 0.47000000 0.00360000 0.00360000 IX, IY, IZ = 142.62343338 281.34067407 296.46596307 eIX,eIY,eIZ = 0.01891744 0.00056383 0.00062609

PX, PY, PZ = 217.59160188 78.87436119 63.74907218

Mass change = 0.99956780

Total mass = 121.02025410

M DM/(M+DM) = 0.99131186

KRAITCHMAN RESULTS:

	a	b	
PLANAR:	0.53517 +- 0.00063	0.19945 +- 0.04794	
+Costain err.	0.53517 +- 0.00287	0.19945 +- 0.04853	

	a	b	c
NONPLANAR:	0.51534 +- 0.00927	0.13739 +- 0.03479	0.14455 +- 0.03315
+Costain err.	0.51534 +- 0.00971	0.13739 +- 0.03647	0.14455 +- 0.03474

R= 0.55258 +- 0.01571

DIX,DIY,DIZ = 0.03935352 0.28399441 0.28204468

DPX,DPY,DPZ = 0.26334278 0.01870189 0.02065163

IXY,IXZ,IYZ = -138.47259980 -153.59983854 -15.12723874

Si-30

----- The parent species:

X, Y, Z = 3544.42800000 1798.13910000 1706.30130000 eX, eY, eZ = 0.00350000 0.00230000 0.00250000 IX, IY, IZ = 142.58407986 281.05667965 296.18391840 eIX,eIY,eIZ = 0.00014080 0.00035950 0.00043396

PX, PY, PZ = 217.32825910 78.85565930 63.72842056

Mass = 120.02068630

The isotopic species:

X, Y, Z = 3544.41000000 1794.55290000 1703.07450000 eX, eY, eZ = 0.37000000 0.00250000 0.00240000 IX, IY, IZ = 142.58480396 281.61833792 296.74509541 eIX,eIY,eIZ = 0.01488439 0.00039232 0.00041818

PX, PY, PZ = 217.88931469 78.85578073 63.72902323

Mass change = 1.99684360

Total mass = 122.01752990

M DM/(M+DM) =

1.96416482

KRAITCHMAN RESULTS:

	a	b	
PLANAR:	0.53474 +- 0.00025	0.01924 +- 0.19775	
+Costain err.	0.53474 +- 0.00282	0.01924 +- 0.21256	

	a	b	c	
NONPLANAR:	0.53446 +- 0.00355	0.00788 +- 0.24179	0.01755 +- 0.10851	
+Costain err.	0.53446 +- 0.00453	0.00788 +- 0.30776	0.01755 +- 0.13814	

R= 0.53480 +- 0.00785

DIX,DIY,DIZ =	0.00072410	0.56165826	0.56117702
DPX,DPY,DPZ =	0.56105559	0.00012143	0.00060267
IXY,IXZ,IYZ =	-138.47259980	-153.59983854	-15.12723874

C-13 1/4

----- The parent species:

X, Y, Z = 3544.42800000 1798.13910000 1706.30130000 eX, eY, eZ = 0.00350000 0.00230000 0.00250000 IX, IY, IZ = 142.58407986 281.05667965 296.18391840 eIX,eIY,eIZ = 0.00014080 0.00035950 0.00043396

PX, PY, PZ = 217.32825910 78.85565930 63.72842056

Mass = 120.02068630

The isotopic species:

X, Y, Z = 3494.65000000 1795.31270000 1692.45100000 eX, eY, eZ = 0.29000000 0.00220000 0.00220000 IX, IY, IZ = 144.61505587 281.49915332 298.60776176 eIX,eIY,eIZ = 0.01200073 0.00034495 0.00038816

PX, PY, PZ = 217.74592961 80.86183215 63.75322372

Mass change = 1.00335484

Total mass = 121.02404114

M DM/(M+DM) = 0.99503648

KRAITCHMAN RESULTS:

	a	b
PLANAR:	0.66194 +- 0.00037	1.43095 +- 0.00423

+Costain err. 0.66194 +- 0.00230 1.43095 +- 0.00436

a b c

NONPLANAR: 0.64312 +- 0.00463 1.42090 +- 0.00215 0.16825 +- 0.02039
+Costain err. 0.64312 +- 0.00518 1.42090 +- 0.00239 0.16825 +- 0.02226

R= 1.56871 +- 0.00386

DIX,DIY,DIZ = 2.03097601 0.44247367 2.42384336
DPX,DPY,DPZ = 0.41767051 2.00617285 0.02480316
IXY,IXZ,IYZ = -138.47259980 -153.59983854 -15.12723874

C-13 2/3

The parent species:

X, Y, Z = 3544.42800000 1798.13910000
1706.30130000 eX, eY, eZ = 0.00350000 0.00230000
0.00250000 IX, IY, IZ = 142.58407986 281.05667965
296.18391840 eIX,eIY,eIZ = 0.00014080 0.00035950
0.00043396
PX, PY, PZ = 217.32825910 78.85565930 63.72842056

Mass = 120.02068630

The isotopic species:

X, Y, Z = 3533.34000000 1773.21460000 1681.42020000 eX, eY, eZ = 0.33000000 0.00220000 0.00200000 IX, IY, IZ = 143.03152400 285.00724334 300.56675006 eIX,eIY,eIZ = 0.01335858 0.00035360 0.00035752

PX, PY, PZ = 221.27123470 79.29551536 63.73600864

Mass change = 1.00335484

Total mass = 121.02404114

M DM/(M+DM) = 0.99503648

KRAITCHMAN RESULTS:

	a	b	
PLANAR:	1.98933 +- 0.00016	0.68008 +- 0.01015	
+Costain err.	1.98933 +- 0.00077	0.68008 +- 0.01039	
	a	b	c
NONPLANAR:	1.98743 +- 0.00169	0.67410 +- 0.00513	0.08972 +- 0.03955
+Costain err.	1.98743 +- 0.00185	0.67410 +- 0.00559	0.08972 +- 0.04294

R= 2.10055 +- 0.00311

DIX,DIY,DIZ = 0.44744414 3.95056369 4.38283166

DPX,DPY,DPZ = 3.94297561 0.43985606 0.00758808

IXY,IXZ,IYZ = -138.47259980 -153.59983854 -15.12723874

```
_____
|                                                       |
|     E V A L   -  Internals and their errors from Cartesians              |
|_____________________________________________________________________
_____|
```

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WARNING:

The EVAL uncertainties are evaluated by assuming that the correlation matrix is a unit matrix.

The EVAL uncertainties may thus differ significantly (but typically by not more than 30% either way) from uncertainties in explicitly fitted internals corresponding to the input Cartesians.

```
!    11dfscp3ene Si-29
!
```

INPUT CARTESIANS:

Si-29	0.51534	0.00971	0.13739	0.03647	0.14455	0.03474
C(1)	-1.98743	0.00185	0.67410	0.00559	-0.08972	0.04294
C(2)	-1.98743	0.00185	-0.67410	0.00559	-0.08972	0.04294
C(3)	-0.64312	0.00518	-1.42090	0.00239	0.16825	0.02226
C(4)	-0.64312	0.00518	1.42090	0.00239	0.16825	0.02226

CALCULATED INTERNALS:

!

! Bond Lengths

!

Si-29 C(3) = 1.94187 +- 0.03006

Si-29 C(4) = 1.72916 +- 0.02811

C(1) C(4) = 1.55930 +- 0.00974

C(1) C(2) = 1.34820 +- 0.00791

C(2) C(3) = 1.55930 +- 0.00974

!

! Bond Angles

!

C(3) Si-29 C(4) = 101.29202 +- 0.53388

Si-29 C(4) C(1) = 102.69831 +- 0.90228

C(4) C(1) C(2) = 118.61565 +- 0.65041

C(1) C(2) C(3) = 118.61565 +- 0.65038

C(2) C(3) Si-29 = 97.35222 +- 0.74091

!

! Dihedral Angles

!

Si-29 C(4) C(1) C(2) = 8.23438 +- 4.22980

C(4) C(1) C(2) C(3) = 0.00000 +- 5.41973

C(1) C(2) C(3) Si-29 = -7.20653 +- 4.02348

C(2) C(3) Si-29 C(4) = 10.63523 +- 2.52151

C(3) Si-29 C(4) C(1) = -10.81436 +- 2.57351

| |

| E V A L - Internals and their errors from Cartesians |

| |

version 19.VI.2017 Zbigniew KISIEL

WARNING:

The EVAL uncertainties are evaluated by assuming that the correlation matrix is a unit matrix.

The EVAL uncertainties may thus differ significantly (but typically by not more than 30% either way) from uncertainties in explicitly fitted internals corresponding to the input Cartesians.

! 11dfscp3ene Si-30

!

INPUT CARTESIANS:

Si-30	0.53446	0.00453	0.00788	0.30776	0.01755	0.13814
C(1)	-1.98743	0.00185	0.67410	0.00559	-0.08972	0.04294
C(2)	-1.98743	0.00185	-0.67410	0.00559	-0.08972	0.04294
C(3)	-0.64312	0.00518	-1.42090	0.00239	0.16825	0.02226
C(4)	-0.64312	0.00518	1.42090	0.00239	0.16825	0.02226

CALCULATED INTERNALS:

!

! Bond Lengths

!

Si-30 C(3) = 1.85764 +- 0.23706

Si-30 C(4) = 1.84554 +- 0.23592

C(1) C(4) = 1.55930 +- 0.00974

C(1) C(2) = 1.34820 +- 0.00791

C(2) C(3) = 1.55930 +- 0.00974

!

! Bond Angles

!

C(3) Si-30 C(4) = 100.24043 +- 0.88606

Si-30 C(4) C(1) = 99.78163 +- 5.96991

C(4) C(1) C(2) = 118.61565 +- 0.65041

C(1) C(2) C(3) = 118.61565 +- 0.65038

C(2) C(3) Si-30 = 99.48121 +- 5.88851

!

! Dihedral Angles

!

Si-30 C(4) C(1) C(2) = 11.73582 +- 6.07476

C(4) C(1) C(2) C(3) = 0.00000 +- 5.41973

C(1) C(2) C(3) Si-30 = -11.64782 +- 6.03921 C(2)

C(3) Si-30 C(4) = 16.10069 +- 6.13063

C(3) Si-30 C(4) C(1) = -16.11541 +- 6.13581

APPENDIX C.

SUPPORTING INFORMATION FOR THE ROTATIONAL SPECTRUM AND RING STRUCTURES OF SILACYCLOHEX-2-ENE AND 1,1-DIFLUOROSILACYCLOHEX-2-ENE

S1-S8: Transition measurements, quantum number assignments, obs-calc, blends, fits and standard errors for all measured isotopologues of silacyclohex-2-ene. Quantum number assignments reported are given in $J'_{Ka', Kc'} \leftarrow J''_{Ka'', Kc''}$ format as is needed for SPFIT.

S9-S16: Transition measurements, quantum number assignments, obs-calc, blends, fits and standard errors for all measured isotopologues of 1,1-difluorosilacyclohex-2-ene. Quantum number assignments reported are given in $J'_{Ka', Kc'} \leftarrow J''_{Ka'', Kc''}$ format as is needed for SPFIT.

S1. Silacyclohex-2-ene Parent

---
obs o-c error

/ instead of : below denotes (o-c)>3*err

1: 1 0 1 0 0 0 4920.0039 -0.0065 0.010
2: 4 2 2 4 2 3 5349.4915 -0.0039 0.010
3: 3 0 3 2 2 0 5691.9866 -0.0115 0.010
4: 3 3 0 3 2 1 5754.4319 -0.0061 0.010
5: 5 3 2 5 2 3 5830.3726 -0.0251 0.010
6: 4 2 2 4 1 3 6019.2006 -0.0013 0.010
7: 2 2 1 2 1 2 6297.4585 -0.0055 0.010
8: 2 2 1 2 0 2 6680.2483 -0.0119 0.010
9: 3 1 2 3 1 3 6732.6610 -0.0061 0.010
10: 6 4 2 6 3 3 6797.2532 0.0013 0.010
11: 3 1 2 3 0 3 6840.4552 -0.0027 0.010
12: 5 4 2 5 3 2 6935.7936 -0.0063 0.010
13: 1 1 0 0 0 0 7019.1643 -0.0043 0.010
14: 6 3 3 6 3 4 7244.6724 -0.0024 0.010
15: 5 4 1 5 3 2 7498.0199 -0.0072 0.010
16: 7 4 3 7 3 4 7617.2442 -0.0148 0.010
17: 3 3 1 3 2 2 7910.7956 0.0002 0.010
18: 7 5 3 7 4 3 8109.0405 -0.0017 0.010
19: 6 3 3 6 2 4 8136.1505 -0.0019 0.010
20: 11 6 5 11 6 6 8136.9983 -0.0165 0.010
21: 3 3 0 3 2 2 8142.1533 -0.0211 0.010
22: 2 0 2 1 1 1 8296.5389 -0.0012 0.010
23: 3 2 2 3 1 3 8355.2229 0.0033 0.010
24: 3 2 2 3 0 3 8463.0001 -0.0100 0.010

25: 2 1 2 1 1 1 8679.3326 -0.0038 0.010
26: 4 4 1 4 3 1 8715.0000 -0.0104 0.010
27: 4 4 0 4 3 1 8787.7399 -0.0051 0.010
28: 5 2 3 5 2 4 9089.3567 -0.0037 0.010
29: 7 5 2 7 4 3 9090.7494 0.0024 0.010
30: 4 3 2 4 2 3 9210.3372 -0.0215 0.010
31: 2 0 2 1 0 1 9235.0189 -0.0002 0.010
32: 5 2 3 5 1 4 9296.4554 -0.0145 0.010
33: 9 5 4 9 4 5 9400.4076 -0.0173 0.010
34: 3 3 1 3 1 2 9533.3451 -0.0025 0.010
35: 2 1 2 1 0 1 9617.8065 -0.0089 0.010
36: 13 7 6 13 7 7 9804.3752 -0.0108 0.010
37: 4 3 2 4 1 3 9880.0566 -0.0086 0.010
38: 10 6 4 10 5 5 9886.7086 -0.0205 0.010
39: 4 4 1 4 3 2 10022.3028 0.0104 0.010
40: 4 4 0 4 3 2 10095.0147 -0.0123 0.010
41: 8 4 4 8 3 5 10250.3115 0.0024 0.010
42: 4 1 3 4 1 4 10299.4171 -0.0057 0.010
43: 4 1 3 4 0 4 10324.3209 0.0049 0.010
44: 4 1 3 3 3 0 10364.5934 0.0047 0.010
45: 9 3 7 8 5 4 10548.8494 -0.0097 0.010
46: 9 6 3 9 5 4 10576.3376 0.0125 0.010
47: 5 4 2 5 3 3 10625.6245 -0.0055 0.010
48: 6 5 1 6 4 2 10667.7124 -0.0141 0.010
49: 7 1 7 6 2 5 10894.9625 -0.0274 0.010
50: 4 2 3 4 1 4 10969.1190 -0.0103 0.010
51: 4 2 3 4 0 4 10994.0263 0.0039 0.010
52: 2 1 1 1 1 0 11000.6802 -0.0088 0.010
53: 5 4 1 5 3 3 11187.8572 0.0000 0.010
54: 10 5 5 10 5 6 11189.7441 0.0015 0.010
55: 11 6 5 11 5 6 11197.9795 0.0099 0.010
56: 5 3 3 5 2 4 11229.9306 0.0025 0.010
57: 4 2 3 3 3 1 11265.6956 0.0212 0.010
58: 7 3 4 7 3 5 11427.7291 -0.0126 0.010
59: 5 3 3 5 1 4 11437.0374 0.0000 0.010
60: 8 1 8 7 2 6 11536.1575 0.0260 0.010
61: 7 3 4 7 2 5 11718.0670 0.0041 0.010
62: 6 4 3 6 3 4 11929.1653 0.0045 0.010
63: 5 5 1 5 4 1 11931.2764 0.0000 0.010
64: 5 5 0 5 4 1 11951.7645 0.0059 0.010
65: 6 1 5 5 3 2 12218.2780 -0.0012 0.010
66: 8 6 2 8 5 3 12376.3618 0.0027 0.010
67: 10 5 5 10 4 6 12378.7306 0.0037 0.010
68: 5 5 1 5 4 2 12493.5006 -0.0030 0.010
69: 5 5 0 5 4 2 12513.9865 0.0007 0.010
70: 3 1 2 2 2 0 12532.4525 -0.0036 0.010

71: 5 1 4 4 3 1 12563.6951 0.0028 0.010
72: 6 5 2 6 4 3 12579.5862 -0.0020 0.010
73: 3 0 3 2 1 2 12594.4518 -0.0031 0.010
74: 3 1 3 2 1 2 12702.2586 0.0130 0.010
75: 5 4 2 5 2 3 12766.2020 0.0044 0.010
76: 5 2 4 4 3 1 12770.7996 -0.0020 0.010
77: 6 4 3 6 2 4 12820.6510 0.0126 0.010
78: 6 2 4 6 2 5 12932.4648 -0.0012 0.010
79: 3 0 3 2 0 2 12977.2517 0.0006 0.010
80: 6 2 4 6 1 5 12986.0318 -0.0049 0.010
81: 3 1 3 2 0 2 13085.0507 0.0088 0.010
82: 2 1 1 1 0 1 13099.8538 0.0064 0.010
83: 3 1 2 2 2 1 13137.4388 -0.0099 0.010
84: 7 5 3 7 4 4 13188.7867 -0.0067 0.010
85: 12 6 6 12 6 7 13249.3492 0.0049 0.010
86: 5 1 4 5 1 5 13699.6657 -0.0060 0.010
87: 5 1 4 5 0 5 13704.8369 -0.0051 0.010
88: 9 4 5 9 4 6 13769.1437 -0.0100 0.010
89: 2 2 1 1 1 0 13816.1121 -0.0091 0.010
90: 6 3 4 6 2 5 13823.9315 -0.0123 0.010
91: 6 3 4 6 1 5 13877.5119 -0.0025 0.010
92: 4 4 1 4 2 2 13883.1541 -0.0015 0.010
93: 5 2 4 5 1 5 13906.7938 0.0126 0.010
94: 5 2 4 5 0 5 13911.9546 0.0031 0.010
95: 7 4 4 7 3 5 13965.2680 0.0184 0.010
96: 7 6 1 7 5 2 14034.6396 0.0079 0.010
97: 5 2 4 4 3 2 14078.0817 -0.0019 0.010
98: 7 4 4 7 2 5 14255.5669 -0.0038 0.010
99: 2 2 0 1 1 0 14421.1189 0.0051 0.010
100: 8 5 4 8 4 5 14527.0156 0.0063 0.010
101: 3 2 2 2 2 1 14760.0029 0.0019 0.010
102/ 5 3 2 5 2 4 14919.8259 0.0676 0.010
103: 7 6 2 7 5 3 14952.5653 -0.0038 0.010
104: 6 6 1 6 5 1 14969.6536 -0.0076 0.010
105: 6 6 0 6 5 1 14975.0567 0.0018 0.010
106: 2 2 1 1 1 1 14976.7966 -0.0038 0.010
107: 8 6 3 8 5 4 15015.3536 0.0052 0.010
108: 7 6 1 7 5 3 15016.3422 0.0058 0.010
109: 6 6 1 6 5 2 15170.5656 0.0002 0.010
110: 6 6 0 6 5 2 15175.9494 -0.0096 0.010
111: 5 3 3 4 4 0 15212.9883 0.0034 0.010
112: 14 7 7 14 7 8 15366.7718 0.0138 0.010
113: 8 6 2 8 5 4 15398.0648 0.0074 0.010
114: 12 8 4 12 7 5 15404.1712 -0.0169 0.010
115: 8 3 5 8 3 6 15518.0486 -0.0119 0.010
116: 2 2 0 1 1 1 15581.7926 -0.0005 0.010

117: 8 5 4 8 3 5 15588.4698 0.0012 0.010
118: 8 3 5 8 2 6 15598.5797 -0.0117 0.010
119: 7 5 3 7 3 4 15726.3061 0.0048 0.010
120: 9 7 2 9 6 3 15950.2116 0.0055 0.010
121: 3 1 2 2 1 1 15952.8706 -0.0102 0.010
122: 11 5 6 11 5 7 16123.0970 0.0047 0.010
123: 7 2 5 7 2 6 16469.0318 0.0133 0.010
124: 7 2 5 7 1 6 16481.4366 -0.0203 0.010
125: 2 2 0 1 0 1 16520.2666 -0.0054 0.010
126: 4 0 4 3 1 3 16537.6592 -0.0075 0.010
127: 3 2 1 2 2 0 16542.7301 -0.0147 0.010
128: 4 1 4 3 1 3 16562.5480 -0.0118 0.010
129: 8 4 5 8 3 6 16579.5425 0.0227 0.010
130: 9 5 5 9 4 6 16607.7500 0.0155 0.010
131: 4 2 2 3 3 1 16615.1959 0.0260 0.010
132: 4 0 4 3 0 3 16645.4335 -0.0239 0.010
133: 8 4 5 8 2 6 16660.0576 0.0067 0.010
134: 4 1 4 3 0 3 16670.3532 0.0026 0.010
135/ 7 3 5 7 2 6 16759.2936 -0.0460 0.010
136: 7 3 5 7 1 6 16771.7862 0.0080 0.010
137: 6 1 5 6 1 6 16928.2514 -0.0237 0.010
138: 9 5 5 9 3 6 16965.0287 -0.0008 0.010
139/ 6 2 5 6 1 6 16981.8810 0.0351 0.010
140: 6 2 5 6 0 6 16982.8692 0.0172 0.010
141: 8 7 1 8 6 2 17222.8654 -0.0031 0.010
142: 6 5 2 6 3 3 17264.0760 0.0018 0.010
143/ 9 7 3 9 6 4 17306.7738 0.0413 0.010
144: 10 7 4 10 6 5 17361.4428 -0.0091 0.010
145: 3 2 2 2 1 1 17575.4415 0.0084 0.010
146: 8 7 2 8 6 3 17586.8335 -0.0103 0.010
147: 6 2 4 5 4 1 17706.2880 -0.0010 0.010
148: 11 8 3 11 7 4 17721.5045 -0.0030 0.010
149: 5 1 4 4 2 2 17731.8436 0.0061 0.010
150/ 7 7 0 7 6 1 17878.6393 0.0344 0.010
151: 7 7 1 7 6 2 17940.9876 -0.0267 0.010
152/ 10 4 6 10 4 7 18074.4655 -0.0356 0.010
153: 10 6 5 10 4 6 18231.0038 0.0142 0.010
154: 9 6 4 9 4 5 18487.9871 -0.0101 0.010
155: 4 1 3 3 2 2 18506.7497 -0.0134 0.010
156: 4 2 3 3 2 2 19176.4830 0.0133 0.010
157: 8 2 6 8 2 7 19763.7503 -0.0197 0.010
158/ 3 2 1 2 1 1 19963.2088 0.0392 0.010
159: 7 1 6 7 1 7 20087.4784 0.0018 0.010
160/ 7 2 6 7 0 7 20100.1455 0.0431 0.010
161: 4 1 3 3 1 2 20129.3215 0.0060 0.010
162: 5 0 5 4 1 4 20345.6155 -0.0048 0.010

163: 5 1 5 4 1 4 20350.8023 0.0117 0.010
164: 5 0 5 4 0 4 20370.5280 0.0146 0.010
165: 5 1 5 4 0 4 20375.6943 0.0105 0.010
166: 4 3 2 3 3 1 20476.0058 -0.0272 0.010
167: 4 3 1 3 3 0 21551.9205 -0.0154 0.010

PARAMETERS IN FIT (values truncated):

10000 A /MHz 3978.8252(4) 1
20000 B /MHz 3040.3459(3) 2
30000 C /MHz 1879.6657(3) 3
200 DJ /kHz 0.326(4) 4
1100 DJK /kHz 0.057(4) 5
2000 DK /kHz 0.644(6) 6
40100 d1 /kHz -0.122(1) 7
50000 d2 /kHz -0.0256(4) 8

MICROWAVE AVG = -0.000902 MHz, IR AVG = 0.00000
MICROWAVE RMS = 0.014178 MHz, IR RMS = 0.00000
END OF ITERATION 1 OLD, NEW RMS ERROR= 1.41776 1.41776

distinct frequency lines in fit: 167
distinct parameters of fit: 8

upper state lower state overall
limits of quantum number 1: 1 14 0 14 0 14
limits of quantum number 2: 0 8 0 7 0 8
limits of quantum number 3: 0 8 0 8 0 8

frequency range: 4920 21551

Standard errors are obtained by muliplying the previous errors by: 1.452989

PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:
(values rounded)

10000 A /MHz 3978.8253(6) 1
20000 B /MHz 3040.3460(5) 2
30000 C /MHz 1879.6657(4) 3
200 DJ /kHz 0.326(6) 4
1100 DJK /kHz 0.058(6) 5
2000 DK /kHz 0.644(9) 6
40100 d1 /kHz -0.122(1) 7
50000 d2 /kHz -0.0256(7) 8

CORRELATION COEFFICIENTS, C.ij:

A B C -DJ -DJK -DK d1 d2

A 1.0000
B 0.7656 1.0000
C 0.6340 0.6763 1.0000
-DJ -0.5482 -0.6939 -0.7377 1.0000
-DJK -0.2900 -0.2848 0.0213 0.1200 1.0000
-DK -0.2336 0.1205 -0.0167 -0.0629 -0.6819 1.0000
d1 -0.3285 -0.5091 0.1521 0.2529 0.4283 -0.1301 1.0000
d2 0.2133 0.3294 -0.0796 -0.2639 0.0138 -0.1648 -0.8140 1.0000

Mean value of |C.ij|, i.ne.j = 0.3417
Mean value of C.ij, i.ne.j = -0.0754

No correlations with absolute value greater than 0.9950

Worst fitted lines (obs-calc/error):

102: 6.8 135: -4.6 160: 4.3 143: 4.1
158: 3.9 152: -3.6 139: 3.5 150: 3.4
49: -2.7 166: -2.7 151: -2.7 60: 2.6
131: 2.6 5: -2.5 132: -2.4 137: -2.4
129: 2.3 30: -2.1 57: 2.1 21: -2.1
38: -2.0 124: -2.0 157: -2.0 95: 1.8
33: -1.7 140: 1.7 114: -1.7 20: -1.7
130: 1.6 167: -1.5 16: -1.5 127: -1.5
164: 1.5 32: -1.4 153: 1.4 48: -1.4
112: 1.4 155: -1.3 123: 1.3 156: 1.3
74: 1.3 77: 1.3 93: 1.3 58: -1.3
46: 1.2 90: -1.2 40: -1.2 115: -1.2
8: -1.2 128: -1.2

102/ 5 3 2 5 2 4 14919.8259 0.0676 0.010
135/ 7 3 5 7 2 6 16759.2936 -0.0460 0.010
160/ 7 2 6 7 0 7 20100.1455 0.0431 0.010
143/ 9 7 3 9 6 4 17306.7738 0.0413 0.010
158/ 3 2 1 2 1 1 19963.2088 0.0392 0.010
152/ 10 4 6 10 4 7 18074.4655 -0.0356 0.010
139/ 6 2 5 6 1 6 16981.8810 0.0351 0.010
150/ 7 7 0 7 6 1 17878.6393 0.0344 0.010
49: 7 1 7 6 2 5 10894.9625 -0.0274 0.010

166: 4 3 2 3 3 1 20476.0058 -0.0272 0.010

S2. Silacyclohex-2-ene Silicon-29

---
obs o-c error

/ instead of : below denotes (o-c)>3*err

1: 3 0 3 2 2 0 5558.5431 -0.0208 0.010
2: 5 3 2 5 2 3 5829.8217 0.0012 0.010
3: 4 2 2 4 1 3 5922.5483 -0.0011 0.010
4: 9 5 4 9 5 5 6010.5635 -0.0029 0.010
5: 3 1 2 3 1 3 6613.7922 -0.0093 0.010
6: 2 2 1 2 0 2 6753.7752 0.0012 0.010
7: 6 3 3 6 3 4 6927.8658 -0.0237 0.010
8: 7 4 3 7 3 4 7579.2118 -0.0117 0.010
9: 3 3 1 3 2 2 8025.6604 0.0057 0.010
10: 3 2 2 3 0 3 8470.3322 0.0016 0.010
11: 2 1 2 1 1 1 8598.2756 -0.0026 0.010
12: 8 4 4 8 4 5 8698.6978 0.0069 0.010
13: 5 2 3 5 2 4 8861.5819 -0.0114 0.010
14: 2 0 2 1 0 1 9161.0362 0.0067 0.010
15: 4 3 2 4 2 3 9266.3667 -0.0174 0.010
16: 4 1 3 3 3 0 10010.4232 -0.0233 0.010
17: 4 3 2 4 1 3 10014.3324 0.0144 0.010
18: 4 1 3 4 1 4 10163.6496 -0.0092 0.010
19: 2 1 1 1 1 0 10873.2177 -0.0276 0.010
20: 4 2 3 4 0 4 10941.0026 0.0120 0.010
21: 5 3 3 5 1 4 11455.1981 -0.0009 0.010
22: 3 0 3 2 1 2 12473.8129 0.0109 0.010
23: 3 1 3 2 1 2 12595.5154 -0.0082 0.010
24: 11 7 4 11 6 5 12606.7744 -0.0056 0.010
25: 6 2 4 6 2 5 12709.8021 0.0048 0.010
26: 6 2 4 6 1 5 12775.5545 0.0107 0.010
27: 3 1 2 2 2 1 12868.8280 0.0091 0.010
28: 3 0 3 2 0 2 12887.0858 0.0161 0.010
29: 3 1 3 2 0 2 13008.7745 -0.0168 0.010
30: 5 1 4 5 0 5 13572.3858 0.0200 0.010
31: 2 2 1 1 1 0 13801.2971 -0.0008 0.010
32: 6 3 4 6 1 5 13804.1452 -0.0020 0.010
33: 5 2 4 5 0 5 13815.0422 0.0018 0.010
34: 4 4 1 4 2 2 14315.0623 -0.0115 0.010
35: 2 2 0 1 1 0 14376.0119 -0.0177 0.010
36: 8 5 4 8 4 5 14586.5824 0.0054 0.010
37: 3 2 2 2 2 1 14603.6398 0.0135 0.010

38: 2 2 1 1 1 1 14938.7909 0.0064 0.010
39: 8 3 5 8 3 6 15193.7539 -0.0090 0.010
40: 2 2 0 1 1 1 15513.5303 0.0140 0.010
41: 3 1 2 2 1 1 15796.8737 0.0023 0.010
42: 4 2 2 3 3 1 16144.0783 -0.0052 0.010
43: 7 5 3 7 3 4 16225.6154 -0.0101 0.010
44: 3 2 1 2 2 0 16320.1857 0.0068 0.010
45: 4 0 4 3 1 3 16402.7524 0.0116 0.010
46: 4 1 4 3 1 3 16432.1473 0.0086 0.010
47: 4 0 4 3 0 3 16524.4613 -0.0011 0.010
48: 4 1 4 3 0 3 16553.8619 0.0015 0.010
49: 6 1 5 6 1 6 16788.4120 -0.0086 0.010
50: 3 2 2 2 1 1 17531.6905 0.0117 0.010
51: 10 7 4 10 6 5 17709.5448 0.0168 0.010
52: 6 5 2 6 3 3 17895.3969 -0.0141 0.010

PARAMETERS IN FIT (values truncated):

10000 A /MHz 3978.705(1) 1
20000 B /MHz 3002.686(1) 2
30000 C /MHz 1865.198(1) 3
200 DJ /kHz 0.28(4) 4
1100 DJK /kHz [0.057561208] 5
2000 DK /kHz 0.60(1) 6
40100 d1 /kHz -0.127(4) 7
50000 d2 /kHz -0.017(1) 8

MICROWAVE AVG = -0.000976 MHz, IR AVG = 0.00000
MICROWAVE RMS = 0.011626 MHz, IR RMS = 0.00000
END OF ITERATION 1 OLD, NEW RMS ERROR= 1.16258 1.16258

distinct frequency lines in fit: 52
distinct parameters of fit: 7

upper state lower state overall
limits of quantum number 1: 2 11 1 11 1 11
limits of quantum number 2: 0 7 0 6 0 7
limits of quantum number 3: 0 5 0 6 0 6

frequency range: 5558 17895

Standard errors are obtained by muliplying the previous errors by: 1.249736

PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:

(values rounded)

10000 A /MHz 3978.706(1) 1
20000 B /MHz 3002.687(1) 2
30000 C /MHz 1865.199(1) 3
200 DJ /kHz 0.29(4) 4
1100 DJK /kHz [0.057561208] 5
2000 DK /kHz 0.60(2) 6
40100 d1 /kHz -0.128(5) 7
50000 d2 /kHz -0.018(2) 8

CORRELATION COEFFICIENTS, C.ij:

A B C -DJ -DK d1 d2

A 1.0000
B 0.8610 1.0000
C 0.7573 0.8011 1.0000
-DJ -0.7722 -0.8737 -0.9024 1.0000
-DK -0.3327 -0.0365 0.2690 -0.1527 1.0000
d1 -0.1901 -0.2806 0.2828 -0.0297 0.5875 1.0000
d2 0.1948 0.1752 -0.2146 0.0340 -0.5344 -0.8426 1.0000

Mean value of |C.ij|, i.ne.j = 0.4345
Mean value of C.ij, i.ne.j = -0.0571

No correlations with absolute value greater than 0.9950

Worst fitted lines (obs-calc/error):

19: -2.8 7: -2.4 16: -2.3 1: -2.1
30: 2.0 35: -1.8 15: -1.7 29: -1.7
51: 1.7 28: 1.6 17: 1.4 52: -1.4
40: 1.4 37: 1.3 20: 1.2 50: 1.2
8: -1.2 45: 1.2 34: -1.1 13: -1.1
22: 1.1 26: 1.1 43: -1.0 5: -0.9
18: -0.9 27: 0.9 39: -0.9 49: -0.9
46: 0.9 23: -0.8 12: 0.7 44: 0.7
14: 0.7 38: 0.6 9: 0.6 24: -0.6
36: 0.5 42: -0.5 25: 0.5 4: -0.3
11: -0.3 41: 0.2 32: -0.2 33: 0.2
10: 0.2 48: 0.1 2: 0.1 6: 0.1
47: -0.1 3: -0.1

19: 2 1 1 1 1 0 10873.2177 -0.0276 0.010
7: 6 3 3 6 3 4 6927.8658 -0.0237 0.010
16: 4 1 3 3 3 0 10010.4232 -0.0233 0.010
1: 3 0 3 2 2 0 5558.5431 -0.0208 0.010
30: 5 1 4 5 0 5 13572.3858 0.0200 0.010
35: 2 2 0 1 1 0 14376.0119 -0.0177 0.010
15: 4 3 2 4 2 3 9266.3667 -0.0174 0.010
29: 3 1 3 2 0 2 13008.7745 -0.0168 0.010
51: 10 7 4 10 6 5 17709.5448 0.0168 0.010
28: 3 0 3 2 0 2 12887.0858 0.0161 0.010

S3. Silacyclohex-2-ene Silicon-30

---
obs o-c error

/ instead of : below denotes (o-c)>3*err

1: 2 1 2 1 1 1 8520.5559 -0.0074 0.010
2: 5 2 3 5 2 4 8640.9986 -0.0037 0.010
3: 2 0 2 1 0 1 9089.1189 -0.0022 0.010
4: 2 1 2 1 0 1 9532.4066 -0.0048 0.010
5: 3 3 1 3 1 2 9979.8572 -0.0120 0.010
6: 4 1 3 4 1 4 10030.4507 0.0058 0.010
7: 4 3 2 4 1 3 10149.5700 -0.0012 0.010
8: 2 1 1 1 1 0 10751.5187 -0.0043 0.010
9: 4 2 3 4 0 4 10891.7740 -0.0034 0.010
10: 5 1 4 4 3 1 12173.4567 -0.0176 0.010
11: 3 0 3 2 1 2 12356.5361 -0.0139 0.010
12: 6 2 4 6 2 5 12488.3592 0.0066 0.010
13: 3 1 3 2 1 2 12492.6440 0.0004 0.010
14: 6 2 4 6 1 5 12567.7059 0.0035 0.010
15: 9 4 5 9 4 6 12745.4338 -0.0069 0.010
16: 3 0 3 2 0 2 12799.8540 0.0136 0.010
17/ 3 1 3 2 0 2 12935.9656 0.0318 0.010
18: 6 3 4 6 1 5 13738.5752 0.0159 0.010
19: 3 2 2 2 2 1 14454.0472 0.0044 0.010
20: 8 3 5 8 3 6 14866.8822 0.0085 0.010
21: 7 6 1 7 5 2 14955.7448 -0.0005 0.010
22: 2 2 0 1 1 1 15449.4500 -0.0163 0.010
23: 3 1 2 2 1 1 15645.7935 -0.0082 0.010
24: 3 2 1 2 2 0 16108.2197 -0.0204 0.010
25: 8 5 4 8 3 5 16136.8242 -0.0019 0.010
26: 4 0 4 3 1 3 16271.9957 -0.0145 0.010
27: 4 1 4 3 1 3 16306.2834 0.0138 0.010
28: 4 0 4 3 0 3 16408.1194 0.0157 0.010

29: 4 1 4 3 0 3 16442.3858 0.0228 0.010
30: 7 3 5 7 1 6 16514.5595 -0.0067 0.010
31: 3 2 2 2 1 1 17489.5766 -0.0054 0.010

PARAMETERS IN FIT (values truncated):

10000 A /MHz 3978.604(1) 1
20000 B /MHz 2966.755(1) 2
30000 C /MHz 1851.272(1) 3
200 DJ /kHz 0.38(3) 4
1100 DJK /kHz [0.057561208] 5
2000 DK /kHz 0.64(2) 6
40100 d1 /kHz -0.125(6) 7
50000 d2 /kHz -0.022(3) 8

MICROWAVE AVG = -0.000283 MHz, IR AVG = 0.00000
MICROWAVE RMS = 0.011998 MHz, IR RMS = 0.00000
END OF ITERATION 1 OLD, NEW RMS ERROR= 1.19985 1.19985

distinct frequency lines in fit: 31
distinct parameters of fit: 7

upper state lower state overall
limits of quantum number 1: 2 9 1 9 1 9
limits of quantum number 2: 0 6 0 5 0 6
limits of quantum number 3: 0 5 0 6 0 6

frequency range: 8520 17489

Standard errors are obtained by muliplying the previous errors by: 1.363648

PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:
(values rounded)

10000 A /MHz 3978.604(1) 1
20000 B /MHz 2966.756(1) 2
30000 C /MHz 1851.272(1) 3
200 DJ /kHz 0.39(4) 4
1100 DJK /kHz [0.057561208] 5
2000 DK /kHz 0.65(3) 6
40100 d1 /kHz -0.125(9) 7
50000 d2 /kHz -0.022(4) 8

Worst fitted constants, with greater than 20% uncertainty: %

50000 d2 /kHz -0.022(4) 8 20.5

CORRELATION COEFFICIENTS, C.ij:

A B C -DJ -DK d1 d2

A 1.0000
B 0.4271 1.0000
C 0.5453 0.4859 1.0000
-DJ -0.5081 -0.6530 -0.8821 1.0000
-DK -0.5569 0.2536 0.1560 -0.2058 1.0000
d1 0.1285 -0.3998 0.5306 -0.2572 -0.0443 1.0000
d2 -0.0430 0.2286 -0.4513 0.2467 -0.0653 -0.8780 1.0000

Mean value of |C.ij|, i.ne.j = 0.3784
Mean value of C.ij, i.ne.j = -0.0925

No correlations with absolute value greater than 0.9950

Worst fitted lines (obs-calc/error):

17: 3.2 29: 2.3 24: -2.0 10: -1.8
22: -1.6 18: 1.6 28: 1.6 26: -1.4
11: -1.4 27: 1.4 16: 1.4 5: -1.2
20: 0.9 23: -0.8 1: -0.7 15: -0.7
30: -0.7 12: 0.7 6: 0.6 31: -0.5
4: -0.5 19: 0.4 8: -0.4 2: -0.4
14: 0.3 9: -0.3 3: -0.2 25: -0.2
7: -0.1 21: -0.1 13: 0.0

17/ 3 1 3 2 0 2 12935.9656 0.0318 0.010
29: 4 1 4 3 0 3 16442.3858 0.0228 0.010
24: 3 2 1 2 2 0 16108.2197 -0.0204 0.010
10: 5 1 4 4 3 1 12173.4567 -0.0176 0.010
22: 2 2 0 1 1 1 15449.4500 -0.0163 0.010
18: 6 3 4 6 1 5 13738.5752 0.0159 0.010
28: 4 0 4 3 0 3 16408.1194 0.0157 0.010
26: 4 0 4 3 1 3 16271.9957 -0.0145 0.010
11: 3 0 3 2 1 2 12356.5361 -0.0139 0.010
27: 4 1 4 3 1 3 16306.2834 0.0138 0.010

S4. Silacyclohex-2-ene Carbon-13 Position 1

---
obs o-c error

/ instead of : below denotes (o-c)>3*err

1: 2 1 2 1 1 1 8631.0310 0.0006 0.010
2: 2 1 1 1 1 0 10980.9170 0.0076 0.010
3: 3 1 3 2 1 2 12613.3611 0.0006 0.010
4: 3 0 3 2 0 2 12861.3135 -0.0016 0.010
5: 3 2 2 2 2 1 14708.9280 -0.0086 0.010
6: 4 1 4 3 1 3 16433.5097 0.0037 0.010
7: 4 0 4 3 0 3 16503.1084 -0.0007 0.010

PARAMETERS IN FIT (values truncated):

10000 A /MHz 3911.48(2) 1
20000 B /MHz 3038.966(2) 2
30000 C /MHz 1864.023(2) 3
200 DJ /kHz [0.326005402] 4
1100 DJK /kHz [0.057561208] 5
2000 DK /kHz [0.644111808] 6
40100 d1 /kHz [-0.122235814] 7
50000 d2 /kHz [-0.025602508] 8

MICROWAVE AVG = 0.000249 MHz, IR AVG = 0.00000
MICROWAVE RMS = 0.004659 MHz, IR RMS = 0.00000
END OF ITERATION 1 OLD, NEW RMS ERROR= 0.46588 0.46588

distinct frequency lines in fit: 7
distinct parameters of fit: 3

upper state lower state overall
limits of quantum number 1: 2 4 1 3 1 4
limits of quantum number 2: 0 2 0 2 0 2
limits of quantum number 3: 1 4 0 3 0 4

frequency range: 8631 16503

Standard errors are obtained by muliplying the previous errors by: 0.616301

PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:
(values rounded)

10000 A /MHz 3911.49(1) 1
20000 B /MHz 3038.967(1) 2
30000 C /MHz 1864.023(1) 3
200 DJ /kHz [0.326005402] 4
1100 DJK /kHz [0.057561208] 5
2000 DK /kHz [0.644111808] 6
40100 d1 /kHz [-0.122235814] 7
50000 d2 /kHz [-0.025602508] 8

CORRELATION COEFFICIENTS, C.ij:

A B C

A 1.0000
B 0.5043 1.0000
C -0.8957 -0.6529 1.0000

Mean value of |C.ij|, i.ne.j = 0.6843
Mean value of C.ij, i.ne.j = -0.3481

No correlations with absolute value greater than 0.9950

Worst fitted lines (obs-calc/error):

5: -0.9 2: 0.8 6: 0.4 4: -0.2
7: -0.1 3: 0.1 1: 0.1

5: 3 2 2 2 2 1 14708.9280 -0.0086 0.010
2: 2 1 1 1 1 0 10980.9170 0.0076 0.010
6: 4 1 4 3 1 3 16433.5097 0.0037 0.010
4: 3 0 3 2 0 2 12861.3135 -0.0016 0.010
7: 4 0 4 3 0 3 16503.1084 -0.0007 0.010
3: 3 1 3 2 1 2 12613.3611 0.0006 0.010
1: 2 1 2 1 1 1 8631.0310 0.0006 0.010

S5. Silacyclohex-2-ene Carbon-13 Position 2

---
obs o-c error

/ instead of : below denotes (o-c)>3*err

1: 2 1 2 1 1 1 8600.5934 0.0015 0.010

2: 3 1 3 2 1 2 12580.2346 -0.0108 0.010
3: 3 0 3 2 0 2 12843.9138 0.0014 0.010
4: 3 2 2 2 2 1 14639.1142 -0.0074 0.010
5: 3 1 2 2 1 1 15817.3594 -0.0022 0.010
6: 4 1 4 3 1 3 16398.3303 -0.0063 0.010
7: 3 2 1 2 2 0 16434.3312 0.0062 0.010
8: 4 0 4 3 0 3 16475.8605 0.0152 0.010

PARAMETERS IN FIT (values truncated):

10000 A /MHz 3928.49(1) 1
20000 B /MHz 3019.278(1) 2
30000 C /MHz 1860.439(1) 3
200 DJ /kHz [0.326005402] 4
1100 DJK /kHz [0.057561208] 5
2000 DK /kHz [0.644111808] 6
40100 d1 /kHz [-0.122235814] 7
50000 d2 /kHz [-0.025602508] 8

MICROWAVE AVG = -0.000302 MHz, IR AVG = 0.00000
MICROWAVE RMS = 0.007851 MHz, IR RMS = 0.00000
END OF ITERATION 1 OLD, NEW RMS ERROR= 0.78510 0.78510

distinct frequency lines in fit: 8
distinct parameters of fit: 3

upper state lower state overall
limits of quantum number 1: 2 4 1 3 1 4
limits of quantum number 2: 0 2 0 2 0 2
limits of quantum number 3: 1 4 0 3 0 4

frequency range: 8600 16475

Standard errors are obtained by muliplying the previous errors by: 0.993082

PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:
(values rounded)

10000 A /MHz 3928.49(1) 1
20000 B /MHz 3019.279(1) 2
30000 C /MHz 1860.440(1) 3
200 DJ /kHz [0.326005402] 4
1100 DJK /kHz [0.057561208] 5
2000 DK /kHz [0.644111808] 6

40100 d1 /kHz [-0.122235814] 7
50000 d2 /kHz [-0.025602508] 8

CORRELATION COEFFICIENTS, C.ij:

A B C

A 1.0000
B 0.5627 1.0000
C -0.7868 -0.6642 1.0000

Mean value of |C.ij|, i.ne.j = 0.6712
Mean value of C.ij, i.ne.j = -0.2961

No correlations with absolute value greater than 0.9950

Worst fitted lines (obs-calc/error):

8: 1.5 2: -1.1 4: -0.7 6: -0.6
7: 0.6 5: -0.2 1: 0.1 3: 0.1

8: 4 0 4 3 0 3 16475.8605 0.0152 0.010
2: 3 1 3 2 1 2 12580.2346 -0.0108 0.010
4: 3 2 2 2 2 1 14639.1142 -0.0074 0.010
6: 4 1 4 3 1 3 16398.3303 -0.0063 0.010
7: 3 2 1 2 2 0 16434.3312 0.0062 0.010
5: 3 1 2 2 1 1 15817.3594 -0.0022 0.010
1: 2 1 2 1 1 1 8600.5934 0.0015 0.010
3: 3 0 3 2 0 2 12843.9138 0.0014 0.010

S6. Silacyclohex-2-ene Carbon-13 Position 3

---
obs o-c error

/ instead of : below denotes (o-c)>3*err

1: 2 1 2 1 1 1 8559.0546 -0.0059 0.010
2: 2 0 2 1 0 1 9124.7802 0.0086 0.010
3: 3 1 3 2 1 2 12543.8113 0.0148 0.010
4: 3 0 3 2 0 2 12843.2782 -0.0041 0.010
5: 3 2 2 2 2 1 14527.5986 -0.0068 0.010
6: 3 1 2 2 1 1 15720.0685 0.0000 0.010
7: 3 2 1 2 2 0 16211.9244 0.0019 0.010

8: 4 1 4 3 1 3 16369.0015 -0.0057 0.010

PARAMETERS IN FIT (values truncated):

10000 A /MHz 3978.37(1) 1
20000 B /MHz 2984.286(1) 2
30000 C /MHz 1858.260(1) 3
200 DJ /kHz [0.326005402] 4
1100 DJK /kHz [0.057561208] 5
2000 DK /kHz [0.644111808] 6
40100 d1 /kHz [-0.122235814] 7
50000 d2 /kHz [-0.025602508] 8

MICROWAVE AVG = 0.000352 MHz, IR AVG = 0.00000
MICROWAVE RMS = 0.007349 MHz, IR RMS = 0.00000
END OF ITERATION 1 OLD, NEW RMS ERROR= 0.73487 0.73487

distinct frequency lines in fit: 8
distinct parameters of fit: 3

upper state lower state overall
limits of quantum number 1: 2 4 1 3 1 4
limits of quantum number 2: 0 2 0 2 0 2
limits of quantum number 3: 1 4 0 3 0 4

frequency range: 8559 16369

Standard errors are obtained by muliplying the previous errors by: 0.929545

PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:
(values rounded)

10000 A /MHz 3978.37(1) 1
20000 B /MHz 2984.286(1) 2
30000 C /MHz 1858.260(1) 3
200 DJ /kHz [0.326005402] 4
1100 DJK /kHz [0.057561208] 5
2000 DK /kHz [0.644111808] 6
40100 d1 /kHz [-0.122235814] 7
50000 d2 /kHz [-0.025602508] 8

CORRELATION COEFFICIENTS, C.ij:

A B C

A 1.0000
B 0.5589 1.0000
C -0.7416 -0.6871 1.0000

Mean value of |C.ij|, i.ne.j = 0.6625
Mean value of C.ij, i.ne.j = -0.2899

No correlations with absolute value greater than 0.9950

Worst fitted lines (obs-calc/error):

3: 1.5 2: 0.9 5: -0.7 1: -0.6
8: -0.6 4: -0.4 7: 0.2 6: 0.0

3: 3 1 3 2 1 2 12543.8113 0.0148 0.010
2: 2 0 2 1 0 1 9124.7802 0.0086 0.010
5: 3 2 2 2 2 1 14527.5986 -0.0068 0.010
1: 2 1 2 1 1 1 8559.0546 -0.0059 0.010
8: 4 1 4 3 1 3 16369.0015 -0.0057 0.010
4: 3 0 3 2 0 2 12843.2782 -0.0041 0.010
7: 3 2 1 2 2 0 16211.9244 0.0019 0.010
6: 3 1 2 2 1 1 15720.0685 0.0000 0.010

S7. Silacyclohex-2-ene Carbon-13 Position 4

---
obs o-c error

/ instead of : below denotes (o-c)>3*err

1: 2 1 2 1 1 1 8607.1932 -0.0028 0.010
2: 2 1 1 1 1 0 10921.6606 -0.0006 0.010
3: 3 1 3 2 1 2 12590.7252 -0.0004 0.010
4: 3 0 3 2 0 2 12854.3545 0.0055 0.010
5: 3 2 2 2 2 1 14646.6218 -0.0029 0.010
6: 4 1 4 3 1 3 16412.8996 0.0073 0.010
7: 3 2 1 2 2 0 16438.8966 0.0018 0.010
8: 4 0 4 3 0 3 16490.4377 -0.0085 0.010

PARAMETERS IN FIT (values truncated):

10000 A /MHz 3928.50(2) 1
20000 B /MHz 3019.728(2) 2
30000 C /MHz 1862.491(1) 3
200 DJ /kHz [0.326005402] 4
1100 DJK /kHz [0.057561208] 5
2000 DK /kHz [0.644111808] 6
40100 d1 /kHz [-0.122235814] 7
50000 d2 /kHz [-0.025602508] 8

MICROWAVE AVG = -0.000093 MHz, IR AVG = 0.00000
MICROWAVE RMS = 0.004735 MHz, IR RMS = 0.00000
END OF ITERATION 1 OLD, NEW RMS ERROR= 0.47351 0.47351

distinct frequency lines in fit: 8
distinct parameters of fit: 3

upper state lower state overall
limits of quantum number 1: 2 4 1 3 1 4
limits of quantum number 2: 0 2 0 2 0 2
limits of quantum number 3: 1 4 0 3 0 4

frequency range: 8607 16490

Standard errors are obtained by muliplying the previous errors by: 0.598948

PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:
(values rounded)

10000 A /MHz 3928.50(1) 1
20000 B /MHz 3019.728(1) 2
30000 C /MHz 1862.492(1) 3
200 DJ /kHz [0.326005402] 4
1100 DJK /kHz [0.057561208] 5
2000 DK /kHz [0.644111808] 6
40100 d1 /kHz [-0.122235814] 7
50000 d2 /kHz [-0.025602508] 8

CORRELATION COEFFICIENTS, C.ij:

A B C

A 1.0000
B 0.8356 1.0000
C -0.9018 -0.8476 1.0000

Mean value of |C.ij|, i.ne.j = 0.8617
Mean value of C.ij, i.ne.j = -0.3046

No correlations with absolute value greater than 0.9950

Worst fitted lines (obs-calc/error):

8: -0.9 6: 0.7 4: 0.5 5: -0.3
1: -0.3 7: 0.2 2: -0.1 3: 0.0

8: 4 0 4 3 0 3 16490.4377 -0.0085 0.010
6: 4 1 4 3 1 3 16412.8996 0.0073 0.010
4: 3 0 3 2 0 2 12854.3545 0.0055 0.010
5: 3 2 2 2 2 1 14646.6218 -0.0029 0.010
1: 2 1 2 1 1 1 8607.1932 -0.0028 0.010
7: 3 2 1 2 2 0 16438.8966 0.0018 0.010
2: 2 1 1 1 1 0 10921.6606 -0.0006 0.010
3: 3 1 3 2 1 2 12590.7252 -0.0004 0.010

S8. Silacyclohex-2-ene Carbon-13 Position 5

---
obs o-c error

/ instead of : below denotes (o-c)>3*err

1: 2 1 2 1 1 1 8629.9841 0.0063 0.010
2: 2 1 1 1 1 0 10972.3768 0.0227 0.010
3: 3 1 3 2 1 2 12614.1392 0.0081 0.010
4: 3 0 3 2 0 2 12864.3059 -0.0071 0.010
5: 3 2 2 2 2 1 14701.7042 -0.0265 0.010
6: 3 1 2 2 1 1 15872.4269 0.0003 0.010
7: 4 1 4 3 1 3 16436.3437 0.0007 0.010
8: 4 0 4 3 0 3 16507.0971 0.0040 0.010
9: 3 2 1 2 2 0 16539.1418 -0.0005 0.010

PARAMETERS IN FIT (values truncated):

10000 A /MHz 3913.31(1) 1
20000 B /MHz 3035.890(1) 2
30000 C /MHz 1864.698(1) 3
200 DJ /kHz [0.326005402] 4

1100 DJK /kHz [0.057561208] 5
2000 DK /kHz [0.644111808] 6
40100 d1 /kHz [-0.122235814] 7
50000 d2 /kHz [-0.025602508] 8

MICROWAVE AVG = 0.000901 MHz, IR AVG = 0.00000
MICROWAVE RMS = 0.012456 MHz, IR RMS = 0.00000
END OF ITERATION 1 OLD, NEW RMS ERROR= 1.24557 1.24557

distinct frequency lines in fit: 9
distinct parameters of fit: 3

upper state lower state overall
limits of quantum number 1: 2 4 1 3 1 4
limits of quantum number 2: 0 2 0 2 0 2
limits of quantum number 3: 1 4 0 3 0 4

frequency range: 8629 16539

Standard errors are obtained by muliplying the previous errors by: 1.525505

PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:
(values rounded)

10000 A /MHz 3913.31(2) 1
20000 B /MHz 3035.890(2) 2
30000 C /MHz 1864.698(2) 3
200 DJ /kHz [0.326005402] 4
1100 DJK /kHz [0.057561208] 5
2000 DK /kHz [0.644111808] 6
40100 d1 /kHz [-0.122235814] 7
50000 d2 /kHz [-0.025602508] 8

CORRELATION COEFFICIENTS, C.ij:

A B C

A 1.0000
B 0.5328 1.0000
C -0.7739 -0.6412 1.0000

Mean value of |C.ij|, i.ne.j = 0.6493
Mean value of C.ij, i.ne.j = -0.2941

No correlations with absolute value greater than 0.9950

Worst fitted lines (obs-calc/error):

5: -2.6 2: 2.3 3: 0.8 4: -0.7
1: 0.6 8: 0.4 7: 0.1 9: -0.1
6: 0.0

5: 3 2 2 2 2 1 14701.7042 -0.0265 0.010
2: 2 1 1 1 1 0 10972.3768 0.0227 0.010
3: 3 1 3 2 1 2 12614.1392 0.0081 0.010
4: 3 0 3 2 0 2 12864.3059 -0.0071 0.010
1: 2 1 2 1 1 1 8629.9841 0.0063 0.010
8: 4 0 4 3 0 3 16507.0971 0.0040 0.010
7: 4 1 4 3 1 3 16436.3437 0.0007 0.010
9: 3 2 1 2 2 0 16539.1418 -0.0005 0.010
6: 3 1 2 2 1 1 15872.4269 0.0003 0.010

S9. 1,1-Difluorosilacyclohex-2-ene Parent

---
obs o-c error

/ instead of : below denotes (o-c)>3*err

1: 2 1 2 1 1 1 5006.2934 0.0047 0.010
2: 2 0 2 1 0 1 5161.4697 -0.0063 0.010
3: 2 1 1 1 1 0 5346.5741 0.0015 0.010
4: 11 2 9 11 2 10 5605.3412 0.0060 0.010
5: 8 3 6 8 2 6 5647.0350 0.0120 0.010
6: 8 1 7 8 1 8 5776.6864 0.0016 0.010
7: 3 2 2 3 0 3 5865.7987 0.0015 0.010
8: 3 0 3 2 1 1 5987.4538 -0.0048 0.010
9: 4 2 3 4 0 4 5997.2148 0.0077 0.010
10: 5 2 3 4 3 1 6100.4863 -0.0064 0.010
11: 5 2 3 5 1 5 6155.2843 0.0088 0.010
12: 7 3 5 7 2 5 6163.2969 0.0025 0.010
13: 6 2 5 6 1 6 6211.0116 0.0015 0.010
14: 5 2 4 5 0 5 6233.5545 -0.0031 0.010
15: 15 3 12 15 3 13 6270.9706 0.0126 0.010
16: 11 2 9 11 1 10 6278.0642 -0.0016 0.010
17: 7 3 4 7 2 5 6327.6635 0.0044 0.010
18: 2 1 2 1 0 1 6369.1592 -0.0043 0.010
19: 5 0 5 4 2 2 6457.1784 -0.0052 0.010
20: 3 0 3 2 1 2 6497.8864 0.0016 0.010

21: 6 3 4 6 2 4 6576.9095 -0.0021 0.010
22: 6 2 5 6 0 6 6597.1263 0.0092 0.010
23: 4 1 3 3 2 1 6743.3735 -0.0077 0.010
24: 5 3 3 5 2 3 6878.0533 -0.0066 0.010
25: 2 1 1 1 0 1 6879.5876 -0.0021 0.010
26: 5 3 2 5 2 3 6900.8788 0.0011 0.010
27: 12 2 10 12 2 11 6927.2978 -0.0033 0.010
28: 9 1 8 9 1 9 6997.0879 0.0072 0.010
29: 4 3 2 4 2 2 7070.8589 0.0074 0.010
30: 4 3 1 4 2 2 7076.5992 -0.0061 0.010
31: 9 1 8 9 0 9 7092.5688 -0.0054 0.010
32: 7 2 6 7 0 7 7093.5711 -0.0023 0.010
33: 13 4 10 13 3 10 7105.4976 -0.0030 0.010
34: 6 2 4 6 1 6 7126.5599 0.0095 0.010
35: 5 1 5 4 2 3 7238.8855 -0.0080 0.010
36: 3 3 1 3 2 2 7248.6863 -0.0029 0.010
37: 3 3 0 3 2 2 7249.5038 -0.0109 0.010
38: 15 4 11 15 3 12 7265.3668 -0.0015 0.010
39: 4 3 2 4 2 3 7287.9196 -0.0026 0.010
40: 4 3 1 4 2 3 7293.6803 0.0041 0.010
41: 5 3 3 5 2 4 7364.4118 -0.0051 0.010
42: 5 3 2 5 2 4 7387.2396 0.0050 0.010
43: 14 4 10 14 3 11 7480.8387 0.0218 0.010
44: 6 3 4 6 2 5 7492.4465 -0.0054 0.010
45: 3 1 3 2 1 2 7500.4509 -0.0082 0.010
46: 8 2 7 8 1 8 7556.5823 -0.0004 0.010
47: 6 3 3 6 2 5 7559.8645 -0.0022 0.010
48: 7 3 5 7 2 6 7685.6903 0.0060 0.010
49: 3 0 3 2 0 2 7705.5733 0.0010 0.010
50: 8 2 7 8 0 8 7713.8048 0.0003 0.010
51: 16 3 13 16 3 14 7733.2596 0.0149 0.010
52: 3 2 2 2 2 1 7764.6364 0.0025 0.010
53: 3 2 1 2 2 0 7823.7020 -0.0036 0.010
54: 13 4 9 13 3 10 7845.1356 -0.0011 0.010
55: 7 3 4 7 2 6 7850.0568 0.0079 0.010
56: 8 4 4 7 5 2 7855.6120 0.0156 0.010
57: 8 4 4 7 5 3 7855.6998 0.0009 0.010
58: 12 4 9 12 3 9 7875.3949 -0.0086 0.010
59: 8 3 6 8 2 7 7955.9337 -0.0018 0.010
60: 3 1 2 2 1 1 8010.0553 -0.0027 0.010
61: 6 2 5 5 3 3 8097.8266 -0.0217 0.010
62: 7 3 5 6 4 3 8105.9406 0.0105 0.010
63: 4 0 4 3 1 2 8187.1623 -0.0081 0.010
64: 7 1 6 6 3 3 8199.7900 -0.0125 0.010
65: 10 1 9 10 1 10 8222.5175 0.0119 0.010
66: 13 2 11 13 2 12 8297.7685 -0.0280 0.010

67: 8 3 5 8 2 7 8303.8226 0.0130 0.010
68: 6 0 6 5 2 3 8378.7846 -0.0066 0.010
69: 9 2 8 9 0 9 8440.2012 0.0010 0.010
70: 11 4 8 11 3 8 8536.5913 0.0067 0.010
71: 3 1 3 2 0 2 8708.1349 -0.0117 0.010
72/ 11 4 7 11 3 8 8755.3490 0.0307 0.010
73: 10 3 8 10 2 9 8760.0227 0.0044 0.010
74/ 9 3 6 9 2 8 8969.8804 0.0692 0.010
75: 6 2 4 5 3 2 8990.5886 0.0177 0.010
76: 10 4 7 10 3 7 9069.5985 0.0104 0.010
77: 11 1 11 10 3 8 9144.8587 0.0148 0.010
78: 4 0 4 3 1 3 9207.1933 -0.0022 0.010
79: 6 1 6 5 2 4 9251.2569 0.0018 0.010
80: 10 2 9 10 0 10 9252.4847 0.0120 0.010
81: 11 1 10 11 1 11 9425.3646 0.0027 0.010
82: 2 2 1 1 1 0 9435.2134 0.0188 0.010
83: 2 2 0 1 1 0 9450.1531 0.0023 0.010
84: 9 4 6 9 3 6 9468.7406 -0.0040 0.010
85: 5 1 4 4 2 2 9551.1078 -0.0092 0.010
86: 2 2 1 1 1 1 9605.3427 0.0059 0.010
87: 2 2 0 1 1 1 9620.2858 -0.0072 0.010
88: 9 3 7 9 1 8 9659.8459 0.0054 0.010
89: 14 2 12 14 2 13 9674.6336 -0.0064 0.010
90: 3 1 2 2 0 2 9728.1770 0.0053 0.010
91: 10 3 8 10 1 9 9733.2998 -0.0048 0.010
92: 8 3 6 8 1 7 9735.8296 -0.0040 0.010
93: 8 4 5 8 3 5 9744.4648 -0.0110 0.010
94: 8 4 4 8 3 5 9762.6588 0.0019 0.010
95: 5 1 4 4 2 3 9768.1888 0.0009 0.010
96: 8 2 6 8 1 8 9865.4970 0.0016 0.010
97/ 10 3 7 10 2 9 9890.4078 -0.0888 0.010
98: 7 4 4 7 3 4 9919.7751 -0.0145 0.010
99: 7 4 3 7 3 4 9925.9244 0.0002 0.010
100: 7 3 5 7 1 6 9928.5946 0.0106 0.010
101: 11 3 9 11 1 10 9973.6682 0.0068 0.010
102: 4 1 4 3 1 3 9984.9657 -0.0064 0.010
103: 7 0 7 6 2 4 9993.4418 -0.0132 0.010
104: 6 4 3 6 3 3 10022.4293 -0.0270 0.010
105: 6 4 2 6 3 3 10024.1580 0.0151 0.010
106: 5 4 2 5 3 2 10077.7394 -0.0267 0.010
107: 5 4 1 5 3 2 10078.0868 -0.0182 0.010
108: 7 4 4 7 3 5 10084.1418 -0.0124 0.010
109: 6 4 3 6 3 4 10089.8645 -0.0065 0.010
110: 7 4 3 7 3 5 10090.2938 0.0050 0.010
111: 6 4 2 6 3 4 10091.5480 -0.0096 0.010
112: 8 4 5 8 3 6 10092.3467 -0.0030 0.010

113: 11 2 10 11 1 11 10098.1092 0.0166 0.010
114: 5 4 2 5 3 3 10100.5966 0.0128 0.010
115: 5 4 1 5 3 3 10100.9240 0.0012 0.010
116: 8 4 4 8 3 6 10110.5115 -0.0193 0.010
117: 9 4 6 9 3 7 10126.3440 0.0026 0.010
118: 11 2 10 11 0 11 10131.1387 0.0060 0.010
119: 9 4 5 9 3 7 10172.7850 0.0025 0.010
120/ 6 3 4 6 1 5 10197.9374 -0.0094 0.010
121: 5 0 5 4 1 3 10197.9374 -0.0875 0.010
122: 10 4 7 10 3 8 10200.0436 -0.0228 0.010
123: 4 0 4 3 0 3 10209.7823 0.0124 0.010
124: 7 1 7 6 2 4 10244.6604 -0.0249 0.010
125: 10 4 6 10 3 8 10305.7475 -0.0021 0.010
126: 11 4 8 11 3 9 10328.2379 0.0139 0.010
127: 4 2 3 3 2 2 10341.1556 -0.0241 0.010
128: 12 3 10 12 1 11 10380.1551 0.0013 0.010
129: 4 3 2 3 3 1 10380.4093 -0.0034 0.010
130: 4 3 1 3 3 0 10385.3332 -0.0079 0.010
131: 7 2 6 6 3 3 10442.7144 0.0123 0.010
132: 4 2 2 3 2 1 10484.2198 -0.0027 0.010
133: 5 3 3 5 1 4 10504.0447 0.0037 0.010
134: 7 2 6 6 3 4 10510.1082 -0.0086 0.010
135/ 11 4 7 11 3 9 10546.9227 -0.0350 0.010
136: 12 3 9 11 5 6 10574.8155 0.0079 0.010
137: 12 1 11 12 1 12 10592.5464 0.0107 0.010
138: 4 1 3 3 1 2 10660.6146 0.0075 0.010
139: 8 3 6 7 4 4 10713.3285 0.0071 0.010
140: 8 1 7 7 3 4 10897.2828 0.0053 0.010
141: 2 2 0 1 0 1 10983.1800 0.0120 0.010
142: 4 1 4 3 0 3 10987.5435 -0.0028 0.010
143: 15 2 13 15 2 14 11022.5281 -0.0097 0.010
144: 12 2 11 12 0 12 11059.1141 0.0000 0.010
145: 3 3 1 3 1 2 11091.9033 0.0163 0.010
146: 11 3 8 11 2 10 11092.5669 -0.0033 0.010
147: 7 1 7 6 2 5 11160.2139 -0.0117 0.010
148: 14 4 11 14 3 12 11168.4748 -0.0128 0.010
149: 8 0 8 7 2 5 11291.0184 -0.0115 0.010
150: 3 2 2 2 1 1 11853.2611 0.0052 0.010
151: 3 2 1 2 1 1 11927.2908 0.0069 0.010
152: 7 2 5 6 3 3 11965.1033 0.0113 0.010
153: 6 0 6 5 1 4 12004.7837 0.0114 0.010
154: 13 2 12 13 0 13 12022.3646 0.0026 0.010
155: 7 2 5 6 3 4 12032.4949 -0.0118 0.010
156: 13 5 9 13 4 9 12050.0396 0.0047 0.010
157/ 13 5 8 13 4 9 12112.5908 -0.0355 0.010
158: 6 1 5 5 2 3 12270.4079 -0.0054 0.010

159: 9 0 9 8 2 6 12286.2759 -0.0034 0.010
160: 19 3 16 19 3 17 12307.6302 -0.0040 0.010
161: 16 2 14 16 2 15 12319.7394 0.0020 0.010
162: 3 2 2 2 1 2 12363.6932 0.0111 0.010
163: 12 5 8 12 4 8 12383.5654 -0.0099 0.010
164: 15 3 13 15 1 14 12408.7740 -0.0054 0.010
165: 3 2 1 2 1 2 12437.7201 0.0100 0.010
166: 5 1 5 4 1 4 12458.3205 -0.0035 0.010
167: 11 5 7 11 4 7 12612.0407 -0.0038 0.010
168: 11 5 6 11 4 7 12624.0096 -0.0052 0.010
169: 5 0 5 4 0 4 12671.4672 0.0056 0.010
170: 8 2 7 7 3 4 12677.1691 -0.0064 0.010
171: 4 1 3 3 0 3 12683.2033 -0.0030 0.010
172: 6 1 5 5 2 4 12756.7702 -0.0001 0.010
173: 10 5 6 10 4 6 12763.2018 -0.0090 0.010
174: 10 5 5 10 4 6 12767.7420 -0.0232 0.010
175: 14 1 13 14 1 14 12822.4967 0.0000 0.010
176: 14 1 13 14 0 14 12828.5486 -0.0043 0.010
177: 12 5 7 12 4 9 12829.3121 -0.0062 0.010
178: 11 5 7 11 4 8 12830.7742 -0.0041 0.010
179: 17 4 14 17 3 15 12835.0674 -0.0173 0.010
180: 8 2 7 7 3 5 12841.5462 0.0060 0.010
181: 11 5 6 11 4 8 12842.7426 -0.0059 0.010
182: 13 5 8 13 4 10 12852.2586 -0.0039 0.010
183/ 9 5 5 9 4 5 12860.8628 -0.0304 0.010
184: 9 5 4 9 4 5 12862.4455 0.0177 0.010
185: 10 5 6 10 4 7 12868.8650 -0.0290 0.010
186: 10 5 5 10 4 7 12873.4506 0.0023 0.010
187: 15 4 12 15 2 13 12904.2326 0.0128 0.010
188: 5 2 4 4 2 3 12907.8246 0.0126 0.010
189: 9 5 4 9 4 6 12908.8712 0.0022 0.010
190: 8 5 4 8 4 4 12923.0017 -0.0250 0.010
191: 14 4 11 14 2 12 12934.5531 -0.0120 0.010
192: 14 5 9 14 4 11 12938.4833 -0.0021 0.010
193: 8 5 4 8 4 5 12941.1964 -0.0113 0.010
194: 8 5 3 8 4 5 12941.6384 -0.0111 0.010
195: 7 5 2 7 4 4 12968.2345 -0.0213 0.010
196: 8 1 8 7 2 6 12970.6329 -0.0086 0.010
197: 5 4 2 4 4 1 12974.2121 0.0120 0.010
198: 5 4 1 4 4 0 12974.4887 -0.0126 0.010
199: 5 3 3 4 3 2 12984.3131 0.0064 0.010
200: 5 3 2 4 3 1 13001.3568 -0.0135 0.010
201: 14 2 13 14 0 14 13009.8795 0.0072 0.010
202: 16 4 13 16 2 14 13072.7922 0.0059 0.010
203/ 13 4 10 13 2 11 13153.0188 0.0305 0.010
204: 5 2 3 4 2 2 13177.1018 0.0037 0.010

205: 5 1 5 4 0 4 13236.1114 0.0108 0.010
206: 16 3 14 16 1 15 13273.9137 0.0290 0.010
207: 5 1 4 4 1 3 13291.9671 0.0087 0.010
208: 9 1 8 8 3 5 13383.9398 -0.0169 0.010
209: 16 5 11 16 4 13 13451.6187 -0.0122 0.010
210: 12 4 9 12 2 10 13530.1048 0.0051 0.010
211: 7 0 7 6 1 5 13614.5052 0.0150 0.010
212: 3 2 1 2 0 2 13645.4011 0.0035 0.010
213/ 6 3 3 6 1 6 13770.9130 0.0362 0.010
214: 11 4 8 11 2 9 14023.8212 0.0016 0.010
215: 4 2 2 3 1 2 14401.4409 -0.0075 0.010
216: 6 0 6 5 1 5 14534.0765 0.0098 0.010
217: 10 4 7 10 2 8 14587.0256 -0.0005 0.010
218: 7 3 4 7 1 7 14692.3930 0.0009 0.010
219: 9 2 8 8 3 5 14731.5587 -0.0238 0.010
220: 7 3 5 7 0 7 14779.2636 0.0058 0.010
221: 7 1 6 6 2 4 14844.1241 -0.0048 0.010
222: 6 1 6 5 1 5 14920.1727 -0.0009 0.010
223: 16 1 15 16 1 16 14957.7320 -0.0101 0.010
224: 8 2 6 7 3 4 14986.0865 -0.0015 0.010
225: 3 3 1 2 2 0 14998.3703 0.0035 0.010
226: 3 3 0 2 2 0 14999.1933 0.0009 0.010
227: 3 3 1 2 2 1 15013.3434 0.0203 0.010
228: 3 3 0 2 2 1 15014.1534 0.0047 0.010
229: 16 2 15 16 0 16 15027.1125 -0.0146 0.010
230: 8 0 8 7 1 6 15056.3250 0.0055 0.010
231: 9 2 8 8 3 6 15079.4657 0.0090 0.010
232: 6 0 6 5 0 5 15098.7050 -0.0008 0.010
233: 8 2 6 7 3 5 15150.4526 0.0000 0.010
234: 18 3 16 18 1 17 15161.1693 0.0050 0.010
235: 9 4 6 9 2 7 15173.2311 0.0104 0.010
236: 15 2 14 14 4 11 15177.6219 0.0216 0.010
237: 4 2 3 3 1 3 15204.4101 0.0074 0.010
238: 4 2 2 3 1 3 15421.4759 0.0024 0.010
239: 6 2 5 5 2 4 15462.2763 0.0111 0.010
240: 6 1 6 5 0 5 15484.7974 -0.0153 0.010
241: 15 6 10 15 5 11 15514.7514 0.0170 0.010
242: 6 5 1 5 5 0 15566.6303 -0.0250 0.010
243: 6 5 2 5 5 1 15566.6303 -0.0094 0.010
244: 6 4 3 5 4 2 15579.5897 0.0021 0.010
245: 6 4 2 5 4 1 15580.9325 -0.0026 0.010
246: 10 1 9 9 3 6 15583.9616 0.0256 0.010
247: 6 3 4 5 3 3 15590.2889 -0.0114 0.010
248: 14 6 8 14 5 10 15593.4126 -0.0091 0.010
249: 6 3 3 5 3 2 15634.8984 0.0011 0.010
250: 11 6 6 11 5 6 15755.0884 0.0076 0.010

251: 5 1 4 4 0 4 15765.3795 -0.0154 0.010
252: 19 2 17 19 2 18 15888.9548 0.0060 0.010
253: 6 2 4 5 2 3 15891.4374 -0.0111 0.010
254: 6 1 5 5 1 4 15896.4133 0.0188 0.010
255: 17 1 16 17 1 17 16005.6577 -0.0058 0.010
256: 17 1 16 17 0 17 16006.6847 -0.0051 0.010
257: 11 4 7 10 5 5 16017.2822 -0.0278 0.010
258: 10 1 10 9 2 8 16331.2482 0.0066 0.010
259: 4 2 2 3 0 3 16424.0519 0.0041 0.010
260: 5 2 4 4 1 3 16431.6026 0.0200 0.010
261: 22 3 19 22 3 20 16441.7053 0.0192 0.010
262: 5 2 3 4 1 3 16917.9412 0.0017 0.010
263: 7 0 7 6 1 6 17119.9998 -0.0056 0.010
264: 8 1 7 7 2 5 17224.9308 -0.0055 0.010
265: 9 3 6 9 1 9 17314.5252 0.0075 0.010
266: 7 1 7 6 1 6 17371.2271 -0.0086 0.010
267/ 11 1 10 10 3 7 17439.7683 0.0410 0.010
268: 7 0 7 6 0 6 17506.1374 0.0250 0.010
269: 4 3 2 3 2 1 17555.0868 0.0127 0.010
270: 4 3 1 3 2 1 17560.8270 -0.0008 0.010
271: 10 0 10 9 1 8 17622.1834 -0.0032 0.010
272: 4 3 2 3 2 2 17629.1074 0.0053 0.010
273: 4 3 1 3 2 2 17634.8654 0.0094 0.010
274: 7 1 7 6 0 6 17757.3168 -0.0258 0.010
275/ 14 6 9 13 7 7 17828.0958 -0.0445 0.010
276: 9 2 7 8 3 5 17996.9280 0.0102 0.010
277: 7 2 6 6 2 5 18002.5508 -0.0179 0.010
278/ 5 2 4 4 1 4 18127.2909 0.0483 0.010
279: 7 5 3 6 5 2 18170.5362 0.0157 0.010
280: 19 7 12 19 6 14 18173.8057 0.0237 0.010
281/ 7 4 4 6 4 3 18190.1358 0.0515 0.010
282: 7 4 3 6 4 2 18194.5214 -0.0108 0.010
283/ 7 3 5 6 3 4 18195.7703 -0.0308 0.010
284: 7 3 4 6 3 3 18292.7728 0.0217 0.010
285: 7 1 6 6 1 5 18465.1413 -0.0227 0.010
286: 7 2 5 6 2 4 18609.4008 -0.0176 0.010
287: 8 1 8 7 1 7 19812.9776 -0.0071 0.010
288: 8 0 8 7 0 7 19907.0027 0.0094 0.010
289: 8 2 7 7 2 6 20527.2231 -0.0012 0.010
290/ 8 6 3 7 6 2 20761.9107 -0.0484 0.010
291: 8 5 4 7 5 3 20778.7351 0.0095 0.010
292: 8 3 6 7 3 5 20797.4759 0.0002 0.010
293: 8 4 5 7 4 4 20805.6697 -0.0015 0.010
294: 8 4 4 7 4 3 20817.7418 0.0241 0.010
295: 8 3 5 7 3 4 20980.9911 0.0061 0.010
296: 8 1 7 7 1 6 20990.2285 0.0026 0.010

297: 8 2 6 7 2 5 21313.7443 -0.0027 0.010
298: 9 1 9 8 1 8 22247.2725 0.0041 0.010
299: 9 0 9 8 0 8 22309.0095 0.0129 0.010
300: 9 2 8 8 2 7 23035.3898 -0.0023 0.010

PARAMETERS IN FIT (values truncated):

10000 A /MHz 2742.0553(2) 1
20000 B /MHz 1379.1798(1) 2
30000 C /MHz 1209.0375(1) 3
200 DJ /kHz 0.084(2) 4
1100 DJK /kHz 0.340(1) 5
2000 DK /kHz -0.095(7) 6
40100 d1 /kHz -0.01194(6) 7
50000 d2 /kHz 0.00725(3) 8
300 HJ /Hz -0.142(6) 9

MICROWAVE AVG = -0.000208 MHz, IR AVG = 0.00000
MICROWAVE RMS = 0.015032 MHz, IR RMS = 0.00000
END OF ITERATION 1 OLD, NEW RMS ERROR= 1.50318 1.50318

distinct frequency lines in fit: 298
distinct parameters of fit: 9

upper state lower state overall
limits of quantum number 1: 2 22 1 22 1 22
limits of quantum number 2: 0 7 0 7 0 7
limits of quantum number 3: 0 19 0 20 0 20

frequency range: 5006 23035

Standard errors are obtained by muliplying the previous errors by: 1.526406

PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:
(values rounded)

10000 A /MHz 2742.0553(4) 1
20000 B /MHz 1379.1798(2) 2
30000 C /MHz 1209.0375(3) 3
200 DJ /kHz 0.084(3) 4
1100 DJK /kHz 0.341(2) 5
2000 DK /kHz -0.10(1) 6
40100 d1 /kHz -0.01195(9) 7
50000 d2 /kHz 0.00725(4) 8

300 HJ /Hz -0.14(1) 9

CORRELATION COEFFICIENTS, C.ij:

A B C -DJ -DJK -DK d1 d2

A 1.0000
B 0.5661 1.0000
C 0.5932 0.9494 1.0000
-DJ -0.4526 -0.8924 -0.9141 1.0000
-DJK -0.2483 0.0395 0.0510 -0.1193 1.0000
-DK -0.3774 0.0526 -0.0018 -0.0271 -0.5346 1.0000
d1 0.1191 -0.0957 0.1836 -0.0965 -0.0640 -0.0907 1.0000
d2 0.0523 0.0165 0.0031 -0.0206 0.2963 -0.2579 -0.0109 1.0000
HJ 0.3711 0.7971 0.8106 -0.9546 0.1088 0.0864 0.0861 0.0332

HJ

HJ 1.0000

Mean value of |C.ij|, i.ne.j = 0.2882
Mean value of C.ij, i.ne.j = 0.0016

No correlations with absolute value greater than 0.9950

Worst fitted lines (obs-calc/error):

97: -8.9 74: 6.9 281: 5.1 120: -4.8
290: -4.8 278: 4.8 275: -4.4 267: 4.1
213: 3.6 157: -3.5 135: -3.5 283: -3.1
72: 3.1 203: 3.0 183: -3.0 185: -2.9
206: 2.9 66: -2.8 257: -2.8 104: -2.7
106: -2.7 274: -2.6 246: 2.6 268: 2.5
190: -2.5 124: -2.5 294: 2.4 127: -2.4
219: -2.4 280: 2.4 174: -2.3 122: -2.3
285: -2.3 43: 2.2 61: -2.2 284: 2.2
236: 2.2 195: -2.1 227: 2.0 260: 2.0
116: -1.9 261: 1.9 82: 1.9 254: 1.9
107: -1.8 277: -1.8 75: 1.8 184: 1.8
286: -1.8 179: -1.7

97/ 10 3 7 10 2 9 9890.4078 -0.0888 0.010
74/ 9 3 6 9 2 8 8969.8804 0.0692 0.010
281/ 7 4 4 6 4 3 18190.1358 0.0515 0.010

120/ 6 3 4 6 1 5 10197.9374 -0.0094 0.010 -0.0485 0.50
290/ 8 6 3 7 6 2 20761.9107 -0.0484 0.010
278/ 5 2 4 4 1 4 18127.2909 0.0483 0.010
275/ 14 6 9 13 7 7 17828.0958 -0.0445 0.010
267/ 11 1 10 10 3 7 17439.7683 0.0410 0.010
213/ 6 3 3 6 1 6 13770.9130 0.0362 0.010
157/ 13 5 8 13 4 9 12112.5908 -0.0355 0.010

S10. 1,1-Difluorosilacyclohex-2-ene Silicon-29

---
obs o-c error

/ instead of : below denotes (o-c)>3*err

1: 2 0 2 1 0 1 5153.6003 -0.0262 0.010
2: 3 1 3 2 1 2 7489.3516 -0.0071 0.010
3: 3 0 3 2 0 2 7694.0532 -0.0097 0.010
4: 3 2 2 2 2 1 7752.6915 0.0044 0.010
5: 3 2 1 2 2 0 7811.3259 -0.0019 0.010
6: 3 1 2 2 1 1 7997.3969 -0.0171 0.010
7: 7 3 5 7 1 6 9946.0968 0.0004 0.010
8: 4 1 4 3 1 3 9970.2712 -0.0101 0.010
9: 5 0 5 4 1 3 10181.7520 0.0051 0.010
10: 4 0 4 3 0 3 10194.8474 -0.0096 0.010
11: 4 2 3 3 2 2 10325.3306 -0.0065 0.010
12: 4 3 2 3 3 1 10364.2813 0.0031 0.010
13: 4 3 1 3 3 0 10369.1525 0.0039 0.010
14: 4 2 2 3 2 1 10467.3663 -0.0066 0.010
15: 4 1 3 3 1 2 10643.8913 -0.0089 0.010
16: 5 1 5 4 1 4 12440.1211 0.0091 0.010
17: 5 0 5 4 0 4 12653.3510 0.0084 0.010
18: 4 1 3 3 0 3 12666.4637 0.0110 0.010
19: 5 2 4 4 2 3 12888.1492 0.0025 0.010
20: 5 4 2 4 4 1 12954.0394 0.0288 0.010
21: 5 4 1 4 4 0 12954.2986 -0.0084 0.010
22: 5 3 3 4 3 2 12964.1035 0.0097 0.010
23: 5 3 2 4 3 1 12980.9600 0.0013 0.010
24: 5 2 3 4 2 2 13155.6451 -0.0108 0.010
25: 5 1 4 4 1 3 13271.3377 -0.0107 0.010
26: 6 1 6 5 1 5 14898.4962 -0.0051 0.010
27: 6 0 6 5 0 5 15077.4363 0.0107 0.010
28: 6 2 5 5 2 4 15438.8711 0.0059 0.010
29: 6 5 1 5 5 0 15542.4024 -0.0121 0.010
30: 6 5 2 5 5 1 15542.4024 0.0031 0.010
31/ 6 4 3 5 4 2 15555.3188 0.0340 0.010

32/ 6 4 2 5 4 1 15556.6417 0.0309 0.010
33: 6 3 4 5 3 3 15566.0305 0.0108 0.010
34: 6 3 3 5 3 2 15610.1135 0.0087 0.010
35: 6 2 4 5 2 3 15865.4486 -0.0210 0.010
36: 6 1 5 5 1 4 15872.0984 -0.0133 0.010
37: 7 1 7 6 1 6 17346.1486 0.0002 0.010
38: 7 0 7 6 0 6 17481.5673 -0.0143 0.010
39: 7 2 6 6 2 5 17975.5624 0.0299 0.010
40: 7 6 1 6 6 0 18130.9092 -0.0260 0.010
41: 7 5 3 6 5 2 18142.1451 -0.0238 0.010
42: 7 5 2 6 5 1 18142.2479 -0.0046 0.010
43: 7 4 3 6 4 2 18166.0355 0.0217 0.010
44: 7 3 5 6 3 4 18167.4785 -0.0151 0.010
45: 7 3 4 6 3 3 18263.3832 0.0226 0.010
46/ 7 1 6 6 1 5 18437.4767 -0.0323 0.010
47: 7 2 5 6 2 4 18579.1313 0.0079 0.010
48: 8 1 8 7 1 7 19784.5066 -0.0024 0.010
49: 8 0 8 7 0 7 19879.0863 -0.0026 0.010

PARAMETERS IN FIT (values truncated):

10000 A /MHz 2742.041(1) 1
20000 B /MHz 1376.9313(7) 2
30000 C /MHz 1207.3058(5) 3
200 DJ /kHz 0.084(5) 4
1100 DJK /kHz 0.60(1) 5
2000 DK /kHz [-0.095727736] 6
40100 d1 /kHz -0.024(4) 7
50000 d2 /kHz [0.007251909801] 8
300 HJ /Hz [-0.142448339] 9

MICROWAVE AVG = -0.000572 MHz, IR AVG = 0.00000
MICROWAVE RMS = 0.015081 MHz, IR RMS = 0.00000
END OF ITERATION 1 OLD, NEW RMS ERROR= 1.50811 1.50811

distinct frequency lines in fit: 48
distinct parameters of fit: 6

upper state lower state overall
limits of quantum number 1: 2 8 1 7 1 8
limits of quantum number 2: 0 6 0 6 0 6
limits of quantum number 3: 1 8 0 7 0 8

frequency range: 5153 19879

Standard errors are obtained by muliplying the previous errors by: 1.612237

PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:
(values rounded)

10000 A /MHz 2742.041(2) 1
20000 B /MHz 1376.931(1) 2
30000 C /MHz 1207.3059(9) 3
200 DJ /kHz 0.084(8) 4
1100 DJK /kHz 0.61(2) 5
2000 DK /kHz [-0.095727736] 6
40100 d1 /kHz -0.024(6) 7
50000 d2 /kHz [0.007251909801] 8
300 HJ /Hz [-0.142448339] 9

Worst fitted constants, with greater than 20% uncertainty: %

40100 d1 /kHz -0.024(6) 7 27.2

CORRELATION COEFFICIENTS, C.ij:

A B C -DJ -DJK d1

A 1.0000
B 0.1364 1.0000
C 0.1060 -0.2587 1.0000
-DJ 0.0398 -0.6696 -0.3860 1.0000
-DJK -0.5802 0.0354 -0.0780 -0.3228 1.0000
d1 0.1699 -0.7784 0.5409 0.4510 -0.2841 1.0000

Mean value of |C.ij|, i.ne.j = 0.3225
Mean value of C.ij, i.ne.j = -0.1252

No correlations with absolute value greater than 0.9950

Worst fitted lines (obs-calc/error):

31: 3.4 46: -3.2 32: 3.1 39: 3.0
20: 2.9 1: -2.6 40: -2.6 41: -2.4
45: 2.3 43: 2.2 35: -2.1 6: -1.7
44: -1.5 38: -1.4 36: -1.3 18: 1.1

33: 1.1 24: -1.1 25: -1.1 27: 1.1
8: -1.0 3: -1.0 22: 1.0 10: -1.0
16: 0.9 15: -0.9 34: 0.9 21: -0.8
17: 0.8 47: 0.8 2: -0.7 14: -0.7
11: -0.6 28: 0.6 26: -0.5 9: 0.5
42: -0.5 29: -0.4 4: 0.4 13: 0.4
12: 0.3 49: -0.3 19: 0.2 48: -0.2
5: -0.2 23: 0.1 7: 0.0 37: 0.0
30: 0.0

31/ 6 4 3 5 4 2 15555.3188 0.0340 0.010
46/ 7 1 6 6 1 5 18437.4767 -0.0323 0.010
32/ 6 4 2 5 4 1 15556.6417 0.0309 0.010
39: 7 2 6 6 2 5 17975.5624 0.0299 0.010
20: 5 4 2 4 4 1 12954.0394 0.0288 0.010
1: 2 0 2 1 0 1 5153.6003 -0.0262 0.010
40: 7 6 1 6 6 0 18130.9092 -0.0260 0.010
41: 7 5 3 6 5 2 18142.1451 -0.0238 0.010
45: 7 3 4 6 3 3 18263.3832 0.0226 0.010
43: 7 4 3 6 4 2 18166.0355 0.0217 0.010

S11. 1,1-Difluorosilacyclohex-2-ene Silicon-30

---
obs o-c error

/ instead of : below denotes (o-c)>3*err

1: 3 1 3 2 1 2 7478.4698 -0.0075 0.010
2: 3 0 3 2 0 2 7682.7700 0.0005 0.010
3: 3 2 2 2 2 1 7740.9689 -0.0009 0.010
4: 3 2 1 2 2 0 7799.1870 0.0059 0.010
5: 3 1 2 2 1 1 7984.9918 0.0006 0.010
6: 4 1 4 3 1 3 9955.8750 -0.0048 0.010
7: 4 0 4 3 0 3 10180.2268 -0.0036 0.010
8: 4 2 3 3 2 2 10309.8092 0.0084 0.010
9: 4 3 2 3 3 1 10348.4698 -0.0011 0.010
10: 4 3 1 3 3 0 10353.2951 0.0110 0.010
11: 7 2 6 6 3 4 10440.2237 0.0000 0.010
12: 4 2 2 3 2 1 10450.8269 -0.0063 0.010
13: 4 1 3 3 1 2 10627.4976 0.0068 0.010
14: 5 1 5 4 1 4 12422.2557 -0.0009 0.010
15: 5 0 5 4 0 4 12635.5781 -0.0002 0.010
16: 5 2 4 4 2 3 12868.8679 0.0041 0.010
17: 5 4 2 4 4 1 12934.2655 -0.0019 0.010
18: 5 4 1 4 4 0 12934.5539 -0.0051 0.010

19: 5 3 3 4 3 2 12944.3034 0.0117 0.010
20: 5 3 2 4 3 1 12960.9502 -0.0092 0.010
21: 5 2 3 4 2 2 13134.6171 0.0122 0.010
22: 5 1 4 4 1 3 13251.1113 -0.0015 0.010
23: 6 1 6 5 1 5 14877.2515 0.0018 0.010
24: 6 0 6 5 0 5 15056.5590 -0.0071 0.010
25: 6 2 5 5 2 4 15415.9259 0.0029 0.010
26: 6 3 4 5 3 3 15542.2377 0.0038 0.010
27: 6 3 3 5 3 2 15585.8048 -0.0071 0.010
28: 6 2 4 5 2 3 15839.9553 -0.0093 0.010
29: 6 1 5 5 1 4 15848.2879 0.0070 0.010
30: 7 1 7 6 1 6 17321.5341 -0.0063 0.010
31: 7 0 7 6 0 6 17457.5304 -0.0027 0.010
32: 7 2 6 6 2 5 17949.0299 0.0015 0.010
33: 7 1 6 6 1 5 18410.3690 -0.0133 0.010
34: 8 1 8 7 1 7 19756.5646 -0.0013 0.010
35: 8 0 8 7 0 7 19851.7369 0.0152 0.010

PARAMETERS IN FIT (values truncated):

10000 A /MHz 2742.078(2) 1
20000 B /MHz 1374.7184(6) 2
30000 C /MHz 1205.6109(7) 3
200 DJ /kHz 0.080(6) 4
1100 DJK /kHz 0.36(4) 5
2000 DK /kHz [-0.095727736] 6
40100 d1 /kHz [-0.011946691] 7
50000 d2 /kHz [0.007251909801] 8
300 HJ /Hz [-0.142448339] 9

MICROWAVE AVG = 0.000090 MHz, IR AVG = 0.00000
MICROWAVE RMS = 0.006696 MHz, IR RMS = 0.00000
END OF ITERATION 1 OLD, NEW RMS ERROR= 0.66963 0.66963

distinct frequency lines in fit: 35
distinct parameters of fit: 5

upper state lower state overall
limits of quantum number 1: 3 8 2 7 2 8
limits of quantum number 2: 0 4 0 4 0 4
limits of quantum number 3: 1 8 0 7 0 8

frequency range: 7478 19851

Standard errors are obtained by muliplying the previous errors by: 0.723283

PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:
(values rounded)

10000 A /MHz 2742.079(2) 1
20000 B /MHz 1374.7185(4) 2
30000 C /MHz 1205.6110(5) 3
200 DJ /kHz 0.080(4) 4
1100 DJK /kHz 0.37(3) 5
2000 DK /kHz [-0.095727736] 6
40100 d1 /kHz [-0.011946691] 7
50000 d2 /kHz [0.007251909801] 8
300 HJ /Hz [-0.142448339] 9

CORRELATION COEFFICIENTS, C.ij:

A B C -DJ -DJK

A 1.0000
B 0.4478 1.0000
C 0.1766 0.0474 1.0000
-DJ -0.1179 -0.2706 -0.8954 1.0000
-DJK -0.6394 -0.6536 -0.0654 0.0551 1.0000

Mean value of |C.ij|, i.ne.j = 0.3369
Mean value of C.ij, i.ne.j = -0.1915

No correlations with absolute value greater than 0.9950

Worst fitted lines (obs-calc/error):

35: 1.5 33: -1.3 21: 1.2 19: 1.2
10: 1.1 28: -0.9 20: -0.9 8: 0.8
1: -0.8 24: -0.7 27: -0.7 29: 0.7
13: 0.7 12: -0.6 30: -0.6 4: 0.6
18: -0.5 6: -0.5 16: 0.4 26: 0.4
7: -0.4 25: 0.3 31: -0.3 17: -0.2
23: 0.2 22: -0.1 32: 0.1 34: -0.1
9: -0.1 3: -0.1 14: -0.1 5: 0.1
2: 0.1 15: 0.0 11: 0.0

35: 8 0 8 7 0 7 19851.7369 0.0152 0.010
33: 7 1 6 6 1 5 18410.3690 -0.0133 0.010

21: 5 2 3 4 2 2 13134.6171 0.0122 0.010
19: 5 3 3 4 3 2 12944.3034 0.0117 0.010
10: 4 3 1 3 3 0 10353.2951 0.0110 0.010
28: 6 2 4 5 2 3 15839.9553 -0.0093 0.010
20: 5 3 2 4 3 1 12960.9502 -0.0092 0.010
8: 4 2 3 3 2 2 10309.8092 0.0084 0.010
1: 3 1 3 2 1 2 7478.4698 -0.0075 0.010
24: 6 0 6 5 0 5 15056.5590 -0.0071 0.010

S12. 1,1-Difluorosilacyclohex-2-ene Carbon-13 1 position

---
obs o-c error

/ instead of : below denotes (o-c)>3*err

1: 3 1 3 2 1 2 7470.2784 -0.0054 0.010
2: 3 0 3 2 0 2 7679.6169 -0.0025 0.010
3: 3 2 2 2 2 1 7743.9414 0.0025 0.010
4: 3 2 1 2 2 0 7808.2585 -0.0112 0.010
5: 3 1 2 2 1 1 7997.1495 0.0121 0.010
6: 4 1 4 3 1 3 9943.4284 0.0031 0.010
7: 4 0 4 3 0 3 10169.9538 0.0000 0.010
8: 4 2 3 3 2 2 10312.5334 0.0046 0.010
9/ 4 3 2 3 3 1 10355.1426 -0.0445 0.010
10: 4 3 1 3 3 0 10360.8506 -0.0045 0.010
11: 4 2 2 3 2 1 10467.7813 -0.0067 0.010
12: 4 1 3 3 1 2 10641.4945 0.0018 0.010
13: 5 1 5 4 1 4 12404.6107 0.0105 0.010
14: 5 0 5 4 0 4 12615.5768 0.0057 0.010
15: 5 2 4 4 2 3 12870.3057 -0.0108 0.010
16: 5 4 2 4 4 1 12942.7239 0.0149 0.010
17/ 5 4 1 4 4 0 12943.1086 0.0341 0.010
18: 5 3 3 4 3 2 12953.2925 0.0065 0.010
19: 5 3 2 4 3 1 12972.8775 -0.0084 0.010
20: 5 2 3 4 2 2 13160.9328 -0.0071 0.010
21: 5 1 4 4 1 3 13264.6715 0.0084 0.010
22: 6 1 6 5 1 5 14853.5842 -0.0026 0.010
23: 6 0 6 5 0 5 15026.4732 -0.0014 0.010
24: 6 2 5 5 2 4 15414.8591 -0.0007 0.010
25: 6 3 4 5 3 3 15553.3206 0.0022 0.010
26: 6 3 3 5 3 2 15604.4361 0.0143 0.010
27: 6 1 5 5 1 4 15858.0395 -0.0154 0.010
28: 6 2 4 5 2 3 15874.6070 0.0053 0.010
29: 7 1 7 6 1 6 17291.3039 -0.0084 0.010
30: 7 0 7 6 0 6 17418.8654 0.0129 0.010

31: 7 2 6 6 2 5 17944.0610 -0.0098 0.010
32/ 7 5 3 6 5 2 18127.0271 -0.0361 0.010
33: 7 5 2 6 5 1 18127.1945 0.0220 0.010
34: 7 2 5 6 2 4 18588.9646 0.0074 0.010

PARAMETERS IN FIT (values truncated):

10000 A /MHz 2709.91(3) 1
20000 B /MHz 1378.6273(7) 2
30000 C /MHz 1202.6919(8) 3
200 DJ /kHz 0.081(6) 4
1100 DJK /kHz 0.38(2) 5
2000 DK /kHz [-0.095727736] 6
40100 d1 /kHz [-0.011946691] 7
50000 d2 /kHz [0.007251909801] 8
300 HJ /Hz [-0.142448339] 9

MICROWAVE AVG = -0.000196 MHz, IR AVG = 0.00000
MICROWAVE RMS = 0.014304 MHz, IR RMS = 0.00000
END OF ITERATION 1 OLD, NEW RMS ERROR= 1.43043 1.43043

distinct frequency lines in fit: 34
distinct parameters of fit: 5

upper state lower state overall
limits of quantum number 1: 3 7 2 6 2 7
limits of quantum number 2: 0 5 0 5 0 5
limits of quantum number 3: 1 7 0 6 0 7

frequency range: 7470 18588

Standard errors are obtained by muliplying the previous errors by: 1.548842

PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:
(values rounded)

10000 A /MHz 2709.92(5) 1
20000 B /MHz 1378.627(1) 2
30000 C /MHz 1202.692(1) 3
200 DJ /kHz 0.08(1) 4
1100 DJK /kHz 0.39(3) 5
2000 DK /kHz [-0.095727736] 6
40100 d1 /kHz [-0.011946691] 7
50000 d2 /kHz [0.007251909801] 8

300 HJ /Hz [-0.142448339] 9

CORRELATION COEFFICIENTS, C.ij:

A B C -DJ -DJK

A 1.0000
B 0.6123 1.0000
C -0.6125 -0.2965 1.0000
-DJ -0.0669 -0.4369 -0.5842 1.0000
-DJK 0.2427 -0.0585 0.0057 -0.3379 1.0000

Mean value of |C.ij|, i.ne.j = 0.3254
Mean value of C.ij, i.ne.j = -0.1533

No correlations with absolute value greater than 0.9950

Worst fitted lines (obs-calc/error):

9: -4.4 32: -3.6 17: 3.4 33: 2.2
27: -1.5 16: 1.5 26: 1.4 30: 1.3
5: 1.2 4: -1.1 15: -1.1 13: 1.1
31: -1.0 21: 0.8 29: -0.8 19: -0.8
34: 0.7 20: -0.7 11: -0.7 18: 0.6
14: 0.6 1: -0.5 28: 0.5 8: 0.5
10: -0.4 6: 0.3 22: -0.3 2: -0.2
3: 0.2 25: 0.2 12: 0.2 23: -0.1
24: -0.1 7: 0.0

9/ 4 3 2 3 3 1 10355.1426 -0.0445 0.010
32/ 7 5 3 6 5 2 18127.0271 -0.0361 0.010
17/ 5 4 1 4 4 0 12943.1086 0.0341 0.010
33: 7 5 2 6 5 1 18127.1945 0.0220 0.010
27: 6 1 5 5 1 4 15858.0395 -0.0154 0.010
16: 5 4 2 4 4 1 12942.7239 0.0149 0.010
26: 6 3 3 5 3 2 15604.4361 0.0143 0.010
30: 7 0 7 6 0 6 17418.8654 0.0129 0.010
5: 3 1 2 2 1 1 7997.1495 0.0121 0.010
4: 3 2 1 2 2 0 7808.2585 -0.0112 0.010

S13. 1,1-Difluorosilacyclohex-2-ene Carbon-13 Position 2

---
obs o-c error

/ instead of : below denotes (o-c)>3*err

1: 3 1 3 2 1 2 7427.7374 0.0033 0.010
2: 3 0 3 2 0 2 7634.6821 -0.0060 0.010
3: 3 2 2 2 2 1 7696.0989 0.0005 0.010
4: 3 2 1 2 2 0 7757.5176 -0.0006 0.010
5: 3 1 2 2 1 1 7944.9564 0.0069 0.010
6: 4 1 4 3 1 3 9887.4150 -0.0021 0.010
7: 4 0 4 3 0 3 10112.9049 -0.0172 0.010
8: 4 2 3 3 2 2 10249.3226 -0.0032 0.010
9: 4 3 2 3 3 1 10290.0925 0.0023 0.010
10: 4 2 2 3 2 1 10397.8404 0.0103 0.010
11: 4 1 3 3 1 2 10572.9467 -0.0067 0.010
12: 5 1 5 4 1 4 12335.5810 0.0041 0.010
13: 5 0 5 4 0 4 12547.6515 0.0061 0.010
14: 5 2 4 4 2 3 12792.2490 0.0071 0.010
15: 5 4 2 4 4 1 12861.3223 0.0078 0.010
16: 5 4 1 4 4 0 12861.6157 -0.0281 0.010
17: 5 3 3 4 3 2 12871.6378 0.0060 0.010
18: 5 3 2 4 3 1 12889.8229 0.0049 0.010
19: 5 2 3 4 2 2 13071.0914 0.0056 0.010
20: 5 1 4 4 1 3 13180.8707 -0.0036 0.010
21: 6 1 6 5 1 5 14771.9275 0.0031 0.010
22: 6 0 6 5 0 5 14947.7869 0.0002 0.010
23: 6 2 5 5 2 4 15322.5184 0.0169 0.010
24: 6 4 3 5 4 2 15444.5250 -0.0035 0.010
25: 6 4 2 5 4 1 15446.0016 0.0001 0.010
26: 6 3 4 5 3 3 15455.2061 0.0061 0.010
27: 6 3 3 5 3 2 15502.6851 0.0054 0.010
28: 6 1 5 5 1 4 15760.6007 -0.0027 0.010
29: 6 2 4 5 2 3 15765.3794 -0.0197 0.010
30: 7 1 7 6 1 6 17197.2520 -0.0164 0.010
31: 7 0 7 6 0 6 17328.6852 0.0034 0.010
32: 7 2 6 6 2 5 17838.0806 0.0000 0.010
33: 7 3 5 6 3 4 18038.0404 0.0080 0.010

PARAMETERS IN FIT (values truncated):

10000 A /MHz 2716.36(3) 1
20000 B /MHz 1369.0359(8) 2
30000 C /MHz 1196.3364(8) 3
200 DJ /kHz 0.095(7) 4
1100 DJK /kHz 0.31(4) 5
2000 DK /kHz [-0.095727736] 6

40100 d1 /kHz [-0.011946691] 7
50000 d2 /kHz [0.007251909801] 8
300 HJ /Hz [-0.142448339] 9

MICROWAVE AVG = -0.000030 MHz, IR AVG = 0.00000
MICROWAVE RMS = 0.009145 MHz, IR RMS = 0.00000
END OF ITERATION 1 OLD, NEW RMS ERROR= 0.91446 0.91446

distinct frequency lines in fit: 33
distinct parameters of fit: 5

upper state lower state overall
limits of quantum number 1: 3 7 2 6 2 7
limits of quantum number 2: 0 4 0 4 0 4
limits of quantum number 3: 1 7 0 6 0 7

frequency range: 7427 18038

Standard errors are obtained by muliplying the previous errors by: 0.992756

PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:
(values rounded)

10000 A /MHz 2716.36(3) 1
20000 B /MHz 1369.0360(7) 2
30000 C /MHz 1196.3364(8) 3
200 DJ /kHz 0.095(7) 4
1100 DJK /kHz 0.32(3) 5
2000 DK /kHz [-0.095727736] 6
40100 d1 /kHz [-0.011946691] 7
50000 d2 /kHz [0.007251909801] 8
300 HJ /Hz [-0.142448339] 9

CORRELATION COEFFICIENTS, C.ij:

A B C -DJ -DJK

A 1.0000
B 0.5033 1.0000
C -0.5504 -0.2216 1.0000
-DJ -0.0912 -0.3787 -0.6442 1.0000
-DJK 0.3166 -0.2675 -0.0801 -0.2073 1.0000

Mean value of |C.ij|, i.ne.j = 0.3261
Mean value of C.ij, i.ne.j = -0.1621

No correlations with absolute value greater than 0.9950

Worst fitted lines (obs-calc/error):

16: -2.8 29: -2.0 7: -1.7 23: 1.7
30: -1.6 10: 1.0 33: 0.8 15: 0.8
14: 0.7 5: 0.7 11: -0.7 26: 0.6
13: 0.6 2: -0.6 17: 0.6 19: 0.6
27: 0.5 18: 0.5 12: 0.4 20: -0.4
24: -0.3 31: 0.3 1: 0.3 8: -0.3
21: 0.3 28: -0.3 9: 0.2 6: -0.2
4: -0.1 3: 0.1 22: 0.0 25: 0.0
32: 0.0

16: 5 4 1 4 4 0 12861.6157 -0.0281 0.010
29: 6 2 4 5 2 3 15765.3794 -0.0197 0.010
7: 4 0 4 3 0 3 10112.9049 -0.0172 0.010
23: 6 2 5 5 2 4 15322.5184 0.0169 0.010
30: 7 1 7 6 1 6 17197.2520 -0.0164 0.010
10: 4 2 2 3 2 1 10397.8404 0.0103 0.010
33: 7 3 5 6 3 4 18038.0404 0.0080 0.010
15: 5 4 2 4 4 1 12861.3223 0.0078 0.010
14: 5 2 4 4 2 3 12792.2490 0.0071 0.010
5: 3 1 2 2 1 1 7944.9564 0.0069 0.010

S14. 1,1-Difluorosilacyclohex-2-ene Carbon-13 Position 3

---
obs o-c error

/ instead of : below denotes (o-c)>3*err

1: 3 1 3 2 1 2 7396.2076 0.0074 0.010
2: 3 0 3 2 0 2 7597.2934 0.0032 0.010
3: 3 2 2 2 2 1 7652.3271 0.0009 0.010
4: 3 2 1 2 2 0 7707.3799 0.0076 0.010
5: 3 1 2 2 1 1 7890.9997 -0.0032 0.010
6: 4 1 4 3 1 3 9846.9713 -0.0041 0.010
7: 4 0 4 3 0 3 10069.4554 -0.0025 0.010
8: 4 2 3 3 2 2 10192.2415 -0.0027 0.010
9: 4 3 2 3 3 1 10228.8576 0.0092 0.010
10: 4 3 1 3 3 0 10233.2521 0.0043 0.010
11: 4 2 2 3 2 1 10325.8577 -0.0040 0.010

12: 4 1 3 3 1 2 10503.2890 -0.0037 0.010
13: 5 1 5 4 1 4 12287.2224 -0.0060 0.010
14: 5 0 5 4 0 4 12501.0250 0.0123 0.010
15: 5 2 4 4 2 3 12722.9315 0.0025 0.010
16/ 5 3 3 4 3 2 12794.3997 -0.0304 0.010
17: 5 3 2 4 3 1 12809.6911 0.0150 0.010
18: 5 2 3 4 2 2 12975.5354 0.0043 0.010
19: 5 1 4 4 1 3 13097.8847 0.0120 0.010
20: 6 1 6 5 1 5 14716.5339 -0.0084 0.010
21: 6 0 6 5 0 5 14898.6005 -0.0061 0.010
22: 6 2 5 5 2 4 15242.2526 -0.0017 0.010
23: 6 4 3 5 4 2 15351.5277 -0.0001 0.010
24: 6 4 2 5 4 1 15352.6681 -0.0132 0.010
25: 6 3 4 5 3 3 15362.2073 0.0058 0.010
26: 6 3 3 5 3 2 15402.1144 -0.0007 0.010
27: 6 2 4 5 2 3 15647.1212 -0.0007 0.010
28: 6 1 5 5 1 4 15667.6709 -0.0083 0.010
29: 7 1 7 6 1 6 17135.4876 0.0063 0.010
30: 7 0 7 6 0 6 17275.5599 0.0051 0.010
31: 7 2 6 6 2 5 17748.3434 -0.0050 0.010
32: 7 5 3 6 5 2 17904.7900 -0.0034 0.010
33/ 7 4 4 6 4 3 17923.1870 0.0446 0.010
34: 7 4 3 6 4 2 17926.9295 -0.0234 0.010
35: 7 3 5 6 3 4 17929.8422 -0.0071 0.010

PARAMETERS IN FIT (values truncated):

10000 A /MHz 2741.70(3) 1
20000 B /MHz 1357.9808(7) 2
30000 C /MHz 1192.8001(8) 3
200 DJ /kHz 0.073(7) 4
1100 DJK /kHz 0.33(3) 5
2000 DK /kHz [-0.095727736] 6
40100 d1 /kHz [-0.011946691] 7
50000 d2 /kHz [0.007251909801] 8
300 HJ /Hz [-0.142448339] 9

MICROWAVE AVG = 0.000160 MHz, IR AVG = 0.00000
MICROWAVE RMS = 0.011832 MHz, IR RMS = 0.00000
END OF ITERATION 1 OLD, NEW RMS ERROR= 1.18322 1.18322

distinct frequency lines in fit: 35
distinct parameters of fit: 5

upper state lower state overall

limits of quantum number 1: 3 7 2 6 2 7
limits of quantum number 2: 0 5 0 5 0 5
limits of quantum number 3: 1 7 0 6 0 7

frequency range: 7396 17929

Standard errors are obtained by muliplying the previous errors by: 1.278024

PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:
(values rounded)

10000 A /MHz 2741.71(4) 1
20000 B /MHz 1357.9809(9) 2
30000 C /MHz 1192.800(1) 3
200 DJ /kHz 0.074(9) 4
1100 DJK /kHz 0.33(4) 5
2000 DK /kHz [-0.095727736] 6
40100 d1 /kHz [-0.011946691] 7
50000 d2 /kHz [0.007251909801] 8
300 HJ /Hz [-0.142448339] 9

CORRELATION COEFFICIENTS, C.ij:

A B C -DJ -DJK

A 1.0000
B 0.5668 1.0000
C -0.5326 -0.3255 1.0000
-DJ -0.1306 -0.3355 -0.6215 1.0000
-DJK 0.3168 -0.0903 0.1616 -0.5286 1.0000

Mean value of |C.ij|, i.ne.j = 0.3610
Mean value of C.ij, i.ne.j = -0.1519

No correlations with absolute value greater than 0.9950

Worst fitted lines (obs-calc/error):

33: 4.5 16: -3.0 34: -2.3 17: 1.5
24: -1.3 14: 1.2 19: 1.2 9: 0.9
20: -0.8 28: -0.8 4: 0.8 1: 0.7
35: -0.7 29: 0.6 21: -0.6 13: -0.6
25: 0.6 30: 0.5 31: -0.5 10: 0.4

18: 0.4 6: -0.4 11: -0.4 12: -0.4
32: -0.3 2: 0.3 5: -0.3 8: -0.3
15: 0.2 7: -0.2 22: -0.2 3: 0.1
27: -0.1 26: -0.1 23: 0.0

33/ 7 4 4 6 4 3 17923.1870 0.0446 0.010
16/ 5 3 3 4 3 2 12794.3997 -0.0304 0.010
34: 7 4 3 6 4 2 17926.9295 -0.0234 0.010
17: 5 3 2 4 3 1 12809.6911 0.0150 0.010
24: 6 4 2 5 4 1 15352.6681 -0.0132 0.010
14: 5 0 5 4 0 4 12501.0250 0.0123 0.010
19: 5 1 4 4 1 3 13097.8847 0.0120 0.010
9: 4 3 2 3 3 1 10228.8576 0.0092 0.010
20: 6 1 6 5 1 5 14716.5339 -0.0084 0.010
28: 6 1 5 5 1 4 15667.6709 -0.0083 0.010

S15. 1,1-Difluorosilacyclohex-2-ene Carbon-13 Position 4

---
obs o-c error

/ instead of : below denotes (o-c)>3*err

1: 3 1 3 2 1 2 7429.8783 -0.0007 0.010
2: 3 0 3 2 0 2 7636.3405 0.0043 0.010
3: 3 2 2 2 2 1 7697.1918 0.0044 0.010
4: 3 2 1 2 2 0 7758.0406 -0.0080 0.010
5: 3 1 2 2 1 1 7945.1627 -0.0014 0.010
6: 4 1 4 3 1 3 9890.4140 -0.0042 0.010
7: 4 0 4 3 0 3 10115.6617 -0.0150 0.010
8: 4 2 3 3 2 2 10250.8909 -0.0005 0.010
9: 4 3 2 3 3 1 10291.2846 -0.0061 0.010
10: 4 2 2 3 2 1 10398.0951 -0.0006 0.010
11: 4 1 3 3 1 2 10573.4374 -0.0034 0.010
12: 5 1 5 4 1 4 12339.5157 -0.0060 0.010
13: 5 0 5 4 0 4 12551.7615 0.0115 0.010
14: 5 2 4 4 2 3 12794.3997 0.0201 0.010
15: 5 3 3 4 3 2 12873.0873 0.0081 0.010
16: 5 3 2 4 3 1 12890.9962 -0.0045 0.010
17: 5 2 3 4 2 2 13070.9523 0.0073 0.010
18: 5 1 4 4 1 3 13181.8517 0.0063 0.010
19: 6 1 6 5 1 5 14776.8793 -0.0094 0.010
20: 6 0 6 5 0 5 14953.2761 -0.0063 0.010
21: 6 2 5 5 2 4 15325.3429 0.0168 0.010
22: 6 5 1 5 5 0 15432.9172 -0.0093 0.010

23: 6 5 2 5 5 1 15432.9217 0.0121 0.010
24: 6 4 3 5 4 2 15446.2185 -0.0138 0.010
25: 6 4 2 5 4 1 15447.6836 0.0079 0.010
26: 6 3 4 5 3 3 15456.9087 -0.0032 0.010
27: 6 3 3 5 3 2 15503.7090 -0.0030 0.010
28: 6 1 5 5 1 4 15762.3587 -0.0029 0.010
29: 6 2 4 5 2 3 15764.9423 -0.0019 0.010
30: 7 1 7 6 1 6 17203.3221 0.0155 0.010
31: 7 0 7 6 0 6 17335.4355 -0.0063 0.010
32: 7 2 6 6 2 5 17841.7138 -0.0058 0.010
33: 7 2 5 6 2 4 18461.5463 -0.0050 0.010

PARAMETERS IN FIT (values truncated):

10000 A /MHz 2719.11(3) 1
20000 B /MHz 1368.8934(7) 2
30000 C /MHz 1196.8416(8) 3
200 DJ /kHz 0.083(7) 4
1100 DJK /kHz 0.33(2) 5
2000 DK /kHz [-0.095727736] 6
40100 d1 /kHz [-0.011946691] 7
50000 d2 /kHz [0.007251909801] 8
300 HJ /Hz [-0.142448339] 9

MICROWAVE AVG = -0.000099 MHz, IR AVG = 0.00000
MICROWAVE RMS = 0.008594 MHz, IR RMS = 0.00000
END OF ITERATION 1 OLD, NEW RMS ERROR= 0.85939 0.85939

distinct frequency lines in fit: 33
distinct parameters of fit: 5

upper state lower state overall
limits of quantum number 1: 3 7 2 6 2 7
limits of quantum number 2: 0 5 0 5 0 5
limits of quantum number 3: 1 7 0 6 0 7

frequency range: 7429 18461

Standard errors are obtained by muliplying the previous errors by: 0.932971

PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:
(values rounded)

10000 A /MHz 2719.12(3) 1

20000 B /MHz 1368.8934(7) 2
30000 C /MHz 1196.8417(8) 3
200 DJ /kHz 0.083(6) 4
1100 DJK /kHz 0.33(2) 5
2000 DK /kHz [-0.095727736] 6
40100 d1 /kHz [-0.011946691] 7
50000 d2 /kHz [0.007251909801] 8
300 HJ /Hz [-0.142448339] 9

CORRELATION COEFFICIENTS, C.ij:

A B C -DJ -DJK

A 1.0000
B 0.5765 1.0000
C -0.6067 -0.1979 1.0000
-DJ -0.0233 -0.4894 -0.6338 1.0000
-DJK 0.2271 -0.1497 -0.1035 -0.1361 1.0000

Mean value of |C.ij|, i.ne.j = 0.3144
Mean value of C.ij, i.ne.j = -0.1537

No correlations with absolute value greater than 0.9950

Worst fitted lines (obs-calc/error):

14: 2.0 21: 1.7 30: 1.6 7: -1.5
24: -1.4 23: 1.2 13: 1.1 19: -0.9
22: -0.9 15: 0.8 4: -0.8 25: 0.8
17: 0.7 20: -0.6 18: 0.6 31: -0.6
9: -0.6 12: -0.6 32: -0.6 33: -0.5
16: -0.4 3: 0.4 2: 0.4 6: -0.4
11: -0.3 26: -0.3 27: -0.3 28: -0.3
29: -0.2 5: -0.1 1: -0.1 10: -0.1
8: -0.1

14: 5 2 4 4 2 3 12794.3997 0.0201 0.010
21: 6 2 5 5 2 4 15325.3429 0.0168 0.010
30: 7 1 7 6 1 6 17203.3221 0.0155 0.010
7: 4 0 4 3 0 3 10115.6617 -0.0150 0.010
24: 6 4 3 5 4 2 15446.2185 -0.0138 0.010
23: 6 5 2 5 5 1 15432.9217 0.0121 0.010
13: 5 0 5 4 0 4 12551.7615 0.0115 0.010
19: 6 1 6 5 1 5 14776.8793 -0.0094 0.010

22: 6 5 1 5 5 0 15432.9172 -0.0093 0.010
15: 5 3 3 4 3 2 12873.0873 0.0081 0.010

S16. 1,1-Difluorosilacyclohex-2-ene Carbon-13 Position 5

---
obs o-c error

/ instead of : below denotes (o-c)>3*err

1: 3 1 3 2 1 2 7472.0647 -0.0003 0.010
2: 3 0 3 2 0 2 7679.9143 0.0001 0.010
3: 3 2 2 2 2 1 7743.0711 0.0060 0.010
4: 3 2 1 2 2 0 7806.2245 -0.0023 0.010
5: 3 1 2 2 1 1 7993.9780 -0.0082 0.010
6: 4 1 4 3 1 3 9946.0974 0.0031 0.010
7: 4 0 4 3 0 3 10171.5140 -0.0060 0.010
8: 4 2 3 3 2 2 10311.6025 0.0045 0.010
9: 4 3 2 3 3 1 10353.4908 -0.0021 0.010
10: 4 3 1 3 3 0 10358.9916 -0.0142 0.010
11: 4 2 2 3 2 1 10464.1282 0.0019 0.010
12: 4 1 3 3 1 2 10637.7118 0.0061 0.010
13: 5 1 5 4 1 4 12408.3442 0.0022 0.010
14: 5 0 5 4 0 4 12618.9520 0.0031 0.010
15: 5 2 4 4 2 3 12869.5280 0.0023 0.010
16: 5 4 2 4 4 1 12940.5912 0.0036 0.010
17: 5 4 1 4 4 0 12940.9313 -0.0086 0.010
18: 5 3 3 4 3 2 12951.0480 0.0027 0.010
19: 5 3 2 4 3 1 12970.1062 -0.0071 0.010
20: 5 2 3 4 2 2 13155.3226 -0.0034 0.010
21: 5 1 4 4 1 3 13260.6788 0.0059 0.010
22: 6 1 6 5 1 5 14858.5632 -0.0015 0.010
23: 6 0 6 5 0 5 15031.8137 -0.0051 0.010
24: 6 2 5 5 2 4 15414.4532 0.0072 0.010
25: 6 4 3 5 4 2 15539.9657 0.0068 0.010
26: 6 3 4 5 3 3 15550.5619 0.0059 0.010
27: 6 3 3 5 3 2 15600.2999 0.0056 0.010
28: 6 1 5 5 1 4 15854.4806 -0.0016 0.010
29: 7 1 7 6 1 6 17297.6468 -0.0009 0.010
30: 7 0 7 6 0 6 17425.9961 0.0061 0.010
31: 7 2 6 6 2 5 17944.2838 -0.0147 0.010

PARAMETERS IN FIT (values truncated):

10000 A /MHz 2709.44(3) 1

20000 B /MHz 1377.6552(8) 2
30000 C /MHz 1203.3726(9) 3
200 DJ /kHz 0.085(8) 4
1100 DJK /kHz 0.36(4) 5
2000 DK /kHz [-0.095727736] 6
40100 d1 /kHz [-0.011946691] 7
50000 d2 /kHz [0.007251909801] 8
300 HJ /Hz [-0.142448339] 9

MICROWAVE AVG = -0.000092 MHz, IR AVG = 0.00000
MICROWAVE RMS = 0.005946 MHz, IR RMS = 0.00000
END OF ITERATION 1 OLD, NEW RMS ERROR= 0.59464 0.59464

distinct frequency lines in fit: 31
distinct parameters of fit: 5

upper state lower state overall
limits of quantum number 1: 3 7 2 6 2 7
limits of quantum number 2: 0 4 0 4 0 4
limits of quantum number 3: 1 7 0 6 0 7

frequency range: 7472 17944

Standard errors are obtained by muliplying the previous errors by: 0.649304

PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:
(values rounded)

10000 A /MHz 2709.44(2) 1
20000 B /MHz 1377.6553(5) 2
30000 C /MHz 1203.3727(5) 3
200 DJ /kHz 0.085(5) 4
1100 DJK /kHz 0.36(3) 5
2000 DK /kHz [-0.095727736] 6
40100 d1 /kHz [-0.011946691] 7
50000 d2 /kHz [0.007251909801] 8
300 HJ /Hz [-0.142448339] 9

CORRELATION COEFFICIENTS, C.ij:

A B C -DJ -DJK

A 1.0000
B 0.3938 1.0000
C -0.4334 -0.2041 1.0000

-DJ -0.2066 -0.2925 -0.6753 1.0000
-DJK 0.4108 -0.3459 -0.0613 -0.2423 1.0000

Mean value of |C.ij|, i.ne.j = 0.3266
Mean value of C.ij, i.ne.j = -0.1657

No correlations with absolute value greater than 0.9950

Worst fitted lines (obs-calc/error):

31: -1.5 10: -1.4 17: -0.9 5: -0.8
24: 0.7 19: -0.7 25: 0.7 30: 0.6
12: 0.6 7: -0.6 3: 0.6 21: 0.6
26: 0.6 27: 0.6 23: -0.5 8: 0.4
16: 0.4 20: -0.3 6: 0.3 14: 0.3
18: 0.3 4: -0.2 15: 0.2 13: 0.2
9: -0.2 11: 0.2 28: -0.2 22: -0.1
29: -0.1 1: 0.0 2: 0.0

31: 7 2 6 6 2 5 17944.2838 -0.0147 0.010
10: 4 3 1 3 3 0 10358.9916 -0.0142 0.010
17: 5 4 1 4 4 0 12940.9313 -0.0086 0.010
5: 3 1 2 2 1 1 7993.9780 -0.0082 0.010
24: 6 2 5 5 2 4 15414.4532 0.0072 0.010
19: 5 3 2 4 3 1 12970.1062 -0.0071 0.010
25: 6 4 3 5 4 2 15539.9657 0.0068 0.010
30: 7 0 7 6 0 6 17425.9961 0.0061 0.010
12: 4 1 3 3 1 2 10637.7118 0.0061 0.010
7: 4 0 4 3 0 3 10171.5140 -0.0060 0.010

APPENDIX D.

SUPPLIMENTARY MATERIAL FOR CONSTRUCTION AND DEMONSTRATION OF A 6-18 GHZ MICROWAVE THREE-WAVE MIXING EXPERIMENT USING MULTIPLE SYNCHRONIZED ARBITRARY WAVEFORM GENERATORS

Alfa Aesar

Certificate of analysis

Product No.:	A13900
Product:	(R)-(-)-Carvone, 98%
Lot No.:	10216199

Appearance:	Clear colourless liquid
Refractive index:	1.4989 @20°C
Assay (GC):	99.3%
Optical rotation:	-61.1° (neat)
Identification (FTIR):	Conforms

ThermoFisher SCIENTIFIC

Certificate of Analysis

Product No.:	L07130
Product:	(S)-(+)-Carvone, 96%
Lot No.:	10220183

Appearance:	Clear pale yellow liquid
Refractive index:	1.4995 @20°C
Assay (GC):	98.9%
Optical rotation:	+56.2° (neat)
Identification (FTIR):	Conforms

APPENDIX E.

SUPPORTING INFORMATION FOR INTERNAL ROTATION ANALYSIS AND STRUCTURE DETERMINATION OF R-CARVONE

INTERNAL ROTATION ANALYSIS AND STRUCTURE DETERMINATION OF R-CARVONE

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SUPPORTING INFORMATION

Table of Contents:

S1. Quality Documentation for R-Carvone

Alfa Aesar

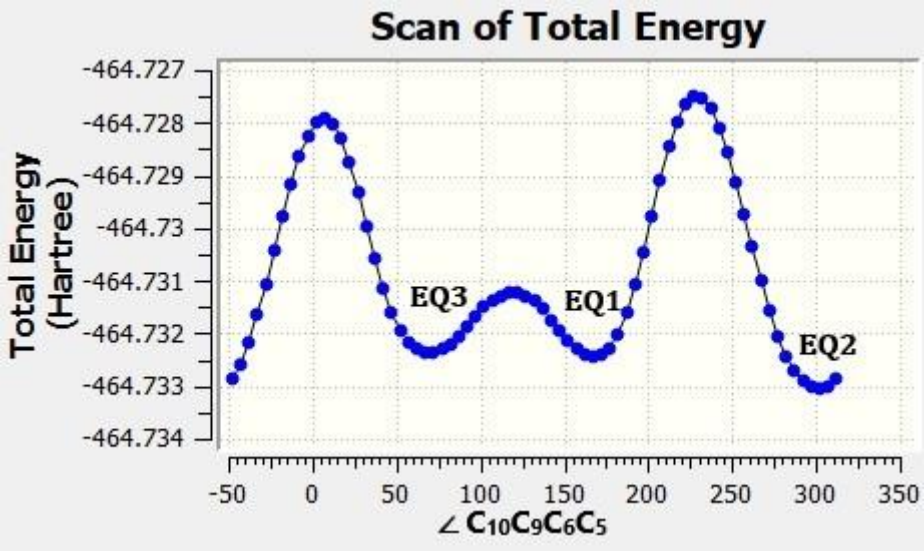
Certificate of analysis

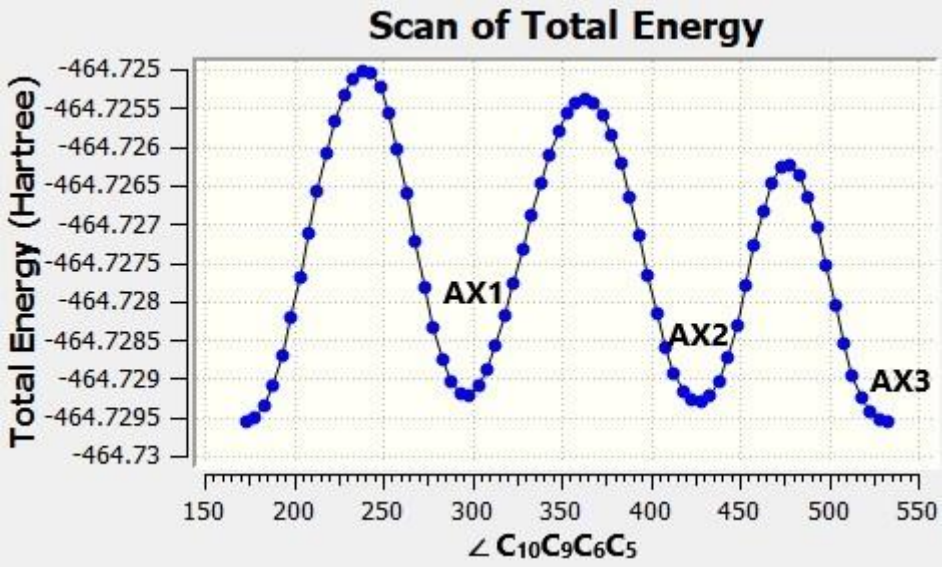
Product No.:	A13900
Product:	(R)-(-)-Carvone, 98%
Lot No.:	10216199

Appearance:	Clear colourless liquid
Refractive index:	1.4989 @20°C
Assay (GC):	99.3%
Optical rotation:	-61.1° (neat)
Identification (FTIR):	Conforms

S2. Interconversion Barriers for Equatorial and Axial Conformers

Interconversion barriers between the conformers of carvone, equatorial (top) and axial (bottom), calculated at the B3LYP/6-31++G(d,p) level of theory.





S3. EQ1 Assignments and Outputs of Structure Evaluation - Isotopologue Overview

Ground Vibrational State	$^{13}C_1$		$^{13}C_2$		$^{13}C_3$		$^{13}C_4$	
	Experiment	Theory	Experiment	Theory	Experiment	Theory	Experiment	Theory
A (MHz)	2,236.89720 (76)	2,236.9	2,232.33843 (95)	2,224.7	2,253.91884 (77)	2,225.9	2,249.8237 (14)	2,244.5
B (MHz)	672.57330 (21)	672.6	671.86307 (16)	647.4	669.66273 (19)	645.3	671.112071 (30)	672.9
C (MHz)	553.27973 (23)	553.28	552.42439 (15)	570.3	552.11950 (19)	570.1	552.86195 (32)	553.8
D_J (kHz)	0.00970 (48)		[0.01120]		0.01339 (62)		0.01330 (73)	
D_{JK} (kHz)	0.0210 (21)		0.0161 (34)		0.0270 (32)		0.0251 (42)	
D_K (kHz)	-0.1722 (34)		[-0.1538]		-0.1538 (42)		-0.1478 (58)	
V_{3_1} (cm^{-1})	535 (5)		[524.61]		525.38 (32)		524.41 (64)	
δ_1 (radian)	1.183 (23)		[1.2260]		1.2225 (18)		[1.2260]	
ε_1 (radian)	[1.476]		[1.476]		[1.476]		[1.476]	
V_{3_2} (cm^{-1})	491 (1)		[492.70]		493.57 (33)		492.62 (13)	
δ_2 (radian)	2.807 (37)		[2.880]		2.918 (14)		[2.880]	
ε_2 (radian)	3.75 (17)		[3.836]		[3.836]		[3.836]	
ν_{RMS} (kHz)	20.4		21.0		19.8		23.5	
Number of Transitions	197		63		203		71	

	$^{13}C_5$		$^{13}C_6$		$^{13}C_7$		$^{13}C_9$	
	Experiment	Theory	Experiment	Theory	Experiment	Theory	Experiment	Theory
A (MHz)	2,244.4545 (18)	2,244.5	2,256.24953 (80)	2256.2	2,251.02460 (83)	2,251.0	2,256.6626 (17)	2,256.7
B (MHz)	672.88935 (66)	672.9	672.11091 (20)	672.1	662.78729 (21)	662.8	667.75736 (31)	667.8
C (MHz)	553.78810 (62)	553.8	554.00602 (23)	554.0	547.27594 (23)	547.3	551.00167 (30)	551.0
D_J (kHz)	0.0122 (15)		0.00827 (54)		0.01119 (70)		0.01205 (66)	
D_{JK} (kHz)	0.0309 (76)		0.0345 (41)		0.0161 (33)		0.0407 (43)	
D_K (kHz)	-0.1561 (11)		-0.1397 (63)		-0.1587 (56)		[-0.1538]	
V_{3_1} (cm^{-1})	[524.61]		524.50 (36)		524.03 (32)		[524.61]	
δ_1 (radian)	[1.2260]		1.2249 (24)		1.2314 (18)		[1.2260]	
ε_1 (radian)	[1.476]		[1.476]		[1.476]		[1.476]	
V_{3_2} (cm^{-1})	[492.70]		493 (1)		492 (1)		[492.70]	
δ_2 (radian)	[2.880]		2.922 (56)		2.895 (53)		[2.880]	
ε_2 (radian)	[3.836]		3.87 (24)		4.00 (27)		[3.836]	
ν_{RMS} (kHz)	21.6		21.9		20.7		22.2	
Number of Transitions	25		151		151		51	

	$^{13}C_{10}$		$^{13}C_{11}$		^{18}O	
	Experiment	Theory	Experiment	Theory	Experiment	Theory
A (MHz)	2,244.39722 (87)	2,244.4	2.239.4735 (11)	2,239.5	2192.64120 (95)	2,171.1
B (MHz)	662.81528 (26)	662.8	664.99315 (25)	665.0	665.22383 (34)	648.7
C (MHz)	547.50145 (23)	547.5	548.53319 (24)	548.5	544.85625 (33)	568.2
D_J (kHz)	0.01620 (67)		0.00982 (73)		[0.01120]	
D_{JK} (kHz)	0.0296 (39)		0.0194 (37)		[0.02291]	
D_K (kHz)	-0.1552 (39)		-0.111 (15)		[-0.1538]	
V_{3_1} (cm^{-1})	524.92 (34)		523.92 (66)		[524.61]	
δ_1 (radian)	1.2205 (22)		1.2294 (31)		[1.2260]	
ε_1 (radian)	[1.476]		[1.476]		[1.476]	
V_{3_2} (cm^{-1})	492 (1)		492.86 (22)		[492.70]	
δ_2 (radian)	2.868 (41)		2.8887 (81)		[2.880]	
ε_2 (radian)	3.80 (14)		[3.836]		[3.836]	
ν_{RMS} (kHz)	22.2		22.7		22.0	
Number of Transitions	128		146		19	

Parent XIAM Output

J K- K+	J K- K+	Sym	calc/GHz	diff/MHz	obs/GHz		
1: 8 2 7	7 2 6	S 3	9.7418447	0.0153	9.7418599	Err 0.1D-04	-
2: 8 1 8	7 0 7	S 1	9.8021820	-0.0437	9.8021383	Err 0.1D-04	-
3: 8 7 1	7 7 0	S 1	9.8391329	-0.0015	9.8391314	Err 0.1D-04	-
4: 8 6 2	7 6 1	S 1	9.8433671	0.0234	9.8433905	Err 0.1D-04	-
5: 8 6 2	7 6 1	S 5	9.8433497	0.0071	9.8433568	Err 0.1D-04	-
6: 8 5 3	7 5 2	S 1	9.8505565	-0.0166	9.8505399	Err 0.1D-04	-
7: 8 4 5	7 4 4	S 1	9.8633253	-0.0012	9.8633242	Err 0.1D-04	-
8: 8 4 4	7 4 3	S 1	9.8652989	-0.0056	9.8652933	Err 0.1D-04	-
9: 8 3 5	7 3 4	S 3	9.9232006	0.0007	9.9232013	Err 0.1D-04	-
10: 14 4 10	14 3 11	S 4	10.0035779	0.0018	10.0035797	Err 0.1D-04	-
11: 14 4 10	14 3 11	S 2	10.0037024	-0.0152	10.0036872	Err 0.1D-04	-
12: 14 4 10	14 3 11	S 3	10.0038143	0.0347	10.0038490	Err 0.1D-04	-
13: 17 2 15	17 1 16	S 1	10.0616141	-0.0223	10.0615918	Err 0.1D-04	-
14: 8 2 6	7 2 5	S 1	10.1683182	-0.0055	10.1683127	Err 0.1D-04	-
15: 6 1 5	5 0 5	S 1	10.3629002	0.0039	10.3629041	Err 0.1D-04	-
16: 9 1 9	8 1 8	S 1	10.3731573	-0.0228	10.3731345	Err 0.1D-04	-
17: 9 0 9	8 0 8	S 1	10.4908638	-0.0254	10.4908384	Err 0.1D-04	-
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33: 5 2 3	4 1 4	S 4	11.8727054	0.0138	11.8727192	Err 0.1D-04	-
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721: 13 1 12 12 1 11 S 2 15.9326257 -0.0052 15.9326204 Err 0.1D-04 -
722: 13 1 12 12 1 11 S 3 15.9326135 0.0069 15.9326204 Err 0.1D-04 -
723: 13 1 12 12 1 11 S 4 15.9325922 0.0282 15.9326204 Err 0.1D-04 -
724: 13 1 12 12 1 11 S 5 15.9325896 0.0308 15.9326204 Err 0.1D-04 -
725: 14 1 13 13 2 12 S 5 15.9562669 0.0142 15.9562811 Err 0.1D-04 -
726: 14 1 13 13 2 12 S 4 15.9562825 -0.0015 15.9562811 Err 0.1D-04 -
727: 14 1 13 13 2 12 S 2 15.9562965 -0.0154 15.9562811 Err 0.1D-04 -
728: 14 1 14 13 1 13 S 2 15.9673971 -0.0375 15.9673595 Err 0.1D-04 -

729: 13 11 2 12 11 1 S 5 15.9895010 0.0170 15.9895179 Err 0.1D-04 -
730: 13 11 2 12 11 1 S 4 15.9895044 0.0136 15.9895179 Err 0.1D-04 -
731: 13 11 2 12 11 1 S 3 15.9895054 0.0126 15.9895179 Err 0.1D-04 -
732: 13 11 2 12 11 1 S 1 15.9895268 -0.0088 15.9895179 Err 0.1D-04 -
733: 13 10 3 12 10 2 S 2 15.9936795 -0.0029 15.9936765 Err 0.1D-04 -
734: 13 10 3 12 10 2 S 3 15.9936631 0.0135 15.9936765 Err 0.1D-04 -
735: 13 10 3 12 10 2 S 4 15.9936616 0.0149 15.9936765 Err 0.1D-04 -
736: 13 10 3 12 10 2 S 5 15.9936582 0.0184 15.9936765 Err 0.1D-04 -
737: 13 9 4 12 9 3 S 2 15.9993186 -0.0091 15.9993095 Err 0.1D-04 -
738: 13 9 4 12 9 3 S 3 15.9993030 0.0065 15.9993095 Err 0.1D-04 -
739: 13 9 4 12 9 3 S 4 15.9993010 0.0085 15.9993095 Err 0.1D-04 -
740: 13 9 4 12 9 3 S 5 15.9992973 0.0122 15.9993095 Err 0.1D-04 -
741: 13 8 5 12 8 4 S 4 16.0072327 0.0026 16.0072353 Err 0.1D-04 -
742: 13 8 5 12 8 4 S 3 16.0072356 -0.0003 16.0072353 Err 0.1D-04 -
743: 13 8 5 12 8 4 S 2 16.0072499 -0.0146 16.0072353 Err 0.1D-04 -
744: 13 8 5 12 8 4 S 1 16.0072569 -0.0215 16.0072353 Err 0.1D-04 -
745: 13 7 6 12 7 5 S 1 16.0189440 -0.0254 16.0189186 Err 0.1D-04 -
746: 13 7 6 12 7 5 S 3 16.0189215 -0.0029 16.0189186 Err 0.1D-04 -
747: 13 7 6 12 7 5 S 4 16.0189174 0.0013 16.0189186 Err 0.1D-04 -
748: 13 7 6 12 7 5 S 5 16.0189124 0.0062 16.0189186 Err 0.1D-04 -
749: 13 3 11 12 3 10 S 2 16.0243754 -0.0237 16.0243517 Err 0.1D-04 -
750: 13 3 11 12 3 10 S 5 16.0243592 -0.0075 16.0243517 Err 0.1D-04 -
751: 13 3 11 12 3 10 S 3 16.0243513 0.0004 16.0243517 Err 0.1D-04 -
752: 13 3 11 12 3 10 S 4 16.0243508 0.0009 16.0243517 Err 0.1D-04 -
753: 13 6 7 12 6 6 S 3 16.0372428 0.0105 16.0372534 Err 0.1D-04 -
754: 13 6 7 12 6 6 S 4 16.0372354 0.0180 16.0372534 Err 0.1D-04 -
755: 13 6 7 12 6 6 S 5 16.0372283 0.0250 16.0372534 Err 0.1D-04 -
756: 13 4 10 12 4 9 S 3 16.1002251 0.0022 16.1002273 Err 0.1D-04 -
757: 12 2 11 11 1 10 S 5 16.2138571 0.0409 16.2138979 Err 0.2D-04 -
758: 12 2 11 11 1 10 S 4 16.2138528 0.0451 16.2138979 Err 0.2D-04 -
759: 13 3 10 12 3 9 S 5 16.4812299 0.0019 16.4812318 Err 0.1D-04 -
760: 13 3 10 12 3 9 S 3 16.4812338 -0.0020 16.4812318 Err 0.1D-04 -
761: 13 3 10 12 3 9 S 4 16.4812381 -0.0063 16.4812318 Err 0.1D-04 -
762: 13 3 10 12 3 9 S 2 16.4812410 -0.0092 16.4812318 Err 0.1D-04 -
763: 13 2 11 12 2 10 S 2 16.6200194 -0.0106 16.6200089 Err 0.1D-04 -
764: 13 2 11 12 2 10 S 3 16.6200133 -0.0044 16.6200089 Err 0.1D-04 -
765: 13 2 11 12 2 10 S 5 16.6200039 0.0050 16.6200089 Err 0.1D-04 -
766: 14 2 13 13 2 12 S 4 16.7602380 0.0195 16.7602576 Err 0.1D-04 -
767: 14 2 13 13 2 12 S 5 16.7602425 0.0151 16.7602576 Err 0.1D-04 -
768: 14 2 13 13 2 12 S 3 16.7602513 0.0062 16.7602576 Err 0.1D-04 -
769: 14 2 13 13 2 12 S 2 16.7602693 -0.0118 16.7602576 Err 0.1D-04 -
770: 13 2 12 12 1 11 S 3 17.0049314 -0.0156 17.0049158 Err 0.1D-04 -
771: 14 1 13 13 1 12 S 1 17.0285811 -0.0477 17.0285333 Err 0.1D-04 -

772: 14 1 13 13 1 12 S 2 17.0285562 -0.0229 17.0285333 Err 0.1D-04 -
773: 14 1 13 13 1 12 S 3 17.0285403 -0.0070 17.0285333 Err 0.1D-04 -
774: 14 1 13 13 1 12 S 5 17.0285133 0.0200 17.0285333 Err 0.1D-04 -
775: 14 12 2 13 12 1 S 1 17.2188952 -0.0268 17.2188684 Err 0.1D-04 -
776: 14 12 3 13 12 2 S 5 17.2188761 -0.0077 17.2188684 Err 0.1D-04 -
777: 14 12 2 13 12 1 S 3 17.2188722 -0.0038 17.2188684 Err 0.1D-04 -
778: 14 12 2 13 12 1 S 4 17.2188714 -0.0030 17.2188684 Err 0.1D-04 -
779: 14 12 2 13 12 1 S 5 17.2188676 0.0008 17.2188684 Err 0.1D-04 -
780: 14 11 3 13 11 2 S 2 17.2228302 -0.0085 17.2228218 Err 0.1D-04 -
781: 14 11 3 13 11 2 S 3 17.2228123 0.0095 17.2228218 Err 0.1D-04 -
782: 14 11 3 13 11 2 S 4 17.2228111 0.0107 17.2228218 Err 0.1D-04 -
783: 14 11 3 13 11 2 S 5 17.2228073 0.0145 17.2228218 Err 0.1D-04 -
784: 14 10 5 13 10 3 S 1 17.2280277 -0.0122 17.2280155 Err 0.1D-04 -
785: 14 10 4 13 10 3 S 3 17.2280048 0.0107 17.2280155 Err 0.1D-04 -
786: 14 10 4 13 10 3 S 4 17.2280031 0.0124 17.2280155 Err 0.1D-04 -
787: 14 10 4 13 10 3 S 5 17.2279992 0.0163 17.2280155 Err 0.1D-04 -
788: 14 9 5 13 9 4 S 3 17.2350512 0.0083 17.2350595 Err 0.1D-04 -
789: 14 9 5 13 9 4 S 4 17.2350488 0.0107 17.2350595 Err 0.1D-04 -
790: 14 9 5 13 9 4 S 5 17.2350446 0.0149 17.2350595 Err 0.1D-04 -
791: 14 9 5 13 9 4 S 2 17.2350675 -0.0080 17.2350595 Err 0.1D-04 -
792: 14 3 12 13 3 11 S 4 17.2365182 0.0263 17.2365445 Err 0.1D-04 -
793: 14 3 12 13 3 11 S 5 17.2365233 0.0211 17.2365445 Err 0.1D-04 -
794: 14 3 12 13 3 11 S 2 17.2365439 0.0006 17.2365445 Err 0.1D-04 -
795: 14 8 6 13 8 5 S 5 17.2449593 0.0140 17.2449733 Err 0.1D-04 -
796: 14 8 6 13 8 5 S 4 17.2449641 0.0092 17.2449733 Err 0.1D-04 -
797: 14 8 6 13 8 5 S 3 17.2449674 0.0058 17.2449733 Err 0.1D-04 -
798: 14 8 6 13 8 5 S 2 17.2449822 -0.0089 17.2449733 Err 0.1D-04 -
799: 14 7 7 13 7 6 S 1 17.2596162 -0.0225 17.2595937 Err 0.1D-04 -
800: 14 7 7 13 7 6 S 2 17.2596022 -0.0085 17.2595937 Err 0.1D-04 -
801: 14 7 7 13 7 6 S 3 17.2595900 0.0037 17.2595937 Err 0.1D-04 -
802: 14 7 7 13 7 6 S 4 17.2595850 0.0087 17.2595937 Err 0.1D-04 -
803: 14 6 8 13 6 7 S 3 17.2825706 -0.0049 17.2825657 Err 0.1D-04 -
804: 14 6 8 13 6 7 S 4 17.2825565 0.0093 17.2825657 Err 0.1D-04 -
805: 14 6 8 13 6 7 S 5 17.2825471 0.0187 17.2825657 Err 0.1D-04 -
806: 15 1 14 14 2 13 S 2 17.3119595 -0.0121 17.3119474 Err 0.1D-04 -
807: 15 1 14 14 2 13 S 4 17.3119330 0.0144 17.3119474 Err 0.1D-04 -
808: 15 1 14 14 2 13 S 5 17.3119060 0.0414 17.3119474 Err 0.1D-04 -
809: 14 4 11 13 4 10 S 3 17.3511079 0.0003 17.3511082 Err 0.1D-04 -
810: 14 4 10 13 4 9 S 1 17.4538846 -0.0435 17.4538411 Err 0.1D-04 -
811: 14 4 10 13 4 9 S 4 17.4537955 0.0456 17.4538411 Err 0.1D-04 -
812: 14 3 11 13 3 10 S 2 17.8258793 -0.0217 17.8258576 Err 0.1D-04 -
813: 14 3 11 13 3 10 S 4 17.8258749 -0.0172 17.8258576 Err 0.1D-04 -
814: 14 3 11 13 3 10 S 3 17.8258689 -0.0113 17.8258576 Err 0.1D-04 -

```
815: 14  3 11 13  3 10   S 5  17.8258700   -0.0124  17.8258576   Err 0.1D-04          -
816: 14  2 12 13  2 11   S 1  17.8519989   -0.0374  17.8519615   Err 0.1D-04          -
817: 14  2 12 13  2 11   S 3  17.8519795   -0.0181  17.8519615   Err 0.1D-04          -
818: 14  2 12 13  2 11   S 5  17.8519658   -0.0044  17.8519615   Err 0.1D-04          -
819: 15  2 14 14  2 13   S 1  17.9006588   -0.0199  17.9006389   Err 0.1D-04          -
820: 15  2 14 14  2 13   S 2  17.9006464   -0.0074  17.9006389   Err 0.1D-04          -
821: 15  2 14 14  2 13   S 5  17.9006199    0.0190  17.9006389   Err 0.1D-04          -
822: 15  2 14 14  2 13   S 4  17.9006128    0.0261  17.9006389   Err 0.1D-04          -
823: 15  1 14 14  1 13   S 5  18.1158815    0.0266  18.1159081   Err 0.1D-04          -
824: 15  1 14 14  1 13   S 3  18.1159111   -0.0030  18.1159081   Err 0.1D-04          -
825: 15  1 14 14  1 13   S 2  18.1159323   -0.0242  18.1159081   Err 0.1D-04          -
826: 15  1 14 14  1 13   S 1  18.1159584   -0.0503  18.1159081   Err 0.1D-04          -
827: 15  3 13 14  3 12   S 4  18.4397364    0.0158  18.4397522   Err 0.2D-04          -
828: 15  3 13 14  3 12   S 5  18.4397398    0.0124  18.4397522   Err 0.2D-04          -
829: 15  3 13 14  3 12   S 1  18.4397694   -0.0172  18.4397522   Err 0.2D-04          -
830: 15  3 13 14  3 12   S 3  18.4397435    0.0087  18.4397522   Err 0.2D-04          -
831: 15 11  4 14 11  3   S 4  18.4568623    0.0112  18.4568736   Err 0.1D-04          -
832: 15 11  4 14 11  3   S 2  18.4568827   -0.0091  18.4568736   Err 0.1D-04          -
833: 15 11  4 14 11  3   S 1  18.4568883   -0.0147  18.4568736   Err 0.1D-04          -
834: 15 10  5 14 10  4   S 5  18.4632447    0.0039  18.4632486   Err 0.1D-04          -
835: 15 10  5 14 10  4   S 4  18.4632491   -0.0005  18.4632486   Err 0.1D-04          -
836: 15 10  5 14 10  4   S 2  18.4632692   -0.0206  18.4632486   Err 0.1D-04          -
837: 15 10  6 14 10  4   S 1  18.4632756   -0.0270  18.4632486   Err 0.1D-04          -
838: 15  9  6 14  9  5   S 3  18.4719228   -0.0079  18.4719149   Err 0.1D-04          -
839: 15  9  6 14  9  5   S 1  18.4719472   -0.0324  18.4719149   Err 0.1D-04          -
840: 15  8  7 14  8  6   S 1  18.4841588   -0.0358  18.4841231   Err 0.1D-04          -
841: 15  8  7 14  8  6   S 2  18.4841491   -0.0261  18.4841231   Err 0.1D-04          -
842: 15  8  7 14  8  6   S 3  18.4841341   -0.0110  18.4841231   Err 0.1D-04          -
843: 15  8  7 14  8  6   S 5  18.4841246   -0.0015  18.4841231   Err 0.1D-04          -
844: 15  7  8 14  7  7   S 2  18.5021746   -0.0182  18.5021565   Err 0.1D-04          -
845: 15  7  8 14  7  7   S 3  18.5021628   -0.0063  18.5021565   Err 0.1D-04          -
846: 15  7  8 14  7  7   S 4  18.5021569   -0.0004  18.5021565   Err 0.1D-04          -
847: 15  4 12 14  4 11   S 1  18.6006429   -0.0404  18.6006026   Err 0.1D-04          -
848: 16  1 15 15  2 14   S 2  18.6119588   -0.0258  18.6119330   Err 0.1D-04          -
849: 16  1 15 15  2 14   S 1  18.6119355   -0.0025  18.6119330   Err 0.1D-04          -
Maximum (obs-calc)/err in line 509   0.0000509

RMS deviations (MHz), B and V sorted
 B  V   n splittings MHz
 B  V   n abs. freq. MHz
 1  1 849         0.018593         0.018834

        Parameters  and  Errors
```

```
 BJ          0.613703223 { 0.000000085}
 BK           1.643208336 { 0.000000634}
 B-          0.059201337 { 0.000000026}
 DJ          0.011205E-6 { 0.000271E-6}
 DJK          0.022912E-6 { 0.000854E-6}
 DK          -0.153866E-6 { 0.027650E-6}
\F12         -0.850495758 {     derived}
\F          158.758072705 {     derived}  160.181537195 {     derived}
 V1n         15727.656407 {   27.734022}   14770.832632 {   22.463053}
\rho         0.005854187 {     derived}    0.013835041 {     derived}
\beta        0.600904303 {     derived}    3.067215413 {     derived}
\gamma         1.455920328 {     derived}   -2.540211310 {     derived}
 epsil       1.476000000 {     fixed  }    3.835947366 { 0.091405936}
 delta       1.225960589 { 0.004294886}    2.879594592 { 0.027139346}

 Standard Deviation       0.018726 MHz

------------------------------------ B =  1
 Rotational Constants and Errors (in GHz)
     B_z       2.256911560       0.000000628
     B_x       0.672904561       0.000000088
     B_y       0.554501886       0.000000089
 Ray's kappa   -0.86090
 F0(calc)     158.000000000       0.000000000
 I_alpha        3.198601709       0.000000000
 <(i,x)  <(i,y)  <(i,z)       84.8892       20.4618       70.2424
d<(i,x) d<(i,y) d<(i,z)        0.0079        0.2368        0.2461

 F0(calc)     158.000000000       0.000000000
 I_alpha        3.198601709       0.000000000
 <(i,x)  <(i,y)  <(i,z)      101.4809       99.5401      164.9886
d<(i,x) d<(i,y) d<(i,z)        2.1111        1.9935        1.5550

 V1n_1      6.275827 kj +/- 0.011067 kj         1.498919 kcal +/- 0.002643 kcal
        524.618074 cm +/-   0.9251 cm    s=  44.029695
 V1n_2      5.894025 kj +/- 0.008963 kj         1.407729 kcal +/- 0.002141 kcal
        492.701873 cm +/-   0.7493 cm    s=  41.351059

F(calc)       158.758072705
F(calc)       160.181537195 XIAM Output for Parent
```

$^{13}C_1$ Isotopologue XIAM Output

	J	K-	K+	J	K-	K+	Sym	calc/GHz	diff/MHz	obs/GHz		
1:	4	2	2	4	1	4	S 1	5.5769923	0.0042	5.5769965	Err 0.1D-04	-
2:	5	1	5	4	1	4	S 2	5.8045928	-0.0135	5.8045794	Err 0.1D-04	-
3:	5	1	5	4	1	4	S 1	5.8045940	-0.0146	5.8045794	Err 0.1D-04	-
4:	5	1	5	4	1	4	S 5	5.8045833	-0.0013	5.8045820	Err 0.1D-04	-
5:	5	1	5	4	1	4	S 4	5.8045819	-0.0025	5.8045794	Err 0.1D-04	-
6:	10	2	8	9	3	7	S 1	5.8874951	-0.0124	5.8874827	Err 0.1D-04	-
7:	10	2	8	9	3	7	S 3	5.8875336	-0.0509	5.8874827	Err 0.1D-04	-
8:	11	3	9	11	2	9	S 1	5.9284642	0.0058	5.9284699	Err 0.1D-04	-
9:	5	0	5	4	0	4	S 2	6.0035710	-0.0040	6.0035670	Err 0.1D-04	-
10:	5	0	5	4	0	4	S 1	6.0035755	-0.0084	6.0035670	Err 0.1D-04	-
11:	5	0	5	4	0	4	S 3	6.0035652	0.0018	6.0035670	Err 0.1D-04	-
12:	5	0	5	4	0	4	S 5	6.0035604	0.0067	6.0035670	Err 0.1D-04	-
13:	5	0	5	4	0	4	S 4	6.0035611	0.0059	6.0035670	Err 0.1D-04	-
14:	19	4	16	19	3	16	S 5	6.0538088	0.0061	6.0538149	Err 0.1D-04	-
15:	19	4	16	19	3	16	S 4	6.0538228	-0.0079	6.0538149	Err 0.1D-04	-
16:	5	2	4	4	2	3	S 3	6.1146760	-0.0016	6.1146744	Err 0.1D-04	-
17:	5	2	4	4	2	3	S 1	6.1146798	-0.0054	6.1146744	Err 0.1D-04	-
18:	6	0	6	5	1	5	S 1	6.2351922	0.0179	6.2352101	Err 0.1D-04	-
19:	6	0	6	5	1	5	S 3	6.2351851	0.0250	6.2352101	Err 0.1D-04	-
20:	6	0	6	5	1	5	S 5	6.2352134	-0.0034	6.2352101	Err 0.1D-04	-
21:	6	0	6	5	1	5	S 2	6.2352220	-0.0120	6.2352101	Err 0.1D-04	-
22:	6	0	6	5	1	5	S 4	6.2352165	-0.0014	6.2352150	Err 0.1D-04	-
23:	11	7	4	12	6	6	S 3	6.2872485	-0.0207	6.2872278	Err 0.1D-04	-
24:	5	1	4	4	1	3	S 5	6.3963170	0.0147	6.3963317	Err 0.1D-04	-
25:	5	1	4	4	1	3	S 4	6.3963178	0.0117	6.3963295	Err 0.1D-04	-
26:	5	1	4	4	1	3	S 3	6.3963213	0.0160	6.3963373	Err 0.1D-04	-
27:	5	1	4	4	1	3	S 2	6.3963218	0.0156	6.3963373	Err 0.1D-04	-
28:	5	1	4	4	1	3	S 1	6.3963257	0.0038	6.3963295	Err 0.1D-04	-
29:	22	6	17	21	7	14	S 1	6.6598747	-0.0274	6.6598473	Err 0.1D-04	-
30:	5	1	5	4	0	4	S 4	6.9127885	0.0157	6.9128042	Err 0.1D-04	-
31:	5	1	5	4	0	4	S 2	6.9128059	-0.0017	6.9128042	Err 0.1D-04	-
32:	5	1	5	4	0	4	S 3	6.9128294	-0.0252	6.9128042	Err 0.1D-04	-
33:	5	1	5	4	0	4	S 5	6.9127893	0.0149	6.9128042	Err 0.1D-04	-
34:	7	0	7	6	1	6	S 2	7.5490510	-0.0129	7.5490381	Err 0.1D-04	-
35:	7	0	7	6	1	6	S 4	7.5490418	0.0003	7.5490421	Err 0.1D-04	-
36:	7	0	7	6	1	6	S 5	7.5490345	0.0076	7.5490421	Err 0.1D-04	-
37:	7	0	7	6	1	6	S 1	7.5490269	0.0106	7.5490375	Err 0.1D-04	-
38:	7	0	7	6	1	6	S 3	7.5490141	0.0234	7.5490375	Err 0.1D-04	-
39:	6	1	5	5	1	4	S 1	7.6539700	0.0070	7.6539770	Err 0.1D-04	-
40:	6	1	5	5	1	4	S 2	7.6539652	0.0156	7.6539807	Err 0.1D-04	-
41:	6	1	5	5	1	4	S 3	7.6539642	0.0166	7.6539807	Err 0.1D-04	-
42:	6	1	5	5	1	4	S 4	7.6539596	0.0211	7.6539807	Err 0.1D-04	-

43: 9 7 3 10 6 5 S 3 8.7830970 0.0343 8.7831313 Err 0.1D-04 -
44: 12 2 10 11 3 8 S 4 8.8210688 0.0282 8.8210970 Err 0.1D-04 -
45: 7 1 6 6 1 5 S 1 8.8977887 -0.0024 8.8977864 Err 0.1D-04 -
46: 7 1 6 6 1 5 S 3 8.8977811 0.0053 8.8977864 Err 0.1D-04 -
47: 7 1 6 6 1 5 S 5 8.8977746 0.0118 8.8977864 Err 0.1D-04 -
48: 7 1 6 6 1 5 S 2 8.8977825 0.0039 8.8977864 Err 0.1D-04 -
49: 10 1 9 9 2 8 S 1 10.0069293 0.0345 10.0069637 Err 0.1D-04 -
50: 10 1 9 9 2 8 S 3 10.0069419 0.0219 10.0069637 Err 0.1D-04 -
51: 9 0 9 8 1 8 S 4 10.0710924 -0.0106 10.0710818 Err 0.1D-04 -
52: 9 0 9 8 1 8 S 5 10.0710648 0.0170 10.0710818 Err 0.1D-04 -
53: 9 0 9 8 1 8 S 1 10.0711021 -0.0203 10.0710818 Err 0.1D-04 -
54: 9 0 9 8 1 8 S 2 10.0711132 -0.0314 10.0710818 Err 0.1D-04 -
55: 4 2 3 3 1 3 S 5 10.1318763 0.0040 10.1318803 Err 0.1D-04 -
56: 8 2 6 7 2 5 S 1 10.1622608 -0.0028 10.1622580 Err 0.1D-04 -
57: 8 2 6 7 2 5 S 2 10.1622562 0.0018 10.1622580 Err 0.1D-04 -
58: 8 2 6 7 2 5 S 4 10.1622539 0.0041 10.1622580 Err 0.1D-04 -
59: 8 2 6 7 2 5 S 5 10.1622490 0.0090 10.1622580 Err 0.1D-04 -
60: 8 2 6 7 2 5 S 3 10.1622560 -0.0017 10.1622543 Err 0.1D-04 -
61: 4 2 2 3 1 3 S 4 10.2292866 -0.0306 10.2292560 Err 0.1D-04 -
62: 13 1 12 12 2 10 S 1 10.4049896 0.0342 10.4050238 Err 0.1D-04 -
63: 13 1 12 12 2 10 S 2 10.4050099 0.0139 10.4050238 Err 0.1D-04 -
64: 9 1 9 8 0 8 S 4 10.7478845 -0.0011 10.7478833 Err 0.1D-04 -
65: 9 1 9 8 0 8 S 2 10.7479074 -0.0241 10.7478833 Err 0.1D-04 -
66: 9 1 9 8 0 8 S 5 10.7479121 -0.0287 10.7478833 Err 0.1D-04 -
67: 9 2 8 8 2 7 S 3 10.9164409 0.0093 10.9164502 Err 0.1D-04 -
68: 9 2 8 8 2 7 S 5 10.9164394 0.0145 10.9164539 Err 0.1D-04 -
69: 9 2 8 8 2 7 S 4 10.9164364 0.0175 10.9164539 Err 0.1D-04 -
70: 9 2 8 8 2 7 S 2 10.9164526 0.0005 10.9164531 Err 0.1D-04 -
71: 9 2 8 8 2 7 S 1 10.9164556 -0.0025 10.9164531 Err 0.1D-04 -
72: 9 6 3 8 6 2 S 1 11.0653412 -0.0078 11.0653334 Err 0.1D-04 -
73: 9 6 3 8 6 2 S 2 11.0653333 0.0001 11.0653334 Err 0.1D-04 -
74: 9 6 3 8 6 2 S 3 11.0653276 0.0058 11.0653334 Err 0.1D-04 -
75: 9 6 3 8 6 2 S 5 11.0653204 0.0130 11.0653334 Err 0.1D-04 -
76: 9 6 3 8 6 2 S 4 11.0653232 0.0102 11.0653334 Err 0.1D-04 -
77: 9 5 5 8 5 4 S 4 11.0758419 0.0194 11.0758614 Err 0.1D-04 -
78: 9 5 5 8 5 4 S 5 11.0758462 0.0152 11.0758614 Err 0.1D-04 -
79: 9 5 5 8 5 4 S 2 11.0758553 0.0061 11.0758614 Err 0.1D-04 -
80: 9 3 6 8 3 5 S 1 11.1930739 0.0149 11.1930887 Err 0.1D-04 -
81: 9 3 6 8 3 5 S 3 11.1930597 0.0290 11.1930887 Err 0.1D-04 -
82: 10 0 10 9 1 9 S 1 11.2803225 -0.0193 11.2803031 Err 0.1D-04 -
83: 10 0 10 9 1 9 S 2 11.2803265 -0.0234 11.2803031 Err 0.1D-04 -
84: 10 0 10 9 1 9 S 4 11.2802967 0.0065 11.2803031 Err 0.1D-04 -
85: 14 2 13 14 0 14 S 1 11.2847496 0.0112 11.2847608 Err 0.1D-04 -

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 86:  6  4  2  6  3  3   S 5  11.3305050   -0.0069  11.3304981   Err 0.1D-04          -
 87:  5  4  1  5  3  2   S 2  11.3482986   -0.0158  11.3482828   Err 0.1D-04          -
 88: 10  0 10  9  0  9   S 5  11.5612622    0.0307  11.5612929   Err 0.1D-04          -
 89: 10  0 10  9  0  9   S 4  11.5612771    0.0158  11.5612929   Err 0.1D-04          -
 90: 10  0 10  9  0  9   S 2  11.5613057   -0.0189  11.5612867   Err 0.1D-04          -
 91: 10  0 10  9  0  9   S 1  11.5613166   -0.0299  11.5612867   Err 0.1D-04          -
 92: 10  0 10  9  0  9   S 4  11.5612771    0.0158  11.5612929   Err 0.1D-04          -
 93: 11  1 10 10  2  9   S 1  11.5724114    0.0415  11.5724529   Err 0.1D-04          -
 94: 11  1 10 10  2  9   S 3  11.5724202    0.0327  11.5724529   Err 0.1D-04          -
 95: 11  1 10 10  2  9   S 2  11.5724976   -0.0447  11.5724529   Err 0.1D-04          -
 96: 11  1 10 10  2  9   S 2  11.5724976   -0.0447  11.5724529   Err 0.1D-04          -
 97: 10  1 10  9  0  9   S 2  11.7560212   -0.0256  11.7559955   Err 0.1D-04          -
 98: 10  1 10  9  0  9   S 4  11.7560016   -0.0061  11.7559955   Err 0.1D-04          -
 99: 10  2  9  9  2  8   S 4  12.0968182    0.0059  12.0968241   Err 0.1D-04          -
100: 10  2  9  9  2  8   S 5  12.0968204    0.0031  12.0968234   Err 0.1D-04          -
101: 10  2  9  9  2  8   S 3  12.0968247   -0.0013  12.0968234   Err 0.1D-04          -
102: 10  2  9  9  2  8   S 2  12.0968363   -0.0128  12.0968234   Err 0.1D-04          -
103: 10  2  9  9  2  8   S 1  12.0968417   -0.0183  12.0968234   Err 0.1D-04          -
104: 11  0 11 10  1 10   S 4  12.4614351    0.0273  12.4614624   Err 0.1D-04          -
105: 11  0 11 10  1 10   S 2  12.4614780   -0.0156  12.4614624   Err 0.1D-04          -
106: 10  3  7  9  3  6   S 3  12.4892822    0.0232  12.4893054   Err 0.1D-04          -
107: 10  3  7  9  3  6   S 1  12.4892924    0.0130  12.4893054   Err 0.1D-04          -
108: 10  1  9  9  1  8   S 5  12.5087746    0.0002  12.5087748   Err 0.1D-04          -
109: 10  1  9  9  1  8   S 3  12.5087888   -0.0139  12.5087748   Err 0.1D-04          -
110: 10  1  9  9  1  8   S 2  12.5087915   -0.0167  12.5087748   Err 0.1D-04          -
111: 10  1  9  9  1  8   S 1  12.5088053   -0.0305  12.5087748   Err 0.1D-04          -
112: 11  1 11 10  0 10   S 2  12.7885249   -0.0319  12.7884930   Err 0.1D-04          -
113: 11  1 11 10  0 10   S 4  12.7885128   -0.0198  12.7884930   Err 0.1D-04          -
114:  4  3  1  3  2  2   S 5  13.0471212    0.0348  13.0471559   Err 0.1D-04          -
115: 11  2 10 10  2  9   S 1  13.2681720    0.0180  13.2681901   Err 0.1D-04          -
116: 11  2 10 10  2  9   S 2  13.2681646    0.0254  13.2681901   Err 0.1D-04          -
117: 11  2 10 10  2  9   S 3  13.2681527    0.0373  13.2681901   Err 0.1D-04          -
118: 20  2 18 20  2 19   S 1  13.4015355   -0.0230  13.4015125   Err 0.1D-04          -
119: 12  1 12 11  0 11   S 1  13.8415502   -0.0237  13.8415266   Err 0.1D-04          -
120: 12  1 12 11  0 11   S 2  13.8415479   -0.0213  13.8415266   Err 0.1D-04          -
121: 11  2  9 10  2  8   S 1  14.0751957   -0.0101  14.0751855   Err 0.1D-04          -
122: 11  2  9 10  2  8   S 2  14.0751900   -0.0045  14.0751855   Err 0.1D-04          -
123: 11  2  9 10  2  8   S 3  14.0751875   -0.0020  14.0751855   Err 0.1D-04          -
124: 11  2  9 10  2  8   S 4  14.0751824    0.0050  14.0751874   Err 0.1D-04          -
125: 11  2  9 10  2  8   S 5  14.0751814    0.0042  14.0751855   Err 0.1D-04          -
126:  8  2  6  7  1  6   S 1  14.2220234   -0.0401  14.2219832   Err 0.1D-04          -
127:  8  2  6  7  1  6   S 3  14.2220111   -0.0279  14.2219832   Err 0.1D-04          -
128:  5  3  3  4  2  3   S 1  14.2911360   -0.0414  14.2910946   Err 0.1D-04          -
```

129: 12 2 11 11 2 10 S 4 14.4303362 0.0196 14.4303558 Err 0.1D-04 -
130: 12 2 11 11 2 10 S 3 14.4303464 0.0094 14.4303558 Err 0.1D-04 -
131: 12 2 11 11 2 10 S 2 14.4303589 -0.0031 14.4303558 Err 0.1D-04 -
132: 12 2 11 11 2 10 S 1 14.4303680 -0.0122 14.4303558 Err 0.1D-04 -
133: 12 2 11 11 2 10 S 5 14.4303384 0.0188 14.4303572 Err 0.1D-04 -
134: 11 5 7 11 4 7 S 3 14.4646779 0.0134 14.4646913 Err 0.1D-04 -
135: 9 5 5 9 4 5 S 4 14.5394630 0.0163 14.5394794 Err 0.1D-04 -
136: 9 5 4 9 4 6 S 1 14.5568623 -0.0308 14.5568315 Err 0.1D-04 -
137: 7 2 6 6 1 6 S 5 14.6948314 -0.0159 14.6948155 Err 0.1D-04 -
138: 7 2 6 6 1 6 S 2 14.6948458 -0.0303 14.6948155 Err 0.1D-04 -
139: 12 10 2 11 10 1 S 5 14.7423827 -0.0183 14.7423645 Err 0.1D-04 -
140: 12 10 2 11 10 1 S 4 14.7423857 -0.0212 14.7423645 Err 0.1D-04 -
141: 12 10 2 11 10 1 S 4 14.7423857 -0.0218 14.7423639 Err 0.1D-04 -
142: 12 10 2 11 10 1 S 3 14.7423893 -0.0248 14.7423645 Err 0.1D-04 -
143: 12 10 2 11 10 1 S 1 14.7424063 -0.0418 14.7423645 Err 0.1D-04 -
144: 12 8 4 11 8 3 S 1 14.7533654 -0.0320 14.7533333 Err 0.1D-04 -
145: 12 8 4 11 8 3 S 2 14.7533572 -0.0239 14.7533333 Err 0.1D-04 -
146: 12 8 4 11 8 3 S 3 14.7533484 -0.0150 14.7533333 Err 0.1D-04 -
147: 12 8 4 11 8 3 S 4 14.7533436 -0.0103 14.7533333 Err 0.1D-04 -
148: 12 8 4 11 8 3 S 5 14.7533402 -0.0069 14.7533333 Err 0.1D-04 -
149: 12 3 10 11 3 9 S 1 14.7853304 0.0000 14.7853304 Err 0.1D-04 -
150: 12 3 10 11 3 9 S 2 14.7853392 -0.0088 14.7853304 Err 0.1D-04 -
151: 12 3 10 11 3 9 S 5 14.7853307 -0.0003 14.7853304 Err 0.1D-04 -
152: 12 3 10 11 3 9 S 3 14.7853151 0.0153 14.7853304 Err 0.1D-04 -
153: 12 3 10 11 3 9 S 4 14.7853171 0.0133 14.7853304 Err 0.1D-04 -
154: 12 1 11 11 1 10 S 2 14.7903568 0.0026 14.7903593 Err 0.1D-04 -
155: 12 1 11 11 1 10 S 3 14.7903519 0.0074 14.7903593 Err 0.1D-04 -
156: 12 1 11 11 1 10 S 5 14.7903305 0.0311 14.7903616 Err 0.1D-04 -
157: 12 1 11 11 1 10 S 4 14.7903322 0.0294 14.7903616 Err 0.1D-04 -
158: 12 5 8 11 5 6 S 3 14.7982927 0.0121 14.7983048 Err 0.1D-04 -
159: 12 3 9 11 3 8 S 1 15.1338013 -0.0085 15.1337928 Err 0.1D-04 -
160: 12 3 9 11 3 8 S 2 15.1337918 0.0010 15.1337928 Err 0.1D-04 -
161: 12 3 9 11 3 8 S 4 15.1337921 0.0007 15.1337928 Err 0.1D-04 -
162: 12 3 9 11 3 8 S 5 15.1337786 0.0142 15.1337928 Err 0.1D-04 -
163: 12 3 9 11 3 8 S 3 15.1337948 -0.0020 15.1337928 Err 0.1D-04 -
164: 12 2 10 11 2 9 S 1 15.3487902 -0.0142 15.3487759 Err 0.1D-04 -
165: 12 2 10 11 2 9 S 2 15.3487818 -0.0059 15.3487759 Err 0.1D-04 -
166: 12 2 10 11 2 9 S 3 15.3487797 -0.0038 15.3487759 Err 0.1D-04 -
167: 12 2 10 11 2 9 S 5 15.3487710 0.0050 15.3487759 Err 0.1D-04 -
168: 12 2 10 11 2 9 S 4 15.3487717 0.0048 15.3487765 Err 0.1D-04 -
169: 11 2 10 10 1 9 S 1 15.3580844 0.0256 15.3581100 Err 0.1D-04 -
170: 11 2 10 10 1 9 S 5 15.3579255 0.0013 15.3579269 Err 0.1D-04 -
171: 13 2 12 12 2 11 S 1 15.5836447 -0.0367 15.5836080 Err 0.1D-04 -

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172: 13  2 12 12  2 11   S 2  15.5836339   -0.0259  15.5836080   Err 0.1D-04          -
173: 13  2 12 12  2 11   S 3  15.5836210   -0.0130  15.5836080   Err 0.1D-04          -
174: 13  2 12 12  2 11   S 4  15.5836087   -0.0007  15.5836080   Err 0.1D-04          -
175: 13  2 12 12  2 11   S 5  15.5836117   -0.0037  15.5836080   Err 0.1D-04          -
176: 14 11  3 15 10  5   S 3  15.6249823    0.0107  15.6249930   Err 0.1D-04          -
177: 14 11  3 15 10  5   S 4  15.6249861    0.0069  15.6249930   Err 0.1D-04          -
178: 19 13  7 20 12  9   S 3  15.9390309   -0.0148  15.9390161   Err 0.1D-04          -
179: 14  1 13 13  2 12   S 4  15.9667797    0.0293  15.9668091   Err 0.1D-04          -
180: 14  1 13 13  2 12   S 2  15.9667893    0.0197  15.9668091   Err 0.1D-04          -
181: 13 12  1 12 12  0   S 1  15.9670173    0.0122  15.9670295   Err 0.1D-04          -
182: 13 12  1 12 12  0   S 2  15.9670107    0.0188  15.9670295   Err 0.1D-04          -
183: 13 12  1 12 12  0   S 3  15.9669988    0.0307  15.9670295   Err 0.1D-04          -
184: 13 12  1 12 12  0   S 4  15.9669955    0.0340  15.9670295   Err 0.1D-04          -
185: 13 12  1 12 12  0   S 5  15.9669922    0.0373  15.9670295   Err 0.1D-04          -
186: 13  2 11 12  2 10   S 1  16.6007089   -0.0087  16.6007002   Err 0.1D-04          -
187: 13  2 11 12  2 10   S 2  16.6006970    0.0031  16.6007002   Err 0.1D-04          -
188: 13  2 11 12  2 10   S 3  16.6006955    0.0047  16.6007002   Err 0.1D-04          -
189: 13  2 11 12  2 10   S 5  16.6006833    0.0147  16.6006979   Err 0.1D-04          -
190: 19  4 16 18  5 13   S 2   8.9529698    0.0281   8.9529979   Err 0.1D-04          -
191: 19  4 16 18  5 13   S 3   8.9530056   -0.0077   8.9529979   Err 0.1D-04          -
192: 19  4 16 18  5 13   S 1   8.9530391    0.0379   8.9530770   Err 0.1D-04          -
193: 19  4 16 18  5 13   S 4   8.9531155   -0.0385   8.9530770   Err 0.1D-04          -
194: 18  3 16 18  1 17   S 3  13.1438169    0.0577  13.1438746   Err 0.1D-04          -
195: 13  5  9 13  4  9   S 2  14.2897952   -0.0103  14.2897849   Err 0.1D-04          -
196: 13  1 13 12  1 12   S 1  14.8220244    0.0080  14.8220323   Err 0.1D-04          -
197: 13  1 13 12  1 12   S 2  14.8220247    0.0077  14.8220323   Err 0.1D-04          -
Maximum (obs-calc)/err in line 194   0.0000577

RMS deviations (MHz), B and V sorted
 B  V   n splittings MHz
 B  V   n abs. freq. MHz
 1  1 197         0.019728         0.020929

          Parameters  and  Errors
 BJ          0.612926515 { 0.000000158}
 BK           1.623970681 { 0.000000739}
 B-          0.059646787 { 0.000000156}
 DJ          0.009699E-6 { 0.000478E-6}
 DJK          0.021032E-6 { 0.002098E-6}
 DK          -0.172219E-6 { 0.003372E-6}
 dj          -0.000328E-6 { 0.000231E-6}
\F12          -0.927279619 {     derived}
\F          158.804607879 {     derived}  160.096888618 {     derived}
```

V1n 16046.749819 { 158.570110} 14720.789634 { 37.762483}
\rho 0.006264629 { derived} 0.013438165 { derived}
\beta 0.545126449 { derived} 3.043026756 { derived}
\gamma 1.455724984 { derived} -2.624568206 { derived}
epsil 1.476000000 { fixed } 3.746400377 { 0.170526445}
delta 1.182773604 { 0.023416200} 2.807104084 { 0.036692996}

Standard Deviation 0.020413 MHz

---------- B = 1
Rotational Constants and Errors (in GHz)
B_z 2.236897196 0.000000755
B_x 0.672573302 0.000000214
B_y 0.553279729 0.000000230
Ray's kappa -0.85829
F0(calc) 158.000000000 0.000000000
I_alpha 3.198601709 0.000000000
<(i,x) <(i,y) <(i,z) 84.9734 22.8532 67.7679
d<(i,x) d<(i,y) d<(i,z) 0.0469 1.2988 1.3416

F0(calc) 158.000000000 0.000000000
I_alpha 3.198601709 0.000000000
<(i,x) <(i,y) <(i,z) 105.6674 100.7582 160.8352
d<(i,x) d<(i,y) d<(i,z) 3.8079 3.6805 2.1024

V1n_1 6.403156 kj +/- 0.063274 kj 1.529330 kcal +/- 0.015112 kcal
535.261883 cm +/- 5.2893 cm s= 44.909835
V1n_2 5.874056 kj +/- 0.015068 kj 1.402960 kcal +/- 0.003599 kcal
491.032619 cm +/- 1.2596 cm s= 41.198887

F(calc) 158.804607879
F(calc) 160.096888618

$^{13}C_2$ Isotopologue XIAM Output

	J K- K+	J K- K+	Sym	calc/GHz	diff/MHz	obs/GHz	
1:	5 1 5	4 1 4	S 1	5.7962851	-0.0010	5.7962841	Err 0.1D-04 -
2:	5 1 4	4 1 3	S 1	6.3887024	0.0025	6.3887049	Err 0.1D-04 -
3:	6 1 6	5 1 5	S 1	6.9406928	-0.0080	6.9406848	Err 0.1D-04 -
4:	6 0 6	5 0 5	S 1	7.1341844	-0.0010	7.1341834	Err 0.1D-04 -
5:	6 2 4	5 2 3	S 1	7.5274042	0.0047	7.5274089	Err 0.1D-04 -
6:	7 0 7	6 1 6	S 1	7.5406415	0.0064	7.5406479	Err 0.1D-04 -

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 7:  6  1  5  5  1  4   S 1   7.6447061    0.0030   7.6447091   Err 0.1D-04          -
 8:  7  1  6  6  1  5   S 1   8.8868053    0.0073   8.8868126   Err 0.1D-04          -
 9:  8  0  8  7  0  7   S 1   9.3557736    0.0031   9.3557767   Err 0.1D-04          -
10:  8  1  7  7  1  6   S 1  10.1112251    0.0045  10.1112296   Err 0.1D-04          -
11:  8  2  6  7  2  5   S 1  10.1508496    0.0079  10.1508576   Err 0.1D-04          -
12:  9  1  9  8  1  8   S 1  10.3368016    0.0171  10.3368187   Err 0.1D-04          -
13:  9  1  9  8  0  8   S 1  10.7297629   -0.0276  10.7297353   Err 0.1D-04          -
14:  9  2  8  8  2  7   S 1  10.9018220    0.0057  10.9018277   Err 0.1D-04          -
15:  9  3  6  8  3  5   S 1  11.1798960    0.0071  11.1799031   Err 0.1D-04          -
16:  6  2  5  5  1  4   S 1  11.3106842   -0.0502  11.3106340   Err 0.2D-04          -
17: 10  0 10  9  0  9   S 1  11.5437385   -0.0076  11.5437309   Err 0.1D-04          -
18: 10  2  9  9  2  8   S 1  12.0804400    0.0139  12.0804540   Err 0.1D-04          -
19: 10  6  4  9  6  3   S 1  12.2853282    0.0107  12.2853389   Err 0.1D-04          -
20: 10  1  9  9  1  8   S 1  12.4920106    0.0127  12.4920233   Err 0.1D-04          -
21: 11  0 11 10  0 10   S 1  12.6369282   -0.0328  12.6368953   Err 0.1D-04          -
22: 10  2  8  9  2  7   S 1  12.7686864    0.0053  12.7686916   Err 0.1D-04          -
23: 11  1 11 10  0 10   S 1  12.7678896   -0.0174  12.7678722   Err 0.1D-04          -
24:  4  3  1  3  2  1   S 1  12.9835728   -0.0274  12.9835454   Err 0.1D-04          -
25: 20  2 18 20  2 19   S 1  13.4113982   -0.0108  13.4113875   Err 0.1D-04          -
26: 11  7  4 10  7  3   S 1  13.5097553   -0.0128  13.5097425   Err 0.1D-04          -
27: 11  6  5 10  6  4   S 1  13.5211591   -0.0241  13.5211350   Err 0.1D-04          -
28:  6  2  4  5  1  5   S 1  13.5309956    0.0026  13.5309982   Err 0.1D-04          -
29: 11  3  9 10  3  8   S 1  13.5435024   -0.0027  13.5434997   Err 0.1D-04          -
30: 11  1 10 10  1  9   S 1  13.6433880   -0.0137  13.6433744   Err 0.1D-04          -
31: 15  3 12 15  2 14   S 1  13.7475728   -0.0184  13.7475544   Err 0.1D-04          -
32:  5  3  3  4  2  2   S 1  14.1669897    0.0272  14.1670169   Err 0.1D-04          -
33: 11  2  9 10  2  8   S 1  14.0587988    0.0195  14.0588183   Err 0.1D-04          -
34: 12  2 11 11  2 10   S 1  14.4103401    0.0111  14.4103513   Err 0.1D-04          -
35: 18  1 17 18  0 18   S 1  14.4653747   -0.0103  14.4653644   Err 0.1D-04          -
36: 12  8  4 11  8  3   S 1  14.7347825    0.0038  14.7347863   Err 0.1D-04          -
37: 13  0 13 12  1 12   S 1  14.7419511   -0.0181  14.7419330   Err 0.1D-04          -
38: 12  7  5 11  7  4   S 1  14.7442545    0.0109  14.7442654   Err 0.1D-04          -
39: 12  6  6 11  6  5   S 1  14.7591080   -0.0090  14.7590990   Err 0.1D-04          -
40: 12  3 10 11  3  9   S 1  14.7664623    0.0102  14.7664725   Err 0.1D-04          -
41: 13  0 13 12  0 12   S 1  14.8294624    0.0447  14.8295071   Err 0.1D-04          -
42: 13  1 13 12  0 12   S 1  14.8871860   -0.0078  14.8871782   Err 0.1D-04          -
43: 22  5 18 22  4 19   S 1  14.9204680   -0.0074  14.9204606   Err 0.1D-04          -
44: 12  3  9 11  3  8   S 1  15.1171559    0.0071  15.1171630   Err 0.1D-04          -
45:  6  3  4  5  2  3   S 1  15.3099369    0.0003  15.3099372   Err 0.1D-04          -
46: 12  2 10 11  2  9   S 1  15.3304822    0.0080  15.3304902   Err 0.1D-04          -
47: 13  2 12 12  2 11   S 1  15.5617705   -0.0088  15.5617617   Err 0.1D-04          -
48: 13  1 12 12  1 11   S 1  15.8739035    0.0033  15.8739068   Err 0.1D-04          -
49: 14  1 14 13  1 13   S 1  15.9087862   -0.0173  15.9087689   Err 0.1D-04          -
```

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 50: 13  3 11 12  3 10   S 1  15.9823770    0.0227  15.9823996   Err 0.1D-04          -
 51:  8  3  5  8  0  8   S 1  16.0370071    0.0257  16.0370328   Err 0.1D-04          -
 52: 13  2 11 12  2 10   S 1  16.5803574   -0.0162  16.5803412   Err 0.1D-04          -
 53: 14  2 13 13  2 12   S 1  16.7047679   -0.0186  16.7047493   Err 0.1D-04          -
 54: 14  8  6 13  8  5   S 1  17.2033082    0.0523  17.2033605   Err 0.1D-04          -
 55: 14  3 11 13  3 10   S 1  17.7992711    0.0518  17.7993228   Err 0.1D-04          -
 56:  7  6  2  7  5  3   S 1  17.8021671    0.0197  17.8021868   Err 0.1D-04          -
 57:  9  2  8  9  1  9   S 1   7.6642517   -0.0426   7.6642092   Err 0.1D-04          -
 58: 22  5 18 22  4 18   S 1  10.0105505   -0.0091  10.0105414   Err 0.1D-04          -
 59: 11  4  7 11  3  9   S 1  11.3701303   -0.0158  11.3701145   Err 0.1D-04          -
 60:  7  2  6  6  1  5   S 1  12.1849461   -0.0414  12.1849047   Err 0.1D-04          -
 61: 16 11  5 17 10  7   S 1  13.0859121    0.0209  13.0859330   Err 0.1D-04          -
 62:  9  2  8  8  1  7   S 1  13.8032056   -0.0194  13.8031862   Err 0.1D-04          -
 63: 11  2 10 10  1  9   S 1  15.3275389   -0.0464  15.3274925   Err 0.1D-04          -
Maximum (obs-calc)/err in line  54   0.0000523

RMS deviations (MHz), B and V sorted
 B  V   n splittings MHz
 B  V   n abs. freq. MHz
 1  1  63         0.020103         0.021379

          Parameters  and  Errors
BJ          0.612143726 { 0.000000143}
BK          1.620194705 { 0.000000902}
B-          0.059719340 { 0.000000057}
DJK         0.016055E-6 { 0.003456E-6}
\F12       -0.841825802 {     derived}
\F        158.753297627 {     derived}  160.157786670 {     derived}
\rho        0.005803898 {     derived}    0.013685069 {     derived}
\beta       0.604277108 {     derived}    3.066568381 {     derived}
\gamma      1.455669015 {     derived}   -2.541239426 {     derived}

Standard Deviation       0.020952 MHz

------------------------------------ B =  1
Rotational Constants and Errors (in GHz)
    B_z       2.232338431       0.000000945
    B_x       0.671863065       0.000000157
    B_y       0.552424386       0.000000151
Ray's kappa   -0.85780
F0(calc)     158.000000000       0.000000000
I_alpha        3.198601709       0.000000000
<(i,x)  <(i,y)  <(i,z)       84.8892       20.4618       70.2424
```

d<(i,x) d<(i,y) d<(i,z) 0.0000 0.0000 0.0000

F0(calc) 158.000000000 0.000000000
I_alpha 3.198601709 0.000000000
<(i,x) <(i,y) <(i,z) 101.4809 99.5401 164.9886
d<(i,x) d<(i,y) d<(i,z) 0.0000 0.0000 0.0000

V1n_1 6.275827 kj +/- 0.000000 kj 1.498919 kcal +/- 0.000000 kcal
524.618074 cm +/- 0.0000 cm s= 44.031019
V1n_2 5.894025 kj +/- 0.000000 kj 1.407729 kcal +/- 0.000000 kcal
492.701873 cm +/- 0.0000 cm s= 41.352303

F(calc) 158.753297627
F(calc) 160.157786670

$^{13}C_3$ Isotopologue XIAM Output

	J K- K+	J K- K+	Sym	calc/GHz	diff/MHz	obs/GHz		
1:	5 1 5	4 1 4	S 1	5.7896268	-0.0150	5.7896118	Err 0.1D-04	-
2:	5 0 5	4 0 4	S 1	5.9880316	-0.0079	5.9880237	Err 0.1D-04	-
3:	5 2 4	4 2 3	S 1	6.0949118	0.0090	6.0949208	Err 0.1D-04	-
4:	6 0 6	5 1 5	S 1	6.1932600	0.0005	6.1932605	Err 0.1D-04	-
5:	6 0 6	5 1 5	S 3	6.1932512	0.0093	6.1932605	Err 0.1D-04	-
6:	5 2 3	4 2 2	S 1	6.2157434	0.0063	6.2157497	Err 0.1D-04	-
7:	5 2 3	4 2 2	S 3	6.2157348	0.0149	6.2157497	Err 0.1D-04	-
8:	5 1 4	4 1 3	S 1	6.3729133	0.0077	6.3729211	Err 0.1D-04	-
9:	5 1 4	4 1 3	S 4	6.3729062	0.0081	6.3729143	Err 0.1D-04	-
10:	5 1 4	4 1 3	S 3	6.3729084	0.0113	6.3729197	Err 0.1D-04	-
11:	5 1 4	4 1 3	S 5	6.3729054	0.0142	6.3729197	Err 0.1D-04	-
12:	5 1 4	4 1 3	S 2	6.3729108	0.0083	6.3729191	Err 0.1D-04	-
13:	2 2 1	1 1 1	S 1	7.4315113	-0.0138	7.4314975	Err 0.1D-04	-
14:	6 1 5	5 1 4	S 1	7.6268354	0.0271	7.6268625	Err 0.1D-04	-
15:	4 3 2	4 2 2	S 3	8.1420518	-0.0192	8.1420326	Err 0.1D-04	-
16:	6 3 4	6 2 5	S 4	8.3258318	0.0262	8.3258580	Err 0.1D-04	-
17:	17 3 15	16 4 13	S 1	8.6422826	0.0139	8.6422965	Err 0.1D-04	-
18:	17 3 15	16 4 13	S 3	8.6422475	0.0490	8.6422965	Err 0.1D-04	-
19:	8 0 8	7 1 7	S 1	8.7868717	-0.0009	8.7868707	Err 0.1D-04	-
20:	8 0 8	7 1 7	S 5	8.7868626	0.0081	8.7868707	Err 0.1D-04	-
21:	8 0 8	7 1 7	S 3	8.7868464	0.0243	8.7868707	Err 0.1D-04	-
22:	8 0 8	7 1 7	S 4	8.7868741	-0.0051	8.7868691	Err 0.1D-04	-
23:	8 0 8	7 1 7	S 2	8.7868937	-0.0246	8.7868691	Err 0.1D-04	-
24:	7 2 5	6 2 4	S 1	8.8086628	0.0155	8.8086783	Err 0.1D-04	-
25:	7 1 6	6 1 5	S 1	8.8675811	-0.0021	8.8675790	Err 0.1D-04	-

26: 7 1 6 6 1 5 S 3 8.8675725 0.0065 8.8675790 Err 0.1D-04 -
27: 7 1 6 6 1 5 S 5 8.8675679 0.0111 8.8675790 Err 0.1D-04 -
28: 7 1 6 6 1 5 S 2 8.8675767 0.0057 8.8675824 Err 0.1D-04 -
29: 19 4 16 18 5 14 S 1 8.8838537 0.0059 8.8838596 Err 0.1D-04 -
30: 14 9 5 15 8 7 S 2 9.4819213 0.0163 9.4819376 Err 0.1D-04 -
31: 17 2 15 17 2 16 S 4 9.6868044 -0.0111 9.6867933 Err 0.1D-04 -
32: 17 2 15 17 2 16 S 3 9.6867674 0.0259 9.6867933 Err 0.1D-04 -
33: 17 2 15 17 2 16 S 5 9.6867638 0.0296 9.6867933 Err 0.1D-04 -
34: 9 0 9 8 1 8 S 3 10.0309604 -0.0324 10.0309280 Err 0.1D-04 -
35: 9 0 9 8 1 8 S 5 10.0309651 -0.0371 10.0309280 Err 0.1D-04 -
36: 8 1 7 7 1 6 S 2 10.0915701 -0.0072 10.0915629 Err 0.1D-04 -
37: 8 1 7 7 1 6 S 4 10.0915591 0.0038 10.0915629 Err 0.1D-04 -
38: 8 1 7 7 1 6 S 1 10.0915763 -0.0134 10.0915629 Err 0.1D-04 -
39: 8 1 7 7 1 6 S 3 10.0915651 0.0009 10.0915660 Err 0.1D-04 -
40: 9 1 9 8 1 8 S 2 10.3281534 -0.0220 10.3281314 Err 0.1D-04 -
41: 9 1 9 8 1 8 S 5 10.3281395 -0.0082 10.3281314 Err 0.1D-04 -
42: 9 1 9 8 1 8 S 4 10.3281330 -0.0016 10.3281314 Err 0.1D-04 -
43: 9 1 9 8 1 8 S 1 10.3281567 -0.0250 10.3281316 Err 0.1D-04 -
44: 5 2 3 4 1 3 S 1 10.6629346 0.0231 10.6629577 Err 0.1D-04 -
45: 5 2 3 4 1 3 S 3 10.6629196 0.0381 10.6629577 Err 0.1D-04 -
46: 9 1 9 8 0 8 S 1 10.7435532 -0.0397 10.7435135 Err 0.1D-04 -
47: 9 2 8 8 2 7 S 1 10.8844003 -0.0098 10.8843906 Err 0.1D-04 -
48: 9 2 8 8 2 7 S 2 10.8843993 -0.0087 10.8843906 Err 0.1D-04 -
49: 9 2 8 8 2 7 S 4 10.8843811 0.0095 10.8843906 Err 0.1D-04 -
50: 9 2 8 8 2 7 S 5 10.8843842 0.0064 10.8843907 Err 0.1D-04 -
51: 9 2 8 8 2 7 S 3 10.8843837 0.0073 10.8843910 Err 0.1D-04 -
52: 18 2 16 18 1 17 S 1 11.1105544 -0.0226 11.1105319 Err 0.1D-04 -
53: 18 2 16 18 1 17 S 2 11.1105345 -0.0026 11.1105319 Err 0.1D-04 -
54: 16 3 13 15 4 12 S 1 11.1640482 -0.0248 11.1640234 Err 0.1D-04 -
55: 10 0 10 9 1 9 S 1 11.2415859 -0.0237 11.2415621 Err 0.1D-04 -
56: 10 0 10 9 1 9 S 2 11.2415950 -0.0329 11.2415621 Err 0.1D-04 -
57: 6 2 5 5 1 4 S 4 11.3780937 0.0294 11.3781230 Err 0.1D-04 -
58: 6 2 5 5 1 4 S 2 11.3781111 0.0120 11.3781230 Err 0.1D-04 -
59: 9 2 7 8 2 6 S 1 11.4294472 -0.0016 11.4294456 Err 0.1D-04 -
60: 9 2 7 8 2 6 S 5 11.4294393 0.0029 11.4294421 Err 0.1D-04 -
61: 9 2 7 8 2 6 S 2 11.4294468 -0.0047 11.4294421 Err 0.1D-04 -
62: 9 2 7 8 2 6 S 3 11.4294411 0.0050 11.4294461 Err 0.1D-04 -
63: 9 2 7 8 2 6 S 4 11.4294421 0.0040 11.4294461 Err 0.1D-04 -
64: 15 1 14 15 1 15 S 5 11.4377138 -0.0185 11.4376953 Err 0.1D-04 -
65: 10 1 10 9 1 9 S 4 11.4490802 0.0083 11.4490885 Err 0.1D-04 -
66: 10 1 10 9 1 9 S 5 11.4490919 -0.0097 11.4490822 Err 0.1D-04 -
67: 10 1 10 9 1 9 S 1 11.4491044 -0.0223 11.4490822 Err 0.1D-04 -
68: 10 1 10 9 1 9 S 3 11.4490897 -0.0021 11.4490876 Err 0.1D-04 -

69: 10 0 10 9 0 9 S 1 11.5387415 -0.0128 11.5387287 Err 0.1D-04 -
70: 20 5 16 20 4 16 S 3 12.0015344 0.0327 12.0015671 Err 0.1D-04 -
71: 10 2 9 9 2 8 S 1 12.0624370 -0.0077 12.0624293 Err 0.1D-04 -
72: 10 2 9 9 2 8 S 2 12.0624335 -0.0043 12.0624293 Err 0.1D-04 -
73: 10 2 9 9 2 8 S 3 12.0624178 0.0114 12.0624293 Err 0.1D-04 -
74: 10 2 9 9 2 8 S 4 12.0624133 0.0160 12.0624293 Err 0.1D-04 -
75: 15 2 14 15 0 15 S 3 12.0656739 0.0120 12.0656860 Err 0.1D-04 -
76: 10 7 3 9 7 2 S 5 12.2501588 0.0127 12.2501715 Err 0.1D-04 -
77: 10 7 3 9 7 2 S 4 12.2501615 0.0100 12.2501715 Err 0.1D-04 -
78: 10 7 3 9 7 2 S 2 12.2501748 -0.0033 12.2501715 Err 0.1D-04 -
79: 10 7 3 9 7 2 S 1 12.2501791 -0.0076 12.2501715 Err 0.1D-04 -
80: 10 6 4 9 6 3 S 5 12.2583211 0.0108 12.2583319 Err 0.1D-04 -
81: 10 6 4 9 6 3 S 3 12.2583271 0.0047 12.2583319 Err 0.1D-04 -
82: 10 6 4 9 6 3 S 2 12.2583373 -0.0054 12.2583319 Err 0.1D-04 -
83: 10 6 4 9 6 3 S 1 12.2583457 -0.0139 12.2583319 Err 0.1D-04 -
84: 10 3 8 9 3 7 S 1 12.2883656 0.0023 12.2883678 Err 0.1D-04 -
85: 11 0 11 10 1 10 S 2 12.4237701 -0.0139 12.4237562 Err 0.1D-04 -
86: 10 1 9 9 1 8 S 1 12.4748067 -0.0386 12.4747681 Err 0.1D-04 -
87: 10 1 9 9 1 8 S 2 12.4747950 -0.0282 12.4747668 Err 0.1D-04 -
88: 10 1 9 9 1 8 S 3 12.4747883 -0.0215 12.4747668 Err 0.1D-04 -
89: 10 1 9 9 1 8 S 5 12.4747763 -0.0095 12.4747668 Err 0.1D-04 -
90: 10 1 9 9 1 8 S 4 12.4747768 -0.0080 12.4747688 Err 0.1D-04 -
91: 11 1 11 10 1 10 S 4 12.5658577 -0.0257 12.5658320 Err 0.1D-04 -
92: 11 0 11 10 0 10 S 1 12.6312859 -0.0338 12.6312522 Err 0.1D-04 -
93: 11 0 11 10 0 10 S 2 12.6312759 -0.0237 12.6312522 Err 0.1D-04 -
94: 11 0 11 10 0 10 S 3 12.6312315 0.0206 12.6312522 Err 0.1D-04 -
95: 10 2 8 9 2 7 S 2 12.7316906 -0.0040 12.7316866 Err 0.1D-04 -
96: 10 2 8 9 2 7 S 1 12.7316911 -0.0052 12.7316859 Err 0.1D-04 -
97: 10 2 8 9 2 7 S 4 12.7316841 0.0018 12.7316859 Err 0.1D-04 -
98: 10 2 8 9 2 7 S 5 12.7316824 0.0035 12.7316859 Err 0.1D-04 -
99: 10 2 8 9 2 7 S 3 12.7316838 0.0067 12.7316906 Err 0.1D-04 -
100: 19 4 16 19 3 17 S 4 13.0745638 -0.0235 13.0745403 Err 0.1D-04 -
101: 19 4 16 19 3 17 S 5 13.0745443 -0.0040 13.0745403 Err 0.1D-04 -
102: 19 4 16 19 3 17 S 2 13.0745220 0.0183 13.0745403 Err 0.1D-04 -
103: 17 3 14 16 4 13 S 1 13.1087306 -0.0250 13.1087056 Err 0.1D-04 -
104: 11 2 10 10 2 9 S 1 13.2316995 -0.0026 13.2316968 Err 0.1D-04 -
105: 11 2 10 10 2 9 S 2 13.2316940 0.0028 13.2316968 Err 0.1D-04 -
106: 11 2 10 10 2 9 S 3 13.2316777 0.0192 13.2316968 Err 0.1D-04 -
107: 11 2 10 10 2 9 S 5 13.2316731 0.0238 13.2316968 Err 0.1D-04 -
108: 11 2 10 10 2 9 S 4 13.2316713 0.0255 13.2316968 Err 0.1D-04 -
109: 11 4 7 10 4 6 S 5 13.5540011 0.0209 13.5540220 Err 0.1D-04 -
110: 11 1 10 10 1 9 S 1 13.6288617 -0.0114 13.6288502 Err 0.1D-04 -
111: 11 1 10 10 1 9 S 2 13.6288464 0.0038 13.6288502 Err 0.1D-04 -

112: 11 1 10 10 1 9 S 3 13.6288386 0.0117 13.6288502 Err 0.1D-04 -
113: 11 1 10 10 1 9 S 4 13.6288237 0.0265 13.6288502 Err 0.1D-04 -
114: 11 1 10 10 1 9 S 5 13.6288229 0.0274 13.6288502 Err 0.1D-04 -
115: 11 3 8 10 3 7 S 1 13.7442488 -0.0006 13.7442482 Err 0.1D-04 -
116: 11 3 8 10 3 7 S 3 13.7442393 0.0090 13.7442482 Err 0.1D-04 -
117: 11 3 8 10 3 7 S 2 13.7442259 0.0223 13.7442482 Err 0.1D-04 -
118: 11 3 8 10 3 7 S 5 13.7442025 0.0457 13.7442482 Err 0.1D-04 -
119: 11 2 9 10 2 8 S 1 14.0206902 -0.0092 14.0206810 Err 0.1D-04 -
120: 11 2 9 10 2 8 S 3 14.0206810 -0.0001 14.0206810 Err 0.1D-04 -
121: 11 2 9 10 2 8 S 5 14.0206784 0.0026 14.0206810 Err 0.1D-04 -
122: 11 2 9 10 2 8 S 2 14.0206881 -0.0130 14.0206750 Err 0.1D-04 -
123: 11 2 9 10 2 8 S 4 14.0206795 0.0004 14.0206799 Err 0.1D-04 -
124: 13 10 3 14 9 5 S 2 14.0279174 0.0144 14.0279318 Err 0.1D-04 -
125: 15 5 11 15 4 11 S 3 14.1680887 0.0195 14.1681083 Err 0.1D-04 -
126: 5 3 2 4 2 2 S 2 14.2795799 0.0106 14.2795905 Err 0.1D-04 -
127: 5 3 3 4 2 3 S 3 14.3642201 -0.0012 14.3642189 Err 0.1D-04 -
128: 12 2 11 11 2 10 S 2 14.3920673 -0.0460 14.3920213 Err 0.2D-04 -
129: 12 2 11 11 2 10 S 3 14.3920502 -0.0289 14.3920213 Err 0.2D-04 -
130: 12 2 11 11 2 10 S 4 14.3920420 -0.0207 14.3920213 Err 0.2D-04 -
131: 12 2 11 11 2 10 S 5 14.3920439 -0.0219 14.3920220 Err 0.2D-04 -
132: 13 1 12 12 2 11 S 1 14.4572492 0.0137 14.4572629 Err 0.1D-04 -
133: 17 5 13 17 4 14 S 4 14.5384727 -0.0134 14.5384593 Err 0.1D-04 -
134: 12 5 8 12 4 8 S 2 14.5704947 -0.0347 14.5704600 Err 0.1D-04 -
135: 12 5 8 12 4 8 S 3 14.5774853 -0.0300 14.5774552 Err 0.1D-04 -
136: 12 5 7 12 4 8 S 1 14.5813348 -0.0165 14.5813183 Err 0.1D-04 -
137: 14 5 10 14 4 11 S 3 14.5845133 0.0091 14.5845225 Err 0.1D-04 -
138: 13 5 8 13 4 10 S 2 14.6291697 -0.0365 14.6291332 Err 0.1D-04 -
139: 12 6 6 11 6 5 S 5 14.7259127 0.0213 14.7259340 Err 0.1D-04 -
140: 12 6 6 11 6 5 S 4 14.7259182 0.0158 14.7259340 Err 0.1D-04 -
141: 12 6 6 11 6 5 S 3 14.7259226 0.0114 14.7259340 Err 0.1D-04 -
142: 12 6 6 11 6 5 S 2 14.7259324 0.0016 14.7259340 Err 0.1D-04 -
143: 12 6 6 11 6 5 S 1 14.7259634 -0.0299 14.7259335 Err 0.1D-04 -
144: 12 3 10 11 3 9 S 2 14.7364910 -0.0211 14.7364699 Err 0.1D-04 -
145: 12 3 10 11 3 9 S 1 14.7364779 -0.0080 14.7364699 Err 0.1D-04 -
146: 12 3 10 11 3 9 S 4 14.7364661 0.0038 14.7364699 Err 0.1D-04 -
147: 12 3 10 11 3 9 S 3 14.7364605 0.0094 14.7364699 Err 0.1D-04 -
148: 12 3 10 11 3 9 S 4 14.7364661 0.0044 14.7364705 Err 0.1D-04 -
149: 12 3 10 11 3 9 S 5 14.7364811 -0.0106 14.7364705 Err 0.1D-04 -
150: 9 5 4 9 4 6 S 4 14.7391661 0.0057 14.7391718 Err 0.1D-04 -
151: 8 5 3 8 4 4 S 3 14.7460280 0.0181 14.7460461 Err 0.1D-04 -
152: 8 5 3 8 4 5 S 1 14.7476946 0.0061 14.7477007 Err 0.1D-04 -
153: 8 5 3 8 4 5 S 3 14.7502500 -0.0120 14.7502380 Err 0.1D-04 -
154: 12 1 11 11 1 10 S 1 14.7578176 -0.0173 14.7578003 Err 0.1D-04 -

155: 12 1 11 11 1 10 S 2 14.7577988 0.0015 14.7578003 Err 0.1D-04 -
156: 12 1 11 11 1 10 S 3 14.7577892 0.0111 14.7578003 Err 0.1D-04 -
157: 12 1 11 11 1 10 S 5 14.7577698 0.0305 14.7578003 Err 0.1D-04 -
158: 12 1 11 11 1 10 S 4 14.7577711 0.0303 14.7578014 Err 0.1D-04 -
159: 5 5 1 5 4 2 S 1 14.7745814 0.0351 14.7746165 Err 0.1D-04 -
160: 5 5 0 5 4 1 S 3 14.7749182 0.0260 14.7749442 Err 0.1D-04 -
161: 15 11 5 16 10 7 S 2 14.8503743 0.0072 14.8503815 Err 0.1D-04 -
162: 12 3 9 11 3 8 S 1 15.0667694 -0.0124 15.0667570 Err 0.1D-04 -
163: 12 3 9 11 3 8 S 4 15.0667620 -0.0050 15.0667570 Err 0.1D-04 -
164: 12 3 9 11 3 8 S 5 15.0667472 0.0098 15.0667570 Err 0.1D-04 -
165: 12 3 9 11 3 8 S 3 15.0667616 -0.0008 15.0667608 Err 0.1D-04 -
166: 12 2 10 11 2 9 S 2 15.2923909 -0.0117 15.2923792 Err 0.1D-04 -
167: 12 2 10 11 2 9 S 2 15.2923909 -0.0077 15.2923832 Err 0.1D-04 -
168: 12 2 10 11 2 9 S 3 15.2923838 -0.0006 15.2923832 Err 0.1D-04 -
169: 12 2 10 11 2 9 S 5 15.2923789 0.0043 15.2923832 Err 0.1D-04 -
170: 12 2 10 11 2 9 S 4 15.2923796 0.0038 15.2923835 Err 0.1D-04 -
171: 13 2 12 12 2 11 S 1 15.5437262 0.0197 15.5437459 Err 0.1D-04 -
172: 13 2 12 12 2 11 S 2 15.5437173 0.0284 15.5437458 Err 0.1D-04 -
173: 14 0 14 13 1 13 S 2 15.8568289 -0.0059 15.8568230 Err 0.1D-04 -
174: 14 0 14 13 1 13 S 1 15.8568547 -0.0317 15.8568230 Err 0.1D-04 -
175: 13 1 12 12 1 11 S 1 15.8652281 -0.0226 15.8652055 Err 0.1D-04 -
176: 13 1 12 12 1 11 S 2 15.8652062 -0.0007 15.8652055 Err 0.1D-04 -
177: 13 3 11 12 3 10 S 1 15.9513464 0.0008 15.9513471 Err 0.1D-04 -
178: 13 3 11 12 3 10 S 2 15.9513512 -0.0041 15.9513471 Err 0.1D-04 -
179: 13 3 11 12 3 10 S 5 15.9513355 0.0116 15.9513471 Err 0.1D-04 -
180: 13 3 11 12 3 10 S 3 15.9513264 0.0207 15.9513471 Err 0.1D-04 -
181: 13 3 11 12 3 10 S 4 15.9513269 0.0202 15.9513471 Err 0.1D-04 -
182: 14 1 14 13 0 13 S 1 15.9625168 -0.0343 15.9624825 Err 0.1D-04 -
183: 14 1 14 13 0 13 S 2 15.9625280 -0.0455 15.9624825 Err 0.1D-04 -
184: 13 6 7 12 6 6 S 1 15.9630109 -0.0499 15.9629610 Err 0.1D-04 -
185: 14 11 3 15 10 5 S 3 16.0899765 -0.0182 16.0899583 Err 0.1D-04 -
186: 20 1 19 20 1 20 S 3 16.2692668 0.0030 16.2692698 Err 0.1D-04 -
187: 14 3 12 13 3 11 S 1 17.1583941 0.0117 17.1584058 Err 0.1D-04 -
188: 14 3 12 13 3 11 S 5 17.1583736 0.0322 17.1584058 Err 0.1D-04 -
189: 14 3 12 13 3 11 S 4 17.1583685 0.0373 17.1584058 Err 0.1D-04 -
190: 5 4 1 4 3 1 S 3 17.6128398 -0.0092 17.6128306 Err 0.1D-04 -
191: 10 6 4 10 5 5 S 2 18.0244248 -0.0286 18.0243961 Err 0.1D-04 -
192: 10 6 4 10 5 5 S 5 18.0247844 -0.0112 18.0247732 Err 0.1D-04 -
193: 9 6 3 9 5 4 S 1 18.0370179 -0.0217 18.0369961 Err 0.1D-04 -
194: 8 6 3 8 5 4 S 1 18.0471964 0.0363 18.0472326 Err 0.1D-04 -
195: 8 6 2 8 5 3 S 2 18.0483775 -0.0126 18.0483649 Err 0.1D-04 -
196: 8 6 2 8 5 3 S 5 18.0487358 -0.0215 18.0487143 Err 0.1D-04 -
197: 12 0 12 11 1 10 S 4 6.3908836 -0.0081 6.3908755 Err 0.2D-04 -

```
 198: 11  1 11 10  0 10   S 2  12.7733819   -0.0412  12.7733407   Err 0.1D-04          -
 199:  7  2  5  6  1  5   S 1  12.9770127    0.0492  12.9770619   Err 0.1D-04          -
 200: 12  1 11 11  2 10   S 2  12.9841806    0.0358  12.9842164   Err 0.1D-04          -
 201: 12  6  6 12  5  7   S 2  17.9815894   -0.0126  17.9815769   Err 0.1D-04          -
 202: 11  6  5 11  5  6   S 3  18.0049562   -0.0001  18.0049560   Err 0.1D-04          -
 203:  8  6  2  8  5  3   S 4  18.0479598    0.0105  18.0479703   Err 0.1D-04          -
 Maximum (obs-calc)/err in line 184   0.0000499

 RMS deviations (MHz), B and V sorted
  B  V   n splittings MHz
  B  V   n abs. freq. MHz
  1  1 203         0.019215         0.020161

          Parameters  and  Errors
 BJ          0.610891115 { 0.000000190}
 BK           1.643027726 { 0.000000730}
 B-          0.058771614 { 0.000000038}
 DJ          0.013393E-6 { 0.000613E-6}
 DJK          0.026994E-6 { 0.003152E-6}
 DK          -0.153775E-6 { 0.004178E-6}
\F12         -0.849109546 {     derived}
\F          158.759326752 {     derived}  160.208738102 {     derived}
 V1n         15750.491355 {    9.506632}   14796.982478 {    9.836135}
\rho          0.005876522 {     derived}    0.013938624 {     derived}
\beta         0.594535117 {     derived}    3.078785442 {     derived}
\gamma        1.455979935 {     derived}   -2.539967012 {     derived}
 delta        1.222540459 { 0.001845476}    2.918296338 { 0.014166621}

 Standard Deviation       0.019757 MHz

------------------------------------ B =  1
 Rotational Constants and Errors (in GHz)
     B_z       2.253918841       0.000000765
     B_x       0.669662729       0.000000194
     B_y       0.552119501       0.000000192
 Ray's kappa   -0.86186
 F0(calc)     158.000000000       0.000000000
 I_alpha        3.198601709       0.000000000
 <(i,x)  <(i,y)  <(i,z)       84.8955       20.6505       70.0464
d<(i,x) d<(i,y) d<(i,z)        0.0034        0.1018        0.1057

 F0(calc)     158.000000000       0.000000000
 I_alpha        3.198601709       0.000000000
```

```
 <(i,x)  <(i,y)  <(i,z)      99.7979      98.1463     167.2061
d<(i,x) d<(i,y) d<(i,z)       0.6177       0.5121      0.8117

 V1n_1      6.284939 kj +/- 0.003793 kj        1.501095 kcal +/- 0.000906 kcal
        525.379766 cm +/-   0.3171 cm    s=  44.093273
 V1n_2      5.904459 kj +/- 0.003925 kj        1.410221 kcal +/- 0.000937 kcal
        493.574138 cm +/-   0.3281 cm    s=  41.423939

F(calc)      158.759326752
F(calc)      160.208738102
```

$^{13}C_4$ Isotopologue XIAM Output

```
  J K- K+  J K- K+    Sym   calc/GHz  diff/MHz     obs/GHz
 1:  5  1  5  4  1  4   S 1   5.7984678    0.0085   5.7984763   Err 0.1D-04          -
 2: 16  1 16 15  2 14   S 1   6.0771596   -0.0366   6.0771230   Err 0.1D-04          -
 3:  6  0  6  5  1  5   S 5   6.2116325    0.0313   6.2116638   Err 0.1D-04          -
 4:  6  0  6  5  1  5   S 4   6.2116354    0.0279   6.2116632   Err 0.1D-04          -
 5:  6  0  6  5  1  5   S 2   6.2116431    0.0201   6.2116632   Err 0.1D-04          -
 6:  5  2  3  4  2  2   S 3   6.2282919   -0.0428   6.2282491   Err 0.1D-04          -
 7:  5  2  3  4  2  2   S 4   6.2282570   -0.0079   6.2282491   Err 0.1D-04          -
 8:  5  1  4  4  1  3   S 1   6.3852230   -0.0090   6.3852140   Err 0.1D-04          -
 9:  6  1  6  5  1  5   S 1   6.9436988    0.0029   6.9437017   Err 0.1D-04          -
10:  8  3  6  8  2  6   S 1   7.3634478    0.0081   7.3634559   Err 0.1D-04          -
11:  6  2  4  5  2  3   S 1   7.5207626    0.0011   7.5207637   Err 0.1D-04          -
12:  7  0  7  6  1  6   S 1   7.5261194    0.0325   7.5261519   Err 0.1D-04          -
13:  6  1  5  5  1  4   S 1   7.6412575   -0.0150   7.6412425   Err 0.1D-04          -
14:  7  0  7  6  0  6   S 1   8.2582079   -0.0004   8.2582075   Err 0.1D-04          -
15:  8  0  8  7  1  7   S 1   8.8067733    0.0236   8.8067969   Err 0.1D-04          -
16: 11  2 10 11  1 11   S 1   8.9748789    0.0446   8.9749235   Err 0.2D-04          -
17: 11  2 10 11  1 11   S 3   8.9748725    0.0510   8.9749235   Err 0.2D-04          -
18:  8  5  3  7  5  2   S 1   9.8231877   -0.0289   9.8231588   Err 0.1D-04          -
19:  9  3  7  8  3  6   S 2  11.0785861    0.0024  11.0785886   Err 0.1D-04          -
20: 10  4  7 10  3  7   S 4  11.0829277    0.0136  11.0829413   Err 0.1D-04          -
21:  7  4  3  7  3  5   S 4  11.4374714   -0.0040  11.4374673   Err 0.1D-04          -
22:  5  4  1  5  3  3   S 5  11.4602023   -0.0112  11.4601911   Err 0.1D-04          -
23: 22  4 19 21  5 16   S 2  11.6361545    0.0053  11.6361599   Err 0.1D-04          -
24: 10  1 10  9  0  9   S 1  11.7569845    0.0410  11.7570255   Err 0.1D-04          -
25: 10  2  9  9  2  8   S 1  12.0821202    0.0102  12.0821304   Err 0.1D-04          -
26: 10  6  4  9  6  3   S 1  12.2809792    0.0012  12.2809804   Err 0.1D-04          -
27: 10  5  5  9  5  4   S 4  12.2950450    0.0080  12.2950530   Err 0.1D-04          -
28: 11  0 11 10  1 10   S 2  12.4446726    0.0135  12.4446862   Err 0.1D-04          -
```

29: 10 1 9 9 1 8 S 1 12.4947580 -0.0220 12.4947359 Err 0.1D-04 -
30: 10 1 9 9 1 8 S 2 12.4947455 -0.0096 12.4947359 Err 0.1D-04 -
31: 10 1 9 9 1 8 S 3 12.4947391 -0.0032 12.4947359 Err 0.1D-04 -
32: 10 1 9 9 1 8 S 4 12.4947270 0.0089 12.4947359 Err 0.1D-04 -
33: 10 1 9 9 1 8 S 5 12.4947263 0.0095 12.4947359 Err 0.1D-04 -
34: 11 1 11 10 1 10 S 1 12.5834342 0.0390 12.5834732 Err 0.1D-04 -
35: 11 0 11 10 0 10 S 1 12.6478394 0.0180 12.6478574 Err 0.1D-04 -
36: 10 2 8 9 2 7 S 4 12.7579652 -0.0420 12.7579232 Err 0.1D-04 -
37: 10 2 8 9 2 7 S 5 12.7579635 -0.0404 12.7579231 Err 0.1D-04 -
38: 10 2 8 9 2 7 S 3 12.7579658 -0.0426 12.7579231 Err 0.1D-04 -
39: 19 5 14 19 4 15 S 1 12.8030275 0.0271 12.8030546 Err 0.1D-04 -
40: 19 5 14 19 4 15 S 4 12.8026402 -0.0188 12.8026215 Err 0.1D-04 -
41: 19 12 7 20 11 9 S 5 13.0306142 0.0017 13.0306159 Err 0.1D-04 -
42: 14 5 10 14 4 10 S 3 14.2956285 -0.0127 14.2956158 Err 0.1D-04 -
43: 12 2 11 11 2 10 S 1 14.4145803 0.0081 14.4145884 Err 0.1D-04 -
44: 10 2 9 9 1 8 S 3 14.6391258 -0.0014 14.6391245 Err 0.1D-04 -
45: 9 5 4 9 4 5 S 1 14.6753055 -0.0001 14.6753054 Err 0.1D-04 -
46: 12 9 3 11 9 2 S 1 14.7235417 -0.0124 14.7235293 Err 0.1D-04 -
47: 12 9 3 11 9 2 S 2 14.7235368 -0.0052 14.7235316 Err 0.1D-04 -
48: 12 9 3 11 9 2 S 3 14.7235221 0.0095 14.7235316 Err 0.1D-04 -
49: 12 9 3 11 9 2 S 4 14.7235204 0.0112 14.7235316 Err 0.1D-04 -
50: 12 9 3 11 9 2 S 5 14.7235173 0.0143 14.7235316 Err 0.1D-04 -
51: 12 8 4 11 8 3 S 1 14.7297835 -0.0070 14.7297765 Err 0.1D-04 -
52: 12 7 5 11 7 4 S 1 14.7389714 -0.0024 14.7389690 Err 0.1D-04 -
53: 12 3 9 11 3 8 S 3 15.0998167 -0.0478 15.0997688 Err 0.1D-04 -
54: 12 3 9 11 3 8 S 4 15.0998164 -0.0475 15.0997689 Err 0.1D-04 -
55: 12 3 9 11 3 8 S 5 15.0998020 -0.0331 15.0997689 Err 0.1D-04 -
56: 12 2 10 11 2 9 S 5 15.3220303 -0.0390 15.3219913 Err 0.1D-04 -
57: 12 2 10 11 2 9 S 4 15.3220311 -0.0398 15.3219913 Err 0.1D-04 -
58: 18 2 16 17 3 14 S 2 15.4129732 0.0353 15.4130085 Err 0.1D-04 -
59: 13 2 12 12 2 11 S 1 15.5675187 0.0157 15.5675344 Err 0.1D-04 -
60: 13 2 12 12 2 11 S 2 15.5675092 0.0281 15.5675373 Err 0.1D-04 -
61: 13 3 11 12 3 10 S 1 15.9795831 0.0025 15.9795856 Err 0.1D-04 -
62: 14 2 13 13 2 12 S 1 16.7121138 0.0186 16.7121324 Err 0.1D-04 -
63: 14 4 10 13 4 9 S 2 17.4062378 -0.0160 17.4062218 Err 0.1D-04 -
64: 8 2 6 7 1 7 S 1 17.5030632 0.0345 17.5030977 Err 0.1D-04 -
65: 15 2 14 14 2 13 S 4 17.8490165 -0.0032 17.8490133 Err 0.1D-04 -
66: 14 2 12 14 2 13 S 2 6.1858170 -0.0074 6.1858096 Err 0.1D-04 -
67: 15 2 13 15 1 14 S 1 7.9243486 0.0210 7.9243696 Err 0.1D-04 -
68: 4 2 2 3 1 3 S 5 10.2579865 0.0055 10.2579919 Err 0.1D-04 -
69: 13 5 9 13 4 10 S 2 14.5630281 -0.0247 14.5630034 Err 0.1D-04 -
70: 15 2 13 14 3 12 S 2 14.7399368 0.0105 14.7399473 Err 0.1D-04 -
71: 16 3 13 16 2 15 S 2 15.1359436 -0.0139 15.1359297 Err 0.1D-04 -

```
 Maximum (obs-calc)/err in line   6   0.0000428

 RMS deviations (MHz), B and V sorted
  B  V   n splittings MHz
  B  V   n abs. freq. MHz
  1  1  71         0.022001         0.024480

          Parameters  and  Errors
 BJ          0.611991331 { 0.000000303}
 BK           1.637832355 { 0.000001327}
 B-          0.059129379 { 0.000000064}
 DJ          0.013304E-6 { 0.000738E-6}
 DJK          0.025107E-6 { 0.004219E-6}
 DK          -0.147754E-6 { 0.005792E-6}
\F12         -0.847797807 {     derived}
\F          158.755759057 {     derived}  160.174593927 {     derived}
 V1n         15721.525802 {   19.315072}   14768.524017 {    4.024298}
\rho         0.005836152 {     derived}    0.013791622 {     derived}
\beta        0.600991805 {     derived}    3.067186315 {     derived}
\gamma       1.455885321 {     derived}   -2.540354702 {     derived}

 Standard Deviation       0.023543 MHz

------------------------------------ B =  1
 Rotational Constants and Errors (in GHz)
     B_z       2.249823686       0.000001413
     B_x       0.671120710       0.000000297
     B_y       0.552861951       0.000000322
 Ray's kappa   -0.86062
 F0(calc)     158.000000000       0.000000000
 I_alpha        3.198601709       0.000000000
 <(i,x)  <(i,y)  <(i,z)       84.8892       20.4618       70.2424
d<(i,x) d<(i,y) d<(i,z)        0.0000        0.0000        0.0000

 F0(calc)     158.000000000       0.000000000
 I_alpha        3.198601709       0.000000000
 <(i,x)  <(i,y)  <(i,z)      101.4809       99.5401      164.9886
d<(i,x) d<(i,y) d<(i,z)        0.0000        0.0000        0.0000

 V1n_1      6.273381 kj +/- 0.007707 kj         1.498334 kcal +/- 0.001841 kcal
        524.413579 cm +/-   0.6443 cm    s=  44.013174
 V1n_2      5.893104 kj +/- 0.001606 kj         1.407509 kcal +/- 0.000384 kcal
        492.624866 cm +/-   0.1342 cm    s=  41.345199
```

F(calc) 158.755759057
F(calc) 160.174593927

$^{13}C_5$ Isotopologue XIAM Output

	J K- K+	J K- K+	Sym	calc/GHz	diff/MHz	obs/GHz	
1:	3 2 2	2 1 1	S 1	8.3948240	0.0117	8.3948357	Err 0.1D-04 -
2:	17 10 8	18 9 9	S 1	8.7365414	0.0029	8.7365443	Err 0.1D-04 -
3:	8 0 8	7 1 7	S 1	8.8312567	0.0094	8.8312661	Err 0.1D-04 -
4:	8 1 7	7 1 6	S 1	10.1312202	-0.0103	10.1312099	Err 0.1D-04 -
5:	10 8 3	11 7 4	S 1	10.9033331	-0.0124	10.9033207	Err 0.1D-04 -
6:	9 2 8	8 2 7	S 1	10.9247257	0.0253	10.9247510	Err 0.1D-04 -
7:	9 7 2	8 7 1	S 1	11.0663481	-0.0017	11.0663464	Err 0.1D-04 -
8:	9 4 5	9 3 6	S 1	11.1866068	-0.0233	11.1865835	Err 0.1D-04 -
9:	14 2 13	14 0 14	S 1	11.2993333	0.0266	11.2993599	Err 0.1D-04 -
10:	9 1 8	8 1 7	S 1	11.3374354	0.0113	11.3374468	Err 0.1D-04 -
11:	6 4 2	6 3 3	S 1	11.3750139	-0.0136	11.3750003	Err 0.1D-04 -
12:	13 4 9	13 3 11	S 1	11.6730208	-0.0074	11.6730134	Err 0.1D-04 -
13:	10 7 3	9 7 2	S 1	12.3002422	0.0082	12.3002504	Err 0.1D-04 -
14:	11 6 5	10 6 4	S 1	13.5467654	-0.0078	13.5467577	Err 0.1D-04 -
15:	11 4 7	10 4 6	S 1	13.6138265	-0.0195	13.6138070	Err 0.1D-04 -
16:	12 0 12	11 1 11	S 1	13.6314002	-0.0274	13.6313729	Err 0.1D-04 -
17:	18 3 15	17 4 13	S 1	14.3736215	0.0125	14.3736340	Err 0.1D-04 -
18:	14 5 9	14 4 11	S 1	14.4884771	-0.0005	14.4884766	Err 0.1D-04 -
19:	4 4 0	3 3 1	S 1	16.3258600	0.0228	16.3258828	Err 0.1D-04 -
20:	14 1 13	13 1 12	S 1	17.0059950	0.0082	17.0060032	Err 0.2D-04 -
21:	14 8 6	13 8 5	S 1	17.2359498	-0.0012	17.2359486	Err 0.1D-04 -
22:	15 1 14	14 2 13	S 1	17.3160263	0.0263	17.3160526	Err 0.1D-04 -
23:	13 6 8	13 5 8	S 1	17.8105993	0.0253	17.8106246	Err 0.1D-04 -
24:	14 3 11	13 3 10	S 1	17.8261126	-0.0423	17.8260703	Err 0.1D-04 -
25:	20 2 18	20 1 19	S 1	13.4811402	-0.0155	13.4811247	Err 0.1D-04 -

Maximum (obs-calc)/err in line 24 0.0000423

RMS deviations (MHz), B and V sorted

B	V	n	splittings MHz	
B	V	n	abs. freq. MHz	
1	1	25	0.018293	0.022683

Parameters and Errors

BJ	0.613338724 { 0.000000630}
BK	1.631115865 { 0.000001545}
B-	0.059550627 { 0.000000098}
DJ	0.012158E-6 { 0.001546E-6}

DJK 0.030913E-6 { 0.007617E-6}
DK -0.156147E-6 { 0.010532E-6}
\F12 -0.846164996 { derived}
\F 158.755957424 { derived} 160.169527370 { derived}
\rho 0.005829838 { derived} 0.013759069 { derived}
\beta 0.602894012 { derived} 3.066835979 { derived}
\gamma 1.455776140 { derived} -2.540801549 { derived}

Standard Deviation 0.021558 MHz

---------- B = 1
Rotational Constants and Errors (in GHz)
B_z 2.244454588 0.000001832
B_x 0.672889351 0.000000655
B_y 0.553788097 0.000000619
Ray's kappa -0.85911
F0(calc) 158.000000000 0.000000000
I_alpha 3.198601709 0.000000000
<(i,x) <(i,y) <(i,z) 84.8892 20.4618 70.2424
d<(i,x) d<(i,y) d<(i,z) 0.0000 0.0000 0.0000

F0(calc) 158.000000000 0.000000000
I_alpha 3.198601709 0.000000000
<(i,x) <(i,y) <(i,z) 101.4809 99.5401 164.9886
d<(i,x) d<(i,y) d<(i,z) 0.0000 0.0000 0.0000

V1n_1 6.275827 kj +/- 0.000000 kj 1.498919 kcal +/- 0.000000 kcal
524.618074 cm +/- 0.0000 cm s= 44.030282
V1n_2 5.894025 kj +/- 0.000000 kj 1.407729 kcal +/- 0.000000 kcal
492.701873 cm +/- 0.0000 cm s= 41.351610

F(calc) 158.755957424
F(calc) 160.169527370

$^{13}C_6$ Isotopologue XIAM Output

	J K- K+	J K- K+	Sym	calc/GHz	diff/MHz	obs/GHz		
1:	5 1 5	4 1 4	S 4	5.8096546	0.0088	5.8096634	Err 0.1D-04	-
2:	5 1 5	4 1 4	S 5	5.8096560	0.0123	5.8096683	Err 0.1D-04	-
3:	5 1 5	4 1 4	S 3	5.8096557	0.0126	5.8096683	Err 0.1D-04	-
4:	5 1 5	4 1 4	S 2	5.8096671	0.0012	5.8096683	Err 0.1D-04	-
5:	5 1 5	4 1 4	S 1	5.8096676	0.0007	5.8096683	Err 0.1D-04	-
6:	16 4 12	15 5 11	S 1	5.8999709	0.0252	5.8999961	Err 0.1D-04	-
7:	5 0 5	4 0 4	S 1	6.0086083	-0.0113	6.0085970	Err 0.1D-04	-

```
 8:  5  0  5  4  0  4   S 3   6.0085965    0.0006   6.0085970   Err 0.1D-04          -
 9:  5  0  5  4  0  4   S 5   6.0085924    0.0046   6.0085970   Err 0.1D-04          -
10:  5  0  5  4  0  4   S 2   6.0086046   -0.0034   6.0086012   Err 0.1D-04          -
11:  5  0  5  4  0  4   S 4   6.0085931    0.0081   6.0086012   Err 0.1D-04          -
12: 14  8  6 15  7  9   S 1   6.0958704    0.0119   6.0958823   Err 0.1D-04          -
13: 14  8  6 15  7  8   S 5   6.0972680   -0.0122   6.0972558   Err 0.1D-04          -
14: 13  2 11 13  1 12   S 1   6.1572263    0.0027   6.1572290   Err 0.1D-04          -
15: 13  2 11 13  1 12   S 4   6.1572633   -0.0302   6.1572332   Err 0.1D-04          -
16: 13  2 11 13  1 12   S 5   6.1572698   -0.0366   6.1572332   Err 0.1D-04          -
17:  6  0  6  5  1  5   S 1   6.2199500    0.0397   6.2199897   Err 0.1D-04          -
18:  5  1  4  4  1  3   S 1   6.3956998    0.0047   6.3957045   Err 0.1D-04          -
19:  5  1  4  4  1  3   S 3   6.3956947    0.0098   6.3957045   Err 0.1D-04          -
20:  5  1  4  4  1  3   S 5   6.3956918    0.0128   6.3957045   Err 0.1D-04          -
21:  5  1  4  4  1  3   S 4   6.3956925    0.0125   6.3957050   Err 0.1D-04          -
22:  5  1  4  4  1  3   S 2   6.3956972    0.0078   6.3957050   Err 0.1D-04          -
23:  6  1  6  5  1  5   S 1   6.9572113   -0.0102   6.9572011   Err 0.1D-04          -
24: 20  1 20 19  2 18   S 1   7.0814557    0.0334   7.0814891   Err 0.1D-04          -
25:  6  0  6  5  0  5   S 1   7.1519421   -0.0061   7.1519360   Err 0.1D-04          -
26:  9  3  6  9  2  7   S 1   7.2080297   -0.0149   7.2080148   Err 0.1D-04          -
27:  6  2  5  5  2  4   S 1   7.3281381   -0.0135   7.3281246   Err 0.1D-04          -
28:  8  3  6  8  2  6   S 1   7.3940001   -0.0257   7.3939744   Err 0.1D-04          -
29:  6  1  5  5  1  4   S 1   7.6539692    0.0078   7.6539770   Err 0.1D-04          -
30:  6  1  5  5  1  4   S 2   7.6539660    0.0141   7.6539801   Err 0.1D-04          -
31:  6  1  5  5  1  4   S 3   7.6539625    0.0176   7.6539801   Err 0.1D-04          -
32:  6  1  5  5  1  4   S 5   7.6539590    0.0210   7.6539801   Err 0.1D-04          -
33:  5  3  2  5  2  3   S 3   8.0609119    0.0062   8.0609181   Err 0.1D-04          -
34:  4  3  1  4  2  2   S 1   8.1443447    0.0205   8.1443652   Err 0.1D-04          -
35:  3  3  1  3  2  2   S 1   8.2199861    0.0076   8.2199937   Err 0.1D-04          -
36:  6  3  4  6  2  5   S 1   8.3286805    0.0228   8.3287033   Err 0.1D-04          -
37:  7  2  6  6  2  5   S 1   8.5335939    0.0180   8.5336119   Err 0.1D-04          -
38: 10  1  9  9  2  8   S 3   9.9432133    0.0372   9.9432504   Err 0.1D-04          -
39: 10  1  9  9  2  8   S 2   9.9433109    0.0246   9.9433355   Err 0.1D-04          -
40: 10  1  9  9  2  8   S 4   9.9433220    0.0135   9.9433355   Err 0.1D-04          -
41: 10  1  9  9  2  8   S 5   9.9433253    0.0102   9.9433355   Err 0.1D-04          -
42:  8  5  3  7  5  2   S 1   9.8400840   -0.0267   9.8400573   Err 0.1D-04          -
43:  8  6  2  7  6  1   S 1   9.8329288    0.0083   9.8329371   Err 0.1D-04          -
44:  9  0  9  8  1  8   S 1  10.0686181   -0.0126  10.0686055   Err 0.1D-04          -
45:  8  2  6  7  2  5   S 1  10.1566443    0.0060  10.1566503   Err 0.1D-04          -
46:  8  2  6  7  2  5   S 2  10.1566421    0.0082  10.1566503   Err 0.1D-04          -
47:  8  2  6  7  2  5   S 3  10.1566387    0.0117  10.1566503   Err 0.1D-04          -
48:  8  2  6  7  2  5   S 5  10.1566339    0.0164  10.1566503   Err 0.1D-04          -
49:  6  1  5  5  0  5   S 1  10.3515134    0.0376  10.3515510   Err 0.1D-04          -
50:  6  1  5  5  0  5   S 3  10.3515215    0.0295  10.3515510   Err 0.1D-04          -
```

51: 19 3 17 18 4 15 S 1 10.4342898 0.0321 10.4343219 Err 0.1D-04 -
52: 9 1 9 8 0 8 S 2 10.7762759 -0.0299 10.7762460 Err 0.1D-04 -
53: 9 1 9 8 0 8 S 4 10.7762557 -0.0097 10.7762460 Err 0.1D-04 -
54: 9 1 9 8 0 8 S 5 10.7762786 -0.0316 10.7762470 Err 0.1D-04 -
55: 9 2 8 8 2 7 S 1 10.9223867 -0.0130 10.9223737 Err 0.1D-04 -
56: 9 5 5 8 5 4 S 1 11.0768152 0.0372 11.0768523 Err 0.1D-04 -
57: 9 3 6 8 3 5 S 1 11.1895398 -0.0363 11.1895034 Err 0.1D-04 -
58: 10 0 10 9 1 9 S 1 11.2825579 -0.0267 11.2825312 Err 0.1D-04 -
59: 6 4 3 6 3 3 S 1 11.4604406 0.0120 11.4604525 Err 0.1D-04 -
60: 8 4 4 8 3 6 S 1 11.4644880 -0.0068 11.4644812 Err 0.1D-04 -
61: 22 4 19 21 5 16 S 1 11.6555524 -0.0025 11.6555499 Err 0.1D-04 -
62: 10 2 9 9 2 8 S 1 12.1043684 -0.0120 12.1043564 Err 0.1D-04 -
63: 10 6 4 9 6 3 S 1 12.3020931 0.0026 12.3020956 Err 0.1D-04 -
64: 10 1 9 9 1 8 S 1 12.5175804 -0.0350 12.5175454 Err 0.1D-04 -
65: 10 2 8 9 2 7 S 2 12.7780967 -0.0250 12.7780718 Err 0.1D-04 -
66: 14 2 12 13 3 11 S 2 12.9205709 -0.0175 12.9205534 Err 0.1D-04 -
67: 12 1 11 11 2 10 S 1 13.0435991 0.0387 13.0436378 Err 0.1D-04 -
68: 12 1 11 11 2 10 S 3 13.0436010 0.0368 13.0436378 Err 0.1D-04 -
69: 8 2 7 7 1 6 S 2 13.1130688 0.0354 13.1131042 Err 0.1D-04 -
70: 11 2 10 10 2 9 S 1 13.2775084 -0.0100 13.2774984 Err 0.1D-04 -
71: 11 6 5 10 6 4 S 1 13.5393385 0.0029 13.5393414 Err 0.1D-04 -
72: 11 6 5 10 6 4 S 2 13.5393229 0.0184 13.5393414 Err 0.1D-04 -
73: 11 6 5 10 6 4 S 3 13.5393125 0.0289 13.5393414 Err 0.1D-04 -
74: 11 6 5 10 6 4 S 4 13.5393091 0.0322 13.5393414 Err 0.1D-04 -
75: 11 6 5 10 6 4 S 5 13.5393047 0.0367 13.5393414 Err 0.1D-04 -
76: 16 11 5 17 10 7 S 2 13.5428866 -0.0061 13.5428805 Err 0.1D-04 -
77: 11 3 8 10 3 7 S 1 13.7951366 0.0031 13.7951397 Err 0.1D-04 -
78: 11 2 9 10 2 8 S 1 14.0713861 -0.0212 14.0713649 Err 0.1D-04 -
79: 11 2 9 10 2 8 S 2 14.0713840 -0.0194 14.0713646 Err 0.1D-04 -
80: 11 2 9 10 2 8 S 3 14.0713767 -0.0122 14.0713646 Err 0.1D-04 -
81: 11 2 9 10 2 8 S 4 14.0713752 -0.0106 14.0713646 Err 0.1D-04 -
82: 11 2 9 10 2 8 S 5 14.0713741 -0.0072 14.0713669 Err 0.1D-04 -
83: 5 3 3 4 2 2 S 1 14.2931229 0.0147 14.2931377 Err 0.1D-04 -
84: 14 5 9 14 4 10 S 1 14.3613545 -0.0362 14.3613182 Err 0.1D-04 -
85: 14 5 9 14 4 10 S 5 14.3661610 -0.0214 14.3661396 Err 0.1D-04 -
86: 5 3 2 4 2 3 S 4 14.3950363 0.0124 14.3950486 Err 0.1D-04 -
87: 21 2 19 21 2 20 S 1 14.4254803 0.0083 14.4254886 Err 0.1D-04 -
88: 18 1 17 18 0 18 S 1 14.4432575 -0.0331 14.4432244 Err 0.1D-04 -
89: 17 5 13 17 4 14 S 1 14.5409866 0.0310 14.5410176 Err 0.1D-04 -
90: 12 5 7 12 4 8 S 1 14.5804888 -0.0035 14.5804853 Err 0.1D-04 -
91: 13 5 8 13 4 10 S 1 14.6239289 0.0329 14.6239618 Err 0.1D-04 -
92: 8 5 4 8 4 5 S 3 14.7474689 -0.0177 14.7474512 Err 0.1D-04 -
93: 12 8 4 11 8 3 S 1 14.7551677 -0.0244 14.7551433 Err 0.1D-04 -

94: 7 5 3 7 4 4 S 1 14.7614906 -0.0128 14.7614778 Err 0.1D-04 -
95: 12 7 5 11 7 4 S 1 14.7643050 0.0279 14.7643329 Err 0.1D-04 -
96: 6 5 1 6 4 2 S 1 14.7700155 -0.0403 14.7699752 Err 0.1D-04 -
97: 6 5 1 6 4 3 S 1 14.7702845 0.0290 14.7703135 Err 0.1D-04 -
98: 6 5 1 6 4 2 S 4 14.7710287 -0.0021 14.7710266 Err 0.1D-04 -
99: 5 5 1 5 4 2 S 2 14.7738383 -0.0034 14.7738349 Err 0.1D-04 -
100: 5 5 1 5 4 2 S 4 14.7742036 -0.0153 14.7741883 Err 0.1D-04 -
101: 5 5 0 5 4 1 S 4 14.7767752 0.0166 14.7767918 Err 0.1D-04 -
102: 19 5 14 19 4 16 S 4 14.8776655 0.0255 14.8776911 Err 0.1D-04 -
103: 12 3 9 11 3 8 S 1 15.1228648 -0.0188 15.1228460 Err 0.1D-04 -
104: 12 3 9 11 3 8 S 4 15.1228576 -0.0116 15.1228460 Err 0.1D-04 -
105: 12 3 9 11 3 8 S 5 15.1228429 0.0031 15.1228460 Err 0.1D-04 -
106: 12 2 10 11 2 9 S 1 15.3471688 -0.0330 15.3471358 Err 0.1D-04 -
107: 12 2 10 11 2 9 S 2 15.3471641 -0.0283 15.3471358 Err 0.1D-04 -
108: 12 2 10 11 2 9 S 5 15.3471519 -0.0161 15.3471358 Err 0.1D-04 -
109: 12 2 10 11 2 9 S 4 15.3471526 -0.0141 15.3471385 Err 0.1D-04 -
110: 12 2 10 11 2 9 S 3 15.3471569 -0.0183 15.3471385 Err 0.1D-04 -
111: 6 3 4 5 2 3 S 1 15.4406987 0.0095 15.4407081 Err 0.1D-04 -
112: 13 2 12 12 2 11 S 1 15.5971145 -0.0354 15.5970791 Err 0.1D-04 -
113: 13 3 11 12 3 10 S 1 16.0076729 -0.0304 16.0076424 Err 0.1D-04 -
114: 14 1 14 13 0 13 S 2 16.0158137 0.0015 16.0158152 Err 0.1D-04 -
115: 14 1 14 13 0 13 S 1 16.0158008 0.0144 16.0158152 Err 0.1D-04 -
116: 13 5 8 12 5 8 S 3 16.0575275 0.0028 16.0575302 Err 0.1D-04 -
117: 20 1 19 20 1 20 S 3 16.3159591 -0.0018 16.3159573 Err 0.1D-04 -
118: 13 2 11 12 2 10 S 1 16.6021274 -0.0326 16.6020948 Err 0.1D-04 -
119: 14 4 10 13 4 9 S 5 17.4340302 0.0213 17.4340515 Err 0.1D-04 -
120: 12 6 7 12 5 8 S 2 17.9793350 0.0086 17.9793436 Err 0.1D-04 -
121: 11 6 6 11 5 7 S 2 18.0036722 0.0267 18.0036989 Err 0.1D-04 -
122: 9 6 3 9 5 4 S 3 18.0388828 -0.0357 18.0388471 Err 0.1D-04 -
123: 8 6 2 8 5 3 S 3 18.0490660 -0.0002 18.0490658 Err 0.1D-04 -
124: 7 6 2 7 5 3 S 1 18.0558497 0.0347 18.0558845 Err 0.1D-04 -
125: 6 6 0 6 5 1 S 1 18.0606217 0.0127 18.0606344 Err 0.1D-04 -
126: 16 0 16 15 0 15 S 3 18.1830923 0.0042 18.1830965 Err 0.1D-04 -
127: 16 0 16 15 0 15 S 4 18.1832308 0.0033 18.1832341 Err 0.1D-04 -
128: 20 3 18 19 4 15 S 5 9.1762381 -0.0361 9.1762021 Err 0.1D-04 -
129: 14 4 10 14 3 11 S 4 10.0105504 -0.0090 10.0105414 Err 0.1D-04 -
130: 7 4 4 7 3 5 S 2 11.4634221 -0.0374 11.4633848 Err 0.1D-04 -
131: 9 2 7 8 2 6 S 1 11.4713632 -0.0022 11.4713610 Err 0.1D-04 -
132: 10 4 6 10 3 8 S 5 11.4849816 0.0147 11.4849963 Err 0.1D-04 -
133: 11 4 8 11 3 9 S 3 11.4861120 -0.0417 11.4860703 Err 0.1D-04 -
134: 4 4 1 4 3 2 S 4 11.4892604 0.0107 11.4892711 Err 0.1D-04 -
135: 11 4 7 11 3 9 S 3 11.5234013 0.0357 11.5234370 Err 0.1D-04 -
136: 19 2 17 19 1 18 S 5 12.2886029 -0.0053 12.2885976 Err 0.1D-04 -

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137:  4  3  1  3  2  2   S 5  13.1438651    0.0100  13.1438751   Err 0.1D-04          -
138: 20  2 18 20  1 19   S 1  13.4023049    0.0027  13.4023076   Err 0.1D-04          -
139: 11  4  7 10  4  7   S 2  13.6254086   -0.0317  13.6253769   Err 0.1D-04          -
140:  5  3  2  4  2  2   S 3  14.2992884    0.0111  14.2992995   Err 0.1D-04          -
141: 14  5  9 14  4 10   S 2  14.3647423   -0.0051  14.3647372   Err 0.1D-04          -
142: 12  2 11 11  2 10   S 1  14.4416994   -0.0261  14.4416734   Err 0.1D-04          -
143: 12  2 11 11  2 10   S 2  14.4416922   -0.0188  14.4416734   Err 0.1D-04          -
144: 12  2 11 11  2 10   S 3  14.4416746   -0.0013  14.4416734   Err 0.1D-04          -
145: 12  2 11 11  2 10   S 4  14.4416664    0.0070  14.4416734   Err 0.1D-04          -
146: 12  2 11 11  2 10   S 5  14.4416683    0.0035  14.4416718   Err 0.1D-04          -
147: 10  2  9  9  1  8   S 2  14.6786224    0.0021  14.6786245   Err 0.1D-04          -
148:  8  5  3  8  4  4   S 2  14.7484435    0.0302  14.7484737   Err 0.1D-04          -
149: 12  4  9 11  4  8   S 4  14.8336380   -0.0085  14.8336295   Err 0.1D-04          -
150: 10  6  4 10  5  6   S 1  18.0247464    0.0270  18.0247734   Err 0.1D-04          -
151:  8  6  3  8  5  4   S 1  18.0487275   -0.0123  18.0487152   Err 0.1D-04          -
Maximum (obs-calc)/err in line 133   0.0000417

 RMS deviations (MHz), B and V sorted
  B  V   n splittings MHz
  B  V   n abs. freq. MHz
  1  1 151         0.020966         0.022493

          Parameters  and  Errors
 BJ          0.613058463 { 0.000000209}
 BK           1.643191069 { 0.000000747}
 B-          0.059052442 { 0.000000057}
 DJ          0.008269E-6 { 0.000535E-6}
 DJK          0.034548E-6 { 0.004117E-6}
 DK          -0.139701E-6 { 0.006277E-6}
\F12         -0.847130554 {     derived}
\F          158.758662501 {     derived}  160.213283522 {     derived}
 V1n         15724.229641 {   10.784525}   14795.552564 {   37.189695}
\rho          0.005862275 {     derived}    0.013962338 {     derived}
\beta         0.599086756 {     derived}    3.079938671 {     derived}
\gamma          1.455952831 {     derived}   -2.509665674 {     derived}
 epsil        1.476000000 {     fixed  }    3.867813971 { 0.240258173}
 delta        1.224910933 { 0.002412435}    2.921571893 { 0.056371715}

 Standard Deviation       0.021852 MHz

------------------------------------ B =  1
 Rotational Constants and Errors (in GHz)
    B_z       2.256249532       0.000000804
```

```
    B_x       0.672110905       0.000000204
    B_y       0.554006021       0.000000228
 Ray's kappa   -0.86124
 F0(calc)     158.000000000       0.000000000
 I_alpha       3.198601709       0.000000000
 <(i,x)  <(i,y)  <(i,z)       84.8911       20.5197       70.1822
d<(i,x) d<(i,y) d<(i,z)        0.0044        0.1331        0.1382

 F0(calc)     158.000000000       0.000000000
 I_alpha       3.198601709       0.000000000
 <(i,x)  <(i,y)  <(i,z)       99.3917       98.3331      167.3937
d<(i,x) d<(i,y) d<(i,z)        4.6631        4.1354        3.2299

 V1n_1      6.274460 kj +/- 0.004303 kj         1.498592 kcal +/- 0.001028 kcal
        524.503770 cm +/-   0.3597 cm    s=  44.019938
 V1n_2      5.903889 kj +/- 0.014840 kj         1.410085 kcal +/- 0.003544 kcal
        493.526441 cm +/-   1.2405 cm    s=  41.420109

F(calc)       158.758662501
F(calc)       160.213283522
```

$^{13}C_7$ Isotopologue XIAM Output

```
   J K- K+  J K- K+    Sym   calc/GHz  diff/MHz     obs/GHz
  1:  6  2  4  5  2  3   S 1   7.4291412    0.0174   7.4291586   Err 0.1D-04          -
  2:  6  1  5  5  1  4   S 1   7.5525725   -0.0053   7.5525671   Err 0.1D-04          -
  3:  6  1  5  5  1  4   S 3   7.5525659    0.0012   7.5525671   Err 0.1D-04          -
  4:  6  1  5  5  1  4   S 5   7.5525625    0.0047   7.5525671   Err 0.1D-04          -
  5:  6  1  5  5  1  4   S 2   7.5525693    0.0013   7.5525706   Err 0.1D-04          -
  6:  7  1  7  6  1  6   S 1   7.9981897   -0.0090   7.9981807   Err 0.1D-04          -
  7:  5  0  5  4  0  4   S 1   5.9336124   -0.0034   5.9336089   Err 0.1D-04          -
  8:  5  0  5  4  0  4   S 3   5.9336008    0.0103   5.9336111   Err 0.1D-04          -
  9:  5  0  5  4  0  4   S 5   5.9335966    0.0145   5.9336111   Err 0.1D-04          -
 10:  5  0  5  4  0  4   S 4   5.9335974    0.0141   5.9336115   Err 0.1D-04          -
 11:  5  0  5  4  0  4   S 2   5.9336086    0.0008   5.9336094   Err 0.1D-04          -
 12:  6  2  5  6  1  6   S 1   6.1885040    0.0194   6.1885234   Err 0.1D-04          -
 13: 19 10 10 20  9 12   S 5   6.8465746    0.0238   6.8465984   Err 0.1D-04          -
 14: 19  3 16 19  2 17   S 3   8.1883752    0.0083   8.1883835   Err 0.1D-04          -
 15: 19  3 16 19  2 17   S 5   8.1883646    0.0141   8.1883787   Err 0.1D-04          -
 16: 19  3 16 19  2 17   S 4   8.1883559    0.0228   8.1883787   Err 0.1D-04          -
 17:  5  3  2  5  2  4   S 5   8.2919201    0.0332   8.2919533   Err 0.1D-04          -
 18: 12  2 10 11  3  8   S 2   8.4578946   -0.0052   8.4578894   Err 0.1D-04          -
 19: 12  2 10 11  3  8   S 4   8.4579321   -0.0427   8.4578894   Err 0.1D-04          -
```

20: 7 3 4 6 3 3 S 2 8.5329158 0.0295 8.5329453 Err 0.1D-04 -
21: 8 0 8 7 1 7 S 1 8.6927845 0.0274 8.6928119 Err 0.1D-04 -
22: 7 1 6 6 1 5 S 1 8.7821496 -0.0022 8.7821474 Err 0.1D-04 -
23: 7 1 6 6 1 5 S 3 8.7821410 0.0064 8.7821474 Err 0.1D-04 -
24: 7 1 6 6 1 5 S 5 8.7821364 0.0110 8.7821474 Err 0.1D-04 -
25: 7 1 6 6 1 5 S 4 8.7821369 0.0106 8.7821475 Err 0.1D-04 -
26: 7 1 6 6 1 5 S 2 8.7821452 0.0023 8.7821475 Err 0.1D-04 -
27: 12 8 5 13 7 7 S 2 8.8558852 -0.0080 8.8558772 Err 0.1D-04 -
28: 12 8 5 13 7 7 S 5 8.8554795 -0.0038 8.8554757 Err 0.1D-04 -
29: 8 1 7 7 1 6 S 1 9.9956633 -0.0004 9.9956628 Err 0.1D-04 -
30: 8 1 7 7 1 6 S 2 9.9956571 0.0057 9.9956628 Err 0.1D-04 -
31: 8 1 7 7 1 6 S 3 9.9956522 0.0107 9.9956628 Err 0.1D-04 -
32: 8 1 7 7 1 6 S 5 9.9956458 0.0170 9.9956628 Err 0.1D-04 -
33: 8 1 7 7 1 6 S 4 9.9956462 0.0178 9.9956641 Err 0.1D-04 -
34: 8 2 6 7 2 5 S 1 10.0160271 0.0046 10.0160317 Err 0.1D-04 -
35: 5 2 4 4 1 3 S 2 10.4091068 -0.0141 10.4090927 Err 0.1D-04 -
36: 5 2 4 4 1 3 S 5 10.4090556 0.0371 10.4090927 Err 0.1D-04 -
37: 9 1 9 8 0 8 S 1 10.6632988 -0.0402 10.6632586 Err 0.1D-04 -
38: 9 1 9 8 0 8 S 3 10.6632891 -0.0305 10.6632586 Err 0.1D-04 -
39: 9 1 9 8 0 8 S 2 10.6632706 -0.0120 10.6632586 Err 0.1D-04 -
40: 9 1 9 8 0 8 S 4 10.6632470 0.0116 10.6632586 Err 0.1D-04 -
41: 9 2 8 8 2 7 S 1 10.7828888 0.0048 10.7828936 Err 0.1D-04 -
42: 9 2 8 8 2 7 S 2 10.7828878 0.0058 10.7828936 Err 0.1D-04 -
43: 9 2 8 8 2 7 S 3 10.7828722 0.0213 10.7828936 Err 0.1D-04 -
44: 9 2 8 8 2 7 S 4 10.7828695 0.0241 10.7828936 Err 0.1D-04 -
45: 9 2 8 8 2 7 S 5 10.7828728 0.0208 10.7828936 Err 0.1D-04 -
46: 14 2 13 14 0 14 S 3 11.1733869 0.0449 11.1734318 Err 0.1D-04 -
47: 14 2 13 14 0 14 S 5 11.1734356 -0.0038 11.1734318 Err 0.1D-04 -
48: 19 1 18 18 2 16 S 1 11.2499322 0.0094 11.2499417 Err 0.1D-04 -
49: 19 1 18 18 2 16 S 5 11.2495576 0.0095 11.2495670 Err 0.1D-04 -
50: 9 2 7 8 2 6 S 1 11.3131412 0.0049 11.3131461 Err 0.1D-04 -
51: 10 0 10 9 0 9 S 1 11.4390306 -0.0130 11.4390176 Err 0.1D-04 -
52: 8 4 4 8 3 6 S 1 11.4848076 -0.0010 11.4848065 Err 0.1D-04 -
53: 10 4 6 10 3 8 S 1 11.4989601 -0.0323 11.4989277 Err 0.1D-04 -
54: 10 1 10 9 0 9 S 1 11.6547884 -0.0400 11.6547484 Err 0.1D-04 -
55: 10 2 9 9 2 8 S 1 11.9507095 -0.0031 11.9507064 Err 0.1D-04 -
56: 10 2 9 9 2 8 S 2 11.9507059 0.0005 11.9507064 Err 0.1D-04 -
57: 10 2 9 9 2 8 S 5 11.9506879 0.0185 11.9507064 Err 0.1D-04 -
58: 10 2 9 9 2 8 S 4 11.9506856 0.0208 11.9507064 Err 0.1D-04 -
59: 10 2 9 9 2 8 S 3 11.9506903 0.0199 11.9507102 Err 0.1D-04 -
60: 10 5 6 9 5 5 S 2 12.1530800 -0.0055 12.1530744 Err 0.1D-04 -
61: 10 5 6 9 5 5 S 4 12.1530627 0.0141 12.1530767 Err 0.1D-04 -
62: 10 5 6 9 5 5 S 5 12.1530687 0.0094 12.1530781 Err 0.1D-04 -

63: 11 0 11 10 1 10 S 1 12.3062181 -0.0129 12.3062052 Err 0.1D-04 -
64: 11 1 11 10 1 10 S 5 12.4547915 -0.0223 12.4547693 Err 0.1D-04 -
65: 11 1 11 10 1 10 S 2 12.4547875 -0.0182 12.4547693 Err 0.1D-04 -
66: 11 1 11 10 1 10 S 3 12.4547822 -0.0129 12.4547693 Err 0.1D-04 -
67: 11 1 11 10 1 10 S 4 12.4547656 0.0036 12.4547693 Err 0.1D-04 -
68: 11 1 11 10 1 10 S 1 12.4547911 -0.0218 12.4547693 Err 0.1D-04 -
69: 9 8 2 10 7 4 S 5 12.5344651 -0.0026 12.5344625 Err 0.1D-04 -
70: 10 2 8 9 2 7 S 2 12.6031907 -0.0189 12.6031717 Err 0.1D-04 -
71: 10 2 8 9 2 7 S 5 12.6031825 -0.0108 12.6031717 Err 0.1D-04 -
72: 10 2 8 9 2 7 S 4 12.6031843 -0.0080 12.6031763 Err 0.1D-04 -
73: 10 2 8 9 2 7 S 1 12.6031912 -0.0142 12.6031770 Err 0.1D-04 -
74: 18 4 15 18 3 16 S 1 12.6406043 -0.0371 12.6405672 Err 0.1D-04 -
75: 18 4 15 18 3 16 S 4 12.6403712 -0.0406 12.6403306 Err 0.1D-04 -
76: 18 4 15 18 3 16 S 5 12.6403439 -0.0133 12.6403306 Err 0.1D-04 -
77: 18 4 15 18 3 16 S 2 12.6403350 -0.0044 12.6403306 Err 0.1D-04 -
78: 11 1 11 10 0 10 S 1 12.6705490 -0.0378 12.6705111 Err 0.1D-04 -
79: 11 1 11 10 0 10 S 4 12.6705278 -0.0215 12.6705063 Err 0.1D-04 -
80: 18 3 16 18 1 17 S 2 13.0474540 0.0025 13.0474566 Err 0.1D-04 -
81: 11 2 10 10 2 9 S 4 13.1099877 -0.0255 13.1099623 Err 0.1D-04 -
82: 11 2 10 10 2 9 S 5 13.1099897 -0.0274 13.1099623 Err 0.1D-04 -
83: 11 2 10 10 2 9 S 3 13.1099943 -0.0321 13.1099623 Err 0.1D-04 -
84: 17 1 16 17 1 17 S 1 13.2886334 0.0056 13.2886390 Err 0.1D-04 -
85: 17 1 16 17 1 17 S 2 13.2883759 0.0184 13.2883943 Err 0.1D-04 -
86: 19 12 8 20 11 10 S 3 13.5035627 -0.0129 13.5035498 Err 0.1D-04 -
87: 12 1 12 11 0 11 S 1 13.7072417 -0.0371 13.7072045 Err 0.1D-04 -
88: 11 2 9 10 2 8 S 1 13.8807824 0.0016 13.8807840 Err 0.1D-04 -
89: 11 2 9 10 2 8 S 2 13.8807805 0.0035 13.8807840 Err 0.1D-04 -
90: 11 2 9 10 2 8 S 3 13.8807733 0.0106 13.8807840 Err 0.1D-04 -
91: 11 2 9 10 2 8 S 4 13.8807720 0.0119 13.8807840 Err 0.1D-04 -
92: 11 2 9 10 2 8 S 5 13.8807709 0.0131 13.8807840 Err 0.1D-04 -
93: 18 1 17 18 0 18 S 1 14.2549294 -0.0243 14.2549051 Err 0.1D-04 -
94: 18 1 17 18 0 18 S 3 14.2570502 -0.0214 14.2570288 Err 0.1D-04 -
95: 12 2 11 11 2 10 S 1 14.2606737 -0.0079 14.2606658 Err 0.1D-04 -
96: 12 2 11 11 2 10 S 2 14.2606662 -0.0005 14.2606658 Err 0.1D-04 -
97: 12 2 11 11 2 10 S 3 14.2606493 0.0223 14.2606716 Err 0.1D-04 -
98: 12 2 11 11 2 10 S 5 14.2606430 0.0286 14.2606716 Err 0.1D-04 -
99: 12 2 11 11 2 10 S 4 14.2606408 0.0308 14.2606716 Err 0.1D-04 -
100: 12 9 3 11 9 2 S 1 14.5547220 -0.0374 14.5546846 Err 0.1D-04 -
101: 12 7 5 11 7 4 S 1 14.5693619 -0.0042 14.5693577 Err 0.1D-04 -
102: 12 7 5 11 7 4 S 2 14.5693549 0.0028 14.5693577 Err 0.1D-04 -
103: 12 7 5 11 7 4 S 3 14.5693423 0.0154 14.5693577 Err 0.1D-04 -
104: 12 7 5 11 7 4 S 4 14.5693395 0.0182 14.5693577 Err 0.1D-04 -
105: 12 7 5 11 7 4 S 5 14.5693356 0.0221 14.5693577 Err 0.1D-04 -

106: 10 2 9 9 1 8 S 3 14.5760413 -0.0119 14.5760294 Err 0.1D-04 -
107: 10 2 9 9 1 8 S 4 14.5759152 0.0420 14.5759572 Err 0.1D-04 -
108: 15 5 11 15 4 12 S 1 14.5876100 -0.0298 14.5875802 Err 0.1D-04 -
109: 13 0 13 12 1 12 S 1 14.5925486 -0.0422 14.5925064 Err 0.1D-04 -
110: 16 5 11 16 4 13 S 1 14.6128156 -0.0251 14.6127904 Err 0.1D-04 -
111: 15 5 10 15 4 12 S 5 14.6147407 -0.0241 14.6147166 Err 0.1D-04 -
112: 12 1 11 11 1 10 S 1 14.6278610 -0.0190 14.6278420 Err 0.1D-04 -
113: 12 1 11 11 1 10 S 2 14.6278422 -0.0002 14.6278420 Err 0.1D-04 -
114: 12 1 11 11 1 10 S 3 14.6278329 0.0091 14.6278420 Err 0.1D-04 -
115: 12 1 11 11 1 10 S 5 14.6278133 0.0287 14.6278420 Err 0.1D-04 -
116: 13 5 9 13 4 10 S 2 14.6422874 -0.0026 14.6422848 Err 0.1D-04 -
117: 17 5 12 17 4 14 S 1 14.6443874 0.0376 14.6444250 Err 0.1D-04 -
118: 17 5 12 17 4 14 S 3 14.6444164 0.0086 14.6444250 Err 0.1D-04 -
119: 13 5 9 13 4 10 S 1 14.6482973 0.0335 14.6483307 Err 0.1D-04 -
120: 11 5 7 11 4 7 S 1 14.6774147 0.0211 14.6774358 Err 0.1D-04 -
121: 11 5 7 11 4 7 S 3 14.6758769 -0.0096 14.6758673 Err 0.1D-04 -
122: 12 2 10 11 2 9 S 5 15.1418895 0.0202 15.1419098 Err 0.1D-04 -
123: 12 2 10 11 2 9 S 2 15.1419014 0.0083 15.1419098 Err 0.1D-04 -
124: 12 2 10 11 2 9 S 1 15.1419057 0.0040 15.1419098 Err 0.1D-04 -
125: 12 2 10 11 2 9 S 3 15.1418943 0.0135 15.1419078 Err 0.1D-04 -
126: 19 2 18 19 0 19 S 1 15.3501249 -0.0311 15.3500939 Err 0.1D-04 -
127: 13 2 12 12 2 11 S 1 15.4028109 -0.0129 15.4027981 Err 0.1D-04 -
128: 13 2 12 12 2 11 S 2 15.4028019 -0.0038 15.4027981 Err 0.1D-04 -
129: 13 2 12 12 2 11 S 3 15.4027842 0.0138 15.4027981 Err 0.1D-04 -
130: 13 2 12 12 2 11 S 4 15.4027736 0.0244 15.4027981 Err 0.1D-04 -
131: 13 2 12 12 2 11 S 5 15.4027766 0.0205 15.4027971 Err 0.1D-04 -
132: 13 1 12 12 1 11 S 1 15.7277569 -0.0039 15.7277530 Err 0.1D-04 -
133: 13 3 10 12 3 9 S 1 16.2299688 -0.0072 16.2299617 Err 0.1D-04 -
134: 7 3 4 6 2 5 S 1 16.8881667 -0.0109 16.8881558 Err 0.1D-04 -
135: 19 6 13 19 5 15 S 1 17.7075578 0.0306 17.7075884 Err 0.1D-04 -
136: 22 1 21 22 0 22 S 3 17.9524234 0.0176 17.9524410 Err 0.1D-04 -
137: 10 6 5 10 5 6 S 5 18.0551155 0.0367 18.0551522 Err 0.1D-04 -
138: 10 6 4 10 5 5 S 5 18.0592504 -0.0072 18.0592432 Err 0.1D-04 -
139: 5 2 4 4 2 3 S 1 6.0368220 -0.0033 6.0368187 Err 0.1D-04 -
140: 5 2 3 4 2 2 S 1 6.1534824 0.0028 6.1534852 Err 0.1D-04 -
141: 5 1 5 4 0 4 S 1 6.8802076 -0.0229 6.8801847 Err 0.1D-04 -
142: 6 0 6 5 0 5 S 1 7.0641374 0.0024 7.0641398 Err 0.1D-04 -
143: 9 3 6 9 2 7 S 2 7.2532278 -0.0170 7.2532108 Err 0.1D-04 -
144: 3 3 0 3 2 2 S 2 8.2391603 0.0077 8.2391681 Err 0.1D-04 -
145: 18 1 17 18 0 18 S 4 14.2559965 -0.0080 14.2559885 Err 0.1D-04 -
146: 13 1 12 12 2 11 S 4 14.2757983 0.0293 14.2758275 Err 0.1D-04 -
147: 12 8 4 11 8 3 S 1 14.5606439 -0.0031 14.5606408 Err 0.1D-04 -
148: 9 5 4 9 4 6 S 3 14.7613532 -0.0117 14.7613414 Err 0.1D-04 -

```
 149:  8  5  4  8  4  4   S 3  14.7704603   -0.0079  14.7704524   Err 0.1D-04          -
 150:  6  5  2  6  4  3   S 4  14.7945278    0.0104  14.7945382   Err 0.1D-04          -
 151:  6  3  4  5  2  4   S 2  15.5693384   -0.0350  15.5693034   Err 0.1D-04          -
 Maximum (obs-calc)/err in line  46   0.0000449

 RMS deviations (MHz), B and V sorted
  B  V   n splittings MHz
  B  V   n abs. freq. MHz
  1  1 151         0.019902         0.021352

          Parameters  and  Errors
 BJ          0.605031619 { 0.000000209}
 BK           1.645992985 { 0.000000757}
 B-          0.057755675 { 0.000000054}
 DJ          0.011192E-6 { 0.000703E-6}
 DJK          0.016102E-6 { 0.003274E-6}
 DK          -0.158695E-6 { 0.005552E-6}
\F12         -0.846354117 {     derived}
\F          158.744951490 {     derived}  160.187088645 {     derived}
 V1n         15710.053364 {    9.650975}   14760.072048 {   40.632480}
\rho         0.005762713 {     derived}    0.013848608 {     derived}
\beta        0.604029191 {     derived}    3.074799767 {     derived}
\gamma        1.456151516 {     derived}   -2.379450569 {     derived}
 epsil       1.476000000 {     fixed  }    3.999224255 { 0.268610887}
 delta       1.231404112 { 0.001804060}    2.895492500 { 0.053488903}

 Standard Deviation       0.020743 MHz

------------------------------------ B =  1
 Rotational Constants and Errors (in GHz)
     B_z       2.251024604       0.000000830
     B_x       0.662787293       0.000000206
     B_y       0.547275944       0.000000225
 Ray's kappa   -0.86440
 F0(calc)     158.000000000       0.000000000
 I_alpha        3.198601709       0.000000000
 <(i,x)  <(i,y)  <(i,z)       84.8792       20.1617       70.5543
d<(i,x) d<(i,y) d<(i,z)        0.0033        0.0994        0.1034

 F0(calc)     158.000000000       0.000000000
 I_alpha        3.198601709       0.000000000
 <(i,x)  <(i,y)  <(i,z)       99.1713      100.6175      165.8995
d<(i,x) d<(i,y) d<(i,z)        5.1342        4.3817        3.0647
```

V1n_1 6.268803 kj +/- 0.003851 kj 1.497241 kcal +/- 0.000920 kcal
524.030900 cm +/- 0.3219 cm s= 43.984050
V1n_2 5.889731 kj +/- 0.016214 kj 1.406703 kcal +/- 0.003872 kcal
492.342939 cm +/- 1.3554 cm s= 41.324351

F(calc) 158.744951490
F(calc) 160.187088645

$^{13}C_9$ Isotopologue XIAM Output

	J K- K+	J K- K+	Sym	calc/GHz	diff/MHz	obs/GHz		
1:	5 1	5 4	1 4	S 1	5.7768657	-0.0038	5.7768619	Err 0.1D-04 -
2:	5 0	5 4	0 4	S 1	5.9747498	-0.0169	5.9747329	Err 0.1D-04 -
3:	5 2	4 4	2 3	S 1	6.0800185	-0.0123	6.0800062	Err 0.1D-04 -
4:	6 0	6 5	1 5	S 1	6.1705712	0.0297	6.1706009	Err 0.1D-04 -
5:	6 1	6 5	1 5	S 1	6.9181705	-0.0221	6.9181484	Err 0.1D-04 -
6:	6 0	6 5	0 5	S 1	7.1125145	-0.0050	7.1125095	Err 0.1D-04 -
7:	6 2	5 5	2 4	S 1	7.2847032	0.0200	7.2847232	Err 0.1D-04 -
8:	7 0	7 6	1 6	S 1	7.4822170	0.0232	7.4822402	Err 0.1D-04 -
9:	6 2	4 5	2 3	S 1	7.4845357	0.0158	7.4845516	Err 0.1D-04 -
10:	18 3	15 18	2 16	S 1	7.5467173	-0.0138	7.5467036	Err 0.1D-04 -
11:	22 4	18 22	3 19	S 1	8.5605769	0.0164	8.5605933	Err 0.1D-04 -
12:	8 0	8 7	1 7	S 1	8.7608784	0.0202	8.7608986	Err 0.1D-04 -
13:	7 1	6 6	1 5	S 1	8.8453157	0.0079	8.8453236	Err 0.1D-04 -
14:	8 1	7 7	1 6	S 1	10.0669007	0.0138	10.0669146	Err 0.1D-04 -
15:	8 2	6 7	2 5	S 1	10.0911210	0.0294	10.0911504	Err 0.1D-04 -
16:	9 0	9 8	0 8	S 1	10.4256196	-0.0329	10.4255867	Err 0.1D-04 -
17:	9 1	8 8	1 7	S 1	11.2683614	0.0048	11.2683662	Err 0.1D-04 -
18:	9 2	7 8	2 6	S 1	11.3977105	0.0288	11.3977393	Err 0.1D-04 -
19:	7 4	4 7	3 4	S 1	11.4561334	0.0094	11.4561428	Err 0.1D-04 -
20:	10 2	9 9	2 8	S 1	12.0346093	0.0018	12.0346111	Err 0.1D-04 -
21:	10 3	7 9	3 6	S 1	12.4035321	0.0096	12.4035417	Err 0.1D-04 -
22:	10 1	9 9	1 8	S 1	12.4464222	0.0056	12.4464279	Err 0.1D-04 -
23:	11 0	11 10	0 10	S 1	12.6061891	-0.0153	12.6061738	Err 0.1D-04 -
24:	10 2	8 9	2 7	S 1	12.6968468	0.0212	12.6968680	Err 0.1D-04 -
25:	11 1	11 10	0 10	S 1	12.7516510	-0.0444	12.7516066	Err 0.1D-04 -
26:	11 2	10 10	2 9	S 1	13.2016200	-0.0059	13.2016141	Err 0.1D-04 -
27:	11 6	5 10	6 4	S 1	13.4570642	-0.0081	13.4570561	Err 0.1D-04 -
28:	12 1	12 11	1 11	S 1	13.6510670	-0.0043	13.6510627	Err 0.1D-04 -
29:	12 1	12 11	0 11	S 1	13.7965289	-0.0327	13.7964962	Err 0.1D-04 -
30:	5 3	3 4	2 2	S 1	14.2781411	-0.0342	14.2781069	Err 0.1D-04 -
31:	18 1	17 18	1 18	S 1	14.3468007	-0.0434	14.3467572	Err 0.1D-04 -

```
 32: 12  2 11 11  2 10   S 1  14.3598440    0.0025  14.3598465   Err 0.1D-04          -
 33: 13  5  8 13  4  9   S 1  14.5347628    0.0389  14.5348017   Err 0.1D-04          -
 34: 12  8  4 11  8  3   S 1  14.6657847    0.0221  14.6658068   Err 0.3D-04          -
 35: 12  7  5 11  7  4   S 1  14.6746939    0.0243  14.6747183   Err 0.1D-04          -
 36: 13  1 13 12  1 12   S 1  14.7596774    0.0064  14.7596839   Err 0.1D-04          -
 37: 13  0 13 12  0 12   S 1  14.7924094   -0.0256  14.7923838   Err 0.1D-04          -
 38: 13  1 13 12  0 12   S 1  14.8579811   -0.0351  14.8579459   Err 0.1D-04          -
 39: 12  3  9 11  3  8   S 1  15.0236408    0.0193  15.0236601   Err 0.1D-04          -
 40: 12  2 10 11  2  9   S 1  15.2524327    0.0131  15.2524457   Err 0.1D-04          -
 41: 13  2 12 12  2 11   S 1  15.5094283   -0.0036  15.5094247   Err 0.1D-04          -
 42: 13  1 12 12  1 11   S 1  15.8331819   -0.0080  15.8331739   Err 0.1D-04          -
 43: 13  4  9 12  4  8   S 1  16.0433141    0.0135  16.0433277   Err 0.1D-04          -
 44: 13  2 11 12  2 10   S 1  16.5015755   -0.0114  16.5015641   Err 0.1D-04          -
 45: 14 13  1 13 13  0   S 1  17.0937029   -0.0088  17.0936941   Err 0.1D-04          -
 46: 19  3 17 18  4 14   S 1   8.9581322   -0.0258   8.9581064   Err 0.1D-04          -
 47: 21  4 18 20  5 15   S 1  10.6790935   -0.0064  10.6790872   Err 0.1D-04          -
 48: 22  4 19 21  5 16   S 1  11.5214395    0.0258  11.5214653   Err 0.1D-04          -
 49: 12  1 11 11  1 10   S 1  14.7269471    0.0270  14.7269741   Err 0.1D-04          -
 50: 16  1 16 15  0 15   S 1  18.1037816    0.0140  18.1037956   Err 0.1D-04          -
 51: 18  3 15 18  2 17   S 1  18.3701406    0.0001  18.3701407   Err 0.1D-04          -
Maximum (obs-calc)/err in line  25   0.0000444

 RMS deviations (MHz), B and V sorted
  B  V   n splittings MHz
  B  V   n abs. freq. MHz
  1  1  51         0.020845         0.022889

          Parameters  and  Errors
 BJ          0.609379518 { 0.000000297}
 BK           1.647283081 { 0.000001742}
 B-          0.058377846 { 0.000000061}
 DJ          0.012045E-6 { 0.000664E-6}
 DJK          0.040708E-6 { 0.004267E-6}
\F12         -0.849746416 {     derived}
\F         158.754893034 {     derived}  160.180982167 {     derived}
\rho          0.005841927 {     derived}    0.013832974 {     derived}
\beta         0.597997724 {     derived}    3.067742423 {     derived}
\gamma        1.456073524 {     derived}   -2.539583102 {     derived}

 Standard Deviation       0.022192 MHz

------------------------------------ B =  1
 Rotational Constants and Errors (in GHz)
```

```
    B_z      2.256662598      0.000001720
    B_x      0.667757364      0.000000305
    B_y      0.551001672      0.000000302
 Ray's kappa   -0.86310
 F0(calc)    158.000000000      0.000000000
 I_alpha      3.198601709      0.000000000
 <(i,x)  <(i,y)  <(i,z)      84.8892      20.4618      70.2424
d<(i,x) d<(i,y) d<(i,z)       0.0000       0.0000       0.0000

 F0(calc)    158.000000000      0.000000000
 I_alpha      3.198601709      0.000000000
 <(i,x)  <(i,y)  <(i,z)     101.4809      99.5401     164.9886
d<(i,x) d<(i,y) d<(i,z)       0.0000       0.0000       0.0000

 V1n_1      6.275827 kj +/- 0.000000 kj        1.498919 kcal +/- 0.000000 kcal
       524.618074 cm +/-   0.0000 cm    s=  44.030577
 V1n_2      5.894025 kj +/- 0.000000 kj        1.407729 kcal +/- 0.000000 kcal
       492.701873 cm +/-   0.0000 cm    s=  41.351888

F(calc)      158.754893034
F(calc)      160.180982167
```

$^{13}C_{10}$ Isotopologue XIAM Output

```
 J K- K+  J K- K+    Sym   calc/GHz  diff/MHz     obs/GHz
  1:  7  5  3  8  4  4   S 1   4.9999754    0.0248   5.0000002   Err 0.1D-04          -
  2:  5  0  5  4  0  4   S 1   5.9348187   -0.0164   5.9348024   Err 0.1D-04          -
  3:  5  0  5  4  0  4   S 2   5.9348149   -0.0146   5.9348003   Err 0.1D-04          -
  4:  5  0  5  4  0  4   S 3   5.9348073   -0.0070   5.9348003   Err 0.1D-04          -
  5:  5  0  5  4  0  4   S 5   5.9348031   -0.0028   5.9348003   Err 0.1D-04          -
  6:  5  0  5  4  0  4   S 4   5.9348038   -0.0011   5.9348028   Err 0.1D-04          -
  7:  5  2  4  4  2  3   S 1   6.0380772    0.0050   6.0380822   Err 0.1D-04          -
  8:  6  0  6  5  1  5   S 2   6.1242062   -0.0028   6.1242034   Err 0.1D-04          -
  9: 11  0 11 10  1  9   S 4   6.2881460    0.0067   6.2881527   Err 0.1D-04          -
 10:  5  1  4  4  1  3   S 1   6.3111031    0.0075   6.3111106   Err 0.1D-04          -
 11: 15  0 15 14  1 13   S 3   6.5805752    0.0075   6.5805827   Err 0.1D-04          -
 12:  5  1  5  4  0  4   S 2   6.8761916   -0.0162   6.8761754   Err 0.1D-04          -
 13:  9  3  7  9  2  7   S 1   7.0441177    0.0051   7.0441228   Err 0.1D-04          -
 14: 17  4 13 16  5 11   S 2   7.1330491   -0.0254   7.1330237   Err 0.1D-04          -
 15:  7  0  7  6  1  6   S 1   7.4276321    0.0138   7.4276459   Err 0.1D-04          -
 16:  6  2  4  5  2  3   S 1   7.4307034   -0.0151   7.4306883   Err 0.1D-04          -
 17: 13  8  5 14  7  8   S 1   7.5195014    0.0113   7.5195127   Err 0.1D-04          -
 18:  6  1  5  5  1  4   S 5   7.5534351    0.0090   7.5534441   Err 0.1D-04          -
 19:  6  1  5  5  1  4   S 3   7.5534391    0.0054   7.5534444   Err 0.1D-04          -
```

20: 6 1 5 5 1 4 S 2 7.5534418 0.0026 7.5534444 Err 0.1D-04 -
21: 6 1 5 5 1 4 S 1 7.5534455 -0.0011 7.5534444 Err 0.1D-04 -
22: 6 1 5 5 1 4 S 4 7.5534356 0.0091 7.5534447 Err 0.1D-04 -
23: 7 1 7 6 1 6 S 1 8.0006274 0.0052 8.0006326 Err 0.1D-04 -
24: 3 3 0 3 2 2 S 2 8.2053294 0.0283 8.2053577 Err 0.1D-04 -
25: 8 0 8 7 1 7 S 1 8.6986972 -0.0042 8.6986930 Err 0.1D-04 -
26: 17 10 8 18 9 10 S 2 9.1948987 -0.0040 9.1948947 Err 0.1D-04 -
27: 9 0 9 8 1 8 S 1 9.9345237 -0.0119 9.9345118 Err 0.1D-04 -
28: 8 1 7 7 1 6 S 1 9.9967327 0.0007 9.9967334 Err 0.1D-04 -
29: 8 1 7 7 1 6 S 2 9.9967261 0.0074 9.9967334 Err 0.1D-04 -
30: 8 1 7 7 1 6 S 3 9.9967218 0.0116 9.9967334 Err 0.1D-04 -
31: 8 1 7 7 1 6 S 5 9.9967149 0.0185 9.9967334 Err 0.1D-04 -
32: 8 1 7 7 1 6 S 4 9.9967153 0.0175 9.9967328 Err 0.1D-04 -
33: 4 2 2 3 1 3 S 2 10.1940400 -0.0150 10.1940250 Err 0.3D-04 -
34: 4 2 2 3 1 3 S 3 10.1940361 -0.0211 10.1940149 Err 0.3D-04 -
35: 4 2 2 3 1 3 S 4 10.1939805 0.0344 10.1940149 Err 0.3D-04 -
36: 9 2 8 8 2 7 S 2 10.7850872 -0.0095 10.7850776 Err 0.1D-04 -
37: 9 2 8 8 2 7 S 5 10.7850725 0.0092 10.7850817 Err 0.1D-04 -
38: 9 2 8 8 2 7 S 4 10.7850692 0.0150 10.7850842 Err 0.1D-04 -
39: 9 2 8 8 2 7 S 1 10.7850887 -0.0044 10.7850842 Err 0.1D-04 -
40: 10 0 10 9 1 9 S 1 11.1371714 -0.0170 11.1371544 Err 0.1D-04 -
41: 9 1 8 8 1 7 S 1 11.1906369 -0.0005 11.1906363 Err 0.1D-04 -
42: 9 4 6 9 3 6 S 1 11.2549084 -0.0254 11.2548830 Err 0.1D-04 -
43: 6 2 5 5 1 4 S 2 11.3146179 -0.0241 11.3145938 Err 0.2D-04 -
44: 6 2 5 5 1 4 S 4 11.3146011 -0.0073 11.3145938 Err 0.2D-04 -
45: 6 2 5 5 1 4 S 5 11.3145753 0.0185 11.3145938 Err 0.2D-04 -
46: 10 1 10 9 1 9 S 1 11.3510564 -0.0382 11.3510182 Err 0.1D-04 -
47: 5 4 1 5 3 2 S 1 11.4534496 0.0245 11.4534741 Err 0.1D-04 -
48: 14 4 11 14 3 12 S 1 11.6718961 -0.0380 11.6718581 Err 0.1D-04 -
49: 10 2 9 9 2 8 S 1 11.9531372 -0.0066 11.9531306 Err 0.1D-04 -
50: 10 2 9 9 2 8 S 2 11.9531333 -0.0026 11.9531306 Err 0.1D-04 -
51: 10 2 9 9 2 8 S 5 11.9531155 0.0151 11.9531306 Err 0.1D-04 -
52: 10 2 9 9 2 8 S 3 11.9531183 0.0129 11.9531312 Err 0.1D-04 -
53: 10 2 9 9 2 8 S 4 11.9531133 0.0181 11.9531314 Err 0.1D-04 -
54: 10 5 6 9 5 5 S 2 12.1556245 0.0022 12.1556268 Err 0.1D-04 -
55: 11 0 11 10 1 10 S 1 12.3114966 -0.0352 12.3114614 Err 0.1D-04 -
56: 11 1 11 10 1 10 S 1 12.4586788 -0.0307 12.4586481 Err 0.1D-04 -
57: 8 2 7 7 1 6 S 3 13.0122101 -0.0278 13.0121823 Err 0.1D-04 -
58: 4 3 2 3 2 1 S 4 13.0189640 0.0278 13.0189917 Err 0.1D-04 -
59: 4 3 2 3 2 1 S 1 13.0226168 -0.0212 13.0225956 Err 0.1D-04 -
60: 11 2 10 10 2 9 S 1 13.1126715 0.0082 13.1126797 Err 0.1D-04 -
61: 11 6 5 10 6 4 S 1 13.3631803 -0.0082 13.3631722 Err 0.1D-04 -
62: 11 3 9 10 3 8 S 5 13.3875922 -0.0111 13.3875811 Err 0.1D-04 -

63: 6 2 4 5 1 5 S 1 13.4417305 -0.0293 13.4417012 Err 0.1D-04 -
64: 11 1 10 10 1 9 S 1 13.5076780 -0.0137 13.5076643 Err 0.1D-04 -
65: 11 1 10 10 1 9 S 2 13.5076626 0.0017 13.5076643 Err 0.1D-04 -
66: 11 1 10 10 1 9 S 3 13.5076554 0.0089 13.5076643 Err 0.1D-04 -
67: 11 1 10 10 1 9 S 5 13.5076395 0.0247 13.5076643 Err 0.1D-04 -
68: 11 1 10 10 1 9 S 4 13.5076405 0.0232 13.5076637 Err 0.1D-04 -
69: 9 2 8 8 1 7 S 2 13.8004782 0.0163 13.8004945 Err 0.1D-04 -
70: 11 2 9 10 2 8 S 1 13.8826994 0.0170 13.8827164 Err 0.1D-04 -
71: 5 3 3 4 2 2 S 3 14.1964784 -0.0390 14.1964393 Err 0.1D-04 -
72: 18 1 17 18 1 18 S 3 14.2078414 -0.0082 14.2078332 Err 0.1D-04 -
73: 18 1 17 18 0 18 S 3 14.2197274 -0.0111 14.2197163 Err 0.1D-04 -
74: 12 2 11 11 2 10 S 1 14.2635596 -0.0020 14.2635576 Err 0.1D-04 -
75: 12 2 11 11 2 10 S 2 14.2635519 0.0095 14.2635614 Err 0.1D-04 -
76: 12 2 11 11 2 10 S 3 14.2635356 0.0258 14.2635614 Err 0.1D-04 -
77: 12 2 11 11 2 10 S 5 14.2635289 0.0325 14.2635614 Err 0.1D-04 -
78: 12 2 11 11 2 10 S 4 14.2635269 0.0345 14.2635614 Err 0.1D-04 -
79: 5 3 3 4 2 3 S 3 14.2865524 0.0038 14.2865561 Err 0.1D-04 -
80: 5 3 2 4 2 3 S 3 14.2926096 -0.0357 14.2925739 Err 0.1D-04 -
81: 5 3 2 4 2 3 S 4 14.2941908 -0.0292 14.2941616 Err 0.1D-04 -
82: 10 2 9 9 1 8 S 2 14.5629836 0.0228 14.5630064 Err 0.1D-04 -
83: 19 5 15 19 4 16 S 2 14.5728586 0.0059 14.5728645 Err 0.1D-04 -
84: 12 6 6 11 6 5 S 1 14.5860638 -0.0094 14.5860544 Err 0.1D-04 -
85: 12 5 7 12 4 9 S 3 14.6238431 -0.0118 14.6238313 Err 0.1D-04 -
86: 20 5 16 20 4 17 S 1 14.6605203 0.0213 14.6605415 Err 0.1D-04 -
87: 13 0 13 12 0 12 S 1 14.6976183 -0.0156 14.6976028 Err 0.1D-04 -
88: 13 0 13 12 0 12 S 1 14.6976183 -0.0255 14.6975928 Err 0.1D-04 -
89: 7 5 3 7 4 4 S 1 14.7271283 -0.0235 14.7271048 Err 0.1D-04 -
90: 7 5 3 7 4 4 S 4 14.7250275 -0.0126 14.7250150 Err 0.1D-04 -
91: 13 1 13 12 0 12 S 1 14.7642488 -0.0435 14.7642053 Err 0.1D-04 -
92: 12 3 9 11 3 8 S 1 14.9140879 0.0103 14.9140982 Err 0.1D-04 -
93: 15 11 5 16 10 6 S 1 14.9604481 -0.0336 14.9604145 Err 0.1D-04 -
94: 15 11 4 16 10 6 S 4 14.9607765 -0.0092 14.9607673 Err 0.1D-04 -
95: 15 11 4 16 10 6 S 3 14.9608051 0.0451 14.9608502 Err 0.1D-04 -
96: 15 11 4 16 10 6 S 2 14.9612020 -0.0036 14.9611984 Err 0.1D-04 -
97: 12 2 10 11 2 9 S 1 15.1437351 0.0162 15.1437513 Err 0.1D-04 -
98: 12 2 10 11 2 9 S 2 15.1437296 0.0217 15.1437513 Err 0.1D-04 -
99: 12 2 10 11 2 9 S 3 15.1437238 0.0275 15.1437513 Err 0.1D-04 -
100: 12 2 10 11 2 9 S 5 15.1437179 0.0334 15.1437513 Err 0.1D-04 -
101: 12 2 10 11 2 9 S 4 15.1437187 0.0346 15.1437533 Err 0.1D-04 -
102: 13 2 12 12 2 11 S 1 15.4059338 0.0014 15.4059353 Err 0.1D-04 -
103: 13 1 12 12 1 11 S 1 15.7292045 -0.0152 15.7291893 Err 0.1D-04 -
104: 14 0 14 13 0 13 S 1 15.7867678 -0.0323 15.7867354 Err 0.1D-04 -
105: 13 3 10 12 3 9 S 1 16.2335449 0.0279 16.2335728 Err 0.1D-04 -

```
106: 13  2 11 12  2 10   S 1  16.3850382   -0.0064  16.3850318   Err 0.1D-04          -
107: 14  3 12 13  3 11   S 1  16.9990637    0.0079  16.9990716   Err 0.1D-04          -
108: 13 11  3 14 10  5   S 5  17.4050126    0.0102  17.4050228   Err 0.1D-04          -
109: 14  2 12 13  2 11   S 1  17.6036814    0.0269  17.6037083   Err 0.1D-04          -
110: 16  6 10 16  5 11   S 5  17.7573216   -0.0092  17.7573124   Err 0.1D-04          -
111: 15  6 10 15  5 10   S 4  17.8061888   -0.0151  17.8061737   Err 0.1D-04          -
112: 10  6  5 10  5  6   S 2  17.9812041   -0.0048  17.9811993   Err 0.1D-04          -
113: 10  6  5 10  5  6   S 5  17.9807811    0.0270  17.9808080   Err 0.1D-04          -
114:  8  6  3  8  5  4   S 4  18.0046757    0.0404  18.0047161   Err 0.1D-04          -
115: 22  6 16 21  7 15   S 1   6.1503970   -0.0017   6.1503953   Err 0.1D-04          -
116: 17  4 14 16  5 12   S 5   6.2866264    0.0331   6.2866594   Err 0.1D-04          -
117: 21  5 17 20  6 15   S 5   8.2057194   -0.0098   8.2057096   Err 0.1D-04          -
118:  8  2  6  7  2  5   S 1  10.0179291    0.0294  10.0179585   Err 0.1D-04          -
119: 14  4 10 14  3 11   S 4  10.0463864    0.0417  10.0464281   Err 0.1D-04          -
120: 14  2 13 14  0 14   S 4  11.1408492    0.0016  11.1408508   Err 0.1D-04          -
121: 14  2 13 14  0 14   S 5  11.1411481    0.0032  11.1411513   Err 0.1D-04          -
122: 14  2 13 14  0 14   S 3  11.1411230    0.0283  11.1411513   Err 0.1D-04          -
123: 14 10  5 15  9  7   S 5  12.8898738   -0.0184  12.8898553   Err 0.1D-04          -
124: 12  8  5 11  8  4   S 5  14.5636449   -0.0467  14.5635982   Err 0.1D-04          -
125:  6  5  1  6  4  2   S 5  14.7370779   -0.0414  14.7370365   Err 0.1D-04          -
126:  6  3  3  5  2  4   S 3  15.5554315    0.0390  15.5554705   Err 0.1D-04          -
127:  7  3  5  6  2  4   S 3  16.4120410    0.0314  16.4120724   Err 0.1D-04          -
128:  7  3  5  6  2  4   S 1  16.4121058   -0.0334  16.4120724   Err 0.1D-04          -
Maximum (obs-calc)/err in line 124   0.0000467

 RMS deviations (MHz), B and V sorted
  B  V   n splittings MHz
  B  V   n abs. freq. MHz
  1  1 128         0.021176         0.022996

          Parameters  and  Errors
 BJ          0.605158362 { 0.000000235}
 BK           1.639238861 { 0.000000824}
 B-          0.057656913 { 0.000000066}
 DJ          0.016198E-6 { 0.000669E-6}
 DJK          0.029556E-6 { 0.003902E-6}
 DK          -0.155151E-6 { 0.003884E-6}
\F12         -0.854259154 {     derived}
\F          158.756361380 {     derived}  160.159305132 {     derived}
 V1n         15736.658943 {   10.335137}   14759.129945 {   34.829163}
\rho          0.005865183 {     derived}    0.013717749 {     derived}
\beta         0.589670990 {     derived}    3.063927658 {     derived}
\gamma        1.456193528 {     derived}   -2.573414237 {     derived}
```

epsil 1.476000000 { fixed } 3.799564759 { 0.136540703}
delta 1.220510556 { 0.002237765} 2.867918955 { 0.041059535}

Standard Deviation 0.022244 MHz

---------- B = 1
Rotational Constants and Errors (in GHz)
B_z 2.244397223 0.000000871
B_x 0.662815275 0.000000255
B_y 0.547501449 0.000000232
Ray's kappa -0.86409
F0(calc) 158.000000000 0.000000000
I_alpha 3.198601709 0.000000000
<(i,x) <(i,y) <(i,z) 84.8993 20.7626 69.9301
d<(i,x) d<(i,y) d<(i,z) 0.0042 0.1235 0.1282

F0(calc) 158.000000000 0.000000000
I_alpha 3.198601709 0.000000000
<(i,x) <(i,y) <(i,z) 102.3479 99.5131 164.3197
d<(i,x) d<(i,y) d<(i,z) 3.2709 3.0150 2.3525

V1n_1 6.279420 kj +/- 0.004124 kj 1.499777 kcal +/- 0.000985 kcal
524.918367 cm +/- 0.3447 cm s= 44.055373
V1n_2 5.889355 kj +/- 0.013898 kj 1.406614 kcal +/- 0.003319 kcal
492.311514 cm +/- 1.1618 cm s= 41.318743

F(calc) 158.756361380
F(calc) 160.159305132

$^{13}C_{11}$ Isotopologue XIAM Output

	J K- K+	J K- K+	Sym	calc/GHz	diff/MHz	obs/GHz		
1:	10 2 8	9 3 7	S 1	5.6541228	-0.0320	5.6540908	Err 0.1D-04	-
2:	5 1 5	4 1 4	S 1	5.7513600	-0.0001	5.7513600	Err 0.1D-04	-
3:	5 0 5	4 0 4	S 1	5.9481933	0.0013	5.9481946	Err 0.1D-04	-
4:	10 1 9	10 0 10	S 3	6.2823014	0.0185	6.2823199	Err 0.1D-04	-
5:	5 1 4	4 1 3	S 1	6.3292970	-0.0083	6.3292887	Err 0.1D-04	-
6:	19 3 16	19 3 17	S 1	6.6656673	-0.0128	6.6656546	Err 0.1D-04	-
7:	5 1 5	4 0 4	S 3	6.8783552	-0.0151	6.8783401	Err 0.1D-04	-
8:	6 1 6	5 1 5	S 1	6.8875284	-0.0308	6.8874976	Err 0.1D-04	-
9:	6 0 6	5 0 5	S 1	7.0805488	-0.0110	7.0805378	Err 0.1D-04	-
10:	6 2 4	5 2 3	S 1	7.4536050	0.0043	7.4536093	Err 0.1D-04	-
11:	7 0 7	6 1 6	S 1	7.4553497	0.0197	7.4553693	Err 0.1D-04	-

12: 6 1 5 5 1 4 S 1 7.5747572 0.0007 7.5747579 Err 0.1D-04 -
13: 6 1 5 5 1 4 S 2 7.5747537 0.0044 7.5747581 Err 0.1D-04 -
14: 6 1 5 5 1 4 S 3 7.5747506 0.0076 7.5747581 Err 0.1D-04 -
15: 6 1 5 5 1 4 S 5 7.5747469 0.0113 7.5747581 Err 0.1D-04 -
16: 6 1 5 5 1 4 S 4 7.5747474 0.0111 7.5747584 Err 0.1D-04 -
17: 16 2 15 15 3 13 S 3 7.9251220 0.0447 7.9251667 Err 0.1D-04 -
18: 7 0 7 6 0 6 S 1 8.1925097 0.0062 8.1925159 Err 0.1D-04 -
19: 7 6 1 8 5 3 S 2 8.2034857 -0.0100 8.2034757 Err 0.1D-04 -
20: 19 4 15 19 3 16 S 1 8.2667700 0.0390 8.2668090 Err 0.1D-04 -
21: 3 2 2 2 1 1 S 1 8.3641157 0.0333 8.3641490 Err 0.1D-04 -
22: 9 3 7 9 2 8 S 4 8.6590830 0.0358 8.6591188 Err 0.1D-04 -
23: 7 2 5 6 2 4 S 1 8.7479893 0.0121 8.7480014 Err 0.1D-04 -
24: 7 1 6 6 1 5 S 1 8.8072114 -0.0016 8.8072098 Err 0.1D-04 -
25: 8 4 4 7 4 3 S 3 9.7525548 0.0170 9.7525718 Err 0.1D-04 -
26: 9 0 9 8 1 8 S 1 9.9635818 0.0094 9.9635912 Err 0.1D-04 -
27: 9 0 9 8 1 8 S 2 9.9635963 -0.0057 9.9635906 Err 0.1D-04 -
28: 9 0 9 8 1 8 S 4 9.9635674 0.0232 9.9635906 Err 0.1D-04 -
29: 9 0 9 8 1 8 S 3 9.9635404 0.0502 9.9635906 Err 0.1D-04 -
30: 9 0 9 8 1 8 S 5 9.9635425 0.0512 9.9635936 Err 0.1D-04 -
31: 8 2 6 7 2 5 S 2 10.0496153 0.0098 10.0496251 Err 0.1D-04 -
32: 8 2 6 7 2 5 S 3 10.0496125 0.0120 10.0496245 Err 0.1D-04 -
33: 8 2 6 7 2 5 S 4 10.0496123 0.0122 10.0496245 Err 0.1D-04 -
34: 8 2 6 7 2 5 S 5 10.0496071 0.0174 10.0496245 Err 0.1D-04 -
35: 8 2 6 7 2 5 S 2 10.0496153 0.0106 10.0496258 Err 0.1D-04 -
36: 13 4 10 13 3 10 S 2 10.2016245 0.0091 10.2016336 Err 0.1D-04 -
37: 9 1 9 8 1 8 S 1 10.2603190 -0.0188 10.2603003 Err 0.1D-04 -
38: 13 2 12 13 1 13 S 2 10.3515649 -0.0097 10.3515552 Err 0.1D-04 -
39: 9 2 8 8 2 7 S 1 10.8114530 -0.0197 10.8114333 Err 0.1D-04 -
40: 9 2 8 8 2 7 S 2 10.8114516 -0.0183 10.8114333 Err 0.1D-04 -
41: 9 2 8 8 2 7 S 5 10.8114365 -0.0028 10.8114337 Err 0.1D-04 -
42: 9 2 8 8 2 7 S 4 10.8114334 0.0006 10.8114340 Err 0.1D-04 -
43: 9 6 3 8 6 2 S 1 10.9526989 -0.0221 10.9526768 Err 0.1D-04 -
44: 9 3 7 8 3 6 S 1 10.9831059 -0.0189 10.9830870 Err 0.1D-04 -
45: 9 3 6 8 3 5 S 1 11.0726093 -0.0148 11.0725945 Err 0.1D-04 -
46: 10 0 10 9 1 9 S 1 11.1666026 -0.0071 11.1665955 Err 0.1D-04 -
47: 8 4 4 8 3 5 S 1 11.2984637 -0.0192 11.2984445 Err 0.1D-04 -
48: 8 4 4 8 3 5 S 3 11.2990945 -0.0065 11.2990880 Err 0.1D-04 -
49: 6 2 5 5 1 4 S 1 11.3058949 0.0022 11.3058971 Err 0.1D-04 -
50: 9 2 7 8 2 6 S 1 11.3506470 0.0050 11.3506521 Err 0.1D-04 -
51: 9 2 7 8 2 6 S 2 11.3506461 0.0062 11.3506523 Err 0.1D-04 -
52: 9 2 7 8 2 6 S 4 11.3506413 0.0110 11.3506523 Err 0.1D-04 -
53: 9 2 7 8 2 6 S 3 11.3506409 0.0115 11.3506523 Err 0.1D-04 -
54: 9 2 7 8 2 6 S 5 11.3506385 0.0140 11.3506525 Err 0.1D-04 -

55: 15 1 14 15 0 15 S 5 11.3714009 -0.0051 11.3713958 Err 0.1D-04 -
56: 10 1 10 9 1 9 S 1 11.3740067 -0.0117 11.3739950 Err 0.1D-04 -
57: 10 0 10 9 0 9 S 1 11.4633398 0.0426 11.4633824 Err 0.1D-04 -
58: 10 0 10 9 0 9 S 4 11.4632947 0.0070 11.4633017 Err 0.1D-04 -
59: 10 0 10 9 0 9 S 5 11.4632814 0.0203 11.4633017 Err 0.1D-04 -
60: 10 0 10 9 0 9 S 3 11.4632980 0.0037 11.4633017 Err 0.1D-04 -
61: 10 1 10 9 0 9 S 1 11.6707440 -0.0138 11.6707302 Err 0.1D-04 -
62: 10 1 10 9 0 9 S 2 11.6707223 0.0079 11.6707302 Err 0.1D-04 -
63: 10 1 10 9 0 9 S 4 11.6707090 0.0212 11.6707302 Err 0.1D-04 -
64: 3 3 0 2 2 0 S 3 11.8030007 -0.0308 11.8029699 Err 0.1D-04 -
65: 3 3 1 2 2 1 S 5 11.8038381 -0.0275 11.8038105 Err 0.1D-04 -
66: 3 3 0 2 2 0 S 4 11.8046634 0.0124 11.8046757 Err 0.1D-04 -
67: 3 3 1 2 2 1 S 2 11.8044177 -0.0338 11.8043839 Err 0.1D-04 -
68: 10 2 9 9 2 8 S 1 11.9817569 -0.0170 11.9817399 Err 0.1D-04 -
69: 10 6 4 9 6 3 S 1 12.1753138 -0.0080 12.1753059 Err 0.1D-04 -
70: 7 2 6 6 1 5 S 2 12.1775062 0.0029 12.1775091 Err 0.1D-04 -
71: 10 3 8 9 3 7 S 1 12.2051323 -0.0077 12.2051246 Err 0.1D-04 -
72: 11 0 11 10 1 10 S 1 12.3414007 -0.0387 12.3413620 Err 0.1D-04 -
73: 10 3 7 9 3 6 S 5 12.3522993 0.0019 12.3523012 Err 0.1D-04 -
74: 10 3 7 9 3 6 S 2 12.3523390 -0.0378 12.3523012 Err 0.1D-04 -
75: 16 1 15 16 0 16 S 1 12.3615806 0.0209 12.3616015 Err 0.1D-04 -
76: 10 1 9 9 1 8 S 1 12.3910281 0.0005 12.3910286 Err 0.1D-04 -
77: 17 3 15 17 1 16 S 2 12.4367479 -0.0061 12.4367418 Err 0.1D-04 -
78: 20 4 16 19 5 15 S 1 12.6414591 -0.0097 12.6414493 Err 0.1D-04 -
79: 10 2 8 9 2 7 S 1 12.6440425 0.0451 12.6440876 Err 0.1D-04 -
80: 4 3 2 3 2 2 S 4 13.0302387 0.0301 13.0302687 Err 0.1D-04 -
81: 4 3 2 3 2 2 S 3 13.0328158 0.0358 13.0328517 Err 0.1D-04 -
82: 4 3 2 3 2 2 S 1 13.0334478 -0.0198 13.0334280 Err 0.1D-04 -
83: 11 6 5 10 6 4 S 1 13.3997283 0.0001 13.3997284 Err 0.1D-04 -
84: 15 3 12 15 2 14 S 2 13.5076613 0.0024 13.5076637 Err 0.1D-04 -
85: 11 1 10 10 1 9 S 1 13.5378475 -0.0231 13.5378244 Err 0.1D-04 -
86: 11 3 8 10 3 7 S 1 13.6495724 -0.0045 13.6495679 Err 0.1D-04 -
87: 11 2 9 10 2 8 S 1 13.9244022 -0.0034 13.9243988 Err 0.1D-04 -
88: 5 3 3 4 2 3 S 1 14.2711035 -0.0426 14.2710609 Err 0.1D-04 -
89: 18 1 17 18 0 18 S 5 14.2865492 0.0070 14.2865561 Err 0.1D-04 -
90: 13 5 8 13 4 9 S 5 14.4083231 0.0153 14.4083384 Err 0.1D-04 -
91: 20 3 18 20 1 19 S 2 14.4356570 0.0208 14.4356779 Err 0.1D-04 -
92: 10 2 9 9 1 8 S 1 14.5545284 0.0111 14.5545395 Err 0.1D-04 -
93: 10 2 9 9 1 8 S 5 14.5543543 0.0027 14.5543570 Err 0.1D-04 -
94: 10 2 9 9 1 8 S 4 14.5543559 0.0009 14.5543568 Err 0.1D-04 -
95: 12 3 10 11 3 9 S 1 14.6368578 -0.0173 14.6368405 Err 0.1D-04 -
96: 12 1 11 11 1 10 S 1 14.6598040 -0.0220 14.6597820 Err 0.1D-04 -
97: 13 0 13 12 0 12 S 1 14.7253645 -0.0076 14.7253569 Err 0.1D-04 -

98: 13 0 13 12 0 12 S 2 14.7253510 0.0058 14.7253569 Err 0.1D-04 -
99: 12 3 9 11 3 8 S 1 14.9626735 -0.0068 14.9626667 Err 0.1D-04 -
100: 12 2 10 11 2 9 S 1 15.1877105 -0.0135 15.1876969 Err 0.1D-04 -
101: 11 2 10 10 1 9 S 2 15.3067686 -0.0262 15.3067424 Err 0.2D-04 -
102: 11 2 10 10 1 9 S 4 15.3067143 0.0281 15.3067424 Err 0.2D-04 -
103: 13 2 12 12 2 11 S 1 15.4404235 -0.0250 15.4403985 Err 0.1D-04 -
104: 9 2 7 8 1 7 S 1 15.4610334 -0.0251 15.4610082 Err 0.1D-04 -
105: 9 2 7 8 1 7 S 3 15.4610261 -0.0179 15.4610082 Err 0.1D-04 -
106: 14 1 13 13 2 12 S 2 15.7599106 0.0141 15.7599247 Err 0.1D-04 -
107: 4 4 0 3 3 1 S 1 16.2843589 0.0346 16.2843935 Err 0.1D-04 -
108: 13 3 10 12 3 9 S 4 16.2871736 0.0010 16.2871746 Err 0.1D-04 -
109: 13 2 11 12 2 10 S 1 16.4307010 -0.0063 16.4306946 Err 0.1D-04 -
110: 20 6 14 20 5 16 S 1 17.5098242 -0.0113 17.5098129 Err 0.1D-04 -
111: 14 3 11 13 3 10 S 1 17.6160014 -0.0216 17.6159798 Err 0.1D-04 -
112: 15 6 9 15 5 11 S 2 17.7754090 -0.0174 17.7753916 Err 0.1D-04 -
113: 14 6 9 14 5 9 S 4 17.7817709 0.0039 17.7817748 Err 0.1D-04 -
114: 14 6 9 14 5 10 S 2 17.7989683 -0.0353 17.7989330 Err 0.1D-04 -
115: 14 6 9 14 5 10 S 1 17.8051242 0.0453 17.8051695 Err 0.1D-04 -
116: 16 0 16 15 0 15 S 1 18.0038186 -0.0393 18.0037793 Err 0.1D-04 -
117: 16 1 16 15 0 15 S 3 18.0229323 0.0075 18.0229398 Err 0.1D-04 -
118: 16 1 16 15 0 15 S 5 18.0236847 -0.0050 18.0236797 Err 0.1D-04 -
119: 4 1 4 3 0 3 S 1 5.9199263 -0.0480 5.9198783 Err 0.1D-04 -
120: 12 3 9 12 2 10 S 4 6.3808390 -0.0019 6.3808371 Err 0.1D-04 -
121: 11 7 4 12 6 6 S 3 6.5547409 -0.0021 6.5547388 Err 0.1D-04 -
122: 11 7 4 12 6 6 S 4 6.5550903 -0.0194 6.5550709 Err 0.1D-04 -
123: 8 1 7 7 2 6 S 4 6.6528347 -0.0247 6.6528100 Err 0.1D-04 -
124: 13 8 6 14 7 8 S 3 7.3730701 0.0132 7.3730833 Err 0.1D-04 -
125: 7 5 2 6 5 1 S 1 8.5167962 -0.0131 8.5167831 Err 0.1D-04 -
126: 13 1 12 13 0 13 S 4 9.3301561 0.0122 9.3301683 Err 0.1D-04 -
127: 11 4 7 11 3 9 S 5 11.4490962 -0.0099 11.4490862 Err 0.1D-04 -
128: 11 1 11 10 1 10 S 4 12.4835327 -0.0015 12.4835312 Err 0.1D-04 -
129: 11 0 11 10 0 10 S 1 12.5488048 -0.0207 12.5487841 Err 0.1D-04 -
130: 15 2 13 14 3 11 S 1 12.6409229 -0.0220 12.6409008 Err 0.1D-04 -
131: 15 2 13 14 3 11 S 4 12.6410365 -0.0101 12.6410264 Err 0.1D-04 -
132: 12 1 12 11 0 11 S 1 13.7319043 -0.0185 13.7318858 Err 0.1D-04 -
133: 12 1 12 11 0 11 S 3 13.7320098 0.0130 13.7320228 Err 0.1D-04 -
134: 12 2 11 11 2 10 S 4 14.2961883 0.0042 14.2961925 Err 0.1D-04 -
135: 14 5 9 14 4 10 S 1 14.2778386 0.0134 14.2778520 Err 0.1D-04 -
136: 14 5 9 14 4 10 S 3 14.2780639 0.0353 14.2780992 Err 0.1D-04 -
137: 13 1 12 12 2 11 S 4 14.3549693 0.0432 14.3550126 Err 0.1D-04 -
138: 17 5 13 17 4 14 S 4 14.4470270 -0.0730 14.4469540 Err 0.1D-04 -
139: 12 6 6 11 6 5 S 4 14.6260924 0.0130 14.6261054 Err 0.1D-04 -
140: 19 2 18 19 1 19 S 5 15.3579275 -0.0006 15.3579269 Err 0.1D-04 -

```
 141: 13  3 11 12  3 10   S 4  15.8436475    0.0020  15.8436495   Err 0.1D-04          -
 142: 13  6  7 12  6  6   S 4  15.8546695    0.0078  15.8546773   Err 0.1D-04          -
 143: 13  4 10 12  4  9   S 2  15.9167372   -0.0393  15.9166979   Err 0.1D-04          -
 144: 16  2 14 15  3 13   S 3  16.3159247    0.0345  16.3159592   Err 0.1D-04          -
 145: 15  0 15 14  0 14   S 4  16.9094787    0.0526  16.9095313   Err 0.1D-04          -
 146: 14  6  8 14  5 10   S 1  17.8055448    0.0159  17.8055607   Err 0.1D-04          -
 Maximum (obs-calc)/err in line 138   0.0000730

 RMS deviations (MHz), B and V sorted
  B  V   n splittings MHz
  B  V   n abs. freq. MHz
  1  1 146         0.021845         0.023341

          Parameters  and  Errors
 BJ          0.606763168 { 0.000000237}
 BK           1.632710310 { 0.000001130}
 B-          0.058229981 { 0.000000044}
 DJ          0.009820E-6 { 0.000729E-6}
 DJK          0.019362E-6 { 0.003740E-6}
 DK          -0.110724E-6 { 0.014993E-6}
\F12         -0.834784880 {     derived}
\F         158.746772884 {     derived}  160.171666070 {     derived}
 V1n         15706.650553 {   19.674684}   14775.634428 {    6.670887}
\rho         0.005767184 {     derived}    0.013758243 {     derived}
\beta        0.604609363 {     derived}    3.070184662 {     derived}
\gamma        1.456034634 {     derived}   -2.539742681 {     derived}
 delta       1.229449307 { 0.003068810}    2.888736777 { 0.008109633}

 Standard Deviation       0.022717 MHz

------------------------------------ B =  1
 Rotational Constants and Errors (in GHz)
     B_z       2.239473477       0.000001125
     B_x       0.664993149       0.000000248
     B_y       0.548533187       0.000000235
 Ray's kappa   -0.86225
 F0(calc)     158.000000000       0.000000000
 I_alpha        3.198601709       0.000000000
 <(i,x)  <(i,y)  <(i,z)       84.8828       20.2694       70.4423
d<(i,x) d<(i,y) d<(i,z)        0.0056        0.1691        0.1758

 F0(calc)     158.000000000       0.000000000
 I_alpha        3.198601709       0.000000000
```

```
 <(i,x)  <(i,y)  <(i,z)      101.0840       99.2116      165.5124
d<(i,x) d<(i,y) d<(i,z)        0.3524        0.2918        0.4646

 V1n_1      6.267446 kj +/- 0.007851 kj         1.496917 kcal +/- 0.001875 kcal
        523.917395 cm +/-   0.6563 cm    s=  43.974019
 V1n_2      5.895941 kj +/- 0.002662 kj         1.408187 kcal +/- 0.000636 kcal
        492.862044 cm +/-   0.2225 cm    s=  41.367447

F(calc)       158.746772884
F(calc)       160.171666070
```

^{18}O Isotopologue XIAM Output

```
    J K- K+  J K- K+    Sym   calc/GHz  diff/MHz     obs/GHz
  1:  7  3  4  7  2  5   S 1   7.4286202    0.0159   7.4286361   Err 0.1D-04          -
  2:  5  3  2  5  2  3   S 1   7.7720297    0.0395   7.7720692   Err 0.1D-04          -
  3:  7  3  5  6  3  4   S 1   8.5131377    0.0182   8.5131559   Err 0.1D-04          -
  4:  7  1  7  6  0  6   S 1   8.6545749   -0.0249   8.6545500   Err 0.1D-04          -
  5: 18 11  7 19 10  9   S 1  10.1716523   -0.0040  10.1716482   Err 0.1D-04          -
  6: 16  3 13 15  4 11   S 1  11.1309363   -0.0037  11.1309326   Err 0.1D-04          -
  7: 10  1 10  9  1  9   S 1  11.3062019    0.0275  11.3062294   Err 0.1D-04          -
  8: 10  8  2  9  8  1   S 1  12.1302634   -0.0141  12.1302493   Err 0.1D-04          -
  9: 18  5 14 18  4 14   S 1  12.4567325    0.0020  12.4567344   Err 0.1D-04          -
 10: 18  4 14 18  3 16   S 1  14.0860565    0.0005  14.0860570   Err 0.1D-04          -
 11:  9  5  4  9  4  5   S 1  14.2182567    0.0126  14.2182693   Err 0.1D-04          -
 12: 22  4 19 22  3 20   S 1  14.5564639   -0.0194  14.5564445   Err 0.1D-04          -
 13: 14  1 14 13  1 13   S 1  15.6949961   -0.0004  15.6949957   Err 0.1D-04          -
 14:  7  3  4  6  2  5   S 1  16.6217879    0.0278  16.6218157   Err 0.1D-04          -
 15:  9  3  7  8  2  6   S 1  18.0238948   -0.0046  18.0238902   Err 0.1D-04          -
 16: 19  4 16 19  3 16   S 1   5.6759472   -0.0225   5.6759247   Err 0.1D-04          -
 17:  7  1  7  6  1  6   S 1   7.9737392   -0.0359   7.9737033   Err 0.1D-04          -
 18: 21  5 16 21  4 17   S 1  11.1765828   -0.0161  11.1765667   Err 0.1D-04          -
 19: 19  2 17 19  2 18   S 1  12.3296210   -0.0104  12.3296105   Err 0.1D-04          -
Maximum (obs-calc)/err in line   2   0.0000395

RMS deviations (MHz), B and V sorted
 B  V   n splittings MHz
 B  V   n abs. freq. MHz
 1  1  19         0.019535         0.022619

          Parameters  and  Errors
BJ          0.605040040 { 0.000000332}
BK          1.587601159 { 0.000000767}
```

```
 B-          0.060183790 { 0.000000069}
\F12         -0.827049468 {     derived}
\F         158.741806534 {     derived}  160.119106670 {     derived}
\rho         0.005708444 {     derived}    0.013442226 {     derived}
\beta        0.606242017 {     derived}    3.066059769 {     derived}
\gamma       1.455227300 {     derived}   -2.543039167 {     derived}

 Standard Deviation       0.021985 MHz

------------------------------------ B =  1
 Rotational Constants and Errors (in GHz)
     B_z      2.192641199       0.000000945
     B_x      0.665223830       0.000000343
     B_y      0.544856250       0.000000334
 Ray's kappa   -0.85390
 F0(calc)    158.000000000       0.000000000
 I_alpha       3.198601709       0.000000000
 <(i,x)  <(i,y)  <(i,z)      84.8892       20.4618       70.2424
d<(i,x) d<(i,y) d<(i,z)       0.0000        0.0000        0.0000

 F0(calc)    158.000000000       0.000000000
 I_alpha       3.198601709       0.000000000
 <(i,x)  <(i,y)  <(i,z)     101.4809       99.5401      164.9886
d<(i,x) d<(i,y) d<(i,z)       0.0000        0.0000        0.0000

 V1n_1      6.275827 kj +/- 0.000000 kj        1.498919 kcal +/- 0.000000 kcal
        524.618074 cm +/-   0.0000 cm    s=  44.034207
 V1n_2      5.894025 kj +/- 0.000000 kj        1.407729 kcal +/- 0.000000 kcal
        492.701873 cm +/-   0.0000 cm    s=  41.355297

F(calc)      158.741806534
F(calc)      160.119106670
```

EQ1 Kraitchman Output

```
_____________________________________________________________________________
____
|                                                                            |
|   KRA  -  SINGLE ISOTOPIC SUBSTITUTION - Various permutations              |
|          of Kraitchman's equations for symmetric/asymmetric tops           |

|____________________________________________________________________________
_____|
```

version 4a.IV.2017 Zbigniew KISIEL

R-Carvon EQ1

---

parent species
Planar calculation will be made from I.a and I.b

C(1)

The parent species:

X, Y, Z =	2256.91160000	672.90456000	554.50189000
eX, eY, eZ =	0.00060000	0.00009000	0.00009000
IX, IY, IZ =	223.92503495	751.04114156	911.41079591
eIX,eIY,eIZ =	0.00005953	0.00010045	0.00014793
PX, PY, PZ =	719.26345126	192.14734465	31.77769029

Mass = 150.10446507

The isotopic species:

X, Y, Z =	2236.89720000	672.57330000	553.27970000
eX, eY, eZ =	0.00080000	0.00020000	0.00020000
IX, IY, IZ =	225.92858040	751.41104903	913.42409436
eIX,eIY,eIZ =	0.00008080	0.00022344	0.00033019
PX, PY, PZ =	719.45328149	193.97081287	31.95776753

Mass change = 1.00335484
Total mass = 151.10781991
M DM/(M+DM) = 0.99669257

KRAITCHMAN RESULTS:

	a	b
PLANAR:	0.60805 +- 0.00020	1.41831 +- 0.00004
+Costain err.	0.60805 +- 0.00248	1.41831 +- 0.00106

	a	b	c

NONPLANAR: 0.43560 +- 0.00026 1.35208 +- 0.00008 0.42753 +- 0.00027
+Costain err. 0.43560 +- 0.00345 1.35208 +- 0.00111 0.42753 +- 0.00352

R= 1.48346 +- 0.00176

DIX,DIY,DIZ = 2.00354546 0.36990747 2.01329845
DPX,DPY,DPZ = 0.18983023 1.82346822 0.18007724
IXY,IXZ,IYZ = -527.11610661 -687.48576097 -160.36965436

C(2)

The parent species:

X, Y, Z = 2256.91160000 672.90456000 554.50189000
eX, eY, eZ = 0.00060000 0.00009000 0.00009000
IX, IY, IZ = 223.92503495 751.04114156 911.41079591
eIX,eIY,eIZ = 0.00005953 0.00010045 0.00014793
PX, PY, PZ = 719.26345126 192.14734465 31.77769029

Mass = 150.10446507

The isotopic species:

X, Y, Z = 2232.33840000 671.86310000 552.42440000
eX, eY, eZ = 0.00090000 0.00020000 0.00020000
IX, IY, IZ = 226.38996350 752.20533603 914.83831797
eIX,eIY,eIZ = 0.00009127 0.00022392 0.00033121
PX, PY, PZ = 720.32684525 194.51147272 31.87849078

Mass change = 1.00335484
Total mass = 151.10781991
M DM/(M+DM) = 0.99669257

KRAITCHMAN RESULTS:

a b

PLANAR: 1.07824 +- 0.00011 1.57435 +- 0.00003
+Costain err. 1.07824 +- 0.00140 1.57435 +- 0.00095

a b c

NONPLANAR: 1.03053 +- 0.00011 1.54119 +- 0.00007 0.32060 +- 0.00036
+Costain err. 1.03053 +- 0.00146 1.54119 +- 0.00098 0.32060 +- 0.00469

R= 1.88150 +- 0.00138

DIX,DIY,DIZ = 2.46492856 1.16419447 3.42752205
DPX,DPY,DPZ = 1.06339399 2.36412807 0.10080049
IXY,IXZ,IYZ = -527.11610661 -687.48576097 -160.36965436

C(3)

The parent species:

X, Y, Z = 2256.91160000 672.90456000 554.50189000
eX, eY, eZ = 0.00060000 0.00009000 0.00009000
IX, IY, IZ = 223.92503495 751.04114156 911.41079591
eIX,eIY,eIZ = 0.00005953 0.00010045 0.00014793
PX, PY, PZ = 719.26345126 192.14734465 31.77769029

Mass = 150.10446507

The isotopic species:

X, Y, Z = 2253.91880000 669.66270000 552.11950000
eX, eY, eZ = 0.00080000 0.00020000 0.00020000
IX, IY, IZ = 224.22236724 754.67695737 915.34352418
eIX,eIY,eIZ = 0.00007958 0.00022539 0.00033157
PX, PY, PZ = 722.89905716 192.44446703 31.77790021

Mass change = 1.00335484
Total mass = 151.10781991
M DM/(M+DM) = 0.99669257

KRAITCHMAN RESULTS:

a b

PLANAR: 1.90940 +- 0.00006 0.54807 +- 0.00009
+Costain err. 1.90940 +- 0.00079 0.54807 +- 0.00274

	a	b	c
NONPLANAR:	1.90935 +- 0.00006	0.54787 +- 0.00021	0.01456 +- 0.00781
+Costain err.	1.90935 +- 0.00079	0.54787 +- 0.00275	0.01456 +- 0.10329

R= 1.98645 +- 0.00131

DIX,DIY,DIZ =	0.29733229	3.63581581	3.93272827
DPX,DPY,DPZ =	3.63560590	0.29712237	0.00020992
IXY,IXZ,IYZ =	-527.11610661	-687.48576097	-160.36965436

C(4)

The parent species:

X, Y, Z =	2256.91160000	672.90456000	554.50189000
eX, eY, eZ =	0.00060000	0.00009000	0.00009000
IX, IY, IZ =	223.92503495	751.04114156	911.41079591
eIX,eIY,eIZ =	0.00005953	0.00010045	0.00014793
PX, PY, PZ =	719.26345126	192.14734465	31.77769029

Mass = 150.10446507

The isotopic species:

X, Y, Z =	2249.82400000	671.12070000	552.86200000
eX, eY, eZ =	0.00200000	0.00030000	0.00030000
IX, IY, IZ =	224.63046394	753.03743261	914.11420734
eIX,eIY,eIZ =	0.00019969	0.00033662	0.00049603
PX, PY, PZ =	721.26058801	192.85361934	31.77684460

Mass change = 1.00335484
Total mass = 151.10781991
M DM/(M+DM) = 0.99669257

KRAITCHMAN RESULTS:

	a	b
PLANAR:	1.41430 +- 0.00012	0.84288 +- 0.00012

+Costain err. 1.41430 +- 0.00107 0.84288 +- 0.00178

a b c

NONPLANAR: 1.41460 +- 0.00012 0.84339 +- 0.00020 0.02924*i+- 0.00570
+Costain err. 1.41460 +- 0.00107 0.84339 +- 0.00179 0.02924*i+- 0.05162

R= 1.64667 +- 0.00159

DIX,DIY,DIZ = 0.70542899 1.99629106 2.70341143
DPX,DPY,DPZ = 1.99713675 0.70627468 -0.00084569
IXY,IXZ,IYZ = -527.11610661 -687.48576097 -160.36965436

C(5)

The parent species:

X, Y, Z = 2256.91160000 672.90456000 554.50189000
eX, eY, eZ = 0.00060000 0.00009000 0.00009000
IX, IY, IZ = 223.92503495 751.04114156 911.41079591
eIX,eIY,eIZ = 0.00005953 0.00010045 0.00014793
PX, PY, PZ = 719.26345126 192.14734465 31.77769029

Mass = 150.10446507

The isotopic species:

X, Y, Z = 2244.45500000 672.88940000 553.78810000
eX, eY, eZ = 0.00200000 0.00070000 0.00060000
IX, IY, IZ = 225.16780639 751.05806229 912.58553389
eIX,eIY,eIZ = 0.00020064 0.00078132 0.00098874
PX, PY, PZ = 719.23789489 193.34763900 31.82016740

Mass change = 1.00335484
Total mass = 151.10781991
M DM/(M+DM) = 0.99669257

KRAITCHMAN RESULTS:

a b

PLANAR: 0.13014 +- 0.00303 1.11666 +- 0.00009
+Costain err. 0.13014 +- 0.01192 1.11666 +- 0.00135

a b c

NONPLANAR: 0.15994*i+- 0.00202 1.09722 +- 0.00029 0.20721 +- 0.00157
+Costain err. 0.15994*i+- 0.00959 1.09722 +- 0.00140 0.20721 +- 0.00741

R= 1.10510 +- 0.00241

DIX,DIY,DIZ = 1.24277145 0.01692074 1.17473798
DPX,DPY,DPZ = -0.02555637 1.20029434 0.04247710
IXY,IXZ,IYZ = -527.11610661 -687.48576097 -160.36965436

C(6)

The parent species:

X, Y, Z = 2256.91160000 672.90456000 554.50189000
eX, eY, eZ = 0.00060000 0.00009000 0.00009000
IX, IY, IZ = 223.92503495 751.04114156 911.41079591
eIX,eIY,eIZ = 0.00005953 0.00010045 0.00014793
PX, PY, PZ = 719.26345126 192.14734465 31.77769029

Mass = 150.10446507

The isotopic species:

X, Y, Z = 2256.24950000 672.11090000 554.00600000
eX, eY, eZ = 0.00080000 0.00020000 0.00020000
IX, IY, IZ = 223.99074610 751.92800608 912.22659845
eIX,eIY,eIZ = 0.00007942 0.00022375 0.00032932
PX, PY, PZ = 720.08192921 192.14466924 31.84607687

Mass change = 1.00335484
Total mass = 151.10781991
M DM/(M+DM) = 0.99669257

KRAITCHMAN RESULTS:

	a	b	
PLANAR:	0.94324 +- 0.00013	0.25698 +- 0.00019	
+Costain err.	0.94324 +- 0.00160	0.25698 +- 0.00584	

	a	b	c
NONPLANAR:	0.90615 +- 0.00012	0.05184*i+- 0.00217	0.26210 +- 0.00043
+Costain err.	0.90615 +- 0.00166	0.05184*i+- 0.02902	0.26210 +- 0.00574

R= 0.94187 +- 0.00277

DIX,DIY,DIZ =	0.06571116	0.88686452	0.81580254
DPX,DPY,DPZ =	0.81847795	-0.00267541	0.06838657
IXY,IXZ,IYZ =	-527.11610661	-687.48576097	-160.36965436

C(7)

The parent species:

X, Y, Z =	2256.91160000	672.90456000	554.50189000
eX, eY, eZ =	0.00060000	0.00009000	0.00009000
IX, IY, IZ =	223.92503495	751.04114156	911.41079591
eIX,eIY,eIZ =	0.00005953	0.00010045	0.00014793
PX, PY, PZ =	719.26345126	192.14734465	31.77769029

Mass = 150.10446507

The isotopic species:

X, Y, Z =	2251.02460000	662.78730000	547.27590000
eX, eY, eZ =	0.00080000	0.00020000	0.00020000
IX, IY, IZ =	224.51065568	762.50557140	923.44466274
eIX,eIY,eIZ =	0.00007979	0.00023009	0.00033747
PX, PY, PZ =	730.71978923	192.72487351	31.78578217

Mass change = 1.00335484
Total mass = 151.10781991
M DM/(M+DM) = 0.99669257

KRAITCHMAN RESULTS:

	a	b	
PLANAR:	3.38965 +- 0.00004	0.77482 +- 0.00007	
+Costain err.	3.38965 +- 0.00044	0.77482 +- 0.00194	
	a	b	c
NONPLANAR:	3.38845 +- 0.00003	0.76942 +- 0.00015	0.09102 +- 0.00128
+Costain err.	3.38845 +- 0.00044	0.76942 +- 0.00196	0.09102 +- 0.01653

R= 3.47591 +- 0.00075

DIX,DIY,DIZ =	0.58562073	11.46442984	12.03386683
DPX,DPY,DPZ =	11.45633797	0.57752886	0.00809188
IXY,IXZ,IYZ =	-527.11610661	-687.48576097	-160.36965436

C(9)

The parent species:

X, Y, Z =	2256.91160000	672.90456000	554.50189000
eX, eY, eZ =	0.00060000	0.00009000	0.00009000
IX, IY, IZ =	223.92503495	751.04114156	911.41079591
eIX,eIY,eIZ =	0.00005953	0.00010045	0.00014793
PX, PY, PZ =	719.26345126	192.14734465	31.77769029

Mass = 150.10446507

The isotopic species:

X, Y, Z =	2256.66300000	667.75740000	551.00170000
eX, eY, eZ =	0.00200000	0.00030000	0.00030000
IX, IY, IZ =	223.94970312	756.83026336	917.20045310
eIX,eIY,eIZ =	0.00019848	0.00034002	0.00049938
PX, PY, PZ =	725.04050667	192.15994643	31.78975669

Mass change = 1.00335484
Total mass = 151.10781991

M DM/(M+DM) = 0.99669257

KRAITCHMAN RESULTS:

	a	b	
PLANAR:	2.40999 +- 0.00007	0.15818 +- 0.00066	
+Costain err.	2.40999 +- 0.00063	0.15818 +- 0.00951	

	a	b	c
NONPLANAR:	2.40749 +- 0.00007	0.11305 +- 0.00149	0.11049 +- 0.00152
+Costain err.	2.40749 +- 0.00063	0.11305 +- 0.01335	0.11049 +- 0.01366

R= 2.41267 +- 0.00108

DIX,DIY,DIZ =	0.02466818	5.78912180	5.78965719
DPX,DPY,DPZ =	5.77705541	0.01260178	0.01206639
IXY,IXZ,IYZ =	-527.11610661	-687.48576097	-160.36965436

C(10)

The parent species:

X, Y, Z =	2256.91160000	672.90456000	554.50189000
eX, eY, eZ =	0.00060000	0.00009000	0.00009000
IX, IY, IZ =	223.92503495	751.04114156	911.41079591
eIX,eIY,eIZ =	0.00005953	0.00010045	0.00014793
PX, PY, PZ =	719.26345126	192.14734465	31.77769029

Mass = 150.10446507

The isotopic species:

X, Y, Z =	2244.39720000	662.81530000	547.50140000
eX, eY, eZ =	0.00090000	0.00030000	0.00020000
IX, IY, IZ =	225.17360514	762.47336007	923.06432258
eIX,eIY,eIZ =	0.00009029	0.00034511	0.00033719
PX, PY, PZ =	730.18203875	192.88228382	32.29132132

Mass change = 1.00335484

Total mass = 151.10781991
M DM/(M+DM) = 0.99669257

KRAITCHMAN RESULTS:

	a	b	
PLANAR:	3.38275 +- 0.00005	1.13132 +- 0.00005	
+Costain err.	3.38275 +- 0.00045	1.13132 +- 0.00133	

	a	b	c
NONPLANAR:	3.30626 +- 0.00004	0.86616 +- 0.00015	0.72520 +- 0.00019
+Costain err.	3.30626 +- 0.00046	0.86616 +- 0.00174	0.72520 +- 0.00208

R= 3.49393 +- 0.00075

DIX,DIY,DIZ =	1.24857020	11.43221852	11.65352666
DPX,DPY,DPZ =	10.91858749	0.73493917	0.51363103
IXY,IXZ,IYZ =	-527.11610661	-687.48576097	-160.36965436

C(11)

The parent species:

X, Y, Z =	2256.91160000	672.90456000	554.50189000
eX, eY, eZ =	0.00060000	0.00009000	0.00009000
IX, IY, IZ =	223.92503495	751.04114156	911.41079591
eIX,eIY,eIZ =	0.00005953	0.00010045	0.00014793
PX, PY, PZ =	719.26345126	192.14734465	31.77769029

Mass = 150.10446507

The isotopic species:

X, Y, Z =	2239.47300000	664.99310000	548.53320000
eX, eY, eZ =	0.00100000	0.00020000	0.00020000
IX, IY, IZ =	225.66872157	759.97631990	921.32802335
eIX,eIY,eIZ =	0.00010077	0.00022857	0.00033592
PX, PY, PZ =	727.81781084	193.51021251	32.15850906

Mass change = 1.00335484
Total mass = 151.10781991
M DM/(M+DM) = 0.99669257

KRAITCHMAN RESULTS:

	a	b	
PLANAR:	2.98918 +- 0.00004	1.33384 +- 0.00004	
+Costain err.	2.98918 +- 0.00050	1.33384 +- 0.00113	

	a	b	c
NONPLANAR:	2.92503 +- 0.00004	1.17740 +- 0.00010	0.62460 +- 0.00019
+Costain err.	2.92503 +- 0.00051	1.17740 +- 0.00128	0.62460 +- 0.00241

R= 3.21438 +- 0.00081

DIX,DIY,DIZ =	1.74368662	8.93517835	9.91722744
DPX,DPY,DPZ =	8.55435958	1.36286786	0.38081877
IXY,IXZ,IYZ =	-527.11610661	-687.48576097	-160.36965436

Oxygen-18

The parent species:

X, Y, Z =	2256.91160000	672.90456000	554.50189000
eX, eY, eZ =	0.00060000	0.00009000	0.00009000
IX, IY, IZ =	223.92503495	751.04114156	911.41079591
eIX,eIY,eIZ =	0.00005953	0.00010045	0.00014793
PX, PY, PZ =	719.26345126	192.14734465	31.77769029

Mass = 150.10446507

The isotopic species:

X, Y, Z =	2192.64120000	665.22380000	544.85630000
eX, eY, eZ =	0.00090000	0.00030000	0.00030000
IX, IY, IZ =	230.48869505	759.71275968	927.54549943
eIX,eIY,eIZ =	0.00009461	0.00034261	0.00051071
PX, PY, PZ =	728.38478203	199.16071740	31.32797765

Mass change = 2.00424499
Total mass = 152.10871006
M DM/(M+DM) = 1.97783626

KRAITCHMAN RESULTS:

	a	b	
PLANAR:	2.08082 +- 0.00004	1.83663 +- 0.00002	
+Costain err.	2.08082 +- 0.00072	1.83663 +- 0.00082	

	a	b	c
NONPLANAR:	2.13387 +- 0.00004	1.90196 +- 0.00004	0.49038*i+- 0.00018
+Costain err.	2.13387 +- 0.00070	1.90196 +- 0.00079	0.49038*i+- 0.00306

R= 2.81609 +- 0.00092

DIX,DIY,DIZ =	6.56366010	8.67161812	16.13470352
DPX,DPY,DPZ =	9.12133077	7.01337275	-0.44971265
IXY,IXZ,IYZ =	-527.11610661	-687.48576097	-160.36965436

EQ1 Eval Output

```
_____________________________________________________________________
____
|                                                                   |
|     E V A L   -  Internals and their errors from Cartesians       |
|___________________________________________________________________
_____|
 version 20.V.2020                          Zbigniew KISIEL
```

WARNING:

The EVAL uncertainties are evaluated by assuming that the correlation matrix is a unit matrix.

The EVAL uncertainties may thus differ significantly

(but typically by not more than 30% either way)
from uncertainties in explicitly fitted internals
corresponding to the input Cartesians.

```
!
! EQ1, KRA coordinates
!

INPUT CARTESIANS:

C(1)      0.43560  0.00345    -1.35208  0.00111     0.42753  0.00352
C(2)     -1.03053  0.00146    -1.54119  0.00098     0.32060  0.00469
C(3)     -1.90935  0.00079    -0.54787  0.00275    -0.01456  0.10329
C(4)     -1.41460  0.00107     0.84339  0.00179     0.00000  0.00000
C(5)      0.00000  0.00000     1.09722  0.00140     0.20721  0.00741
C(6)      0.90615  0.00166     0.00000  0.00000    -0.26210  0.00574
C(7)     -3.38845  0.00044    -0.76942  0.00196    -0.09102  0.01653
C(9)      2.40749  0.00063     0.11305  0.01335    -0.11049  0.01366
C(10)     3.30626  0.00046     0.86616  0.00174     0.72520  0.00208
C(11)     2.92503  0.00051     1.17740  0.00128    -0.62460  0.00241
Oxygen   -2.13387  0.00070     1.90196  0.00079     0.00000  0.00000

CALCULATED INTERNALS:

!
!  Bond lengths
!
        C(1)  C(2)   =   1.48214 +- 0.00373
        C(2)  C(3)   =   1.36797 +- 0.02541
        C(3)  C(4)   =   1.47668 +- 0.00327
        C(4)  C(5)   =   1.45205 +- 0.00154
        C(5)  C(6)   =   1.49842 +- 0.00327
        C(6)  C(1)   =   1.58906 +- 0.00327
        C(3)  C(7)   =   1.49755 +- 0.00547
        C(6)  C(9)   =   1.51320 +- 0.00251
        C(9)  C(10)  =   1.43991 +- 0.01068
        C(9)  C(11)  =   1.29035 +- 0.01237
        C(4)  Oxygen =   1.27981 +- 0.00177
!
!  Bond angles
!
    C(1)  C(2)  C(3)   =  124.09144 +- 0.36574
```

C(2) C(3) C(4) = 117.80520 +- 1.73661
C(3) C(4) C(5) = 119.50515 +- 0.64804
C(4) C(5) C(6) = 114.61017 +- 0.24277
C(5) C(6) C(1) = 107.94171 +- 0.30395
C(6) C(1) C(2) = 111.72630 +- 0.20818
C(2) C(3) C(7) = 122.65608 +- 1.45563
C(4) C(3) C(7) = 118.08619 +- 0.32567
C(1) C(6) C(9) = 108.29331 +- 0.54913
C(5) C(6) C(9) = 120.92467 +- 0.53852
C(6) C(9) C(11) = 114.81224 +- 0.76273
C(6) C(9) C(10) = 135.76745 +- 0.85961

!
! Dihedral Angles
!
C(1) C(2) C(3) C(4) = -12.98029 +- 9.37950
C(2) C(3) C(4) C(5) = 7.27787 +- 8.96958
C(3) C(4) C(5) C(6) = 28.48479 +- 4.58653
C(4) C(5) C(6) C(1) = -54.39474 +- 0.58900
C(5) C(6) C(1) C(2) = 47.57613 +- 0.46485
C(6) C(1) C(2) C(3) = -15.47667 +- 5.07621
C(1) C(2) C(3) C(7) = -178.95131 +- 4.44319
C(5) C(4) C(3) C(7) = 173.90218 +- 4.43990
C(4) C(5) C(6) C(9) = -179.74517 +- 0.70040
C(2) C(1) C(6) C(9) = -179.89395 +- 0.60962
C(5) C(6) C(9) C(11) = -54.48595 +- 1.23017
C(1) C(6) C(9) C(11) = -179.67372 +- 0.76184
C(1) C(6) C(9) C(10) = -103.36357 +- 1.27824
C(5) C(6) C(9) C(10) = 21.82420 +- 1.69280
C(2) C(3) C(4) Oxygen = -164.02234 +- 3.79222
C(6) C(5) C(4) Oxygen = -159.17656 +- 0.35174

S4. EQ2 Assignments and Outputs of Structure Evaluation - Isotopologue Overview

	$^{13}C_1$		$^{13}C_2$		$^{13}C_3$		$^{13}C_4$	
	Experiment	Theory	Experiment	Theory	Experiment	Theory	Experiment	Theory
A (MHz)	2,216.1959 (16)	2,207.4	2,213.2346 (10)	2,204.7	2,234.6711 (64)	2,225.9	2,229.8382 (12)	2,221.1
B (MHz)	656.11032 (53)	648.2	655.27755 (32)	647.4	653.18526 (26)	645.3	654.69211 (46)	646.8
C (MHz)	578.14251 (67)	571.2	577.25614 (29)	570.3	577.03856 (26)	570.1	577.91425 (47)	570.9
D_J (kHz)	0.0217 (26)		0.021445 (56)		0.00896 (57)		0.03000 (95)	
D_{JK} (kHz)	[0.0597]		0.0588 (42)		0.0716 (21)		0.0640 (45)	
D_K (kHz)	[0.0225]		[0.0225]		0.0176 (33)		[0.0225]	
d_J (kHz)	[-0.00278]		-0.00303 (15)		-0.00141 (24)		[-0.00278]	
d_K (kHz)	[0.00189]		[0.00189]		0.001939 (72)		[0.00189]	
V_{3_1} (cm^{-1})	[599]		[599]		585 (6)		[599]	
δ_1 (radian)	[0.55]		[0.55]		0.718 (63)		[0.55]	
ε_1 (radian)	[3.91]		[3.91]		[3.91]		[3.91]	
V_{3_2} (cm^{-1})	[485.67]		[485.67]		490 (1)		[485.67]	
δ_2 (radian)	[2.838]		[2.838]		3.09 (22)		[2.838]	
ε_2 (radian)	[3.032]		[3.032]		[3.032]		[3.032]	
ν_{RMS} (kHz)	22.8		22.0		22.4		22.7	
Number of Transitions	30		64		146		39	
	$^{13}C_5$		$^{13}C_6$		$^{13}C_7$		$^{13}C_9$	
A (MHz)	2,226.0769 (10)	2,217.4	2,235.9401 (14)	2,227.2	2,232.93640 (64)	2,224.2	2,236.90972 (70)	2,228.2
B (MHz)	656.21840(39)	648.3	655.48585 (48)	647.6	646.53884 (20)	638.8	651.36220 (27)	643.5
C (MHz)	578.95689 (40)	572.0	579.09795 (54)	572.1	571.77591 (22)	564.9	575.1409 (23)	568.8
D_J (kHz)	0.01873 (74)		0.0214 (10)		0.02441 (53)		0.02482 (33)	
D_{JK} (kHz)	[0.0597]		0.0620 (46)		[0.0597]		0.0491 (22)	
D_K (kHz)	[0.0225]		[0.0225]		0.0363 (43)		0.0268 (29)	
d_J (kHz)	[-0.00278]		-0.00246 (36)		-0.00284 (15)		-0.00502 (23)	
d_K (kHz)	[0.00189]		[0.00189]		0.00166 (11)		0.001982 (68)	
V_{3_1} (cm^{-1})	[599]		[599]		[599]		603 (3)	
δ_1 (radian)	[0.55]		[0.55]		[0.55]		0.505 (53)	
ε_1 (radian)	[3.91]		[3.91]		[3.91]		[3.91]	
V_{3_2} (cm^{-1})	[485.67]		[485.67]		[485.67]		485.36 (77)	
δ_2 (radian)	[2.838]		[2.838]		[2.838]		2.840 (25)	
ε_2 (radian)	[3.032]		[3.032]		[3.032]		[3.032]	
ν_{RMS} (kHz)	25.5		25.9		23.3		22.1	
Number of Transitions	36		49		175		255	
	$^{13}C_{10}$		$^{13}C_{11}$		^{18}O			
A (MHz)	2,222.1928 (14)	2,213.4	2,222.3986 (18)	2,213.9	2,176.1986 (12)	2,165.0		
B (MHz)	647.70150 (52)	639.9	646.30140 (43)	638.6	647.86971 (32)	641.0		
C (MHz)	573.87388 (58)	567.0	572.81601 (13)	565.9	569.92069 (39)	562.7		
D_J (kHz)	0.02548 (98)		0.0314 (14)		0.02421 (86)			
D_{JK} (kHz)	0.0623 (57)		[0.0597]		0.0606 (27)			
D_K (kHz)	0.0291 (38)		[0.0225]		0.0314 (87)			
d_J (kHz)	-0.00694 (58)		[-0.00278]		-0.00306 (12)			
d_K (kHz)	0.002039 (88)		[0.00189]		0.001858 (80)			
V_{3_1} (cm^{-1})	[599]		[599]		602.07 (51)			
δ_1 (radian)	[0.55]		[0.55]		[0.55]			
ε_1 (radian)	[3.91]		[3.91]		[3.91]			
V_{3_2} (cm^{-1})	[485.67]		[485.67]		486.11 (12)			
δ_2 (radian)	[2.838]		[2.838]		[2.838]			
ε_2 (radian)	[3.032]		[3.032]		[3.032]			
ν_{RMS} (kHz)	23.4		25.4		24.0			
Number of Transitions	53		41		99			

Parent XIAM Output

	J	K-	K+	J	K-	K+	Sym	calc/GHz	diff/MHz	obs/GHz		
1:	8	1	8	7	1	7	S 1	9.5335304	-0.0060	9.5335244	Err 0.1D-04	-
2:	8	0	8	7	0	7	S 1	9.6829429	-0.0080	9.6829349	Err 0.1D-04	-
3:	8	2	7	7	2	6	S 2	9.8542036	-0.0340	9.8541696	Err 0.1D-04	-
4:	8	7	2	7	7	0	S 1	9.8957167	-0.0103	9.8957064	Err 0.1D-04	-
5:	8	6	2	7	6	1	S 1	9.8975263	-0.0100	9.8975164	Err 0.1D-04	-
6:	8	3	6	7	3	4	S 2	9.8972115	0.0425	9.8972540	Err 0.1D-04	-
7:	8	5	3	7	5	2	S 1	9.9005824	-0.0113	9.9005711	Err 0.1D-04	-
8:	8	4	5	7	4	4	S 1	9.9062320	0.0007	9.9062327	Err 0.1D-04	-
9:	8	4	4	7	4	3	S 1	9.9065968	-0.0044	9.9065924	Err 0.1D-04	-
10:	8	4	4	7	4	3	S 2	9.9064117	0.0097	9.9064215	Err 0.1D-04	-
11:	8	2	6	7	2	5	S 1	10.0581905	0.0110	10.0582015	Err 0.1D-04	-
12:	8	1	7	7	1	6	S 1	10.1317130	0.0054	10.1317184	Err 0.1D-04	-
13:	9	0	9	8	1	8	S 1	10.1928793	-0.0075	10.1928718	Err 0.1D-04	-
14:	8	1	8	7	0	7	S 1	10.3371996	-0.0156	10.3371840	Err 0.1D-04	-
15:	8	1	8	7	0	7	S 2	10.3371620	-0.0008	10.3371612	Err 0.1D-04	-
16:	22	2	20	22	2	21	S 2	10.5156164	-0.0084	10.5156080	Err 0.1D-04	-
17:	5	2	4	4	1	3	S 1	10.6533228	-0.0318	10.6532909	Err 0.2D-04	-
18:	9	1	9	8	1	8	S 2	10.7127140	-0.0052	10.7127088	Err 0.1D-04	-
19:	9	0	9	8	0	8	S 1	10.8471360	-0.0134	10.8471226	Err 0.1D-04	-
20:	9	2	8	8	2	7	S 1	11.0745829	-0.0107	11.0745721	Err 0.1D-04	-
21:	9	8	1	8	8	0	S 2	11.1324520	-0.0273	11.1324247	Err 0.1D-04	-
22:	9	7	2	8	7	1	S 2	11.1341080	-0.0092	11.1340988	Err 0.1D-04	-
23:	9	6	3	8	6	2	S 1	11.1366863	-0.0142	11.1366721	Err 0.2D-04	-
24:	9	5	4	8	5	3	S 1	11.1410417	-0.0233	11.1410184	Err 0.1D-04	-
25:	9	4	6	8	4	5	S 1	11.1489247	0.0007	11.1489254	Err 0.1D-04	-
26:	9	4	5	8	4	4	S 1	11.1497971	-0.0024	11.1497947	Err 0.1D-04	-
27:	9	4	6	8	4	5	S 4	11.1493203	-0.0135	11.1493068	Err 0.3D-04	-
28:	9	4	5	9	3	6	S 3	11.2524909	-0.0016	11.2524892	Err 0.1D-04	-
29:	9	4	5	9	3	6	S 1	11.2513609	-0.0035	11.2513573	Err 0.1D-04	-
30:	9	2	7	8	2	6	S 1	11.3497813	0.0162	11.3497975	Err 0.1D-04	-
31:	9	1	8	8	1	7	S 1	11.3754105	0.0021	11.3754126	Err 0.1D-04	-
32:	10	0	10	9	0	9	S 1	12.0045022	-0.0042	12.0044980	Err 0.1D-04	-
33:	10	2	9	9	2	8	S 1	12.2910964	-0.0150	12.2910814	Err 0.2D-04	-
34:	10	9	1	9	9	0	S 2	12.3691908	0.0047	12.3691955	Err 0.1D-04	-
35:	10	8	2	9	8	1	S 1	12.3707456	-0.0057	12.3707399	Err 0.1D-04	-
36:	10	7	3	9	7	2	S 1	12.3730139	-0.0029	12.3730110	Err 0.1D-04	-
37:	10	6	4	9	6	3	S 1	12.3765427	-0.0032	12.3765395	Err 0.1D-04	-
38:	10	5	5	9	5	4	S 1	12.3825307	-0.0267	12.3825040	Err 0.1D-04	-
39:	10	4	7	9	4	6	S 1	12.3930332	0.0008	12.3930340	Err 0.1D-04	-
40:	10	4	6	9	4	5	S 1	12.3949143	-0.0009	12.3949133	Err 0.1D-04	-

41: 10 1 10 9 0 9 S 1 12.4086151 -0.0129 12.4086022 Err 0.1D-04 -
42: 10 3 7 9 3 6 S 1 12.4441494 0.0136 12.4441630 Err 0.1D-04 -
43: 10 1 9 9 1 8 S 1 12.6095494 -0.0146 12.6095348 Err 0.1D-04 -
44: 11 0 11 10 1 10 S 1 12.7537100 0.0021 12.7537120 Err 0.1D-04 -
45: 11 1 11 10 1 10 S 1 13.0619275 -0.0096 13.0619179 Err 0.1D-04 -
46: 11 0 11 10 0 10 S 1 13.1578229 -0.0084 13.1578145 Err 0.1D-04 -
47: 11 1 11 10 0 10 S 1 13.4660405 -0.0191 13.4660214 Err 0.1D-04 -
48: 11 2 10 10 2 9 S 2 13.5034183 -0.0243 13.5033940 Err 0.1D-04 -
49: 11 9 2 10 9 1 S 1 13.6074026 -0.0049 13.6073977 Err 0.1D-04 -
50: 11 10 2 10 10 0 S 1 13.6059295 -0.0093 13.6059201 Err 0.1D-04 -
51: 11 8 4 10 8 2 S 1 13.6094615 -0.0101 13.6094514 Err 0.1D-04 -
52: 11 7 4 10 7 3 S 1 13.6124775 0.0031 13.6124807 Err 0.1D-04 -
53: 11 6 5 10 6 4 S 1 13.6171745 0.0025 13.6171769 Err 0.1D-04 -
54: 11 5 6 10 5 5 S 1 13.6251762 -0.0409 13.6251352 Err 0.1D-04 -
55: 11 1 10 10 1 9 S 1 13.8325207 -0.0089 13.8325118 Err 0.1D-04 -
56: 12 0 12 11 1 11 S 1 14.0011743 -0.0050 14.0011693 Err 0.1D-04 -
57: 12 1 12 11 1 11 S 1 14.2324484 -0.0078 14.2324406 Err 0.1D-04 -
58: 12 0 12 11 0 11 S 1 14.3093919 -0.0090 14.3093829 Err 0.1D-04 -
59: 13 5 8 13 4 9 S 1 14.4618600 -0.0187 14.4618414 Err 0.1D-04 -
60: 14 5 10 14 4 11 S 1 14.4645417 0.0099 14.4645516 Err 0.1D-04 -
61: 13 5 8 13 4 9 S 4 14.4665750 -0.0011 14.4665739 Err 0.1D-04 -
62: 11 5 7 11 4 8 S 4 14.5195677 0.0028 14.5195705 Err 0.1D-04 -
63: 11 5 6 11 4 7 S 1 14.5168704 0.0049 14.5168752 Err 0.1D-04 -
64: 11 5 7 11 4 8 S 1 14.5237614 0.0032 14.5237646 Err 0.1D-04 -
65: 10 5 5 10 4 6 S 4 14.5362458 -0.0221 14.5362238 Err 0.1D-04 -
66: 10 5 6 10 4 7 S 1 14.5372717 0.0079 14.5372796 Err 0.1D-04 -
67: 10 5 5 10 4 6 S 1 14.5340259 0.0109 14.5340367 Err 0.1D-04 -
68: 12 1 12 11 0 11 S 1 14.5406660 -0.0049 14.5406610 Err 0.1D-04 -
69: 8 5 3 8 4 4 S 4 14.5562721 0.0210 14.5562931 Err 0.1D-04 -
70: 6 5 2 6 4 3 S 1 14.5651985 -0.0220 14.5651765 Err 0.1D-04 -
71: 12 11 1 11 11 0 S 1 14.8426549 -0.0104 14.8426445 Err 0.1D-04 -
72: 12 10 2 11 10 1 S 2 14.8440647 0.0024 14.8440671 Err 0.1D-04 -
73: 12 9 3 11 9 2 S 2 14.8459720 0.0019 14.8459739 Err 0.1D-04 -
74: 12 8 4 11 8 3 S 1 14.8486469 -0.0017 14.8486452 Err 0.1D-04 -
75: 12 7 5 11 7 4 S 1 14.8525603 -0.0000 14.8525603 Err 0.1D-04 -
76: 12 6 6 11 6 5 S 1 14.8586616 0.0005 14.8586620 Err 0.1D-04 -
77: 12 3 10 11 3 9 S 1 14.8823573 -0.0004 14.8823569 Err 0.1D-04 -
78: 12 1 11 11 1 10 S 1 15.0429082 -0.0193 15.0428889 Err 0.1D-04 -
79: 12 1 11 11 1 10 S 5 15.0428911 -0.0022 15.0428889 Err 0.1D-04 -
80: 13 0 13 12 1 12 S 2 15.2295154 -0.0123 15.2295031 Err 0.2D-04 -
81: 13 1 13 12 1 12 S 1 15.4006668 -0.0010 15.4006658 Err 0.1D-04 -
82: 13 0 13 12 0 12 S 1 15.4607813 -0.0049 15.4607764 Err 0.1D-04 -
83: 10 2 9 9 1 8 S 5 15.5388214 0.0710 15.5388924 Err 0.2D-04 -

84: 13 1 13 12 0 12 S 1 15.6319408 0.0031 15.6319439 Err 0.1D-04 -
85: 13 12 1 12 12 0 S 1 16.0793690 -0.0106 16.0793584 Err 0.1D-04 -
86: 13 11 2 12 11 1 S 1 16.0807401 -0.0042 16.0807360 Err 0.1D-04 -
87: 13 10 3 12 10 2 S 1 16.0825342 -0.0056 16.0825286 Err 0.1D-04 -
88: 13 9 4 12 9 3 S 1 16.0849549 -0.0011 16.0849537 Err 0.1D-04 -
89: 13 8 5 12 8 4 S 1 16.0883449 -0.0059 16.0883389 Err 0.1D-04 -
90: 13 7 6 12 7 5 S 1 16.0933195 -0.0052 16.0933143 Err 0.1D-04 -
91: 13 6 7 12 6 6 S 1 16.1010857 -0.0136 16.1010721 Err 0.1D-04 -
92: 13 5 9 12 5 8 S 1 16.1140576 0.0113 16.1140689 Err 0.1D-04 -
93: 13 5 8 12 5 7 S 1 16.1144999 0.0091 16.1145090 Err 0.1D-04 -
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97: 13 3 10 12 3 9 S 1 16.2786496 -0.0515 16.2785981 Err 0.1D-04 -
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104: 14 10 4 13 10 3 S 1 17.3213484 -0.0054 17.3213430 Err 0.1D-04 -
105: 14 9 6 13 9 4 S 1 17.3243674 -0.0036 17.3243638 Err 0.1D-04 -
106: 14 8 6 13 8 5 S 1 17.3285987 0.0375 17.3286362 Err 0.1D-04 -
107: 14 8 6 13 8 5 S 2 17.3285907 0.0033 17.3285940 Err 0.1D-04 -
108: 14 7 7 13 7 6 S 1 17.3348132 0.0060 17.3348192 Err 0.1D-04 -
109: 14 6 8 13 6 7 S 1 17.3445308 -0.0071 17.3445237 Err 0.1D-04 -
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116: 5 4 1 4 3 2 S 1 17.5155577 -0.0500 17.5155077 Err 0.1D-04 -
117: 15 0 15 14 1 14 S 1 17.6408638 0.0041 17.6408679 Err 0.1D-04 -
118: 15 6 10 15 5 11 S 1 17.7230717 -0.0173 17.7230544 Err 0.1D-04 -
119: 15 6 9 15 5 10 S 4 17.7219842 -0.0051 17.7219791 Err 0.1D-04 -
120: 15 6 10 15 5 11 S 3 17.7214320 0.0554 17.7214875 Err 0.1D-04 -
121: 15 6 9 15 5 10 S 1 17.7198197 -0.0211 17.7197986 Err 0.1D-04 -
122: 15 1 15 14 1 14 S 2 17.7315474 0.0000 17.7315475 Err 0.1D-04 -
123: 14 2 12 13 2 11 S 1 17.7824574 0.0318 17.7824892 Err 0.1D-04 -
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125: 8 3 5 7 2 5 S 1 17.7983092 0.0104 17.7983196 Err 0.1D-04 -
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127: 15 1 15 14 0 14 S 1 17.8567553 0.0098 17.8567651 Err 0.1D-04 -
128: 16 1 15 15 2 14 S 1 18.4055741 -0.0082 18.4055659 Err 0.1D-04 -
129: 15 11 4 14 11 3 S 1 18.5577953 -0.0133 18.5577820 Err 0.1D-04 -
130: 15 10 6 14 10 4 S 1 18.5605398 -0.0182 18.5605216 Err 0.1D-04 -
131: 15 9 6 14 9 5 S 1 18.5642492 -0.0072 18.5642421 Err 0.1D-04 -
132: 15 8 7 14 8 6 S 1 18.5694521 -0.0015 18.5694506 Err 0.1D-04 -
133: 15 7 8 14 7 7 S 1 18.5771000 -0.0020 18.5770979 Err 0.1D-04 -
134: 15 6 9 14 6 8 S 1 18.5890848 -0.0259 18.5890588 Err 0.1D-04 -
135: 15 3 13 14 3 12 S 1 18.5931185 -0.0321 18.5930864 Err 0.1D-04 -
136: 15 5 10 14 5 9 S 1 18.6103414 -0.0294 18.6103120 Err 0.1D-04 -
137: 15 5 10 14 5 9 S 4 18.6096480 0.0341 18.6096821 Err 0.1D-04 -
138: 15 5 11 14 5 10 S 1 18.6086833 -0.0181 18.6086652 Err 0.1D-04 -
139: 15 4 12 14 4 11 S 1 18.6336177 -0.0079 18.6336098 Err 0.1D-04 -
140: 6 4 3 5 3 3 S 3 18.7508545 0.0406 18.7508951 Err 0.1D-04 -
141: 16 1 16 15 1 15 S 1 18.8948590 0.0094 18.8948685 Err 0.1D-04 -
142: 16 1 16 15 0 15 S 4 18.9855331 0.0180 18.9855511 Err 0.1D-04 -
143: 6 2 5 6 1 6 S 1 5.6804136 -0.0273 5.6803863 Err 0.2D-04 -
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153: 5 3 3 4 3 2 S 1 6.1883035 -0.0063 6.1882972 Err 0.1D-04 -
154: 5 3 2 4 3 1 S 1 6.1895679 -0.0015 6.1895663 Err 0.1D-04 -
155: 5 3 2 4 3 1 S 4 6.1890132 0.0369 6.1890502 Err 0.1D-04 -
156: 5 3 3 4 3 2 S 4 6.1888521 -0.0335 6.1888186 Err 0.1D-04 -
157: 6 0 6 5 1 5 S 1 6.2036950 -0.0000 6.2036949 Err 0.1D-04 -
158: 5 2 3 4 2 2 S 1 6.2269084 0.0110 6.2269194 Err 0.1D-04 -
159: 5 2 3 4 2 2 S 4 6.2268080 0.0075 6.2268155 Err 0.1D-04 -
160: 5 2 3 4 2 2 S 2 6.2267316 -0.0081 6.2267235 Err 0.1D-04 -
161: 5 2 3 4 2 2 S 5 6.2266313 0.0035 6.2266348 Err 0.1D-04 -
162: 8 2 7 8 1 8 S 1 6.2802542 -0.0359 6.2802183 Err 0.2D-04 -
163: 8 2 7 8 1 8 S 2 6.2800967 -0.0656 6.2800311 Err 0.2D-04 -
164: 8 2 7 8 1 8 S 4 6.2800758 -0.0699 6.2800059 Err 0.2D-04 -
165: 15 3 12 15 2 13 S 1 6.3107240 0.0004 6.3107244 Err 0.2D-04 -
166: 15 3 12 15 2 13 S 2 6.3105542 -0.0526 6.3105016 Err 0.2D-04 -
167: 5 1 4 4 1 3 S 1 6.3586352 -0.0123 6.3586230 Err 0.1D-04 -
168: 14 3 11 14 2 12 S 3 6.4781512 0.0116 6.4781628 Err 0.3D-04 -
169: 9 2 8 9 1 9 S 1 6.6421207 -0.0454 6.6420754 Err 0.2D-04 -

170: 13 3 10 13 2 11 S 2 6.6854676 0.0384 6.6855060 Err 0.2D-04 -
171: 12 3 9 12 2 10 S 2 6.9151985 0.0512 6.9152497 Err 0.2D-04 -
172: 10 2 9 10 1 10 S 1 7.0444391 -0.0554 7.0443837 Err 0.2D-04 -
173: 11 3 8 11 2 9 S 2 7.1497688 0.0044 7.1497731 Err 0.1D-04 -
174: 6 1 6 5 1 5 S 2 7.1654497 -0.0135 7.1654361 Err 0.1D-04 -
175: 18 10 9 19 9 11 S 5 7.1946793 -0.0044 7.1946749 Err 0.1D-04 -
176: 18 10 8 19 9 10 S 2 7.1987662 0.0344 7.1988006 Err 0.1D-04 -
177: 5 1 5 4 0 4 S 1 7.2463800 -0.0184 7.2463617 Err 0.1D-04 -
178: 2 2 1 1 1 0 S 1 7.2912701 -0.0090 7.2912611 Err 0.1D-04 -
179: 9 1 8 8 2 6 S 1 7.2950968 0.0103 7.2951071 Err 0.1D-04 -
180: 6 0 6 5 0 5 S 1 7.3238765 -0.0038 7.3238727 Err 0.1D-04 -
181: 6 5 1 5 5 0 S 2 7.4222711 0.0032 7.4222743 Err 0.1D-04 -
182: 6 4 2 5 4 1 S 1 7.4247516 -0.0233 7.4247283 Err 0.1D-04 -
183: 6 3 4 5 3 3 S 1 7.4287998 -0.0033 7.4287964 Err 0.1D-04 -
184: 6 2 4 5 2 3 S 1 7.4948350 -0.0064 7.4948285 Err 0.1D-04 -
185: 14 1 13 14 0 14 S 1 7.5164091 -0.0279 7.5163811 Err 0.1D-04 -
186: 7 0 7 6 1 6 S 1 7.5474373 0.0004 7.5474377 Err 0.1D-04 -
187: 6 1 5 5 1 4 S 1 7.6219279 -0.0158 7.6219121 Err 0.1D-04 -
188: 6 1 6 5 0 5 S 1 8.2856319 -0.0214 8.2856105 Err 0.1D-04 -
189: 15 1 14 15 0 15 S 1 8.3437388 -0.0668 8.3436719 Err 0.2D-04 -
190: 7 1 7 6 1 6 S 2 8.3511052 -0.0074 8.3510978 Err 0.1D-04 -
191: 7 0 7 6 0 6 S 1 8.5091926 -0.0004 8.5091922 Err 0.1D-04 -
192: 10 1 9 9 2 7 S 1 8.5548649 -0.0215 8.5548434 Err 0.1D-04 -
193: 7 2 6 6 2 5 S 1 8.6302852 -0.0080 8.6302772 Err 0.1D-04 -
194: 7 6 1 6 6 0 S 1 8.6589846 -0.0081 8.6589765 Err 0.1D-04 -
195: 7 5 2 6 5 1 S 1 8.6610322 -0.0044 8.6610278 Err 0.1D-04 -
196: 7 2 5 6 2 4 S 1 8.7723607 0.0050 8.7723657 Err 0.1D-04 -
197: 8 0 8 7 1 7 S 1 8.8792737 0.0011 8.8792748 Err 0.1D-04 -
198: 7 1 6 6 1 5 S 1 8.8800585 -0.0035 8.8800550 Err 0.1D-04 -
199: 8 1 8 7 1 7 S 2 9.5335285 -0.0030 9.5335256 Err 0.1D-04 -
200: 8 1 8 7 1 7 S 4 9.5335262 -0.0006 9.5335256 Err 0.1D-04 -
201: 8 0 8 7 0 7 S 3 9.6829398 -0.0059 9.6829339 Err 0.1D-04 -
202: 8 0 8 7 0 7 S 2 9.6829372 0.0007 9.6829379 Err 0.1D-04 -
203: 8 0 8 7 0 7 S 4 9.6829342 0.0037 9.6829379 Err 0.1D-04 -
204: 8 2 7 7 2 6 S 5 9.8542097 -0.0410 9.8541687 Err 0.1D-04 -
205: 8 2 7 7 2 6 S 2 9.8542036 -0.0349 9.8541687 Err 0.1D-04 -
206: 8 2 7 7 2 6 S 4 9.8541946 -0.0259 9.8541687 Err 0.1D-04 -
207: 8 2 7 7 2 6 S 3 9.8541908 -0.0222 9.8541687 Err 0.1D-04 -
208: 8 7 1 7 7 0 S 2 9.8957128 -0.0064 9.8957064 Err 0.1D-04 -
209: 8 7 2 7 7 1 S 5 9.8957133 -0.0069 9.8957064 Err 0.1D-04 -
210: 8 7 1 7 7 0 S 3 9.8957141 -0.0077 9.8957064 Err 0.1D-04 -
211: 8 7 1 7 7 0 S 4 9.8957111 -0.0047 9.8957064 Err 0.1D-04 -
212: 8 7 1 7 7 0 S 5 9.8957102 -0.0038 9.8957064 Err 0.1D-04 -

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215:	8	6	2	7	6	1	S 4	9.8975204	-0.0040	9.8975164	Err 0.1D-04	-	
216:	8	6	2	7	6	1	S 5	9.8975194	-0.0030	9.8975164	Err 0.1D-04	-	
217:	8	5	3	7	5	2	S 5	9.9005723	-0.0013	9.9005711	Err 0.1D-04	-	
218:	8	5	3	7	5	2	S 4	9.9005738	-0.0027	9.9005711	Err 0.1D-04	-	
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220:	8	5	3	7	5	2	S 2	9.9005752	-0.0041	9.9005711	Err 0.1D-04	-	
221:	8	4	4	7	4	3	S 4	9.9064125	0.0090	9.9064215	Err 0.1D-04	-	
222:	8	4	5	7	4	4	S 5	9.9064120	0.0095	9.9064215	Err 0.1D-04	-	
223:	8	4	4	7	4	3	S 5	9.9064074	0.0141	9.9064215	Err 0.1D-04	-	
224:	8	4	5	7	4	4	S 4	9.9064069	0.0146	9.9064215	Err 0.1D-04	-	
225:	8	4	5	7	4	4	S 3	9.9063953	0.0262	9.9064215	Err 0.1D-04	-	
226:	8	2	6	7	2	5	S 3	10.0581879	0.0148	10.0582027	Err 0.1D-04	-	
227:	8	2	6	7	2	5	S 4	10.0581799	0.0228	10.0582027	Err 0.1D-04	-	
228:	8	2	6	7	2	5	S 2	10.0581749	0.0278	10.0582027	Err 0.1D-04	-	
229:	8	2	6	7	2	5	S 5	10.0581648	0.0379	10.0582027	Err 0.1D-04	-	
230:	8	1	7	7	1	6	S 2	10.1317070	0.0132	10.1317202	Err 0.1D-04	-	
231:	8	1	7	7	1	6	S 3	10.1317102	0.0103	10.1317205	Err 0.1D-04	-	
232:	8	1	7	7	1	6	S 5	10.1317041	0.0165	10.1317205	Err 0.1D-04	-	
233:	9	0	9	8	1	8	S 4	10.1929080	-0.0373	10.1928707	Err 0.1D-04	-	
234:	9	0	9	8	1	8	S 2	10.1929048	-0.0341	10.1928707	Err 0.1D-04	-	
235:	8	1	8	7	0	7	S 5	10.3371515	0.0205	10.3371720	Err 0.1D-04	-	
236:	8	1	8	7	0	7	S 4	10.3371524	0.0196	10.3371720	Err 0.1D-04	-	
237:	8	1	8	7	0	7	S 3	10.3371896	-0.0176	10.3371720	Err 0.1D-04	-	
238:	22	2	20	22	2	21	S 2	10.5156164	-0.0076	10.5156089	Err 0.1D-04	-	
239:	22	2	20	22	2	21	S 5	10.5156056	0.0032	10.5156089	Err 0.1D-04	-	
240:	22	2	20	22	2	21	S 3	10.5156493	-0.0403	10.5156090	Err 0.1D-04	-	
241:	22	2	20	22	2	21	S 4	10.5156097	-0.0007	10.5156090	Err 0.1D-04	-	
242:	5	2	4	4	1	3	S 3	10.6532832	0.0078	10.6532909	Err 0.2D-04	-	
243:	9	1	9	8	1	8	S 2	10.7127140	-0.0024	10.7127117	Err 0.1D-04	-	
244:	9	1	9	8	1	8	S 3	10.7127140	-0.0023	10.7127117	Err 0.1D-04	-	
245:	9	1	9	8	1	8	S 5	10.7127118	-0.0002	10.7127117	Err 0.1D-04	-	
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949: 13 1 12 13 0 13 S 1 6.7063148 0.0002 6.7063150 Err 0.1D-04 -
950: 7 3 4 7 2 5 S 1 7.8706514 0.0071 7.8706585 Err 0.1D-04 -
951: 8 3 6 8 2 7 S 1 8.2442093 0.0428 8.2442521 Err 0.1D-04 -
952: 10 5 6 10 4 6 S 4 14.5230151 -0.0506 14.5229645 Err 0.1D-04 -
Maximum (obs-calc)/err in line 891 0.0001145

RMS deviations (MHz), B and V sorted
B V n splittings MHz
B V n abs. freq. MHz
1 1 952 0.023708 0.024057

Parameters and Errors

BJ	0.617958959 { 0.000000108}	
BK	1.619216488 { 0.000000373}	
B-	0.038321111 { 0.000000070}	
DJ	0.023666E-6 { 0.000330E-6}	
DJK	0.059705E-6 { 0.001065E-6}	
DK	0.022450E-6 { 0.005620E-6}	
dj	-0.002777E-6 { 0.000089E-6}	
dk	0.001892E-6 { 0.000047E-6}	
\F12	-1.802391119 { derived}	
\F	159.841807616 { derived}	160.143850881 { derived}
V1n	17968.833217 { 118.743164}	14560.069841 { 23.998196}
\rho	0.012270601 { derived}	0.013566715 { derived}
\beta	0.166975867 { derived}	3.049912779 { derived}
\gamma	-2.434682496 { derived}	3.044967510 { derived}
epsil	3.910273646 { 0.190306177}	3.032286976 { 0.132408704}
delta	0.546101996 { 0.061725155}	2.837510643 { 0.026001067}

Standard Deviation 0.023897 MHz

---------- B = 1
Rotational Constants and Errors (in GHz)

B_z	2.237175446	0.000000383
B_x	0.656280069	0.000000129
B_y	0.579637848	0.000000130

Ray's kappa -0.90752

F0(calc)	158.000000000	0.000000000
I_alpha	3.198601709	0.000000000

```
 <(i,x)  <(i,y)  <(i,z)      111.9212      111.1649      31.2893
d<(i,x) d<(i,y) d<(i,z)       6.8818       6.2221       3.5366

 F0(calc)     158.000000000       0.000000000
 I_alpha        3.198601709       0.000000000
 <(i,x)  <(i,y)  <(i,z)      107.3153      88.1282     162.5774
d<(i,x) d<(i,y) d<(i,z)       1.5825       2.4238       1.4898

 V1n_1      7.170127 kj +/- 0.047382 kj        1.712513 kcal +/- 0.011317 kcal
        599.375675 cm +/-   3.9608 cm    s=  49.962824
 V1n_2      5.809924 kj +/- 0.009576 kj        1.387642 kcal +/- 0.002287 kcal
        485.671584 cm +/-   0.8005 cm    s=  40.484666

F(calc)       159.841807616
F(calc)       160.143850881Parent XIAM Output
```

$^{13}C_1$ Isotopologue XIAM Output

```
  J K- K+  J K- K+    Sym   calc/GHz  diff/MHz     obs/GHz
  1:  5  1  5  4  1  4   S 1   5.9645394   -0.0188   5.9645207   Err 0.1D-04          -
  2:  5  2  3  4  2  2   S 1   6.2207883    0.0194   6.2208077   Err 0.1D-04          -
  3:  6  1  6  5  1  5   S 1   7.1505706   -0.0154   7.1505552   Err 0.1D-04          -
  4:  7  0  7  6  1  6   S 1   7.5567767    0.0333   7.5568100   Err 0.1D-04          -
  5: 12  2 10 11  3  9   S 1   8.3798963   -0.0178   8.3798785   Err 0.1D-04          -
  6: 15  2 14 14  3 11   S 1   8.4341131    0.0086   8.4341217   Err 0.1D-04          -
  7:  7  2  5  6  2  4   S 1   8.7659218    0.0147   8.7659365   Err 0.1D-04          -
  8:  7  1  6  6  1  5   S 1   8.8710260    0.0073   8.8710332   Err 0.1D-04          -
  9:  8  3  6  7  3  5   S 1   9.9004218   -0.0019   9.9004199   Err 0.1D-04          -
 10:  8  2  6  7  2  5   S 1  10.0517656    0.0327  10.0517983   Err 0.1D-04          -
 11:  9  2  8  8  2  7   S 1  11.0572963   -0.0020  11.0572942   Err 0.1D-04          -
 12:  9  4  6  9  3  6   S 1  11.1039349    0.0050  11.1039399   Err 0.1D-04          -
 13:  9  5  4  8  5  3   S 1  11.1269197    0.0047  11.1269244   Err 0.1D-04          -
 14: 11  4  8 11  3  9   S 1  11.1557423    0.0018  11.1557441   Err 0.1D-04          -
 15:  9  1  8  8  1  7   S 1  11.3615264    0.0053  11.3615318   Err 0.1D-04          -
 16:  5  2  3  4  1  4   S 1  11.4554618   -0.0208  11.4554410   Err 0.1D-04          -
 17: 10  0 10  9  1  9   S 1  11.4790030   -0.0085  11.4789945   Err 0.1D-04          -
 18: 13  1 12 12  2 10   S 1  11.8455847    0.0060  11.8455907   Err 0.1D-04          -
 19: 10  5  6  9  5  5   S 1  12.3669740   -0.0062  12.3669678   Err 0.1D-04          -
 20: 10  1  9  9  1  8   S 1  12.5924806   -0.0191  12.5924615   Err 0.1D-04          -
 21: 12  0 12 11  1 11   S 1  13.9831009    0.0207  13.9831216   Err 0.1D-04          -
 22:  9  5  5  9  4  6   S 1  14.3653033   -0.0039  14.3652994   Err 0.1D-04          -
 23: 17  1 16 16  2 14   S 1  14.7787008   -0.0047  14.7786961   Err 0.1D-04          -
 24: 12 10  2 11 10  1   S 1  14.8247431    0.0639  14.8248070   Err 0.1D-04          -
```

```
 25: 12  7  5 11  7  4   S 1  14.8336371   -0.0076  14.8336295   Err 0.1D-04          -
 26: 12  6  6 11  6  5   S 1  14.8400313    0.0066  14.8400379   Err 0.1D-04          -
 27: 12  3 10 11  3  9   S 1  14.8635415   -0.0105  14.8635311   Err 0.1D-04          -
 28: 12  1 11 11  1 10   S 1  15.0176682   -0.0269  15.0176414   Err 0.1D-04          -
 29:  8  3  6  7  3  5   S 1   9.9004218    0.0011   9.9004229   Err 0.1D-04          -
 30:  9  0  9  8  0  8   S 1  10.8213743   -0.0488  10.8213256   Err 0.1D-04          -
Maximum (obs-calc)/err in line  24   0.0000639

 RMS deviations (MHz), B and V sorted
  B  V   n splittings MHz
  B  V   n abs. freq. MHz
  1  1  30         0.020782         0.023553

          Parameters  and  Errors
 BJ          0.617126411 { 0.000000637}
 BK           1.599069515 { 0.000001522}
 B-          0.038983904 { 0.000000204}
 DJ          0.021707E-6 { 0.002556E-6}
\F12         -1.784453966 {     derived}
\F          159.825510378 {     derived}  160.123820213 {     derived}
\rho          0.012158301 {     derived}    0.013440530 {     derived}
\beta         0.168322341 {     derived}    3.049075606 {     derived}
\gamma       -2.435830207 {     derived}    3.045190458 {     derived}

 Standard Deviation       0.022765 MHz

------------------------------------ B =  1
 Rotational Constants and Errors (in GHz)
     B_z       2.216195926       0.000001554
     B_x       0.656110315       0.000000526
     B_y       0.578142508       0.000000787
 Ray's kappa   -0.90480
 F0(calc)     158.000000000       0.000000000
 I_alpha        3.198601709       0.000000000
 <(i,x)  <(i,y)  <(i,z)      111.9212      111.1649       31.2893
d<(i,x) d<(i,y) d<(i,z)        0.0000        0.0000        0.0000

 F0(calc)     158.000000000       0.000000000
 I_alpha        3.198601709       0.000000000
 <(i,x)  <(i,y)  <(i,z)      107.3153       88.1282      162.5774
d<(i,x) d<(i,y) d<(i,z)        0.0000        0.0000        0.0000

 V1n_1      7.170127 kj +/- 0.000000 kj         1.712513 kcal +/- 0.000000 kcal
```

599.375675 cm +/- 0.0000 cm s= 49.967919
V1n_2 5.809924 kj +/- 0.000000 kj 1.387642 kcal +/- 0.000000 kcal
485.671584 cm +/- 0.0000 cm s= 40.488794

F(calc) 159.825510378
F(calc) 160.123820213

$^{13}C_2$ Isotopologue XIAM Output

	J K- K+	J K- K+	Sym	calc/GHz	diff/MHz	obs/GHz	
1:	5 0 5	4 0 4	S 1	6.1066376	0.0093	6.1066469	Err 0.1D-04 -
2:	6 1 6	5 1 5	S 1	7.1400422	-0.0119	7.1400303	Err 0.1D-04 -
3:	6 2 5	5 2 4	S 1	7.3823357	0.0020	7.3823377	Err 0.1D-04 -
4:	6 5 1	5 5 0	S 1	7.4023165	0.0109	7.4023274	Err 0.1D-04 -
5:	6 2 4	5 2 3	S 1	7.4783248	0.0052	7.4783300	Err 0.1D-04 -
6:	14 1 13	14 1 14	S 1	7.4868495	0.0075	7.4868571	Err 0.1D-04 -
7:	16 4 12	16 3 13	S 1	10.0496505	-0.0254	10.0496251	Err 0.1D-04 -
8:	22 5 18	21 6 15	S 1	10.0512320	0.0222	10.0512543	Err 0.1D-04 -
9:	8 1 7	7 1 6	S 1	10.1067481	0.0359	10.1067840	Err 0.1D-04 -
10:	16 2 15	16 0 16	S 1	10.2819436	-0.0145	10.2819291	Err 0.1D-04 -
11:	9 2 8	8 2 7	S 1	11.0416894	-0.0078	11.0416816	Err 0.1D-04 -
12:	9 6 3	8 6 2	S 1	11.1069221	-0.0088	11.1069134	Err 0.1D-04 -
13:	9 5 4	8 5 3	S 1	11.1114991	0.0047	11.1115038	Err 0.1D-04 -
14:	9 4 5	9 3 7	S 1	11.1495711	0.0164	11.1495875	Err 0.1D-04 -
15:	17 11 7	18 10 8	S 1	11.2877665	0.0191	11.2877856	Err 0.1D-04 -
16:	10 0 10	9 1 9	S 1	11.4629254	-0.0024	11.4629230	Err 0.1D-04 -
17:	10 1 10	9 1 9	S 1	11.8442708	-0.0245	11.8442463	Err 0.1D-04 -
18:	10 0 10	9 0 9	S 1	11.9570822	-0.0279	11.9570544	Err 0.1D-04 -
19:	10 7 3	9 7 2	S 1	12.3398913	0.0233	12.3399146	Err 0.1D-04 -
20:	10 5 5	9 5 4	S 1	12.3498927	0.0029	12.3498956	Err 0.1D-04 -
21:	10 4 7	9 4 6	S 1	12.3608700	-0.0170	12.3608530	Err 0.1D-04 -
22:	10 1 9	9 1 8	S 1	12.5751341	0.0418	12.5751758	Err 0.1D-04 -
23:	4 3 1	3 2 1	S 1	12.9086078	0.0411	12.9086489	Err 0.1D-04 -
24:	22 4 19	21 5 16	S 1	13.0464557	-0.0101	13.0464455	Err 0.1D-04 -
25:	20 2 19	19 3 17	S 1	13.0962620	-0.0186	13.0962434	Err 0.1D-04 -
26:	18 12 7	19 11 8	S 1	13.2499566	0.0056	13.2499622	Err 0.1D-04 -
27:	11 2 10	10 2 9	S 1	13.4616647	-0.0183	13.4616464	Err 0.1D-04 -
28:	21 2 20	21 1 21	S 1	13.5378266	-0.0022	13.5378244	Err 0.1D-04 -
29:	11 6 5	10 6 4	S 1	13.5810906	0.0251	13.5811157	Err 0.1D-04 -
30:	19 5 15	19 4 15	S 1	13.6253695	0.0010	13.6253705	Err 0.1D-04 -
31:	11 1 10	10 1 9	S 1	13.7924641	0.0058	13.7924699	Err 0.1D-04 -
32:	18 5 13	18 4 14	S 1	13.8338027	-0.0019	13.8338008	Err 0.1D-04 -
33:	16 1 15	15 2 13	S 1	14.1718717	0.0423	14.1719139	Err 0.1D-04 -
34:	12 1 12	11 0 11	S 1	14.4666514	0.0418	14.4666931	Err 0.1D-04 -

```
 35:  9  2  8  8  1  7   S 1  14.5029115   -0.0203  14.5028912   Err 0.1D-04          -
 36: 12  2 11 11  2 10   S 1  14.6648362   -0.0165  14.6648198   Err 0.1D-04          -
 37: 12  1 11 11  1 10   S 1  14.9965678   -0.0007  14.9965671   Err 0.1D-04          -
 38: 19  1 18 18  2 16   S 1  15.6275426    0.0054  15.6275480   Err 0.1D-04          -
 39: 13  8  5 12  8  4   S 1  16.0454735    0.0238  16.0454973   Err 0.1D-04          -
 40: 13  6  7 12  6  6   S 1  16.0588616    0.0106  16.0588722   Err 0.1D-04          -
 41: 10  2  8  9  1  8   S 1  16.6195515    0.0289  16.6195804   Err 0.1D-04          -
 42: 15  0 15 14  0 14   S 1  17.6942607   -0.0272  17.6942335   Err 0.1D-04          -
 43: 13  3 10 13  0 13   S 1  17.9805730   -0.0068  17.9805661   Err 0.1D-04          -
 44: 16  4 12 15  5 11   S 1   5.7449991   -0.0108   5.7449883   Err 0.1D-04          -
 45:  5  1  5  4  1  4   S 1   5.9557795    0.0080   5.9557874   Err 0.1D-04          -
 46:  4  1  4  3  0  3   S 1   6.1440182   -0.0238   6.1439944   Err 0.1D-04          -
 47:  6  4  2  5  4  1   S 1   7.4049205   -0.0096   7.4049109   Err 0.1D-04          -
 48: 22  3 19 22  2 20   S 1   7.4585188    0.0189   7.4585377   Err 0.1D-04          -
 49: 15  1 14 15  0 15   S 1   8.4329780    0.0065   8.4329845   Err 0.1D-04          -
 50:  7  5  2  6  5  1   S 1   8.6378362    0.0162   8.6378524   Err 0.1D-04          -
 51:  7  1  6  6  1  5   S 1   8.8590592    0.0417   8.8591009   Err 0.1D-04          -
 52: 18  4 15 18  3 15   S 1   9.0802619   -0.0038   9.0802581   Err 0.1D-04          -
 53: 19  4 16 18  5 13   S 1   9.3900097    0.0011   9.3900108   Err 0.1D-04          -
 54: 22  2 21 21  3 18   S 1   9.7417036    0.0105   9.7417141   Err 0.1D-04          -
 55:  9  0  9  8  0  8   S 1  10.8052997   -0.0306  10.8052690   Err 0.1D-04          -
 56: 13  4 10 13  3 11   S 1  11.1598747   -0.0290  11.1598457   Err 0.1D-04          -
 57:  5  4  1  5  3  2   S 1  11.1693262   -0.0360  11.1692902   Err 0.1D-04          -
 58:  4  4  1  4  3  2   S 1  11.1739505    0.0043  11.1739548   Err 0.1D-04          -
 59: 10  9  1  9  9  0   S 1  12.3358815   -0.0152  12.3358663   Err 0.1D-04          -
 60: 10  2  8  9  2  7   S 1  12.6199499    0.0184  12.6199683   Err 0.1D-04          -
 61: 11  1 11 10  1 10   S 1  13.0124463   -0.0214  13.0124250   Err 0.1D-04          -
 62: 12  1 12 11  1 11   S 1  14.1779601   -0.0300  14.1779300   Err 0.1D-04          -
 63: 13  2 12 12  2 11   S 1  15.8632150   -0.0387  15.8631763   Err 0.1D-04          -
 64:  7  3  4  6  2  5   S 1  16.6979159   -0.0149  16.6979010   Err 0.1D-04          -
Maximum (obs-calc)/err in line  33   0.0000423

RMS deviations (MHz), B and V sorted
 B  V   n splittings MHz
 B  V   n abs. freq. MHz
 1  1  64         0.020702         0.022643

         Parameters  and  Errors
BJ          0.616266826 { 0.000000281}
BK          1.596967844 { 0.000000957}
B-          0.039010695 { 0.000000121}
DJ          0.021427E-6 { 0.000557E-6}
DJK         0.058689E-6 { 0.004203E-6}
```

```
 dj          -0.003032E-6 { 0.000153E-6}
\F12          -1.757142738 {     derived}
\F          159.801035705 {     derived}  160.115027576 {     derived}
\rho          0.012044505 {     derived}    0.013400166 {     derived}
\beta         0.173528823 {     derived}    3.047114457 {     derived}
\gamma       -2.425323318 {     derived}    3.076748203 {     derived}

 Standard Deviation       0.021937 MHz

------------------------------------ B =  1
 Rotational Constants and Errors (in GHz)
     B_z       2.213234669       0.000001043
     B_x       0.655277520       0.000000322
     B_y       0.577256131       0.000000289
 Ray's kappa   -0.90462
 F0(calc)     158.000000000       0.000000000
 I_alpha        3.198601709       0.000000000
 <(i,x)  <(i,y)  <(i,z)      112.2228      111.9455       32.1209
d<(i,x) d<(i,y) d<(i,z)        0.0000        0.0000        0.0000

 F0(calc)     158.000000000       0.000000000
 I_alpha        3.198601709       0.000000000
 <(i,x)  <(i,y)  <(i,z)      107.7081       88.7153      162.2422
d<(i,x) d<(i,y) d<(i,z)        0.0000        0.0000        0.0000

 V1n_1      7.155838 kj +/- 0.000000 kj         1.709100 kcal +/- 0.000000 kcal
         598.181169 cm +/-   0.0000 cm    s=  49.875974
 V1n_2      5.808392 kj +/- 0.000000 kj         1.387277 kcal +/- 0.000000 kcal
         485.543541 cm +/-   0.0000 cm    s=  40.484319

F(calc)       159.801035705
F(calc)       160.115027576
```

$^{13}C_3$ Isotopologue XIAM Output

```
J K- K+  J K- K+    Sym   calc/GHz  diff/MHz     obs/GHz
  1:  5  1  5  4  1  4   S 4   5.9496159   -0.0001   5.9496158   Err 0.1D-04          -
  2:  5  1  5  4  1  4   S 2   5.9496189   -0.0031   5.9496158   Err 0.1D-04          -
  3:  5  1  5  4  1  4   S 3   5.9496156    0.0002   5.9496158   Err 0.1D-04          -
  4: 13  3 11 13  2 11   S 1   6.2669417   -0.0238   6.2669179   Err 0.1D-04          -
  5: 13  3 11 13  2 11   S 3   6.2668928    0.0251   6.2669179   Err 0.1D-04          -
  6: 13  3 11 13  2 11   S 2   6.2666230   -0.0347   6.2665883   Err 0.1D-04          -
  7: 13  3 11 13  2 11   S 4   6.2666076   -0.0193   6.2665883   Err 0.1D-04          -
  8:  8  2  7  8  1  8   S 1   6.2719021   -0.0261   6.2718760   Err 0.1D-04          -
```

```
 9:  8  2  7  8  1  8   S 3   6.2718732    0.0027   6.2718760   Err 0.1D-04          -
10:  8  2  7  8  1  8   S 2   6.2717438    0.0207   6.2717645   Err 0.1D-04          -
11: 14  1 13 14  1 14   S 1   7.3510051   -0.0441   7.3509611   Err 0.2D-04          -
12: 14  1 13 14  1 14   S 3   7.3509854   -0.0243   7.3509611   Err 0.2D-04          -
13: 14  1 13 14  1 14   S 2   7.3509735   -0.0125   7.3509611   Err 0.2D-04          -
14: 14  1 13 14  1 14   S 4   7.3509538    0.0081   7.3509619   Err 0.2D-04          -
15: 14  1 13 14  1 14   S 5   7.3509538    0.0081   7.3509619   Err 0.2D-04          -
16:  6  3  4  5  3  3   S 1   7.3944823    0.0158   7.3944981   Err 0.1D-04          -
17:  7  1  7  6  1  6   S 5   8.3133936    0.0137   8.3134073   Err 0.1D-04          -
18:  7  1  7  6  1  6   S 4   8.3133931    0.0142   8.3134073   Err 0.1D-04          -
19:  7  1  7  6  1  6   S 3   8.3133936    0.0137   8.3134073   Err 0.1D-04          -
20:  7  1  7  6  1  6   S 2   8.3133966    0.0107   8.3134073   Err 0.1D-04          -
21:  7  1  7  6  1  6   S 1   8.3133969    0.0104   8.3134073   Err 0.1D-04          -
22:  7  0  7  6  0  6   S 3   8.4710920   -0.0266   8.4710654   Err 0.1D-04          -
23:  7  0  7  6  0  6   S 1   8.4710961   -0.0301   8.4710661   Err 0.1D-04          -
24:  7  0  7  6  0  6   S 2   8.4710926   -0.0265   8.4710661   Err 0.1D-04          -
25:  7  0  7  6  0  6   S 4   8.4710885   -0.0225   8.4710661   Err 0.1D-04          -
26:  7  5  2  6  5  1   S 5   8.6210565   -0.0001   8.6210564   Err 0.1D-04          -
27:  7  5  2  6  5  1   S 4   8.6210578   -0.0014   8.6210564   Err 0.1D-04          -
28:  7  5  2  6  5  1   S 3   8.6210578   -0.0014   8.6210564   Err 0.1D-04          -
29:  7  5  2  6  5  1   S 2   8.6210607   -0.0043   8.6210564   Err 0.1D-04          -
30:  7  5  2  6  5  1   S 1   8.6210625   -0.0061   8.6210564   Err 0.1D-04          -
31:  3  2  1  2  1  2   S 1   8.6770874   -0.0320   8.6770554   Err 0.1D-04          -
32: 16  3 13 15  4 12   S 1   9.6398507   -0.0349   9.6398158   Err 0.1D-04          -
33:  9  0  9  8  1  8   S 1  10.1405781   -0.0402  10.1405379   Err 0.1D-04          -
34:  8  1  8  7  0  7   S 1  10.2982840    0.0284  10.2983123   Err 0.1D-04          -
35:  9  0  9  8  0  8   S 2  10.7990281   -0.0089  10.7990193   Err 0.1D-04          -
36:  9  0  9  8  0  8   S 1  10.7990338   -0.0145  10.7990193   Err 0.1D-04          -
37:  9  0  9  8  0  8   S 3  10.7990283   -0.0091  10.7990193   Err 0.1D-04          -
38:  9  0  9  8  0  8   S 5  10.7990227   -0.0034  10.7990193   Err 0.1D-04          -
39: 16  3 13 16  2 15   S 1  11.0744467   -0.0102  11.0744365   Err 0.1D-04          -
40:  8  4  4  8  3  5   S 1  11.2874221   -0.0210  11.2874011   Err 0.1D-04          -
41:  9  2  7  8  2  6   S 1  11.2961277    0.0426  11.2961703   Err 0.1D-04          -
42: 10  4  7 10  3  8   S 1  11.3015787   -0.0454  11.3015333   Err 0.1D-04          -
43:  7  4  4  7  3  4   S 1  11.3079831   -0.0203  11.3079628   Err 0.1D-04          -
44:  9  4  5  9  3  7   S 1  11.3085470    0.0248  11.3085718   Err 0.1D-04          -
45:  9  4  5  9  3  7   S 5  11.3172702   -0.0186  11.3172516   Err 0.1D-04          -
46:  9  1  9  8  0  8   S 1  11.3229748    0.0429  11.3230177   Err 0.1D-04          -
47:  5  4  2  5  3  2   S 3  11.3254691    0.0112  11.3254803   Err 0.1D-04          -
48:  6  4  3  6  3  4   S 1  11.3257355   -0.0443  11.3256912   Err 0.1D-04          -
49:  5  4  1  5  3  2   S 4  11.3298200    0.0181  11.3298381   Err 0.1D-04          -
50:  4  4  1  4  3  2   S 4  11.3305356   -0.0271  11.3305085   Err 0.1D-04          -
51: 14  4 11 14  3 12   S 2  11.3356637    0.0215  11.3356852   Err 0.1D-04          -
```

52: 14 4 11 14 3 12 S 4 11.3360564 0.0120 11.3360684 Err 0.1D-04 -
53: 15 4 12 15 3 13 S 2 11.3755696 -0.0008 11.3755689 Err 0.1D-04 -
54: 18 2 17 18 0 18 S 1 11.4652969 0.0095 11.4653064 Err 0.1D-04 -
55: 20 3 18 20 2 19 S 1 11.4892729 -0.0229 11.4892500 Err 0.1D-04 -
56: 6 2 5 5 1 4 S 1 11.6685570 0.0247 11.6685817 Err 0.1D-04 -
57: 10 0 10 9 0 9 S 1 11.9513967 -0.0066 11.9513902 Err 0.1D-04 -
58: 10 3 7 9 3 6 S 5 12.3856321 0.0183 12.3856504 Err 0.1D-04 -
59: 7 2 6 6 1 5 S 1 12.6726696 -0.0071 12.6726625 Err 0.1D-04 -
60: 7 2 6 6 1 5 S 3 12.6726385 0.0240 12.6726625 Err 0.1D-04 -
61: 7 2 6 6 1 5 S 2 12.6724924 0.0165 12.6725089 Err 0.1D-04 -
62: 7 2 6 6 1 5 S 4 12.6724817 0.0272 12.6725089 Err 0.1D-04 -
63: 22 4 19 21 5 17 S 1 12.8998196 -0.0049 12.8998147 Err 0.1D-04 -
64: 16 11 6 17 10 8 S 4 13.0438453 0.0093 13.0438546 Err 0.1D-04 -
65: 12 1 12 11 1 11 S 1 14.1687185 0.0283 14.1687468 Err 0.2D-04 -
66: 12 1 12 11 1 11 S 3 14.1687136 0.0332 14.1687468 Err 0.2D-04 -
67: 12 1 12 11 1 11 S 5 14.1687111 0.0357 14.1687468 Err 0.2D-04 -
68: 12 1 12 11 1 11 S 4 14.1687108 0.0360 14.1687468 Err 0.2D-04 -
69: 17 5 13 17 4 13 S 3 14.1910072 0.0099 14.1910171 Err 0.1D-04 -
70: 17 5 13 17 4 13 S 1 14.1915414 -0.0099 14.1915315 Err 0.1D-04 -
71: 12 0 12 11 0 11 S 1 14.2461431 -0.0022 14.2461409 Err 0.1D-04 -
72: 12 0 12 11 0 11 S 2 14.2461362 0.0047 14.2461409 Err 0.1D-04 -
73: 12 0 12 11 0 11 S 3 14.2461354 0.0055 14.2461409 Err 0.1D-04 -
74: 12 0 12 11 0 11 S 5 14.2461284 0.0125 14.2461409 Err 0.1D-04 -
75: 5 3 3 4 2 3 S 5 14.2609283 -0.0396 14.2608887 Err 0.1D-04 -
76: 5 3 3 4 2 3 S 3 14.2658602 -0.0084 14.2658518 Err 0.1D-04 -
77: 15 11 5 16 10 7 S 4 14.2814617 -0.0346 14.2814271 Err 0.1D-04 -
78: 20 5 16 20 4 17 S 4 14.3392184 0.0232 14.3392416 Err 0.1D-04 -
79: 22 5 18 22 4 19 S 5 14.3568305 0.0216 14.3568521 Err 0.1D-04 -
80: 22 5 18 22 4 19 S 2 14.3572006 -0.0186 14.3571819 Err 0.1D-04 -
81: 19 5 14 19 4 16 S 2 14.3856521 0.0140 14.3856661 Err 0.1D-04 -
82: 19 5 14 19 4 16 S 5 14.3867818 -0.0181 14.3867637 Err 0.1D-04 -
83: 15 5 10 15 4 12 S 5 14.4574314 0.0068 14.4574382 Err 0.1D-04 -
84: 13 5 9 13 4 9 S 2 14.4551066 0.0098 14.4551164 Err 0.1D-04 -
85: 13 5 8 13 4 9 S 3 14.4683385 -0.0179 14.4683206 Err 0.1D-04 -
86: 22 5 17 22 4 19 S 4 14.4927527 -0.0110 14.4927417 Err 0.1D-04 -
87: 12 5 7 12 4 9 S 4 14.5191062 -0.0006 14.5191055 Err 0.1D-04 -
88: 11 5 7 11 4 7 S 1 14.5206472 0.0321 14.5206793 Err 0.1D-04 -
89: 10 5 5 10 4 6 S 2 14.5404737 0.0108 14.5404845 Err 0.1D-04 -
90: 9 5 5 9 4 5 S 3 14.5462799 0.0008 14.5462807 Err 0.1D-04 -
91: 8 5 4 8 4 5 S 4 14.5570033 -0.0401 14.5569631 Err 0.1D-04 -
92: 8 5 4 8 4 5 S 2 14.5566216 -0.0047 14.5566169 Err 0.1D-04 -
93: 8 5 4 8 4 5 S 5 14.5560862 0.0402 14.5561264 Err 0.1D-04 -
94: 8 5 3 8 4 4 S 2 14.5601711 0.0179 14.5601890 Err 0.1D-04 -

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 95:  7  5  2  7  4  3   S 4  14.5653986   -0.0364  14.5653622   Err 0.1D-04          -
 96:  7  5  2  7  4  3   S 5  14.5663121    0.0095  14.5663216   Err 0.1D-04          -
 97:  6  5  2  6  4  3   S 3  14.5678880   -0.0379  14.5678501   Err 0.1D-04          -
 98:  5  5  1  5  4  2   S 5  14.5681282   -0.0040  14.5681242   Err 0.1D-04          -
 99:  9  2  8  8  1  7   S 1  14.5816739    0.0262  14.5817000   Err 0.1D-04          -
100: 20 13  8 21 12 10   S 5  14.5844121   -0.0111  14.5844010   Err 0.1D-04          -
101: 19  3 16 18  4 15   S 3  14.6294167    0.0191  14.6294358   Err 0.1D-04          -
102:  9  1  8  8  0  8   S 1  14.6959740    0.0016  14.6959756   Err 0.1D-04          -
103:  9  1  8  8  0  8   S 3  14.6959599    0.0157  14.6959756   Err 0.1D-04          -
104:  9  1  8  8  0  8   S 2  14.6959345    0.0411  14.6959756   Err 0.1D-04          -
105: 12 10  3 13  9  5   S 4  14.7461531    0.0159  14.7461689   Err 0.1D-04          -
106: 12 10  3 13  9  5   S 3  14.7478363    0.0209  14.7478572   Err 0.1D-04          -
107: 12 10  2 13  9  4   S 1  14.7484413    0.0276  14.7484689   Err 0.1D-04          -
108: 12  8  5 11  8  3   S 1  14.7801664   -0.0237  14.7801426   Err 0.1D-04          -
109: 12  8  5 11  8  4   S 2  14.7801685   -0.0274  14.7801411   Err 0.1D-04          -
110: 12  8  5 11  8  4   S 3  14.7801614   -0.0187  14.7801427   Err 0.1D-04          -
111: 13  0 13 12  0 12   S 1  15.3923929   -0.0215  15.3923714   Err 0.1D-04          -
112: 13  0 13 12  0 12   S 3  15.3923842   -0.0128  15.3923714   Err 0.1D-04          -
113: 13  0 13 12  0 12   S 4  15.3923775   -0.0061  15.3923714   Err 0.1D-04          -
114: 10  3  7 10  0 10   S 2  15.9674963    0.0148  15.9675111   Err 0.1D-04          -
115: 10  3  7 10  0 10   S 3  15.9675376   -0.0265  15.9675111   Err 0.1D-04          -
116: 13  7  6 12  7  5   S 1  16.0190607   -0.0107  16.0190500   Err 0.1D-04          -
117: 13  7  6 12  7  5   S 2  16.0190580   -0.0080  16.0190500   Err 0.1D-04          -
118: 13  7  6 12  7  5   S 3  16.0190527   -0.0027  16.0190500   Err 0.1D-04          -
119: 13  7  6 12  7  5   S 4  16.0190529   -0.0029  16.0190500   Err 0.1D-04          -
120: 13  7  6 12  7  5   S 5  16.0190500    0.0000  16.0190500   Err 0.1D-04          -
121: 13  4  9 12  4  8   S 5  16.0694531    0.0453  16.0694984   Err 0.1D-04          -
122: 19  6 13 19  5 14   S 2  17.5853099    0.0044  17.5853143   Err 0.1D-04          -
123: 19  6 13 19  5 14   S 5  17.5867726    0.0225  17.5867951   Err 0.1D-04          -
124: 18  6 13 18  5 14   S 1  17.6457037   -0.0149  17.6456888   Err 0.1D-04          -
125: 15  6 10 15  5 10   S 3  17.7208481   -0.0094  17.7208387   Err 0.1D-04          -
126:  8  6  3  8  5  4   S 2  17.8019834    0.0086  17.8019920   Err 0.1D-04          -
127:  8  6  3  8  5  4   S 4  17.8023444    0.0251  17.8023695   Err 0.1D-04          -
128:  8  6  2  8  5  3   S 1  17.8042517   -0.0245  17.8042272   Err 0.1D-04          -
129:  8  6  2  8  5  3   S 2  17.8055204    0.0363  17.8055567   Err 0.1D-04          -
130: 14  3 11 13  4  9   S 5   6.5804538   -0.0056   6.5804482   Err 0.1D-04          -
131: 17  4 14 16  5 12   S 3   6.6199614    0.0070   6.6199684   Err 0.1D-04          -
132:  3  2  1  2  1  2   S 4   8.6774390    0.0143   8.6774533   Err 0.1D-04          -
133:  6  6  0  7  5  2   S 2   9.1894966   -0.0339   9.1894627   Err 0.1D-04          -
134:  6  1  5  5  0  5   S 3   9.8503806    0.0140   9.8503946   Err 0.1D-04          -
135:  6  1  5  5  0  5   S 1   9.8503927    0.0019   9.8503946   Err 0.1D-04          -
136:  8  7  2  9  6  3   S 1   9.9605807   -0.0334   9.9605472   Err 0.1D-04          -
137:  9  1  9  8  1  8   S 2  10.6645178   -0.0181  10.6644997   Err 0.1D-04          -
```

```
 138:  9  1  9  8  1  8   S 4  10.6645135   -0.0138  10.6644997   Err 0.1D-04          -
 139:  9  1  9  8  1  8   S 5  10.6645137   -0.0140  10.6644997   Err 0.1D-04          -
 140:  9  1  9  8  1  8   S 3  10.6645149   -0.0138  10.6645010   Err 0.1D-04          -
 141:  9  1  9  8  1  8   S 2  10.6645178   -0.0181  10.6644997   Err 0.1D-04          -
 142: 10  8  2 11  7  4   S 4  10.7329317    0.0094  10.7329410   Err 0.1D-04          -
 143: 18  3 16 18  1 17   S 2  11.2512233   -0.0171  11.2512063   Err 0.1D-04          -
 144: 18  3 16 18  1 17   S 4  11.2511794    0.0269  11.2512063   Err 0.1D-04          -
 145: 18  3 16 18  1 17   S 5  11.2511700    0.0363  11.2512063   Err 0.1D-04          -
 146:  6  5  1  6  4  2   S 3  14.5688002    0.0342  14.5688344   Err 0.1D-04          -
 Maximum (obs-calc)/err in line  42   0.0000454

 RMS deviations (MHz), B and V sorted
  B  V   n splittings MHz
  B  V   n abs. freq. MHz
  1  1 146         0.021393         0.023152

          Parameters  and  Errors
 BJ          0.615111913 { 0.000000224}
 BK          1.619565198 { 0.000000556}
 B-          0.038073353 { 0.000000134}
 DJ          0.008958E-6 { 0.000568E-6}
 DJK         0.071632E-6 { 0.002148E-6}
 DK          0.017643E-6 { 0.003310E-6}
 dj         -0.001411E-6 { 0.000240E-6}
 dk          0.001939E-6 { 0.000072E-6}
\F12         -1.707645956 {     derived}
\F          159.567889700 {     derived}  160.280797315 {     derived}
 V1n         17547.638530 {  169.697929}   14683.233397 {   32.999432}
\rho         0.010959736 {     derived}    0.014126771 {     derived}
\beta        0.236764475 {     derived}    3.126723015 {     derived}
\gamma      -2.434567715 {     derived}    3.044945190 {     derived}
 delta       0.717767161 { 0.062885579}    3.090694306 { 0.217071185}

 Standard Deviation       0.022415 MHz

------------------------------------ B =  1
 Rotational Constants and Errors (in GHz)
     B_z       2.234677111       0.000000640
     B_x       0.653185266       0.000000258
     B_y       0.577038561       0.000000263
 Ray's kappa   -0.90813
 F0(calc)     158.000000000       0.000000000
 I_alpha        3.198601709       0.000000000
```

```
 <(i,x)  <(i,y)  <(i,z)      118.2147      117.2084       41.1250
d<(i,x) d<(i,y) d<(i,z)       2.1745        2.0818        3.6031

 F0(calc)     158.000000000       0.000000000
 I_alpha        3.198601709       0.000000000
 <(i,x)  <(i,y)  <(i,z)       92.8988       89.6820      177.0837
d<(i,x) d<(i,y) d<(i,z)       6.5648        0.7159       12.4373

 V1n_1      7.002057 kj +/- 0.067715 kj         1.672372 kcal +/- 0.016173 kcal
        585.326135 cm +/-   5.6605 cm    s=  48.875438
 V1n_2      5.859070 kj +/- 0.013168 kj         1.399380 kcal +/- 0.003145 kcal
        489.779878 cm +/-   1.1007 cm    s=  40.897210

F(calc)       159.567889700
F(calc)       160.280797315
```

$^{13}C_4$ Isotopologue XIAM Output

```
J K- K+  J K- K+    Sym   calc/GHz  diff/MHz     obs/GHz
  1:  7  2  6  7  1  7   S 1   5.9446220    0.0103   5.9446323   Err 0.1D-04          -
  2:  5  1  5  4  1  4   S 1   5.9597232    0.0050   5.9597282   Err 0.1D-04          -
  3: 16  2 14 16  1 15   S 1   6.0086054   -0.0062   6.0085992   Err 0.1D-04          -
  4:  5  0  5  4  0  4   S 1   6.1092713   -0.0373   6.1092340   Err 0.1D-04          -
  5:  5  2  4  4  2  3   S 1   6.1569314    0.0294   6.1569608   Err 0.1D-04          -
  6:  6  2  5  5  2  4   S 1   7.3832984   -0.0067   7.3832917   Err 0.1D-04          -
  7:  6  2  4  5  2  3   S 1   7.4754865   -0.0252   7.4754613   Err 0.1D-04          -
  8:  6  3  3  6  2  4   S 1   7.9358698    0.0233   7.9358931   Err 0.1D-04          -
  9:  7  1  6  6  1  5   S 1   8.8570443    0.0047   8.8570490   Err 0.1D-04          -
 10:  8  0  8  7  1  7   S 1   8.8574145    0.0173   8.8574318   Err 0.1D-04          -
 11:  9  0  9  8  1  8   S 1  10.1670033    0.0140  10.1670173   Err 0.1D-04          -
 12: 11  4  7 11  3  8   S 1  11.0894894   -0.0316  11.0894578   Err 0.1D-04          -
 13:  9  5  4  8  5  3   S 1  11.1113447   -0.0042  11.1113406   Err 0.1D-04          -
 14:  7  4  3  7  3  4   S 1  11.2652760   -0.0383  11.2652377   Err 0.1D-04          -
 15: 13  4 10 13  3 11   S 1  11.2725789    0.0268  11.2726057   Err 0.1D-04          -
 16:  7  4  4  7  3  5   S 1  11.2778165    0.0280  11.2778445   Err 0.1D-04          -
 17:  9  1  8  8  1  7   S 1  11.3454705    0.0100  11.3454805   Err 0.1D-04          -
 18: 10  0 10  9  1  9   S 1  11.4546697   -0.0062  11.4546635   Err 0.1D-04          -
 19: 10  5  5  9  5  4   S 1  12.3495544   -0.0058  12.3495486   Err 0.1D-04          -
 20: 10  1  9  9  1  8   S 1  12.5760294   -0.0115  12.5760179   Err 0.1D-04          -
 21: 11  0 11 10  0 10   S 1  13.1193250   -0.0113  13.1193137   Err 0.1D-04          -
 22: 11  2 10 10  2  9   S 1  13.4663261    0.0219  13.4663480   Err 0.1D-04          -
 23: 11  6  5 10  6  4   S 1  13.5808673    0.0143  13.5808816   Err 0.1D-04          -
 24: 11  1 10 10  1  9   S 1  13.7953287   -0.0200  13.7953087   Err 0.1D-04          -
 25: 15  5 11 15  4 11   S 1  14.3070132    0.0060  14.3070192   Err 0.1D-04          -
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 26: 12  5  7 12  4  8   S 1  14.4416721    0.0012  14.4416734   Err 0.1D-04          -
 27: 12  5  8 12  4  9   S 1  14.4555360   -0.0319  14.4555041   Err 0.1D-04          -
 28: 12 10  2 11 10  1   S 1  14.8043722   -0.0107  14.8043615   Err 0.1D-04          -
 29: 13  2 12 12  2 11   S 1  15.8704462    0.0048  15.8704510   Err 0.1D-04          -
 30: 13 11  2 12 11  1   S 1  16.0377207    0.0222  16.0377429   Err 0.1D-04          -
 31: 13 10  3 12 10  2   S 1  16.0395290   -0.0280  16.0395010   Err 0.1D-04          -
 32: 13  7  6 12  7  5   S 1  16.0503943    0.0372  16.0504316   Err 0.1D-04          -
 33: 13  6  8 13  5  9   S 1  17.6959577   -0.0164  17.6959413   Err 0.1D-04          -
 34: 20  5 15 19  6 14   S 1   7.3235900   -0.0044   7.3235856   Err 0.1D-04          -
 35: 10  7  4 11  6  5   S 1   7.3802780    0.0199   7.3802980   Err 0.1D-04          -
 36:  4  4  0  3  3  1   S 1  16.2258438    0.0005  16.2258443   Err 0.1D-04          -
 Maximum (obs-calc)/err in line   4   0.0000373

 RMS deviations (MHz), B and V sorted
  B  V   n splittings MHz
  B  V   n abs. freq. MHz
  1  1  36         0.019636         0.022363

          Parameters  and  Errors
 BJ          0.616303344 { 0.000000434}
 BK           1.613534845 { 0.000000995}
 B-          0.038389031 { 0.000000159}
 DJ          0.030991E-6 { 0.001075E-6}
 DJK          0.062779E-6 { 0.004381E-6}
\F12         -1.796270761 {     derived}
\F          159.835732497 {     derived}  160.136707605 {     derived}
\rho          0.012230570 {     derived}    0.013522317 {     derived}
\beta         0.167078913 {     derived}    3.049834548 {     derived}
\gamma       -2.434956935 {     derived}    3.045020860 {     derived}

 Standard Deviation       0.021510 MHz

---------------------------------- B =  1
 Rotational Constants and Errors (in GHz)
     B_z       2.229838189       0.000001171
     B_x       0.654692375       0.000000471
     B_y       0.577914312       0.000000453
 Ray's kappa   -0.90704
 F0(calc)     158.000000000       0.000000000
 I_alpha        3.198601709       0.000000000
 <(i,x)  <(i,y)  <(i,z)      111.9212      111.1649       31.2893
d<(i,x) d<(i,y) d<(i,z)        0.0000        0.0000        0.0000
```

F0(calc) 158.000000000 0.000000000
I_alpha 3.198601709 0.000000000
<(i,x) <(i,y) <(i,z) 107.3153 88.1282 162.5774
d<(i,x) d<(i,y) d<(i,z) 0.0000 0.0000 0.0000

V1n_1 7.170127 kj +/- 0.000000 kj 1.712513 kcal +/- 0.000000 kcal
599.375675 cm +/- 0.0000 cm s= 49.964723
V1n_2 5.809924 kj +/- 0.000000 kj 1.387642 kcal +/- 0.000000 kcal
485.671584 cm +/- 0.0000 cm s= 40.486204

F(calc) 159.835732497
F(calc) 160.136707605

$^{13}C_5$ Isotopologue XIAM Output

	J K- K+	J K- K+	Sym	calc/GHz	diff/MHz	obs/GHz		
1:	7 2 6	7 1 7	S 1	5.9366573	-0.0011	5.9366563	Err 0.1D-04	-
2:	5 1 5	4 1 4	S 1	5.9711901	-0.0471	5.9711430	Err 0.1D-04	-
3:	18 2 16	18 2 17	S 1	6.7562268	-0.0190	6.7562078	Err 0.1D-04	-
4:	6 0 6	5 0 5	S 1	7.3174208	-0.0249	7.3173959	Err 0.1D-04	-
5:	6 3 3	5 3 2	S 1	7.4281193	0.0009	7.4281202	Err 0.1D-04	-
6:	3 2 1	2 1 2	S 1	8.6608715	0.0087	8.6608803	Err 0.1D-04	-
7:	14 9 6	15 8 7	S 1	8.7623676	-0.0217	8.7623459	Err 0.1D-04	-
8:	7 1 6	6 1 5	S 1	8.8760653	0.0026	8.8760679	Err 0.1D-04	-
9:	8 0 8	7 1 7	S 1	8.8830625	0.0212	8.8830838	Err 0.1D-04	-
10:	8 2 7	7 2 6	S 1	9.8475045	0.0231	9.8475277	Err 0.1D-04	-
11:	8 4 5	7 4 4	S 1	9.9007323	-0.0278	9.9007044	Err 0.1D-04	-
12:	4 2 2	3 1 3	S 1	10.0390804	-0.0472	10.0390332	Err 0.1D-04	-
13:	8 2 6	7 2 5	S 1	10.0555690	0.0208	10.0555898	Err 0.1D-04	-
14:	9 0 9	8 1 8	S 1	10.1942161	-0.0044	10.1942116	Err 0.1D-04	-
15:	9 5 4	8 5 3	S 1	11.1347843	-0.0311	11.1347532	Err 0.1D-04	-
16:	7 4 4	7 3 5	S 1	11.2422825	-0.0079	11.2422747	Err 0.1D-04	-
17:	9 2 7	8 2 6	S 1	11.3471339	0.0143	11.3471482	Err 0.1D-04	-
18:	9 1 8	8 1 7	S 1	11.3691908	-0.0119	11.3691790	Err 0.1D-04	-
19:	17 4 14	17 3 15	S 1	11.4588482	0.0528	11.4589010	Err 0.1D-04	-
20:	19 1 18	19 1 19	S 1	11.6446451	0.0277	11.6446728	Err 0.1D-04	-
21:	10 6 4	9 6 3	S 1	12.3695389	-0.0194	12.3695195	Err 0.1D-04	-
22:	10 5 5	9 5 4	S 1	12.3756658	-0.0177	12.3756480	Err 0.1D-04	-
23:	10 3 8	9 3 7	S 1	12.3917869	0.0161	12.3918030	Err 0.1D-04	-
24:	19 2 18	18 3 16	S 1	12.4428097	-0.0122	12.4427975	Err 0.1D-04	-
25:	16 11 5	17 10 7	S 1	12.7277470	-0.0081	12.7277389	Err 0.1D-04	-
26:	11 0 11	10 1 10	S 1	12.7492713	-0.0365	12.7492348	Err 0.1D-04	-
27:	11 2 9	10 2 8	S 1	13.9335091	0.0293	13.9335384	Err 0.1D-04	-
28:	10 5 5	10 4 6	S 1	14.4365215	0.0006	14.4365221	Err 0.1D-04	-
29:	12 10 2	11 10 1	S 1	14.8355002	0.0459	14.8355461	Err 0.1D-04	-

```
 30: 19  3 16 18  4 15   S 1  14.8921140   -0.0250  14.8920890   Err 0.1D-04          -
 31: 12  3  9 11  3  8   S 1  14.9867973    0.0016  14.9867989   Err 0.1D-04          -
 32: 12  2 10 11  2  9   S 1  15.2217405    0.0186  15.2217592   Err 0.1D-04          -
 33:  6  3  3  5  2  3   S 1  15.4007769    0.0123  15.4007891   Err 0.1D-04          -
 34: 13  2 11 12  2 10   S 1  16.5031919   -0.0037  16.5031882   Err 0.1D-04          -
 35: 20  3 18 19  4 15   S 1  12.4616701    0.0197  12.4616898   Err 0.1D-04          -
 36: 22  4 19 21  5 17   S 1  13.1063203   -0.0071  13.1063132   Err 0.1D-04          -
Maximum (obs-calc)/err in line  19   0.0000528

RMS deviations (MHz), B and V sorted
 B  V   n splittings MHz
 B  V   n abs. freq. MHz
 1  1  36         0.023669         0.026299

          Parameters  and  Errors
 BJ          0.617587642 { 0.000000387}
 BK           1.608489262 { 0.000000954}
 B-          0.038630753 { 0.000000070}
 DJ          0.018729E-6 { 0.000741E-6}
\F12        -1.792899406 {     derived}
\F         159.833203839 {     derived}  160.133255825 {     derived}
\rho         0.012211225 {     derived}    0.013499964 {     derived}
\beta        0.167702331 {     derived}    3.049467798 {     derived}
\gamma      -2.435216557 {     derived}    3.045071307 {     derived}

 Standard Deviation       0.025506 MHz

------------------------------------ B =  1
 Rotational Constants and Errors (in GHz)
     B_z       2.226076904       0.000001018
     B_x       0.656218395       0.000000388
     B_y       0.578956889       0.000000399
 Ray's kappa   -0.90619
 F0(calc)     158.000000000       0.000000000
 I_alpha        3.198601709       0.000000000
 <(i,x)  <(i,y)  <(i,z)      111.9212      111.1649       31.2893
d<(i,x) d<(i,y) d<(i,z)        0.0000        0.0000        0.0000

 F0(calc)     158.000000000       0.000000000
 I_alpha        3.198601709       0.000000000
 <(i,x)  <(i,y)  <(i,z)      107.3153       88.1282      162.5774
d<(i,x) d<(i,y) d<(i,z)        0.0000        0.0000        0.0000
```

V1n_1 7.170127 kj +/- 0.000000 kj 1.712513 kcal +/- 0.000000 kcal
599.375675 cm +/- 0.0000 cm s= 49.965513
V1n_2 5.809924 kj +/- 0.000000 kj 1.387642 kcal +/- 0.000000 kcal
485.671584 cm +/- 0.0000 cm s= 40.486845

F(calc) 159.833203839
F(calc) 160.133255825

$^{13}C_6$ Isotopologue XIAM Output

J K- K+	J K- K+	Sym	calc/GHz	diff/MHz	obs/GHz	
1: 8 2 7	8 1 8	S 1	6.2735303	0.2126	6.2737429	Err 0.1D-04 -
2: 18 2 16	18 2 17	S 1	6.6481375	-0.0285	6.6481090	Err 0.1D-04 -
3: 4 1 3	3 0 3	S 1	6.9450752	0.0955	6.9451707	Err 0.1D-04 -
4: 5 1 5	4 0 4	S 1	7.2408561	0.1015	7.2409576	Err 0.1D-04 -
5: 6 2 4	5 2 3	S 1	7.4863788	-0.0107	7.4863681	Err 0.1D-04 -
6: 7 0 7	6 1 6	S 1	7.5378217	-0.0311	7.5377906	Err 0.1D-04 -
7: 9 3 6	9 2 7	S 1	7.5725541	0.2807	7.5728348	Err 0.1D-04 -
8: 8 0 8	7 1 7	S 1	8.8683961	-0.0437	8.8683524	Err 0.1D-04 -
9: 7 1 6	6 1 5	S 1	8.8701094	0.0017	8.8701111	Err 0.1D-04 -
10: 7 1 6	6 1 5	S 1	8.8701094	0.0017	8.8701111	Err 0.1D-04 -
11: 8 2 6	7 2 5	S 1	10.0465898	-0.0568	10.0465330	Err 0.1D-04 -
12: 9 0 9	8 1 8	S 1	10.1808639	-0.0283	10.1808356	Err 0.1D-04 -
13: 18 1 17	18 1 18	S 1	10.7638985	-0.0335	10.7638650	Err 0.1D-04 -
14: 9 2 8	8 2 7	S 1	11.0628866	-0.0331	11.0628535	Err 0.1D-04 -
15: 12 4 9	12 3 10	S 1	11.2951749	0.2655	11.2954403	Err 0.1D-04 -
16: 9 1 8	8 1 7	S 1	11.3628871	-0.0044	11.3628826	Err 0.1D-04 -
17: 10 0 10	9 1 9	S 1	11.4716160	-0.0251	11.4715909	Err 0.1D-04 -
18: 18 2 17	17 3 15	S 1	11.6776890	-0.1439	11.6775451	Err 0.1D-04 -
19: 19 2 18	19 0 19	S 1	12.1291201	-0.0142	12.1291059	Err 0.1D-04 -
20: 10 2 9	9 2 8	S 1	12.2781743	-0.0417	12.2781326	Err 0.1D-04 -
21: 11 1 10	10 1 9	S 1	13.8176753	0.0049	13.8176802	Err 0.1D-04 -
22: 12 4 9	11 4 8	S 1	14.8692185	-0.0573	14.8691612	Err 0.1D-04 -
23: 18 2 16	17 3 14	S 1	16.5834468	-0.1489	16.5832979	Err 0.1D-04 -
24: 9 2 8	8 1 8	S 1	17.3364169	0.1397	17.3365566	Err 0.1D-04 -
25: 8 3 6	7 2 5	S 1	17.7582347	0.2676	17.7585023	Err 0.1D-04 -
26: 19 4 16	18 5 14	S 1	9.2482016	-0.1961	9.2480055	Err 0.1D-04 -
27: 7 1 7	6 0 6	S 1	9.3057525	0.0502	9.3058027	Err 0.1D-04 -
28: 8 2 7	7 2 6	S 1	9.8437415	-0.0212	9.8437203	Err 0.1D-04 -
29: 9 3 6	8 3 5	S 1	11.1702615	-0.0023	11.1702592	Err 0.1D-04 -
30: 10 3 8	9 3 7	S 1	12.3850424	-0.0196	12.3850229	Err 0.1D-04 -
31: 19 12 7	20 11 9	S 1	12.4684537	-0.3850	12.4680688	Err 0.1D-04 -

Maximum (obs-calc)/err in line 31 0.0003850

```
 RMS deviations (MHz), B and V sorted
  B  V   n splittings MHz
  B  V   n abs. freq. MHz
  1  1  31         0.133662         0.150909

           Parameters  and  Errors
 BJ          0.617294829 { 0.000002760}
 BK           1.618576482 { 0.000008585}
 B-          0.038194124 { 0.000000401}
 DJ          0.038200E-6 { 0.007087E-6}
\F12         -1.801356714 {     derived}
\F         159.840625599 {     derived}  160.142535809 {     derived}
\rho         0.012263277 {     derived}    0.013558736 {     derived}
\beta        0.166893067 {     derived}    3.049969329 {     derived}
\gamma      -2.434544676 {     derived}    3.044940709 {     derived}

 Standard Deviation       0.145949 MHz

------------------------------------ B =  1
 Rotational Constants and Errors (in GHz)
     B_z       2.235871310       0.000007825
     B_x       0.655488953       0.000002783
     B_y       0.579100704       0.000002795
 Ray's kappa   -0.90779
 F0(calc)     158.000000000       0.000000000
 I_alpha        3.198601709       0.000000000
 <(i,x)  <(i,y)  <(i,z)      111.9212      111.1649       31.2893
d<(i,x) d<(i,y) d<(i,z)        0.0000        0.0000        0.0000

 F0(calc)     158.000000000       0.000000000
 I_alpha        3.198601709       0.000000000
 <(i,x)  <(i,y)  <(i,z)      107.3153       88.1282      162.5774
d<(i,x) d<(i,y) d<(i,z)        0.0000        0.0000        0.0000

 V1n_1      7.170127 kj +/- 0.000000 kj         1.712513 kcal +/- 0.000000 kcal
        599.375675 cm +/-   0.0000 cm    s=  49.963193
 V1n_2      5.809924 kj +/- 0.000000 kj         1.387642 kcal +/- 0.000000 kcal
        485.671584 cm +/-   0.0000 cm    s=  40.484965

F(calc)       159.840625599
F(calc)       160.142535809
```

$^{13}C_7$ Isotopologue XIAM Output

	J K- K+	J K- K+	Sym	calc/GHz	diff/MHz	obs/GHz		
1:	5 2 4	5 1 5	S 1	5.4417055	-0.0076	5.4416979	Err 0.1D-04	-
2:	6 2 5	6 1 6	S 1	5.6735132	-0.0339	5.6734793	Err 0.1D-04	-
3:	6 2 5	6 1 6	S 3	5.6734808	-0.0015	5.6734793	Err 0.1D-04	-
4:	14 3 12	13 4 9	S 2	5.7456122	-0.0212	5.7455910	Err 0.1D-04	-
5:	14 3 12	13 4 9	S 4	5.7465243	0.0231	5.7465475	Err 0.1D-04	-
6:	14 3 12	14 2 12	S 2	5.9267530	0.0039	5.9267569	Err 0.1D-04	-
7:	14 3 12	14 2 12	S 4	5.9267257	0.0312	5.9267569	Err 0.1D-04	-
8:	5 0 5	4 0 4	S 1	6.0408598	-0.0110	6.0408488	Err 0.1D-04	-
9:	5 0 5	4 0 4	S 3	6.0408575	-0.0073	6.0408501	Err 0.1D-04	-
10:	5 0 5	4 0 4	S 2	6.0408575	-0.0088	6.0408488	Err 0.1D-04	-
11:	5 0 5	4 0 4	S 4	6.0408552	-0.0064	6.0408488	Err 0.1D-04	-
12:	5 4 1	4 4 0	S 1	6.0972960	-0.0402	6.0972558	Err 0.1D-04	-
13:	5 4 1	4 4 0	S 2	6.0972898	-0.0328	6.0972570	Err 0.1D-04	-
14:	5 4 1	4 4 0	S 3	6.0972896	-0.0338	6.0972558	Err 0.1D-04	-
15:	5 4 2	4 4 1	S 2	6.0972921	-0.0400	6.0972521	Err 0.1D-04	-
16:	8 1 7	7 2 6	S 2	6.1229560	0.0136	6.1229696	Err 0.1D-04	-
17:	8 1 7	7 2 6	S 4	6.1229602	0.0095	6.1229696	Err 0.1D-04	-
18:	13 1 12	13 1 13	S 2	6.3956899	0.0117	6.3957016	Err 0.1D-04	-
19:	13 1 12	13 1 13	S 3	6.3957144	-0.0128	6.3957016	Err 0.1D-04	-
20:	13 1 12	13 1 13	S 1	6.3957267	-0.0252	6.3957016	Err 0.1D-04	-
21:	13 3 10	13 2 11	S 2	6.7458570	0.0372	6.7458943	Err 0.1D-04	-
22:	8 6 3	9 5 5	S 2	6.8670864	-0.0288	6.8670576	Err 0.1D-04	-
23:	8 6 2	9 5 4	S 2	6.8706261	-0.0620	6.8705641	Err 0.1D-04	-
24:	6 0 6	5 0 5	S 1	7.2227661	-0.0286	7.2227375	Err 0.1D-04	-
25:	6 0 6	5 0 5	S 3	7.2227632	-0.0266	7.2227367	Err 0.1D-04	-
26:	6 0 6	5 0 5	S 2	7.2227630	-0.0263	7.2227367	Err 0.1D-04	-
27:	6 3 3	5 3 2	S 1	7.3256443	0.0019	7.3256462	Err 0.1D-04	-
28:	6 1 5	5 1 4	S 2	7.5119120	0.0220	7.5119340	Err 0.1D-04	-
29:	6 1 5	5 1 4	S 1	7.5119154	0.0186	7.5119340	Err 0.1D-04	-
30:	6 1 5	5 1 4	S 3	7.5119125	0.0215	7.5119340	Err 0.1D-04	-
31:	6 1 5	5 1 4	S 4	7.5119095	0.0245	7.5119340	Err 0.1D-04	-
32:	16 3 14	15 4 12	S 4	8.1445134	0.0158	8.1445292	Err 0.1D-04	-
33:	16 3 14	15 4 12	S 2	8.1447516	-0.0047	8.1447469	Err 0.1D-04	-
34:	7 0 7	6 0 6	S 1	8.3927715	0.0289	8.3928004	Err 0.1D-04	-
35:	7 0 7	6 0 6	S 3	8.3927680	0.0324	8.3928004	Err 0.1D-04	-
36:	7 0 7	6 0 6	S 2	8.3927673	0.0331	8.3928004	Err 0.1D-04	-
37:	7 4 3	6 4 2	S 3	8.5410167	0.0018	8.5410185	Err 0.1D-04	-
38:	7 4 3	6 4 2	S 2	8.5410148	0.0037	8.5410185	Err 0.1D-04	-
39:	7 4 3	6 4 2	S 4	8.5410130	0.0055	8.5410185	Err 0.1D-04	-
40:	11 3 9	11 2 10	S 2	8.5705614	-0.0317	8.5705297	Err 0.1D-04	-
41:	8 0 8	7 1 7	S 2	8.7296147	0.0202	8.7296349	Err 0.1D-04	-

42: 8 0 8 7 1 7 S 4 8.7296170 0.0179 8.7296349 Err 0.1D-04 -
43: 7 1 6 6 1 5 S 1 8.7523811 0.0071 8.7523881 Err 0.1D-04 -
44: 7 1 6 6 1 5 S 3 8.7523777 0.0104 8.7523881 Err 0.1D-04 -
45: 7 1 6 6 1 5 S 2 8.7523772 0.0109 8.7523881 Err 0.1D-04 -
46: 7 1 6 6 1 5 S 4 8.7523741 0.0140 8.7523881 Err 0.1D-04 -
47: 17 10 8 18 9 10 S 4 8.8513395 0.0134 8.8513529 Err 0.1D-04 -
48: 17 10 8 18 9 10 S 2 8.8510531 -0.0212 8.8510319 Err 0.1D-04 -
49: 9 7 3 10 6 4 S 1 8.8989233 -0.0043 8.8989190 Err 0.1D-04 -
50: 20 4 16 20 3 17 S 3 9.1226905 0.0076 9.1226981 Err 0.1D-04 -
51: 21 2 19 21 2 20 S 1 9.2860652 -0.0012 9.2860640 Err 0.1D-04 -
52: 21 2 19 21 2 20 S 1 9.2860652 -0.0012 9.2860640 Err 0.1D-04 -
53: 21 2 19 21 2 20 S 3 9.2860581 0.0035 9.2860616 Err 0.1D-04 -
54: 21 2 19 21 2 20 S 2 9.2860622 -0.0043 9.2860579 Err 0.1D-04 -
55: 21 2 19 21 2 20 S 4 9.2860556 0.0023 9.2860579 Err 0.1D-04 -
56: 8 2 7 7 2 6 S 1 9.7150500 -0.0044 9.7150456 Err 0.1D-04 -
57: 8 2 7 7 2 6 S 2 9.7150631 -0.0175 9.7150456 Err 0.1D-04 -
58: 8 2 7 7 2 6 S 4 9.7150526 -0.0070 9.7150456 Err 0.1D-04 -
59: 8 2 7 7 2 6 S 3 9.7150475 -0.0019 9.7150456 Err 0.1D-04 -
60: 8 1 7 7 1 6 S 1 9.9867434 0.0165 9.9867599 Err 0.1D-04 -
61: 8 1 7 7 1 6 S 3 9.9867395 0.0204 9.9867599 Err 0.1D-04 -
62: 8 1 7 7 1 6 S 2 9.9867389 0.0233 9.9867622 Err 0.1D-04 -
63: 8 1 7 7 1 6 S 4 9.9867351 0.0248 9.9867599 Err 0.1D-04 -
64: 17 4 13 17 3 14 S 1 10.0733743 -0.0055 10.0733688 Err 0.1D-04 -
65: 21 2 20 20 3 17 S 1 10.1898975 0.0095 10.1899070 Err 0.1D-04 -
66: 21 2 20 20 3 17 S 3 10.1899151 -0.0082 10.1899070 Err 0.1D-04 -
67: 9 0 9 8 0 8 S 1 10.7008135 -0.0507 10.7007629 Err 0.1D-04 -
68: 9 0 9 8 0 8 S 3 10.7008089 -0.0449 10.7007639 Err 0.1D-04 -
69: 9 0 9 8 0 8 S 2 10.7008075 -0.0436 10.7007639 Err 0.1D-04 -
70: 18 11 8 19 10 9 S 1 10.8853690 0.0393 10.8854083 Err 0.1D-04 -
71: 9 2 8 8 2 7 S 1 10.9186188 -0.0293 10.9185895 Err 0.1D-04 -
72: 9 2 8 8 2 7 S 3 10.9186154 -0.0259 10.9185895 Err 0.1D-04 -
73: 9 2 8 8 2 7 S 2 10.9186243 -0.0316 10.9185927 Err 0.1D-04 -
74: 19 3 17 19 2 18 S 3 10.9415414 -0.0068 10.9415347 Err 0.1D-04 -
75: 9 5 4 8 5 3 S 1 10.9816964 -0.0103 10.9816861 Err 0.1D-04 -
76: 9 5 4 8 5 3 S 3 10.9816860 0.0037 10.9816897 Err 0.1D-04 -
77: 9 5 4 8 5 3 S 2 10.9816858 0.0003 10.9816861 Err 0.1D-04 -
78: 9 5 4 8 5 3 S 4 10.9816831 0.0066 10.9816897 Err 0.1D-04 -
79: 9 2 7 8 2 6 S 1 11.1817966 0.0338 11.1818305 Err 0.1D-04 -
80: 9 2 7 8 2 6 S 3 11.1817928 0.0377 11.1818305 Err 0.1D-04 -
81: 9 2 7 8 2 6 S 4 11.1817894 0.0410 11.1818305 Err 0.1D-04 -
82: 9 2 7 8 2 6 S 2 11.1817889 0.0416 11.1818305 Err 0.1D-04 -
83: 7 1 6 6 0 6 S 4 11.2963399 -0.0310 11.2963088 Err 0.1D-04 -
84: 7 1 6 6 0 6 S 2 11.2963530 -0.0365 11.2963165 Err 0.1D-04 -

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 85: 10  2  9  9  2  8   S 3  12.1184940   -0.0258  12.1184681   Err 0.1D-04          -
 86: 10  2  9  9  2  8   S 4  12.1184927   -0.0246  12.1184681   Err 0.1D-04          -
 87: 10  6  4  9  6  3   S 3  12.1996082    0.0023  12.1996105   Err 0.1D-04          -
 88: 10  6  4  9  6  3   S 1  12.1996134    0.0009  12.1996143   Err 0.1D-04          -
 89: 10  6  4  9  6  3   S 2  12.1996087    0.0041  12.1996128   Err 0.1D-04          -
 90: 10  6  4  9  6  3   S 4  12.1996056    0.0073  12.1996128   Err 0.1D-04          -
 91: 10  5  6  9  5  5   S 1  12.2052614    0.0022  12.2052636   Err 0.1D-04          -
 92: 10  5  6  9  5  5   S 4  12.2052745   -0.0109  12.2052636   Err 0.1D-04          -
 93: 10  5  6  9  5  5   S 2  12.2052800   -0.0163  12.2052636   Err 0.1D-04          -
 94: 10  5  6  9  5  5   S 3  12.2052747   -0.0112  12.2052635   Err 0.1D-04          -
 95: 10  1  9  9  1  8   S 1  12.4314762   -0.0010  12.4314751   Err 0.1D-04          -
 96: 10  1  9  9  1  8   S 3  12.4314710    0.0041  12.4314751   Err 0.1D-04          -
 97: 10  1  9  9  1  8   S 2  12.4314693    0.0058  12.4314751   Err 0.1D-04          -
 98: 11  0 11 10  1 10   S 4  12.5606183   -0.0209  12.5605974   Err 0.1D-04          -
 99: 11  0 11 10  1 10   S 3  12.5605993   -0.0019  12.5605974   Err 0.1D-04          -
100: 11  0 11 10  1 10   S 1  12.5606016   -0.0042  12.5605974   Err 0.1D-04          -
101:  7  2  6  6  1  5   S 2  12.6161600   -0.0208  12.6161393   Err 0.1D-04          -
102:  7  2  6  6  1  5   S 4  12.6161490   -0.0097  12.6161393   Err 0.1D-04          -
103: 22  3 20 22  1 21   S 1  12.7047589   -0.0126  12.7047463   Err 0.1D-04          -
104: 22  3 20 22  1 21   S 3  12.7047192    0.0271  12.7047463   Err 0.1D-04          -
105: 11  1 10 10  1  9   S 1  13.6388004    0.0102  13.6388106   Err 0.1D-04          -
106: 11  1 10 10  1  9   S 2  13.6387919    0.0184  13.6388104   Err 0.1D-04          -
107: 11  1 10 10  1  9   S 3  13.6387945    0.0189  13.6388134   Err 0.1D-04          -
108: 12  0 12 11  1 11   S 2  13.7945752   -0.0135  13.7945617   Err 0.1D-04          -
109: 12  0 12 11  1 11   S 1  13.7945609    0.0008  13.7945617   Err 0.1D-04          -
110: 12  0 12 11  1 11   S 3  13.7945562    0.0055  13.7945617   Err 0.1D-04          -
111: 12  0 12 11  1 11   S 4  13.7945715   -0.0098  13.7945617   Err 0.1D-04          -
112: 12  1 12 11  1 11   S 3  14.0384641   -0.0143  14.0384498   Err 0.1D-04          -
113: 12  1 12 11  1 11   S 1  14.0384683   -0.0185  14.0384498   Err 0.1D-04          -
114: 12  1 12 11  1 11   S 4  14.0384606   -0.0108  14.0384498   Err 0.1D-04          -
115: 10  9  1 11  8  3   S 2  14.1806787   -0.0382  14.1806405   Err 0.1D-04          -
116: 16  5 12 16  4 13   S 1  14.4603283    0.0424  14.4603708   Err 0.1D-04          -
117: 16  5 11 16  4 13   S 4  14.4699613    0.0206  14.4699819   Err 0.1D-04          -
118: 15  5 10 15  4 12   S 2  14.4966670   -0.0057  14.4966613   Err 0.1D-04          -
119: 12  6  6 11  6  5   S 3  14.6459852    0.0115  14.6459967   Err 0.1D-04          -
120: 12  6  6 11  6  5   S 4  14.6459815    0.0152  14.6459967   Err 0.1D-04          -
121: 12  6  6 11  6  5   S 2  14.6459850    0.0106  14.6459956   Err 0.1D-04          -
122: 12  6  6 11  6  5   S 3  14.6459852    0.0104  14.6459956   Err 0.1D-04          -
123: 12  6  6 11  6  5   S 1  14.6459930    0.0026  14.6459956   Err 0.1D-04          -
124: 12  5  7 11  5  6   S 3  14.6558074    0.0126  14.6558200   Err 0.1D-04          -
125: 12  5  7 11  5  6   S 4  14.6557994    0.0194  14.6558189   Err 0.1D-04          -
126: 12  5  7 11  5  6   S 3  14.6558074    0.0115  14.6558189   Err 0.1D-04          -
127: 12  3  9 11  3  8   S 2  14.7706929   -0.0051  14.7706878   Err 0.1D-04          -
```

128: 12 3 9 11 3 8 S 4 14.7707193 -0.0315 14.7706878 Err 0.1D-04 -
129: 13 3 10 12 3 9 S 2 16.0375990 -0.0006 16.0375984 Err 0.1D-04 -
130: 13 3 10 12 3 9 S 4 16.0376118 -0.0134 16.0375984 Err 0.1D-04 -
131: 13 3 10 12 3 9 S 3 16.0376283 -0.0299 16.0375984 Err 0.1D-04 -
132: 14 8 6 13 8 5 S 1 17.0808111 0.0119 17.0808230 Err 0.1D-04 -
133: 14 8 6 13 8 5 S 2 17.0808054 0.0176 17.0808230 Err 0.1D-04 -
134: 14 8 6 13 8 5 S 3 17.0808042 0.0188 17.0808230 Err 0.1D-04 -
135: 14 8 6 13 8 5 S 4 17.0808010 0.0220 17.0808230 Err 0.1D-04 -
136: 18 6 13 18 5 14 S 3 17.6960322 0.0530 17.6960852 Err 0.1D-04 -
137: 17 6 12 17 5 12 S 4 17.7072916 0.0410 17.7073326 Err 0.1D-04 -
138: 16 6 10 16 5 12 S 3 17.7588153 0.0214 17.7588367 Err 0.1D-04 -
139: 15 6 9 15 5 11 S 4 17.7903285 0.0413 17.7903698 Err 0.1D-04 -
140: 14 6 8 14 5 9 S 1 17.7949485 0.0226 17.7949711 Err 0.1D-04 -
141: 14 6 8 14 5 9 S 4 17.7963647 -0.0243 17.7963404 Err 0.1D-04 -
142: 12 6 7 12 5 8 S 3 17.8233211 0.0359 17.8233570 Err 0.1D-04 -
143: 9 2 7 8 1 8 S 2 17.9461103 0.0320 17.9461423 Err 0.1D-04 -
144: 10 3 7 10 2 8 S 1 7.4245773 0.0050 7.4245823 Err 0.1D-04 -
145: 7 3 5 7 2 6 S 3 8.2038661 0.0039 8.2038700 Err 0.1D-04 -
146: 7 1 7 6 1 6 S 2 8.2360078 -0.0040 8.2360038 Err 0.1D-04 -
147: 7 1 7 6 1 6 S 1 8.2360087 -0.0049 8.2360038 Err 0.1D-04 -
148: 7 1 7 6 1 6 S 4 8.2360048 -0.0010 8.2360038 Err 0.1D-04 -
149: 7 1 7 6 1 6 S 3 8.2360060 -0.0022 8.2360038 Err 0.1D-04 -
150: 7 5 2 6 5 1 S 1 8.5373153 -0.0010 8.5373143 Err 0.1D-04 -
151: 7 5 2 6 5 1 S 2 8.5373118 0.0048 8.5373167 Err 0.1D-04 -
152: 7 5 2 6 5 1 S 4 8.5373095 0.0071 8.5373167 Err 0.1D-04 -
153: 7 2 5 6 2 4 S 1 8.6434248 0.0094 8.6434342 Err 0.1D-04 -
154: 7 2 5 6 2 4 S 3 8.6434202 0.0140 8.6434342 Err 0.1D-04 -
155: 7 2 5 6 2 4 S 4 8.6434053 0.0289 8.6434342 Err 0.1D-04 -
156: 22 5 18 21 6 15 S 3 9.4017320 0.0004 9.4017323 Err 0.1D-04 -
157: 9 1 9 8 1 8 S 1 10.5657906 -0.0399 10.5657507 Err 0.1D-04 -
158: 9 1 9 8 1 8 S 2 10.5657887 -0.0380 10.5657507 Err 0.1D-04 -
159: 9 1 9 8 1 8 S 3 10.5657871 -0.0364 10.5657507 Err 0.1D-04 -
160: 9 1 8 8 1 7 S 2 11.2136065 0.0266 11.2136331 Err 0.1D-04 -
161: 9 1 8 8 1 7 S 1 11.2136121 0.0225 11.2136346 Err 0.1D-04 -
162: 9 1 8 8 1 7 S 3 11.2136076 0.0270 11.2136346 Err 0.1D-04 -
163: 9 1 8 8 1 7 S 4 11.2136021 0.0325 11.2136346 Err 0.1D-04 -
164: 9 4 5 9 3 6 S 2 11.2938712 -0.0375 11.2938337 Err 0.1D-04 -
165: 18 3 15 17 4 13 S 1 12.3957450 0.0133 12.3957584 Err 0.1D-04 -
166: 8 2 7 7 1 6 S 4 13.5788276 -0.0564 13.5787712 Err 0.1D-04 -
167: 7 2 5 6 1 6 S 4 14.4930724 -0.0228 14.4930496 Err 0.1D-04 -
168: 12 2 11 11 2 10 S 1 14.5060340 -0.0346 14.5059994 Err 0.1D-04 -
169: 12 2 11 11 2 10 S 2 14.5060309 -0.0315 14.5059994 Err 0.1D-04 -
170: 12 2 11 11 2 10 S 4 14.5060246 -0.0252 14.5059994 Err 0.1D-04 -

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 171: 12  2 11 11  2 10   S 3  14.5060287   -0.0293  14.5059994   Err 0.1D-04          -
 172: 13  5  8 13  4 10   S 4  14.5397533   -0.0083  14.5397450   Err 0.1D-04          -
 173: 11  5  7 11  4  7   S 2  14.5470508   -0.0272  14.5470236   Err 0.1D-04          -
 174: 15 11  5 16 10  7   S 2  14.5621270    0.0065  14.5621335   Err 0.1D-04          -
 175: 15 11  5 16 10  7   S 3  14.5641220   -0.0308  14.5640912   Err 0.1D-04          -
 Maximum (obs-calc)/err in line  23   0.0000620

 RMS deviations (MHz), B and V sorted
  B  V   n splittings MHz
  B  V   n abs. freq. MHz
  1  1 175         0.022698         0.023736

          Parameters  and  Errors
 BJ          0.609157376 { 0.000000177}
 BK           1.623779013 { 0.000000627}
 B-          0.037381462 { 0.000000115}
 DJ          0.024408E-6 { 0.000525E-6}
 DK           0.036382E-6 { 0.004296E-6}
 dj          -0.002842E-6 { 0.000151E-6}
 dk          0.001663E-6 { 0.000111E-6}
\F12         -1.687567236 {     derived}
\F         159.656860469 {     derived}  160.185687856 {     derived}
 V1n         17688.950575 {     fixed  }   14598.459775 {    1.765844}
\rho         0.011410230 {     derived}    0.013741891 {     derived}
\beta        0.209641700 {     derived}    3.068993667 {     derived}
\gamma       -2.434041405 {     derived}    3.044842789 {     derived}

 Standard Deviation       0.023306 MHz

------------------------------------ B =  1
 Rotational Constants and Errors (in GHz)
     B_z       2.232936389       0.000000640
     B_x       0.646538838       0.000000199
     B_y       0.571775914       0.000000223
 Ray's kappa   -0.90999
 F0(calc)     158.000000000       0.000000000
 I_alpha        3.198601709       0.000000000
 <(i,x)  <(i,y)  <(i,z)      116.1676      115.2453       37.8427
d<(i,x) d<(i,y) d<(i,z)        0.0000        0.0000        0.0000

 F0(calc)     158.000000000       0.000000000
 I_alpha        3.198601709       0.000000000
 <(i,x)  <(i,y)  <(i,z)      104.0312       88.4753      165.8828
```

d<(i,x) d<(i,y) d<(i,z) 0.0000 0.0000 0.0000

V1n_1 7.058445 kj +/- 0.000000 kj 1.685839 kcal +/- 0.000000 kcal
590.039797 cm +/- 0.0000 cm s= 49.241578
V1n_2 5.825243 kj +/- 0.000705 kj 1.391301 kcal +/- 0.000168 kcal
486.952134 cm +/- 0.0589 cm s= 40.638431

F(calc) 159.656860469
F(calc) 160.185687856

$^{13}C_9$ Isotopologue XIAM Output

	J K- K+	J K- K+	Sym	calc/GHz	diff/MHz	obs/GHz		
1:	5 1 5	4 1 4	S 2	5.9360733	-0.0255	5.9360478	Err 0.1D-04	-
2:	5 1 5	4 1 4	S 5	5.9360721	-0.0258	5.9360463	Err 0.1D-04	-
3:	5 1 5	4 1 4	S 3	5.9360711	-0.0233	5.9360478	Err 0.1D-04	-
4:	4 1 4	3 0 3	S 2	6.1607297	-0.0260	6.1607037	Err 0.1D-04	-
5:	4 1 4	3 0 3	S 4	6.1607214	-0.0177	6.1607037	Err 0.1D-04	-
6:	4 1 4	3 0 3	S 5	6.1607171	-0.0134	6.1607037	Err 0.1D-04	-
7:	19 10 10	20 9 11	S 1	6.2035634	-0.0181	6.2035454	Err 0.1D-04	-
8:	19 10 9	20 9 11	S 3	6.2038457	-0.0131	6.2038326	Err 0.1D-04	-
9:	19 10 9	20 9 11	S 2	6.2044864	0.0164	6.2045028	Err 0.1D-04	-
10:	5 1 4	4 1 3	S 3	6.3125736	0.0238	6.3125973	Err 0.1D-04	-
11:	5 1 4	4 1 3	S 1	6.3125759	0.0201	6.3125961	Err 0.1D-04	-
12:	5 1 4	4 1 3	S 2	6.3125717	0.0244	6.3125961	Err 0.1D-04	-
13:	5 1 4	4 1 3	S 4	6.3125700	0.0260	6.3125961	Err 0.1D-04	-
14:	5 1 4	4 1 3	S 5	6.3125686	0.0275	6.3125961	Err 0.1D-04	-
15:	6 1 6	5 1 5	S 1	7.1168881	-0.0208	7.1168673	Err 0.1D-04	-
16:	6 1 6	5 1 5	S 3	7.1168858	-0.0185	7.1168673	Err 0.1D-04	-
17:	6 1 6	5 1 5	S 4	7.1168848	-0.0175	7.1168673	Err 0.1D-04	-
18:	6 1 6	5 1 5	S 2	7.1168875	-0.0178	7.1168698	Err 0.1D-04	-
19:	5 5 0	6 4 2	S 5	7.2345021	0.0589	7.2345609	Err 0.1D-04	-
20:	5 5 0	6 4 2	S 3	7.2331135	-0.0125	7.2331010	Err 0.1D-04	-
21:	6 0 6	5 0 5	S 3	7.2741423	0.0167	7.2741590	Err 0.1D-04	-
22:	6 0 6	5 0 5	S 1	7.2741452	0.0138	7.2741590	Err 0.1D-04	-
23:	6 0 6	5 0 5	S 2	7.2741416	0.0174	7.2741590	Err 0.1D-04	-
24:	6 0 6	5 0 5	S 4	7.2741387	0.0203	7.2741590	Err 0.1D-04	-
25:	7 0 7	6 1 6	S 5	7.4791853	0.0021	7.4791874	Err 0.1D-04	-
26:	7 0 7	6 1 6	S 2	7.4791802	0.0072	7.4791874	Err 0.1D-04	-
27:	7 0 7	6 1 6	S 1	7.4791451	0.0422	7.4791874	Err 0.1D-04	-
28:	7 0 7	6 1 6	S 3	7.4791493	0.0381	7.4791874	Err 0.1D-04	-
29:	7 0 7	6 1 6	S 4	7.4791833	-0.0062	7.4791772	Err 0.1D-04	-
30:	6 1 5	5 1 4	S 1	7.5669326	0.0289	7.5669615	Err 0.1D-04	-
31:	6 1 5	5 1 4	S 2	7.5669283	0.0332	7.5669615	Err 0.1D-04	-

32: 6 1 5 5 1 4 S 5 7.5669250 0.0365 7.5669615 Err 0.1D-04 -
33: 6 1 5 5 1 4 S 4 7.5669258 0.0369 7.5669627 Err 0.1D-04 -
34: 6 1 5 5 1 4 S 3 7.5669298 0.0317 7.5669615 Err 0.1D-04 -
35: 8 3 5 8 2 6 S 5 7.7716026 0.0199 7.7716225 Err 0.1D-04 -
36: 7 3 4 7 2 6 S 4 8.2164871 0.0556 8.2165428 Err 0.1D-04 -
37: 7 1 7 6 1 6 S 1 8.2946890 -0.0153 8.2946737 Err 0.1D-04 -
38: 7 1 7 6 1 6 S 2 8.2946878 -0.0141 8.2946737 Err 0.1D-04 -
39: 7 1 7 6 1 6 S 3 8.2946863 -0.0162 8.2946701 Err 0.1D-04 -
40: 7 1 7 6 1 6 S 4 8.2946848 -0.0110 8.2946737 Err 0.1D-04 -
41: 21 5 16 20 6 15 S 2 8.4178504 0.0079 8.4178583 Err 0.1D-04 -
42: 7 2 6 6 2 5 S 3 8.5697389 0.0166 8.5697555 Err 0.1D-04 -
43: 7 2 6 6 2 5 S 4 8.5697515 0.0040 8.5697555 Err 0.1D-04 -
44: 7 2 6 6 2 5 S 2 8.5697680 -0.0125 8.5697555 Err 0.1D-04 -
45: 7 2 6 6 2 5 S 5 8.5697823 -0.0268 8.5697555 Err 0.1D-04 -
46: 21 4 17 21 3 18 S 3 8.7841407 0.0020 8.7841427 Err 0.1D-04 -
47: 21 4 17 21 3 18 S 1 8.7842000 -0.0552 8.7841449 Err 0.1D-04 -
48: 8 0 8 7 1 7 S 1 8.8031194 0.0405 8.8031599 Err 0.1D-04 -
49: 8 0 8 7 1 7 S 2 8.8031502 0.0097 8.8031599 Err 0.1D-04 -
50: 7 1 6 6 1 5 S 2 8.8162991 0.0268 8.8163259 Err 0.1D-04 -
51: 7 1 6 6 1 5 S 5 8.8162955 0.0304 8.8163259 Err 0.1D-04 -
52: 7 1 6 6 1 5 S 3 8.8163007 0.0252 8.8163259 Err 0.1D-04 -
53: 7 1 6 6 1 5 S 1 8.8163041 0.0218 8.8163259 Err 0.1D-04 -
54: 13 3 11 13 2 12 S 5 8.9457168 0.0293 8.9457461 Err 0.1D-04 -
55: 14 3 12 14 2 13 S 5 9.1855584 0.0366 9.1855950 Err 0.1D-04 -
56: 19 4 15 18 5 13 S 2 9.4806900 0.0119 9.4807019 Err 0.1D-04 -
57: 4 2 3 3 1 3 S 2 10.0045071 0.0109 10.0045180 Err 0.1D-04 -
58: 4 2 3 3 1 3 S 4 10.0046158 -0.0083 10.0046075 Err 0.1D-04 -
59: 8 7 1 9 6 3 S 2 10.0384622 0.0060 10.0384682 Err 0.1D-04 -
60: 8 1 7 7 1 6 S 5 10.0594160 0.0364 10.0594524 Err 0.1D-04 -
61: 8 1 7 7 1 6 S 1 10.0594258 0.0266 10.0594524 Err 0.1D-04 -
62: 8 1 7 7 1 6 S 3 10.0594220 0.0238 10.0594457 Err 0.1D-04 -
63: 8 1 7 7 1 6 S 2 10.0594201 0.0260 10.0594461 Err 0.1D-04 -
64: 9 0 9 8 1 8 S 5 10.1095380 -0.0123 10.1095257 Err 0.1D-04 -
65: 9 0 9 8 1 8 S 4 10.1095375 -0.0118 10.1095257 Err 0.1D-04 -
66: 9 0 9 8 1 8 S 2 10.1095365 -0.0108 10.1095257 Err 0.1D-04 -
67: 9 0 9 8 1 8 S 3 10.1095116 0.0141 10.1095257 Err 0.1D-04 -
68: 9 0 9 8 1 8 S 1 10.1095103 0.0173 10.1095276 Err 0.1D-04 -
69: 22 2 21 21 3 18 S 5 10.1107708 0.0298 10.1108006 Err 0.1D-04 -
70: 22 2 21 21 3 18 S 2 10.1107549 0.0457 10.1108006 Err 0.1D-04 -
71: 8 1 8 7 0 7 S 5 10.2848310 -0.0473 10.2847837 Err 0.1D-04 -
72: 8 1 8 7 0 7 S 2 10.2848415 -0.0578 10.2847837 Err 0.1D-04 -
73: 9 1 9 8 1 8 S 1 10.6408144 -0.0245 10.6407900 Err 0.1D-04 -
74: 9 1 9 8 1 8 S 5 10.6408089 -0.0189 10.6407900 Err 0.1D-04 -

75: 9 1 9 8 1 8 S 3 10.6408109 -0.0210 10.6407900 Err 0.1D-04 -
76: 9 1 9 8 1 8 S 2 10.6408122 -0.0222 10.6407900 Err 0.1D-04 -
77: 9 0 9 8 0 8 S 1 10.7757265 -0.0293 10.7756972 Err 0.1D-04 -
78: 9 0 9 8 0 8 S 3 10.7757218 -0.0246 10.7756972 Err 0.1D-04 -
79: 9 0 9 8 0 8 S 2 10.7757202 -0.0230 10.7756972 Err 0.1D-04 -
80: 9 0 9 8 0 8 S 4 10.7757156 -0.0160 10.7756996 Err 0.1D-04 -
81: 10 8 2 11 7 4 S 3 10.8232063 0.0312 10.8232374 Err 0.1D-04 -
82: 9 2 8 8 2 7 S 2 10.9973968 -0.0096 10.9973871 Err 0.1D-04 -
83: 9 2 8 8 2 7 S 5 10.9973976 -0.0170 10.9973806 Err 0.1D-04 -
84: 9 2 8 8 2 7 S 1 10.9973923 -0.0117 10.9973806 Err 0.1D-04 -
85: 9 2 8 8 2 7 S 4 10.9973891 -0.0020 10.9973871 Err 0.1D-04 -
86: 9 6 3 8 6 2 S 1 11.0575965 -0.0035 11.0575930 Err 0.1D-04 -
87: 9 6 3 8 6 2 S 3 11.0575920 0.0010 11.0575930 Err 0.1D-04 -
88: 9 6 3 8 6 2 S 2 11.0575915 -0.0012 11.0575903 Err 0.1D-04 -
89: 9 6 3 8 6 2 S 4 11.0575886 0.0044 11.0575930 Err 0.1D-04 -
90: 9 6 3 8 6 2 S 5 11.0575871 0.0032 11.0575903 Err 0.1D-04 -
91: 9 5 4 8 5 3 S 1 11.0618138 -0.0011 11.0618127 Err 0.1D-04 -
92: 9 5 4 8 5 3 S 3 11.0618030 0.0096 11.0618126 Err 0.1D-04 -
93: 9 5 4 8 5 3 S 2 11.0618015 0.0111 11.0618127 Err 0.1D-04 -
94: 9 5 4 8 5 3 S 4 11.0617989 0.0137 11.0618127 Err 0.1D-04 -
95: 9 5 4 8 5 3 S 5 11.0617968 0.0158 11.0618127 Err 0.1D-04 -
96: 15 10 6 16 9 8 S 4 11.1558933 -0.0053 11.1558880 Err 0.1D-04 -
97: 18 3 16 18 1 17 S 3 11.2539606 0.0380 11.2539986 Err 0.1D-04 -
98: 18 3 16 18 1 17 S 1 11.2540107 -0.0121 11.2539986 Err 0.1D-04 -
99: 9 4 5 9 3 6 S 4 11.2871423 -0.0056 11.2871367 Err 0.1D-04 -
100: 8 4 4 8 3 5 S 2 11.3202771 -0.0215 11.3202556 Err 0.1D-04 -
101: 8 4 5 8 3 6 S 4 11.3355730 -0.0277 11.3355453 Err 0.1D-04 -
102: 20 3 18 20 2 19 S 3 11.4633627 0.0197 11.4633824 Err 0.1D-04 -
103: 5 2 3 4 1 4 S 5 11.4735905 0.0295 11.4736200 Err 0.1D-04 -
104: 20 12 8 21 11 10 S 3 11.4905208 -0.0400 11.4904808 Err 0.1D-04 -
105: 10 1 10 9 1 9 S 1 11.8092280 -0.0257 11.8092022 Err 0.1D-04 -
106: 10 1 10 9 1 9 S 3 11.8092241 -0.0219 11.8092022 Err 0.1D-04 -
107: 10 1 10 9 1 9 S 5 11.8092216 -0.0194 11.8092022 Err 0.1D-04 -
108: 10 1 10 9 1 9 S 4 11.8092212 -0.0192 11.8092020 Err 0.1D-04 -
109: 10 0 10 9 0 9 S 1 11.9259056 -0.0403 11.9258653 Err 0.1D-04 -
110: 10 0 10 9 0 9 S 3 11.9259003 -0.0336 11.9258667 Err 0.1D-04 -
111: 10 0 10 9 0 9 S 2 11.9258987 -0.0320 11.9258667 Err 0.1D-04 -
112: 10 0 10 9 0 9 S 5 11.9258932 -0.0265 11.9258667 Err 0.1D-04 -
113: 10 2 9 9 2 8 S 4 12.2057423 -0.0062 12.2057361 Err 0.1D-04 -
114: 10 2 9 9 2 8 S 3 12.2057445 -0.0069 12.2057375 Err 0.1D-04 -
115: 10 2 9 9 2 8 S 5 12.2057472 -0.0111 12.2057361 Err 0.1D-04 -
116: 10 8 2 9 8 1 S 1 12.2829788 -0.0011 12.2829777 Err 0.1D-04 -
117: 10 8 2 9 8 1 S 3 12.2829740 0.0028 12.2829768 Err 0.1D-04 -

118: 10 8 2 9 8 1 S 2 12.2829741 0.0035 12.2829777 Err 0.1D-04 -
119: 10 8 2 9 8 1 S 4 12.2829708 0.0060 12.2829768 Err 0.1D-04 -
120: 10 8 2 9 8 1 S 5 12.2829694 0.0074 12.2829768 Err 0.1D-04 -
121: 10 6 4 9 6 3 S 1 12.2885883 0.0060 12.2885943 Err 0.1D-04 -
122: 10 6 4 9 6 3 S 3 12.2885831 0.0144 12.2885976 Err 0.1D-04 -
123: 10 6 4 9 6 3 S 2 12.2885823 0.0158 12.2885981 Err 0.1D-04 -
124: 10 6 4 9 6 3 S 4 12.2885792 0.0184 12.2885976 Err 0.1D-04 -
125: 10 6 4 9 6 3 S 5 12.2885773 0.0203 12.2885976 Err 0.1D-04 -
126: 10 5 5 9 5 4 S 1 12.2943865 -0.0029 12.2943836 Err 0.1D-04 -
127: 10 5 5 9 5 4 S 3 12.2943643 0.0183 12.2943826 Err 0.1D-04 -
128: 10 5 5 9 5 4 S 2 12.2943620 0.0205 12.2943826 Err 0.1D-04 -
129: 10 5 5 9 5 4 S 4 12.2943593 0.0233 12.2943826 Err 0.1D-04 -
130: 10 5 5 9 5 4 S 5 12.2943566 0.0260 12.2943826 Err 0.1D-04 -
131: 21 3 19 21 1 20 S 1 12.2938259 0.0251 12.2938510 Err 0.1D-04 -
132: 12 1 11 11 2 10 S 3 12.3007334 0.0384 12.3007718 Err 0.1D-04 -
133: 12 1 11 11 2 10 S 1 12.3007164 0.0554 12.3007718 Err 0.1D-04 -
134: 15 2 13 14 3 11 S 1 12.3909847 0.0439 12.3910286 Err 0.1D-04 -
135: 11 2 10 10 2 9 S 1 13.4100343 -0.0205 13.4100138 Err 0.1D-04 -
136: 11 2 10 10 2 9 S 2 13.4100319 -0.0182 13.4100138 Err 0.1D-04 -
137: 11 2 10 10 2 9 S 3 13.4100296 -0.0158 13.4100138 Err 0.1D-04 -
138: 11 2 10 10 2 9 S 5 13.4100287 -0.0173 13.4100114 Err 0.1D-04 -
139: 11 2 10 10 2 9 S 4 13.4100257 -0.0119 13.4100138 Err 0.1D-04 -
140: 8 2 7 7 1 6 S 2 13.6376646 -0.0094 13.6376552 Err 0.1D-04 -
141: 11 1 10 10 1 9 S 1 13.7365329 0.0120 13.7365450 Err 0.1D-04 -
142: 11 1 10 10 1 9 S 3 13.7365271 0.0178 13.7365450 Err 0.1D-04 -
143: 11 1 10 10 1 9 S 2 13.7365231 0.0228 13.7365459 Err 0.1D-04 -
144: 11 1 10 10 1 9 S 5 13.7365173 0.0277 13.7365450 Err 0.1D-04 -
145: 22 2 21 22 0 22 S 5 14.0903525 -0.1025 14.0902500 Err 0.1D-04 -
146: 12 1 12 11 1 11 S 3 14.1377210 -0.0299 14.1376912 Err 0.1D-04 -
147: 12 1 12 11 1 11 S 3 14.1377210 -0.0323 14.1376888 Err 0.1D-04 -
148: 12 1 12 11 1 11 S 2 14.1377218 -0.0330 14.1376888 Err 0.1D-04 -
149: 12 1 12 11 1 11 S 5 14.1377180 -0.0292 14.1376888 Err 0.1D-04 -
150: 12 0 12 11 0 11 S 1 14.2160360 -0.0279 14.2160081 Err 0.2D-04 -
151: 12 0 12 11 0 11 S 5 14.2160217 -0.0152 14.2160065 Err 0.2D-04 -
152: 12 0 12 11 0 11 S 2 14.2160287 -0.0205 14.2160081 Err 0.2D-04 -
153: 12 0 12 11 0 11 S 3 14.2160294 -0.0229 14.2160065 Err 0.2D-04 -
154: 12 0 12 11 0 11 S 4 14.2160225 -0.0144 14.2160081 Err 0.2D-04 -
155: 5 3 2 4 2 2 S 1 14.2321657 0.0326 14.2321983 Err 0.1D-04 -
156: 7 2 6 6 1 6 S 2 14.2502407 0.0502 14.2502908 Err 0.1D-04 -
157: 19 5 15 19 4 16 S 2 14.3832683 -0.0396 14.3832287 Err 0.1D-04 -
158: 18 5 14 18 4 15 S 2 14.4009835 0.0099 14.4009934 Err 0.1D-04 -
159: 15 11 4 16 10 6 S 2 14.4133293 0.0509 14.4133802 Err 0.1D-04 -
160: 20 5 15 20 4 17 S 5 14.4280923 -0.0173 14.4280749 Err 0.1D-04 -

161: 12 5 8 12 4 9 S 4 14.5408027 -0.0166 14.5407860 Err 0.1D-04 -
162: 12 5 8 12 4 9 S 1 14.5458977 -0.0321 14.5458656 Err 0.1D-04 -
163: 11 5 7 11 4 7 S 1 14.5555477 0.0316 14.5555793 Err 0.1D-04 -
164: 11 5 7 11 4 8 S 3 14.5603502 0.0128 14.5603631 Err 0.1D-04 -
165: 10 5 6 10 4 6 S 4 14.5610517 0.0248 14.5610765 Err 0.1D-04 -
166: 12 5 7 12 4 9 S 5 14.5611914 0.0338 14.5612252 Err 0.1D-04 -
167: 11 5 6 11 4 8 S 3 14.5648147 0.0361 14.5648508 Err 0.1D-04 -
168: 10 5 6 10 4 7 S 1 14.5752835 0.0008 14.5752843 Err 0.1D-04 -
169: 9 5 5 9 4 6 S 5 14.5821808 -0.0220 14.5821588 Err 0.1D-04 -
170: 12 2 11 11 2 10 S 1 14.6100022 -0.0116 14.6099906 Err 0.1D-04 -
171: 12 2 11 11 2 10 S 3 14.6099969 -0.0063 14.6099906 Err 0.1D-04 -
172: 12 2 11 11 2 10 S 2 14.6099980 -0.0074 14.6099906 Err 0.1D-04 -
173: 12 2 11 11 2 10 S 5 14.6099937 -0.0031 14.6099906 Err 0.1D-04 -
174: 12 2 11 11 2 10 S 4 14.6099917 -0.0011 14.6099906 Err 0.1D-04 -
175: 12 9 3 11 9 2 S 1 14.7406273 0.0086 14.7406359 Err 0.1D-04 -
176: 12 9 3 11 9 2 S 2 14.7406217 0.0168 14.7406386 Err 0.1D-04 -
177: 12 9 3 11 9 2 S 4 14.7406178 0.0208 14.7406386 Err 0.1D-04 -
178: 12 9 3 11 9 2 S 5 14.7406160 0.0226 14.7406386 Err 0.1D-04 -
179: 12 8 4 11 8 3 S 1 14.7432078 0.0216 14.7432294 Err 0.1D-04 -
180: 12 8 4 11 8 3 S 3 14.7432020 0.0274 14.7432294 Err 0.1D-04 -
181: 12 8 4 11 8 3 S 2 14.7432018 0.0276 14.7432294 Err 0.1D-04 -
182: 12 8 4 11 8 3 S 4 14.7431979 0.0315 14.7432294 Err 0.1D-04 -
183: 12 8 4 11 8 3 S 5 14.7431960 0.0334 14.7432294 Err 0.1D-04 -
184: 12 7 5 11 7 4 S 1 14.7469948 -0.0002 14.7469946 Err 0.1D-04 -
185: 12 7 5 11 7 4 S 3 14.7469888 0.0058 14.7469946 Err 0.1D-04 -
186: 12 7 5 11 7 4 S 2 14.7469880 0.0066 14.7469946 Err 0.1D-04 -
187: 12 7 5 11 7 4 S 4 14.7469843 0.0103 14.7469946 Err 0.1D-04 -
188: 12 7 5 11 7 4 S 5 14.7469821 0.0125 14.7469946 Err 0.1D-04 -
189: 12 6 6 11 6 5 S 1 14.7529022 0.0066 14.7529089 Err 0.1D-04 -
190: 12 6 6 11 6 5 S 3 14.7528943 0.0145 14.7529089 Err 0.1D-04 -
191: 12 6 6 11 6 5 S 2 14.7528925 0.0162 14.7529086 Err 0.1D-04 -
192: 12 6 6 11 6 5 S 4 14.7528890 0.0196 14.7529086 Err 0.1D-04 -
193: 12 6 6 11 6 5 S 5 14.7528861 0.0227 14.7529089 Err 0.1D-04 -
194: 12 4 9 11 4 7 S 5 14.7618114 0.0021 14.7618134 Err 0.1D-04 -
195: 12 3 9 11 3 8 S 5 14.8806519 0.0443 14.8806962 Err 0.1D-04 -
196: 12 3 9 11 3 8 S 2 14.8806936 0.0026 14.8806962 Err 0.1D-04 -
197: 12 3 9 11 3 8 S 4 14.8807186 -0.0224 14.8806962 Err 0.1D-04 -
198: 12 1 11 11 1 10 S 1 14.9397829 -0.0071 14.9397759 Err 0.1D-04 -
199: 12 1 11 11 1 10 S 3 14.9397764 -0.0005 14.9397759 Err 0.1D-04 -
200: 12 1 11 11 1 10 S 2 14.9397713 0.0046 14.9397759 Err 0.1D-04 -
201: 12 1 11 11 1 10 S 5 14.9397647 0.0112 14.9397759 Err 0.1D-04 -
202: 17 12 5 18 11 7 S 4 15.1977369 0.0141 15.1977509 Err 0.1D-04 -
203: 13 0 13 12 0 12 S 2 15.3598516 -0.0608 15.3597907 Err 0.1D-04 -

204: 13 0 13 12 0 12   S 3 15.3598515   -0.0611 15.3597904   Err 0.1D-04   -
205: 13 0 13 12 0 12   S 4 15.3598448   -0.0545 15.3597904   Err 0.1D-04   -
206: 13 0 13 12 0 12   S 5 15.3598436   -0.0528 15.3597907   Err 0.1D-04   -
207: 13 6 7 12 6 6   S 1 15.9863805   -0.0323 15.9863483   Err 0.1D-04   -
208: 13 6 7 12 6 6   S 3 15.9863694   -0.0210 15.9863484   Err 0.1D-04   -
209: 13 6 7 12 6 6   S 4 15.9863633   -0.0150 15.9863483   Err 0.1D-04   -
210: 13 6 7 12 6 6   S 5 15.9863598   -0.0115 15.9863483   Err 0.1D-04   -
211: 13 4 9 12 4 8   S 1 16.0297738   0.0256 16.0297995   Err 0.1D-04   -
212: 16 12 5 17 11 7   S 3 16.4308310   0.0070 16.4308381   Err 0.1D-04   -
213: 14 1 14 13 0 13   S 5 16.6348008   -0.0621 16.6347387   Err 0.1D-04   -
214: 14 4 11 13 4 10   S 2 17.2594829   -0.0283 17.2594546   Err 0.1D-04   -
215: 14 4 11 13 4 10   S 5 17.2598383   -0.0142 17.2598241   Err 0.1D-04   -
216: 14 4 10 13 4 9   S 4 17.2774151   0.0386 17.2774537   Err 0.1D-04   -
217: 14 6 9 14 5 10   S 3 17.7888270   -0.0170 17.7888100   Err 0.1D-04   -
218: 13 6 7 13 5 8   S 4 17.8060140   -0.0156 17.8059984   Err 0.1D-04   -
219: 8 6 2 8 5 3   S 5 17.8474096   -0.0263 17.8473833   Err 0.1D-04   -
220: 15 3 13 14 3 12   S 2 18.4619162   -0.0277 18.4618885   Err 0.1D-04   -
221: 15 3 13 14 3 12   S 5 18.4619174   -0.0289 18.4618885   Err 0.1D-04   -
222: 15 3 13 14 3 12   S 1 18.4619090   -0.0205 18.4618885   Err 0.1D-04   -
223: 15 3 13 14 3 12   S 3 18.4619033   -0.0148 18.4618885   Err 0.1D-04   -
224: 15 3 13 14 3 12   S 4 18.4619037   -0.0152 18.4618885   Err 0.1D-04   -
225: 15 4 11 14 4 10   S 2 18.5303187   0.0257 18.5303444   Err 0.1D-04   -
226: 9 3 6 8 2 6   S 1 18.8722350   0.0228 18.8722578   Err 0.1D-04   -
227: 9 3 6 8 2 6   S 4 18.8722520   0.0045 18.8722565   Err 0.1D-04   -
228: 9 3 6 8 2 6   S 3 18.8722189   0.0376 18.8722565   Err 0.1D-04   -
229: 22 6 16 21 7 14   S 5   6.2270726   -0.0015   6.2270711   Err 0.1D-04   -
230: 21 5 16 20 6 15   S 5   8.4210757   -0.0439   8.4210318   Err 0.1D-04   -
231: 7 3 4 6 3 3   S 2   8.6143628   0.0557   8.6144184   Err 0.1D-04   -
232: 13 9 5 14 8 7   S 3 10.3729506   0.0075 10.3729581   Err 0.1D-04   -
233: 12 4 8 12 3 9   S 3 11.0723368   -0.0550 11.0722818   Err 0.1D-04   -
234: 9 3 7 8 3 6   S 1 11.0761352   0.0238 11.0761590   Err 0.1D-04   -
235: 9 4 6 9 3 6   S 5 11.2722812   0.0024 11.2722836   Err 0.1D-04   -
236: 20 3 18 20 1 19   S 4 11.8829120   0.0506 11.8829626   Err 0.1D-04   -
237: 20 3 18 20 1 19   S 5 11.8829092   0.0534 11.8829626   Err 0.1D-04   -
238: 20 3 18 20 1 19   S 2 11.8829547   0.0079 11.8829626   Err 0.1D-04   -
239: 20 3 18 19 4 16   S 2 12.7433365   -0.0055 12.7433310   Err 0.1D-04   -
240: 20 3 18 19 4 16   S 4 12.7433409   -0.0098 12.7433310   Err 0.1D-04   -
241: 22 4 19 21 5 17   S 5 12.8000606   0.0527 12.8001133   Err 0.1D-04   -
242: 22 4 18 21 5 16   S 1 13.9533903   -0.0183 13.9533720   Err 0.1D-04   -
243: 22 4 18 21 5 16   S 3 13.9534154   -0.0433 13.9533720   Err 0.1D-04   -
244: 21 5 16 21 4 18   S 3 14.4569017   -0.0988 14.4568029   Err 0.1D-04   -
245: 12 5 7 12 4 9   S 4 14.5541454   0.0081 14.5541535   Err 0.1D-04   -
246: 12 5 8 11 5 7   S 1 14.7628287   -0.0494 14.7627793   Err 0.1D-04   -

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 247: 12  5  8 11  5  7   S 4  14.7629205    0.0386  14.7629591   Err 0.1D-04          -
 248: 12  5  8 11  5  7   S 2  14.7629280    0.0311  14.7629591   Err 0.1D-04          -
 249: 12  4  9 11  4  7   S 2  14.7648316   -0.0019  14.7648297   Err 0.1D-04          -
 250: 12 10  2 13  9  4   S 2  14.8610001   -0.0302  14.8609699   Err 0.1D-04          -
 251: 13  0 13 12  1 12   S 1  15.1206839   -0.0025  15.1206813   Err 0.1D-04          -
 252: 13  0 13 12  1 12   S 2  15.1206928   -0.0115  15.1206813   Err 0.1D-04          -
 253: 13  0 13 12  1 12   S 3  15.1206758    0.0056  15.1206813   Err 0.1D-04          -
 254: 13  0 13 12  1 12   S 4  15.1206871   -0.0058  15.1206813   Err 0.1D-04          -
 255: 13  3 11 12  3 10   S 3  16.0075082   -0.0348  16.0074734   Err 0.1D-04          -
 Maximum (obs-calc)/err in line 145   0.0001025

 RMS deviations (MHz), B and V sorted
  B  V   n splittings MHz
  B  V   n abs. freq. MHz
  1  1 255         0.027324         0.028396

          Parameters  and  Errors
 BJ          0.613587792 { 0.000000182}
 BK           1.623320329 { 0.000000797}
 B-          0.037771796 { 0.000000049}
 DJ          0.024259E-6 { 0.000407E-6}
 DJK          0.043344E-6 { 0.002719E-6}
 DK           0.024643E-6 { 0.003597E-6}
 dk          0.002174E-6 { 0.000054E-6}
\F12         -1.648058960 {     derived}
\F          159.655502896 {     derived}  160.144965560 {     derived}
 V1n         17749.040113 {    8.545625}   14553.885677 {   28.677644}
\rho         0.011410750 {     derived}    0.013585529 {     derived}
\beta        0.211666678 {     derived}    3.052341156 {     derived}
\gamma       -2.423590060 {     derived}    3.044880047 {     derived}
 delta       0.663258496 {     fixed  }    2.843063364 { 0.031553391}

 Standard Deviation       0.027933 MHz

------------------------------------ B =  1
 Rotational Constants and Errors (in GHz)
     B_z       2.236908121       0.000000863
     B_x       0.651359588       0.000000187
     B_y       0.575815995       0.000000190
 Ray's kappa   -0.90904
 F0(calc)     158.000000000       0.000000000
 I_alpha        3.198601709       0.000000000
 <(i,x)  <(i,y)  <(i,z)      115.9729      115.6424       38.0019
```

d<(i,x) d<(i,y) d<(i,z) 0.0000 0.0000 0.0000

F0(calc) 158.000000000 0.000000000
I_alpha 3.198601709 0.000000000
<(i,x) <(i,y) <(i,z) 106.9993 88.1614 162.8955
d<(i,x) d<(i,y) d<(i,z) 1.7962 0.1895 1.8079

V1n_1 7.082423 kj +/- 0.003410 kj 1.691566 kcal +/- 0.000814 kcal
592.044168 cm +/- 0.2851 cm s= 49.409273
V1n_2 5.807456 kj +/- 0.011443 kj 1.387053 kcal +/- 0.002733 kcal
485.465303 cm +/- 0.9566 cm s= 40.514693

F(calc) 159.655502896
F(calc) 160.144965560

$^{13}C_{10}$ Isotopologue XIAM Output

	J K- K+	J K- K+	Sym	calc/GHz	diff/MHz	obs/GHz	
1:	5 0 5	4 0 4	S 1	6.0580354	-0.0105	6.0580249	Err 0.1D-04 -
2:	17 3 14	17 2 15	S 1	6.1343664	0.0405	6.1344069	Err 0.1D-04 -
3:	22 6 16	21 7 14	S 1	6.2503071	0.0213	6.2503284	Err 0.1D-04 -
4:	4 1 3	3 0 3	S 1	6.8726706	-0.0218	6.8726488	Err 0.1D-04 -
5:	6 1 6	5 1 5	S 1	7.0891535	-0.0100	7.0891434	Err 0.1D-04 -
6:	6 0 6	5 0 5	S 1	7.2438147	0.0030	7.2438177	Err 0.1D-04 -
7:	6 3 3	5 3 2	S 1	7.3449245	0.0471	7.3449716	Err 0.1D-04 -
8:	6 2 4	5 2 3	S 1	7.4036140	-0.0219	7.4035921	Err 0.1D-04 -
9:	7 0 7	6 1 6	S 1	7.4441223	0.0120	7.4441343	Err 0.1D-04 -
10:	6 1 5	5 1 4	S 1	7.5290633	-0.0042	7.5290591	Err 0.1D-04 -
11:	7 1 7	6 0 6	S 1	9.2363750	-0.0005	9.2363745	Err 0.1D-04 -
12:	8 0 8	7 0 7	S 1	9.5808175	0.0066	9.5808241	Err 0.1D-04 -
13:	8 1 7	7 1 6	S 1	10.0101343	0.0108	10.0101451	Err 0.1D-04 -
14:	9 0 9	8 1 8	S 1	10.0636789	0.0066	10.0636855	Err 0.1D-04 -
15:	18 1 17	18 1 18	S 1	10.4906255	-0.0248	10.4906007	Err 0.1D-04 -
16:	9 0 9	8 0 8	S 1	10.7344100	0.0005	10.7344106	Err 0.1D-04 -
17:	9 2 8	8 2 7	S 1	10.9487608	0.0272	10.9487881	Err 0.1D-04 -
18:	9 6 3	8 6 2	S 1	11.0066809	0.0045	11.0066854	Err 0.1D-04 -
19:	9 5 4	8 5 3	S 1	11.0107419	-0.0043	11.0107375	Err 0.1D-04 -
20:	9 4 6	9 3 6	S 1	11.2018517	-0.0056	11.2018461	Err 0.1D-04 -
21:	9 1 8	8 1 7	S 1	11.2403208	0.0127	11.2403336	Err 0.1D-04 -
22:	8 4 5	8 3 6	S 1	11.2577247	0.0034	11.2577281	Err 0.1D-04 -
23:	13 4 9	13 3 11	S 1	11.2769225	-0.0236	11.2768989	Err 0.1D-04 -
24:	19 1 18	19 1 19	S 1	11.2934968	0.0247	11.2935215	Err 0.1D-04 -
25:	10 0 10	9 1 9	S 1	11.3444294	0.0375	11.3444669	Err 0.1D-04 -
26:	13 1 12	12 2 10	S 1	11.7462246	0.0077	11.7462324	Err 0.1D-04 -

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 27: 10  5  5  9  5  4   S 1  12.2375052   -0.0226  12.2374827   Err 0.1D-04          -
 28:  4  3  1  3  2  2   S 1  12.9503388   -0.0148  12.9503240   Err 0.1D-04          -
 29: 11  9  2 10  9  1   S 1  13.4487720    0.0033  13.4487753   Err 0.1D-04          -
 30: 11  6  5 10  6  4   S 1  13.4578882    0.0391  13.4579273   Err 0.1D-04          -
 31: 11  5  6 10  5  5   S 1  13.4653437   -0.0213  13.4653224   Err 0.1D-04          -
 32: 12  1 12 11  1 11   S 1  14.0853537   -0.0227  14.0853310   Err 0.1D-04          -
 33: 19  3 16 18  4 14   S 1  14.1021088    0.0008  14.1021095   Err 0.1D-04          -
 34: 12  0 12 11  0 11   S 1  14.1641424   -0.0300  14.1641124   Err 0.1D-04          -
 35:  5  3  2  4  2  3   S 1  14.1831763   -0.0077  14.1831686   Err 0.1D-04          -
 36: 13  5  8 13  4 10   S 1  14.4228138   -0.0304  14.4227834   Err 0.1D-04          -
 37: 11  5  7 11  4  8   S 1  14.4566215    0.0207  14.4566422   Err 0.1D-04          -
 38:  6  5  2  6  4  3   S 1  14.4954303    0.0343  14.4954645   Err 0.1D-04          -
 39: 12 11  1 11 11  0   S 1  14.6697139   -0.0225  14.6696913   Err 0.1D-04          -
 40: 12  6  6 11  6  5   S 1  14.6846486    0.0130  14.6846615   Err 0.1D-04          -
 41: 12  1 11 11  1 10   S 1  14.8719666    0.0079  14.8719745   Err 0.1D-04          -
 42: 13  0 13 12  1 12   S 1  15.0600216    0.0077  15.0600293   Err 0.1D-04          -
 43: 14  1 13 13  2 12   S 1  15.2286281   -0.0254  15.2286027   Err 0.1D-04          -
 44: 13  1 13 12  0 12   S 1  15.4863647   -0.0074  15.4863573   Err 0.1D-04          -
 45: 20  3 17 19  4 15   S 1  15.7037368   -0.0228  15.7037141   Err 0.1D-04          -
 46: 13  6  7 12  6  6   S 1  15.9122806    0.0532  15.9123338   Err 0.1D-04          -
 47: 13  1 12 12  1 11   S 1  16.0585639   -0.0005  16.0585634   Err 0.1D-04          -
 48:  8  2  6  7  1  7   S 1  16.1343234   -0.0470  16.1342763   Err 0.2D-04          -
 49: 10  2  8  9  1  8   S 1  16.5209443    0.0063  16.5209506   Err 0.1D-04          -
 50:  7  2  5  6  2  4   S 1   8.6643223   -0.0084   8.6643139   Err 0.1D-04          -
 51: 17  2 16 16  3 13   S 1   9.5931084   -0.0119   9.5930966   Err 0.1D-04          -
 52: 10  1 10  9  0  9   S 1  12.3014680   -0.0359  12.3014321   Err 0.1D-04          -
 53: 20 14  7 21 13  8   S 1  17.8000563    0.0014  17.8000576   Err 0.1D-04          -
Maximum (obs-calc)/err in line  46   0.0000532

RMS deviations (MHz), B and V sorted
 B  V   n splittings MHz
 B  V   n abs. freq. MHz
 1  1  53         0.021296         0.024511

          Parameters  and  Errors
BJ          0.610787679 { 0.000000381}
BK           1.611405224 { 0.000001332}
B-          0.036913798 { 0.000000393}
DJ          0.025480E-6 { 0.000979E-6}
DJK          0.062345E-6 { 0.005672E-6}
DK          0.029139E-6 { 0.003843E-6}
dj         -0.006943E-6 { 0.000584E-6}
dk          0.002039E-6 { 0.000088E-6}
```

\F12 -1.765552745 { derived}
\F 159.806199924 { derived} 160.122833214 { derived}
\rho 0.012088565 { derived} 0.013452560 { derived}
\beta 0.171301131 { derived} 3.048572466 { derived}
\gamma -2.422473391 { derived} 3.076375166 { derived}

Standard Deviation 0.023373 MHz

---------- B = 1
Rotational Constants and Errors (in GHz)
B_z 2.222192903 0.000001410
B_x 0.647701476 0.000000518
B_y 0.573873881 0.000000575
Ray's kappa -0.91042
F0(calc) 158.000000000 0.000000000
I_alpha 3.198601709 0.000000000
<(i,x) <(i,y) <(i,z) 112.2228 111.9455 32.1209
d<(i,x) d<(i,y) d<(i,z) 0.0000 0.0000 0.0000

F0(calc) 158.000000000 0.000000000
I_alpha 3.198601709 0.000000000
<(i,x) <(i,y) <(i,z) 107.7081 88.7153 162.2422
d<(i,x) d<(i,y) d<(i,z) 0.0000 0.0000 0.0000

V1n_1 7.155838 kj +/- 0.000000 kj 1.709100 kcal +/- 0.000000 kcal
598.181169 cm +/- 0.0000 cm s= 49.874363
V1n_2 5.808392 kj +/- 0.000000 kj 1.387277 kcal +/- 0.000000 kcal
485.543541 cm +/- 0.0000 cm s= 40.483011

F(calc) 159.806199924
F(calc) 160.122833214

$^{13}C_{11}$ Isotopologue XIAM Output

	J K- K+	J K- K+	Sym	calc/GHz	diff/MHz	obs/GHz		
1:	5 0 5	4 0 4	S 1	6.0462380	-0.0121	6.0462258	Err 0.1D-04	-
2:	6 0 6	5 1 5	S 1	6.0982049	0.0209	6.0982258	Err 0.1D-04	-
3:	5 1 4	4 1 3	S 1	6.2677359	-0.0041	6.2677318	Err 0.1D-04	-
4:	6 0 6	5 0 5	S 1	7.2298944	-0.0056	7.2298888	Err 0.1D-04	-
5:	6 1 5	5 1 4	S 1	7.5135278	-0.0038	7.5135240	Err 0.1D-04	-
6:	3 3 1	3 2 2	S 1	8.0659610	0.0259	8.0659869	Err 0.1D-04	-
7:	7 2 5	6 2 4	S 1	8.6460638	0.0225	8.6460863	Err 0.1D-04	-
8:	7 1 6	6 1 5	S 1	8.7545903	-0.0079	8.7545825	Err 0.1D-04	-
9:	16 2 15	15 3 13	S 1	9.8912396	0.0225	9.8912621	Err 0.1D-04	-

```
 10:  8  1  7  7  1  6   S 1   9.9897297    0.0065   9.9897362   Err 0.1D-04          -
 11:  9  0  9  8  1  8   S 1  10.0398741    0.0203  10.0398944   Err 0.1D-04          -
 12:  9  0  9  8  0  8   S 1  10.7145065   -0.0336  10.7144729   Err 0.1D-04          -
 13:  9  6  3  8  6  2   S 1  10.9843892    0.0241  10.9844133   Err 0.1D-04          -
 14:  9  5  4  8  5  3   S 1  10.9884205    0.0014  10.9884220   Err 0.1D-04          -
 15:  9  3  7  8  3  6   S 1  11.0023084   -0.0193  11.0022891   Err 0.1D-04          -
 16:  9  2  7  8  2  6   S 1  11.1838172    0.0252  11.1838424   Err 0.1D-04          -
 17:  9  1  8  8  1  7   S 1  11.2175988    0.0012  11.2176000   Err 0.1D-04          -
 18: 10  0 10  9  1  9   S 1  11.3187922    0.0102  11.3188024   Err 0.1D-04          -
 19: 10  0 10  9  0  9   S 1  11.8592583   -0.0376  11.8592208   Err 0.1D-04          -
 20: 10  6  4  9  6  3   S 1  12.2071283   -0.0116  12.2071168   Err 0.1D-04          -
 21: 10  5  5  9  5  4   S 1  12.2126661    0.0098  12.2126758   Err 0.1D-04          -
 22: 10  3  7  9  3  6   S 1  12.2688034   -0.0309  12.2687726   Err 0.1D-04          -
 23: 10  1  9  9  1  8   S 1  12.4367316    0.0102  12.4367418   Err 0.1D-04          -
 24: 11  1 11 10  1 10   S 1  12.9020301   -0.0354  12.9019947   Err 0.1D-04          -
 25: 11  5  6 10  5  5   S 1  13.4379744   -0.0024  13.4379720   Err 0.1D-04          -
 26: 19  3 16 19  2 18   S 1  13.4942313    0.0093  13.4942407   Err 0.1D-04          -
 27: 11  1 10 10  1  9   S 1  13.6456324    0.0064  13.6456387   Err 0.1D-04          -
 28: 12  1 12 11  1 11   S 1  14.0589513   -0.0022  14.0589491   Err 0.1D-04          -
 29: 19  5 15 19  4 16   S 1  14.2964673    0.0046  14.2964719   Err 0.1D-04          -
 30: 11  5  6 11  4  7   S 1  14.4641498   -0.0299  14.4641199   Err 0.1D-04          -
 31: 10  5  5 10  4  7   S 1  14.4826873    0.0241  14.4827114   Err 0.1D-04          -
 32: 12  7  5 11  7  4   S 1  14.6491700    0.0258  14.6491957   Err 0.1D-04          -
 33: 12  3 10 11  3  9   S 1  14.6781945    0.0315  14.6782260   Err 0.1D-04          -
 34: 12  1 11 11  1 10   S 1  14.8429391    0.0078  14.8429469   Err 0.1D-04          -
 35: 13  0 13 12  1 12   S 1  15.0293260   -0.0030  15.0293230   Err 0.1D-04          -
 36:  6  3  4  5  2  3   S 1  15.3266491    0.0395  15.3266886   Err 0.1D-04          -
 37: 13  2 12 12  2 11   S 1  15.7075096   -0.0195  15.7074901   Err 0.1D-04          -
 38: 19  1 18 18  2 16   S 1  15.8436470    0.0035  15.8436506   Err 0.1D-04          -
 39: 13  1 12 12  1 11   S 1  16.0276647   -0.0120  16.0276527   Err 0.1D-04          -
 40: 14  2 13 13  2 12   S 1  16.8919393   -0.0300  16.8919093   Err 0.1D-04          -
 41: 22  6 17 22  5 18   S 1  17.4231733   -0.0037  17.4231696   Err 0.1D-04          -
 42: 22  3 19 22  2 20   S 1   7.1444488   -0.0064   7.1444424   Err 0.1D-04          -
 43: 10  3  7 10  2  9   S 1   8.4657482   -0.0397   8.4657085   Err 0.1D-04          -
 44: 15  2 14 15  1 15   S 1   9.3909229   -0.0088   9.3909140   Err 0.1D-04          -
 45: 21  5 17 21  4 18   S 1  14.2806521    0.0046  14.2806567   Err 0.1D-04          -
 46: 12  5  7 11  5  6   S 1  14.6644695   -0.0002  14.6644693   Err 0.1D-04          -
 47:  4  4  1  3  3  0   S 1  16.1670098    0.0053  16.1670151   Err 0.1D-04          -
Maximum (obs-calc)/err in line  43   0.0000397

RMS deviations (MHz), B and V sorted
 B  V   n splittings MHz
 B  V   n abs. freq. MHz
```

```
 1  1  47         0.019409         0.022713

          Parameters  and  Errors
 BJ          0.609559113 { 0.000000380}
 BK           1.612847423 { 0.000002591}
 B-          0.036744354 { 0.000000651}
 DJ          0.030557E-6 { 0.001253E-6}
 DJK          0.118252E-6 { 0.006955E-6}
 DK          -0.202168E-6 { 0.085871E-6}
 dj          -0.005333E-6 { 0.001047E-6}
 dk          0.002391E-6 { 0.000247E-6}
\F12         -1.765883684 {     derived}
\F          159.806008121 {     derived}  160.122906150 {     derived}
\rho         0.012088984 {     derived}    0.013453592 {     derived}
\beta        0.170945251 {     derived}    3.048780839 {     derived}
\gamma       -2.422318024 {     derived}    3.076354777 {     derived}

 Standard Deviation       0.021585 MHz

------------------------------------ B =  1
 Rotational Constants and Errors (in GHz)
     B_z       2.222406536       0.000002608
     B_x       0.646303467       0.000000694
     B_y       0.572814759       0.000000809
 Ray's kappa   -0.91090
 F0(calc)     158.000000000       0.000000000
 I_alpha        3.198601709       0.000000000
 <(i,x)  <(i,y)  <(i,z)      112.2228      111.9455       32.1209
d<(i,x) d<(i,y) d<(i,z)        0.0000        0.0000        0.0000

 F0(calc)     158.000000000       0.000000000
 I_alpha        3.198601709       0.000000000
 <(i,x)  <(i,y)  <(i,z)      107.7081       88.7153      162.2422
d<(i,x) d<(i,y) d<(i,z)        0.0000        0.0000        0.0000

 V1n_1      7.155838 kj +/- 0.000000 kj         1.709100 kcal +/- 0.000000 kcal
         598.181169 cm +/-   0.0000 cm    s=  49.874422
 V1n_2      5.808392 kj +/- 0.000000 kj         1.387277 kcal +/- 0.000000 kcal
         485.543541 cm +/-   0.0000 cm    s=  40.483059

F(calc)       159.806008121
F(calc)       160.122906150
```

^{18}O Isotopologue XIAM Output

	J K- K+	J K- K+	Sym	calc/GHz	diff/MHz	obs/GHz		
1:	19 5	15 18 6	12 S 4	6.2135821	0.0233	6.2136054	Err 0.1D-04	-
2:	19 5	15 18 6	13 S 4	6.2289476	0.0183	6.2289659	Err 0.1D-04	-
3:	8 1	7 7 2	6 S 1	6.3318295	-0.0330	6.3317965	Err 0.1D-04	-
4:	10 2	9 10 1	10 S 1	6.9278697	0.0259	6.9278956	Err 0.1D-04	-
5:	10 2	9 10 1	10 S 4	6.9277055	0.0158	6.9277214	Err 0.1D-04	-
6:	10 2	9 10 1	10 S 2	6.9277305	-0.0091	6.9277214	Err 0.1D-04	-
7:	10 2	9 10 1	10 S 5	6.9276974	0.0239	6.9277214	Err 0.1D-04	-
8:	10 2	9 10 1	10 S 3	6.9278407	0.0475	6.9278882	Err 0.1D-04	-
9:	4 3	2 4 2	3 S 1	7.8463345	-0.0062	7.8463283	Err 0.1D-04	-
10:	3 2	2 2 1	1 S 1	8.2384555	-0.0205	8.2384350	Err 0.1D-04	-
11:	13 3	11 13 2	12 S 1	8.7372447	-0.0061	8.7372386	Err 0.1D-04	-
12:	16 2	15 16 0	16 S 1	10.1790409	-0.0119	10.1790290	Err 0.1D-04	-
13:	16 2	15 16 0	16 S 3	10.1790180	0.0110	10.1790290	Err 0.1D-04	-
14:	12 9	4 13 8	5 S 1	10.7741816	-0.0087	10.7741729	Err 0.1D-04	-
15:	19 3	17 19 1	18 S 1	11.3507666	0.0086	11.3507752	Err 0.1D-04	-
16:	17 4	13 17 3	15 S 1	11.4372648	-0.0300	11.4372348	Err 0.1D-04	-
17:	17 4	13 17 3	15 S 5	11.4372520	-0.0172	11.4372348	Err 0.1D-04	-
18:	17 4	13 17 3	15 S 3	11.4372207	0.0141	11.4372348	Err 0.1D-04	-
19:	17 4	13 17 3	15 S 2	11.4372002	0.0345	11.4372348	Err 0.1D-04	-
20:	3 3	1 2 2	1 S 3	11.4907667	0.0086	11.4907754	Err 0.1D-04	-
21:	10 0	10 9 0	9 S 1	11.8059380	0.0120	11.8059500	Err 0.1D-04	-
22:	10 0	10 9 0	9 S 3	11.8059342	0.0158	11.8059500	Err 0.1D-04	-
23:	10 0	10 9 0	9 S 2	11.8059312	0.0188	11.8059500	Err 0.1D-04	-
24:	10 0	10 9 0	9 S 5	11.8059272	0.0228	11.8059500	Err 0.1D-04	-
25:	10 0	10 9 0	9 S 4	11.8059275	0.0225	11.8059500	Err 0.1D-04	-
26:	10 5	5 9 5	4 S 1	12.2028702	-0.0402	12.2028301	Err 0.1D-04	-
27:	10 5	5 9 5	4 S 5	12.2028356	-0.0055	12.2028301	Err 0.1D-04	-
28:	10 5	5 9 5	4 S 4	12.2028383	-0.0082	12.2028301	Err 0.1D-04	-
29:	10 5	5 9 5	4 S 2	12.2028395	-0.0094	12.2028301	Err 0.1D-04	-
30:	10 5	5 9 5	4 S 3	12.2028438	-0.0137	12.2028301	Err 0.1D-04	-
31:	12 1	11 11 2	10 S 1	12.3890433	-0.0182	12.3890252	Err 0.1D-04	-
32:	12 1	11 11 2	10 S 3	12.3890624	-0.0372	12.3890252	Err 0.1D-04	-
33:	10 2	8 9 2	7 S 1	12.4749089	0.0124	12.4749213	Err 0.1D-04	-
34:	10 2	8 9 2	7 S 4	12.4749029	0.0184	12.4749213	Err 0.1D-04	-
35:	10 2	8 9 2	7 S 5	12.4748989	0.0224	12.4749213	Err 0.1D-04	-
36:	10 2	8 9 2	7 S 3	12.4749066	0.0147	12.4749213	Err 0.1D-04	-
37:	22 5	17 22 4	18 S 1	12.5916237	0.0217	12.5916454	Err 0.1D-04	-
38:	4 3	1 3 2	2 S 4	12.7195428	-0.0075	12.7195353	Err 0.1D-04	-
39:	11 4	7 10 4	6 S 1	13.4464138	-0.0157	13.4463981	Err 0.1D-04	-
40:	16 5	11 16 4	12 S 4	13.7988318	0.0059	13.7988378	Err 0.1D-04	-
41:	12 5	8 12 4	8 S 3	14.0172996	0.0007	14.0173003	Err 0.1D-04	-

42: 8 5 3 8 4 4 S 1 14.0866496 -0.0328 14.0866168 Err 0.1D-04 -
43: 8 5 4 8 4 5 S 3 14.0864911 0.0400 14.0865311 Err 0.1D-04 -
44: 17 1 16 16 2 14 S 1 14.5062610 -0.0201 14.5062409 Err 0.1D-04 -
45: 12 7 5 11 7 4 S 5 14.6365098 0.0351 14.6365449 Err 0.1D-04 -
46: 12 7 5 11 7 4 S 4 14.6365118 0.0331 14.6365449 Err 0.1D-04 -
47: 12 7 5 11 7 4 S 2 14.6365139 0.0310 14.6365449 Err 0.1D-04 -
48: 12 7 5 11 7 4 S 3 14.6365169 0.0280 14.6365449 Err 0.1D-04 -
49: 12 7 5 11 7 4 S 1 14.6365210 0.0239 14.6365449 Err 0.1D-04 -
50: 12 5 8 11 5 7 S 1 14.6539798 -0.0183 14.6539614 Err 0.1D-04 -
51: 4 4 1 3 3 1 S 3 15.8424489 -0.0271 15.8424218 Err 0.1D-04 -
52: 13 8 5 12 8 4 S 1 15.8541721 -0.0019 15.8541702 Err 0.1D-04 -
53: 13 8 5 12 8 4 S 3 15.8541679 0.0023 15.8541702 Err 0.1D-04 -
54: 13 8 5 12 8 4 S 2 15.8541651 0.0051 15.8541702 Err 0.1D-04 -
55: 13 8 5 12 8 4 S 4 15.8541627 0.0075 15.8541702 Err 0.1D-04 -
56: 13 8 5 12 8 4 S 5 15.8541608 0.0094 15.8541702 Err 0.1D-04 -
57: 13 4 9 12 4 8 S 1 15.9166442 0.0516 15.9166959 Err 0.1D-04 -
58: 10 1 9 9 0 9 S 1 16.3457789 0.0020 16.3457809 Err 0.1D-04 -
59: 10 1 9 9 0 9 S 3 16.3457674 0.0135 16.3457809 Err 0.1D-04 -
60: 10 1 9 9 0 9 S 5 16.3457179 -0.0302 16.3456877 Err 0.1D-04 -
61: 10 1 9 9 0 9 S 2 16.3457288 -0.0411 16.3456877 Err 0.1D-04 -
62: 10 1 9 9 0 9 S 4 16.3457166 -0.0289 16.3456877 Err 0.1D-04 -
63: 20 6 14 20 5 15 S 1 16.9123615 0.0043 16.9123658 Err 0.1D-04 -
64: 9 6 3 9 5 4 S 5 17.2253430 0.0059 17.2253489 Err 0.1D-04 -
65: 8 3 6 7 2 6 S 5 17.6995193 -0.0058 17.6995136 Err 0.1D-04 -
66: 15 10 5 14 10 4 S 1 18.2901457 -0.0228 18.2901229 Err 0.1D-04 -
67: 15 10 5 14 10 4 S 3 18.2901409 -0.0180 18.2901229 Err 0.1D-04 -
68: 15 10 5 14 10 4 S 2 18.2901383 -0.0154 18.2901229 Err 0.1D-04 -
69: 15 10 5 14 10 4 S 4 18.2901355 -0.0126 18.2901229 Err 0.1D-04 -
70: 15 10 5 14 10 4 S 5 18.2901335 -0.0106 18.2901229 Err 0.1D-04 -
71: 14 3 12 13 4 9 S 5 6.1175164 0.0302 6.1175466 Err 0.1D-04 -
72: 14 3 12 13 4 9 S 4 6.1189072 0.0020 6.1189092 Err 0.1D-04 -
73: 14 3 12 13 4 10 S 4 6.1513512 0.0243 6.1513755 Err 0.1D-04 -
74: 15 1 14 15 1 15 S 1 8.3132308 0.0087 8.3132396 Err 0.1D-04 -
75: 12 3 10 12 2 11 S 5 8.5189509 0.0242 8.5189751 Err 0.1D-04 -
76: 7 3 5 6 3 4 S 5 8.5462690 0.0035 8.5462725 Err 0.1D-04 -
77: 15 3 13 15 2 14 S 2 9.2939325 -0.0360 9.2938965 Err 0.1D-04 -
78: 15 3 13 15 2 14 S 4 9.2939006 -0.0041 9.2938965 Err 0.1D-04 -
79: 15 3 13 15 2 14 S 5 9.2938804 0.0161 9.2938965 Err 0.1D-04 -
80: 19 2 18 18 3 15 S 1 9.7390396 -0.0082 9.7390314 Err 0.1D-04 -
81: 19 2 18 18 3 15 S 3 9.7390571 -0.0257 9.7390314 Err 0.1D-04 -
82: 22 2 20 22 2 21 S 1 10.7022044 -0.0392 10.7021652 Err 0.1D-04 -
83: 22 2 20 22 2 21 S 3 10.7021940 -0.0289 10.7021652 Err 0.1D-04 -
84: 22 2 20 22 2 21 S 2 10.7021557 0.0094 10.7021652 Err 0.1D-04 -

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 85: 22  2 20 22  2 21   S 4  10.7021474    0.0178  10.7021652   Err 0.1D-04          -
 86: 22  2 20 22  2 21   S 5  10.7021433    0.0219  10.7021652   Err 0.1D-04          -
 87: 12  1 11 11  2  9   S 4  10.7132598    0.0022  10.7132620   Err 0.1D-04          -
 88: 12  1 11 11  2  9   S 4  10.7132598    0.0072  10.7132671   Err 0.1D-04          -
 89: 12  1 11 11  2  9   S 5  10.7132549    0.0105  10.7132653   Err 0.1D-04          -
 90: 11  4  7 11  3  8   S 4  10.7517885    0.0179  10.7518064   Err 0.1D-04          -
 91: 10  4  7 10  3  7   S 5  10.8157274   -0.0336  10.8156938   Err 0.1D-04          -
 92: 14  2 12 13  3 10   S 2  11.1365029    0.0159  11.1365188   Err 0.1D-04          -
 93: 14  2 12 13  3 10   S 5  11.1365164    0.0134  11.1365299   Err 0.1D-04          -
 94: 14  2 12 13  3 10   S 4  11.1365636   -0.0448  11.1365188   Err 0.1D-04          -
 95: 19  4 16 19  3 17   S 2  11.4842012   -0.0165  11.4841847   Err 0.1D-04          -
 96: 13 10  3 14  9  5   S 5  12.6916164    0.0091  12.6916255   Err 0.1D-04          -
 97: 12  5  8 12  4  9   S 2  14.0296823    0.0500  14.0297323   Err 0.1D-04          -
 98: 12  4  8 11  4  7   S 4  14.6786685   -0.0452  14.6786233   Err 0.1D-04          -
 99:  4  4  0  3  3  0   S 5  15.8447296   -0.0275  15.8447021   Err 0.1D-04          -
Maximum (obs-calc)/err in line  57   0.0000516

 RMS deviations (MHz), B and V sorted
  B  V   n splittings MHz
  B  V   n abs. freq. MHz
  1  1  99         0.022650         0.024938

          Parameters  and  Errors
 BJ          0.608895198 { 0.000000340}
 BK          1.567303446 { 0.000001071}
 B-          0.038974513 { 0.000000104}
 DJ          0.024211E-6 { 0.000862E-6}
 DJK         0.060632E-6 { 0.002689E-6}
 DK          0.031350E-6 { 0.008691E-6}
 dj         -0.003060E-6 { 0.000124E-6}
 dk          0.001858E-6 { 0.000080E-6}
\F12         -1.751087702 {     derived}
\F          159.792633373 {     derived}  160.084948935 {     derived}
 V1n         18049.678645 {   15.269148}   14573.172607 {    3.683868}
\rho         0.011940510 {     derived}    0.013198588 {     derived}
\beta        0.169127784 {     derived}    3.048562957 {     derived}
\gamma      -2.436661372 {     derived}    3.045351649 {     derived}

 Standard Deviation       0.024024 MHz

------------------------------------ B =  1
 Rotational Constants and Errors (in GHz)
    B_z       2.176198644       0.000001152
```

```
     B_x       0.647869711       0.000000320
     B_y       0.569920685       0.000000387
 Ray's kappa   -0.90294
 F0(calc)     158.000000000       0.000000000
 I_alpha        3.198601709       0.000000000
 <(i,x)  <(i,y)  <(i,z)      111.9212      111.1649       31.2893
d<(i,x) d<(i,y) d<(i,z)        0.0000        0.0000        0.0000

 F0(calc)     158.000000000       0.000000000
 I_alpha        3.198601709       0.000000000
 <(i,x)  <(i,y)  <(i,z)      107.3153       88.1282      162.5774
d<(i,x) d<(i,y) d<(i,z)        0.0000        0.0000        0.0000

 V1n_1      7.202387 kj +/- 0.006093 kj         1.720218 kcal +/- 0.001455 kcal
         602.072388 cm +/-   0.5093 cm    s=  50.203061
 V1n_2      5.815152 kj +/- 0.001470 kj         1.388891 kcal +/- 0.000351 kcal
         486.108645 cm +/-   0.1229 cm    s=  40.533568

F(calc)       159.792633373
F(calc)       160.084948935
```

EQ2 Kraitchman Output

```
_____________________________________________________________________________
____
|                                                     |
|   KRA  -  SINGLE ISOTOPIC SUBSTITUTION - Various permutations           |
|          of Kraitchman's equations for symmetric/asymmetric tops        |

|_____________________________________________________________________________
_____|
 version 4a.IV.2017                              Zbigniew KISIEL

 ---------------------------------------------------------------------------
    R-Carvon EQ2
 ---------------------------------------------------------------------------

  parent species
 Planar calculation will be made from I.a and I.b

 ---------------------------------------------------------------------------
  C(1)
 ---------------------------------------------------------------------------
```

The parent species:

X, Y, Z =	2237.17540000	656.28010000	579.63780000
eX, eY, eZ =	0.00040000	0.00010000	0.00010000
IX, IY, IZ =	225.90048545	770.06602653	871.88759757
eIX,eIY,eIZ =	0.00004039	0.00011734	0.00015042
PX, PY, PZ =	708.02656932	163.86102824	62.03945721

Mass = 150.10446507

The isotopic species:

X, Y, Z =	2216.19300000	656.11010000	578.14200000
eX, eY, eZ =	0.00200000	0.00040000	0.00070000
IX, IY, IZ =	228.03925872	770.26555284	874.14339193
eIX,eIY,eIZ =	0.00020579	0.00046960	0.00105839
PX, PY, PZ =	708.18484303	165.95854891	62.08070981

Mass change = 1.00335484
Total mass = 151.10781991
M DM/(M+DM) = 0.99669257

KRAITCHMAN RESULTS:

	a	b			
PLANAR:	0.44654	+- 0.00054	1.46515	+- 0.00007	
+Costain err.	0.44654	+- 0.00340	1.46515	+- 0.00103	

	a	b	c			
NONPLANAR:	0.39771	+- 0.00075	1.45060	+- 0.00021	0.20555	+- 0.00148
+Costain err.	0.39771	+- 0.00385	1.45060	+- 0.00105	0.20555	+- 0.00745

R= 1.51811 +- 0.00175

DIX,DIY,DIZ =	2.13877327	0.19952631	2.25579437
DPX,DPY,DPZ =	0.15827370	2.09752067	0.04125260
IXY,IXZ,IYZ =	-544.16554108	-645.98711211	-101.82157103

C(2)

The parent species:

X, Y, Z =	2237.17540000	656.28010000	579.63780000
eX, eY, eZ =	0.00040000	0.00010000	0.00010000
IX, IY, IZ =	225.90048545	770.06602653	871.88759757
eIX,eIY,eIZ =	0.00004039	0.00011734	0.00015042
PX, PY, PZ =	708.02656932	163.86102824	62.03945721

Mass = 150.10446507

The isotopic species:

X, Y, Z =	2213.23500000	655.27750000	577.25610000
eX, eY, eZ =	0.00100000	0.00030000	0.00030000
IX, IY, IZ =	228.34403437	771.24425743	875.48491718
eIX,eIY,eIZ =	0.00010317	0.00035309	0.00045499
PX, PY, PZ =	709.19257012	166.29234706	62.05168731

Mass change = 1.00335484
Total mass = 151.10781991
M DM/(M+DM) = 0.99669257

KRAITCHMAN RESULTS:

	a	b	
PLANAR:	1.08482 +- 0.00017	1.56747 +- 0.00004	
+Costain err.	1.08482 +- 0.00139	1.56747 +- 0.00096	

	a	b	c
NONPLANAR:	1.07918 +- 0.00014	1.56343 +- 0.00010	0.11219 +- 0.00141
+Costain err.	1.07918 +- 0.00140	1.56343 +- 0.00096	0.11219 +- 0.01344

R= 1.90303 +- 0.00137

DIX,DIY,DIZ =	2.44354891	1.17823090	3.59731961
DPX,DPY,DPZ =	1.16600080	2.43131881	0.01223010
IXY,IXZ,IYZ =	-544.16554108	-645.98711211	-101.82157103

C(3)

The parent species:

X, Y, Z =	2237.17540000	656.28010000	579.63780000
eX, eY, eZ =	0.00040000	0.00010000	0.00010000
IX, IY, IZ =	225.90048545	770.06602653	871.88759757
eIX,eIY,eIZ =	0.00004039	0.00011734	0.00015042
PX, PY, PZ =	708.02656932	163.86102824	62.03945721

Mass = 150.10446507

The isotopic species:

X, Y, Z =	2234.67710000	653.18530000	577.03860000
eX, eY, eZ =	0.00060000	0.00030000	0.00030000
IX, IY, IZ =	226.15303522	773.71460886	875.81490892
eIX,eIY,eIZ =	0.00006072	0.00035536	0.00045533
PX, PY, PZ =	711.68824128	164.12666764	62.02636758

Mass change = 1.00335484
Total mass = 151.10781991
M DM/(M+DM) = 0.99669257

KRAITCHMAN RESULTS:

	a	b
PLANAR:	1.91285 +- 0.00010	0.50506 +- 0.00007
+Costain err.	1.91285 +- 0.00079	0.50506 +- 0.00297

	a	b	c
NONPLANAR:	1.91627 +- 0.00008	0.51802 +- 0.00030	0.11507*i+- 0.00135
+Costain err.	1.91627 +- 0.00079	0.51802 +- 0.00291	0.11507*i+- 0.01310

R= 1.98172 +- 0.00132

DIX,DIY,DIZ =	0.25254977	3.64858232	3.92731135
DPX,DPY,DPZ =	3.66167195	0.26563940	-0.01308963
IXY,IXZ,IYZ =	-544.16554108	-645.98711211	-101.82157103

C(4)

The parent species:

X, Y, Z =	2237.17540000	656.28010000	579.63780000
eX, eY, eZ =	0.00040000	0.00010000	0.00010000
IX, IY, IZ =	225.90048545	770.06602653	871.88759757
eIX,eIY,eIZ =	0.00004039	0.00011734	0.00015042
PX, PY, PZ =	708.02656932	163.86102824	62.03945721

Mass = 150.10446507

The isotopic species:

X, Y, Z =	2229.83800000	654.69210000	577.91430000
eX, eY, eZ =	0.00100000	0.00050000	0.00050000
IX, IY, IZ =	226.64382296	771.93387380	874.48780710
eIX,eIY,eIZ =	0.00010164	0.00058954	0.00075659
PX, PY, PZ =	709.88892897	164.59887813	62.04494483

Mass change = 1.00335484
Total mass = 151.10781991
M DM/(M+DM) = 0.99669257

KRAITCHMAN RESULTS:

	a	b			
PLANAR:	1.36802	+- 0.00022	0.86508	+- 0.00006	
+Costain err.	1.36802	+- 0.00112	0.86508	+- 0.00174	

	a	b	c			
NONPLANAR:	1.36601	+- 0.00018	0.86185	+- 0.00029	0.07458	+- 0.00334
+Costain err.	1.36601	+- 0.00111	0.86185	+- 0.00176	0.07458	+- 0.02039

R= 1.61689 +- 0.00163

DIX,DIY,DIZ =	0.74333751	1.86784727	2.60020954
DPX,DPY,DPZ =	1.86235965	0.73784989	0.00548762

IXY,IXZ,IYZ = -544.16554108 -645.98711211 -101.82157103

C(5)

The parent species:

X, Y, Z =	2237.17540000	656.28010000	579.63780000
eX, eY, eZ =	0.00040000	0.00010000	0.00010000
IX, IY, IZ =	225.90048545	770.06602653	871.88759757
eIX,eIY,eIZ =	0.00004039	0.00011734	0.00015042
PX, PY, PZ =	708.02656932	163.86102824	62.03945721

Mass = 150.10446507

The isotopic species:

X, Y, Z =	2226.07300000	656.21750000	578.95600000
eX, eY, eZ =	0.00200000	0.00040000	0.00040000
IX, IY, IZ =	227.02715001	770.13948714	872.91436465
eIX,eIY,eIZ =	0.00020397	0.00046944	0.00060310
PX, PY, PZ =	708.01335089	164.90101376	62.12613625

Mass change = 1.00335484
Total mass = 151.10781991
M DM/(M+DM) = 0.99669257

KRAITCHMAN RESULTS:

	a	b	
PLANAR:	0.27120 +- 0.00089	1.06328 +- 0.00010	
+Costain err.	0.27120 +- 0.00560	1.06328 +- 0.00141	

	a	b	c
NONPLANAR:	0.11504*i+- 0.00177	1.02104 +- 0.00020	0.29640 +- 0.00070
+Costain err.	0.11504*i+- 0.01316	1.02104 +- 0.00148	0.29640 +- 0.00511

R= 1.05695 +- 0.00248

DIX,DIY,DIZ = 1.12666456 0.07346060 1.02676708
DPX,DPY,DPZ = -0.01321843 1.03998552 0.08667904
IXY,IXZ,IYZ = -544.16554108 -645.98711211 -101.82157103

C(6)

The parent species:

X, Y, Z = 2237.17540000 656.28010000 579.63780000
eX, eY, eZ = 0.00040000 0.00010000 0.00010000
IX, IY, IZ = 225.90048545 770.06602653 871.88759757
eIX,eIY,eIZ = 0.00004039 0.00011734 0.00015042
PX, PY, PZ = 708.02656932 163.86102824 62.03945721

Mass = 150.10446507

The isotopic species:

X, Y, Z = 2235.87100000 655.48900000 579.10100000
eX, eY, eZ = 0.00800000 0.00300000 0.00300000
IX, IY, IZ = 226.03227507 770.99540786 872.69579728
eIX,eIY,eIZ = 0.00080875 0.00352864 0.00452095
PX, PY, PZ = 708.82946503 163.86633225 62.16594283

Mass change = 1.00335484
Total mass = 151.10781991
M DM/(M+DM) = 0.99669257

KRAITCHMAN RESULTS:

a b

PLANAR: 0.96553 +- 0.00183 0.36394 +- 0.00112
+Costain err. 0.96553 +- 0.00240 0.36394 +- 0.00427

a b c

NONPLANAR: 0.89744 +- 0.00162 0.07296 +- 0.01993 0.35647 +- 0.00408
+Costain err. 0.89744 +- 0.00233 0.07296 +- 0.02863 0.35647 +- 0.00586

R= 0.96839 +- 0.00374

DIX,DIY,DIZ = 0.13178962 0.92938132 0.80819971
DPX,DPY,DPZ = 0.80289571 0.00530401 0.12648562
IXY,IXZ,IYZ = -544.16554108 -645.98711211 -101.82157103

C(7)

The parent species:

X, Y, Z = 2237.17540000 656.28010000 579.63780000
eX, eY, eZ = 0.00040000 0.00010000 0.00010000
IX, IY, IZ = 225.90048545 770.06602653 871.88759757
eIX,eIY,eIZ = 0.00004039 0.00011734 0.00015042
PX, PY, PZ = 708.02656932 163.86102824 62.03945721

Mass = 150.10446507

The isotopic species:

X, Y, Z = 2232.92900000 646.53830000 571.77510000
eX, eY, eZ = 0.00100000 0.00020000 0.00030000
IX, IY, IZ = 226.33008434 781.66909663 883.87726031
eIX,eIY,eIZ = 0.00010136 0.00024180 0.00046375
PX, PY, PZ = 719.60813630 164.26912401 62.06096033

Mass change = 1.00335484
Total mass = 151.10781991
M DM/(M+DM) = 0.99669257

KRAITCHMAN RESULTS:

a b

PLANAR: 3.41063 +- 0.00004 0.66349 +- 0.00008
+Costain err. 3.41063 +- 0.00044 0.66349 +- 0.00226

a b c

NONPLANAR: 3.40748 +- 0.00004 0.64659 +- 0.00022 0.14849 +- 0.00098
+Costain err. 3.40748 +- 0.00044 0.64659 +- 0.00233 0.14849 +- 0.01015

R= 3.47146 +- 0.00075

DIX,DIY,DIZ =	0.42959889	11.60307010	11.98966274
DPX,DPY,DPZ =	11.58156698	0.40809577	0.02150312
IXY,IXZ,IYZ =	-544.16554108	-645.98711211	-101.82157103

C(9)

The parent species:

X, Y, Z =	2237.17540000	656.28010000	579.63780000
eX, eY, eZ =	0.00040000	0.00010000	0.00010000
IX, IY, IZ =	225.90048545	770.06602653	871.88759757
eIX,eIY,eIZ =	0.00004039	0.00011734	0.00015042
PX, PY, PZ =	708.02656932	163.86102824	62.03945721

Mass = 150.10446507

The isotopic species:

X, Y, Z =	2236.90960000	651.36280000	575.81370000
eX, eY, eZ =	0.00070000	0.00020000	0.00020000
IX, IY, IZ =	225.92732800	775.87944675	877.67798665
eIX,eIY,eIZ =	0.00007070	0.00023823	0.00030485
PX, PY, PZ =	713.81505270	163.86293395	62.06439405

Mass change = 1.00335484
Total mass = 151.10781991
M DM/(M+DM) = 0.99669257

KRAITCHMAN RESULTS:

	a	b	
PLANAR:	2.41504 +- 0.00006	0.16498 +- 0.00025	
+Costain err.	2.41504 +- 0.00062	0.16498 +- 0.00910	

	a	b	c	
NONPLANAR:	2.40986 +- 0.00005	0.04395 +- 0.00253	0.15888 +- 0.00070	
+Costain err.	2.40986 +- 0.00062	0.04395 +- 0.03422	0.15888 +- 0.00947	

R= 2.41550 +- 0.00108

DIX,DIY,DIZ =	0.02684255	5.81342022	5.79038908
DPX,DPY,DPZ =	5.78848338	0.00190570	0.02493684
IXY,IXZ,IYZ =	-544.16554108	-645.98711211	-101.82157103

C(10)

The parent species:

X, Y, Z =	2237.17540000	656.28010000	579.63780000
eX, eY, eZ =	0.00040000	0.00010000	0.00010000
IX, IY, IZ =	225.90048545	770.06602653	871.88759757
eIX,eIY,eIZ =	0.00004039	0.00011734	0.00015042
PX, PY, PZ =	708.02656932	163.86102824	62.03945721

Mass = 150.10446507

The isotopic species:

X, Y, Z =	2222.19300000	647.70150000	573.87390000
eX, eY, eZ =	0.00100000	0.00050000	0.00060000
IX, IY, IZ =	227.42354462	780.26530570	880.64470069
eIX,eIY,eIZ =	0.00010234	0.00060233	0.00092074
PX, PY, PZ =	716.74323088	163.90146981	63.52207482

Mass change = 1.00335484
Total mass = 151.10781991
M DM/(M+DM) = 0.99669257

KRAITCHMAN RESULTS:

	a	b	
PLANAR:	3.19445 +- 0.00010	1.24770 +- 0.00005	
+Costain err.	3.19445 +- 0.00048	1.24770 +- 0.00120	

	a	b	c
NONPLANAR:	2.95379 +- 0.00010	0.20156 +- 0.00140	1.22809 +- 0.00023

+Costain err. 2.95379 +- 0.00052 0.20156 +- 0.00757 1.22809 +- 0.00124

R= 3.20526 +- 0.00082

DIX,DIY,DIZ = 1.52305917 10.19927917 8.75710313
DPX,DPY,DPZ = 8.71666156 0.04044157 1.48261761
IXY,IXZ,IYZ = -544.16554108 -645.98711211 -101.82157103

C(11)

The parent species:

X, Y, Z = 2237.17540000 656.28010000 579.63780000
eX, eY, eZ = 0.00040000 0.00010000 0.00010000
IX, IY, IZ = 225.90048545 770.06602653 871.88759757
eIX,eIY,eIZ = 0.00004039 0.00011734 0.00015042
PX, PY, PZ = 708.02656932 163.86102824 62.03945721

Mass = 150.10446507

The isotopic species:

X, Y, Z = 2222.39900000 646.30140000 572.81600000
eX, eY, eZ = 0.00200000 0.00040000 0.00050000
IX, IY, IZ = 227.40246414 781.95561529 882.27111132
eIX,eIY,eIZ = 0.00020465 0.00048396 0.00077012
PX, PY, PZ = 718.41213123 163.85898008 63.54348406

Mass change = 1.00335484
Total mass = 151.10781991
M DM/(M+DM) = 0.99669257

KRAITCHMAN RESULTS:

a b

PLANAR: 3.44907 +- 0.00007 1.24092 +- 0.00009
+Costain err. 3.44907 +- 0.00044 1.24092 +- 0.00121

a b c

NONPLANAR: 3.22425 +- 0.00007 0.04542*i+- 0.00528 1.23824 +- 0.00020
+Costain err. 3.22425 +- 0.00047 0.04542*i+- 0.03344 1.23824 +- 0.00123

R= 3.45355 +- 0.00076

DIX,DIY,DIZ = 1.50197869 11.88958876 10.38351375
DPX,DPY,DPZ = 10.38556191 -0.00204816 1.50402685
IXY,IXZ,IYZ = -544.16554108 -645.98711211 -101.82157103

Oxygen-18

The parent species:

X, Y, Z = 2237.17540000 656.28010000 579.63780000
eX, eY, eZ = 0.00040000 0.00010000 0.00010000
IX, IY, IZ = 225.90048545 770.06602653 871.88759757
eIX,eIY,eIZ = 0.00004039 0.00011734 0.00015042
PX, PY, PZ = 708.02656932 163.86102824 62.03945721

Mass = 150.10446507

The isotopic species:

X, Y, Z = 2176.19900000 647.86970000 569.92070000
eX, eY, eZ = 0.00100000 0.00030000 0.00040000
IX, IY, IZ = 232.23014481 780.06273314 886.75320777
eIX,eIY,eIZ = 0.00010671 0.00036121 0.00062237
PX, PY, PZ = 717.29289805 169.46030972 62.76983509

Mass change = 2.00424499
Total mass = 152.10871006
M DM/(M+DM) = 1.97783626

KRAITCHMAN RESULTS:

a b

PLANAR: 2.23508 +- 0.00004 1.80529 +- 0.00002
+Costain err. 2.23508 +- 0.00067 1.80529 +- 0.00083

a b c

NONPLANAR: 2.15212 +- 0.00004 1.69073 +- 0.00006 0.62863 +- 0.00016
+Costain err. 2.15212 +- 0.00070 1.69073 +- 0.00089 0.62863 +- 0.00239

R= 2.80809 +- 0.00093

DIX,DIY,DIZ = 6.32965936 9.99670661 14.86561021
DPX,DPY,DPZ = 9.26632873 5.59928148 0.73037788
IXY,IXZ,IYZ = -544.16554108 -645.98711211 -101.82157103

EQ2 EVAL Output

| E V A L - Internals and their errors from Cartesians |

version 20.V.2020 Zbigniew KISIEL

WARNING:

The EVAL uncertainties are evaluated by assuming that
the correlation matrix is a unit matrix.

The EVAL uncertainties may thus differ significantly
(but typically by not more than 30% either way)
from uncertainties in explicitly fitted internals
corresponding to the input Cartesians.

!
! EQ2, KRA coordinates
!

INPUT CARTESIANS:

C(1)	-0.39729	0.00387	1.45046	0.00106	0.20582	0.00749
C(2)	1.07918	0.00140	1.56343	0.00096	0.11219	0.01344
C(3)	1.91627	0.00079	0.51802	0.00291	0.00000	0.00000
C(4)	1.36601	0.00111	-0.86185	0.00176	-0.07458	0.02039

C(5)	0.00000	0.00000	-1.02087	0.00148	0.29631	0.00511
C(6)	-0.90170	0.00169	0.04693	0.03239	-0.35097	0.00433
C(7)	3.40740	0.00044	0.64606	0.00233	-0.14836	0.01014
C(9)	-2.40988	0.00062	0.00000	0.00000	-0.17036	0.00883
C(10)	-2.95379	0.00052	0.20156	0.00757	-1.22809	0.00124
C(11)	-3.22425	0.00047	0.00000	0.00000	1.23824	0.00123
Oxygen	2.15212	0.00070	-1.69073	0.00089	-0.62863	0.00239

CALCULATED INTERNALS:

```
!
!  Bond lengths
!
        C(1)  C(2)   =    1.48374 +- 0.00421
        C(2)  C(3)   =    1.34395 +- 0.00282
        C(3)  C(4)   =    1.48741 +- 0.00335
        C(4)  C(5)   =    1.42437 +- 0.00558
        C(5)  C(6)   =    1.54020 +- 0.02268
        C(6)  C(1)   =    1.59196 +- 0.02876
        C(3)  C(7)   =    1.50395 +- 0.00138
        C(6)  C(9)   =    1.51968 +- 0.00236
        C(9)  C(10)  =    1.51398 +- 0.00830
        C(9)  C(11)  =    1.62707 +- 0.00773
        C(4)  Oxygen =    1.26964 +- 0.00909
!
!  Bond angles
!
    C(1)  C(2)  C(3)   =  124.46130 +- 0.12209
    C(2)  C(3)  C(4)   =  119.69535 +- 0.11037
    C(3)  C(4)  C(5)   =  116.44265 +- 0.42035
    C(4)  C(5)  C(6)   =  112.00112 +- 0.70615
    C(5)  C(6)  C(1)   =  106.18522 +- 0.41849
    C(6)  C(1)  C(2)   =  111.12175 +- 0.43585
    C(2)  C(3)  C(7)   =  124.02541 +- 0.21937
    C(4)  C(3)  C(7)   =  116.15653 +- 0.21493
    C(1)  C(6)  C(9)   =  107.46418 +- 1.42113
    C(5)  C(6)  C(9)   =  120.64086 +- 1.56590
    C(6)  C(9)  C(11)  =  126.84235 +- 0.51433
    C(6)  C(9)  C(10)  =  118.06221 +- 0.50381
!
! Dihedral Angles
!
C(1)  C(2)  C(3)  C(4)   =   1.68820 +- 1.65596
```

C(2) C(3) C(4) C(5) = -14.55460 +- 1.82206
C(3) C(4) C(5) C(6) = 46.41695 +- 1.70900
C(4) C(5) C(6) C(1) = -62.17360 +- 0.83649
C(5) C(6) C(1) C(2) = 47.63105 +- 0.78328
C(6) C(1) C(2) C(3) = -20.25726 +- 1.44948
C(1) C(2) C(3) C(7) = 177.50124 +- 0.85989
C(5) C(4) C(3) C(7) = 169.31091 +- 0.98167
C(4) C(5) C(6) C(9) = 175.47316 +- 1.21604
C(2) C(1) C(6) C(9) = 177.99556 +- 0.84219
C(5) C(6) C(9) C(11) = 56.86185 +- 2.14002
C(1) C(6) C(9) C(11) = -64.87351 +- 1.59972
C(1) C(6) C(9) C(10) = -73.92797 +- 1.36987
C(5) C(6) C(9) C(10) = 47.80739 +- 1.91255
C(2) C(3) C(4) Oxygen = 156.83784 +- 1.00277
C(6) C(5) C(4) Oxygen = -123.35270 +- 1.63016

S5. EQ3 Assignments and Outputs of Structure Evaluation - Isotopologue Overview

Ground Vibrational State	$^{13}C_1$		$^{13}C_2$		$^{13}C_3$		$^{13}C_4$	
	Experiment	Theory	Experiment	Theory	Experiment	Theory	Experiment	Theory
A (MHz)	2,190.5411 (15)	2,183.2	2,189.3269 (13)	2,182.0	2,210.42070 (97)	2,203.0	2,205.50445 (97)	2198.1
B (MHz)	684.40670 (51)	673.6	683.31181 (54)	672.5	681.06329 (36)	670.3	682.78659 (39)	672.0
C (MHz)	553.25447 (48)	548.7	552.48059 (59)	547.9	552.30343 (33)	547.8	553.17679 (40)	548.6
V_{3_1} (cm^{-1})	[539]		[539]		539 (2)		539 (1)	
δ_1 (radian)	[1.988]		[1.988]		[1.988]		[1.988]	
ε_1 (radian)	[0.518]		[0.518]		[0.518]		[0.518]	
V_{3_2} (cm^{-1})	[484.85]		[484.85]		484.64 (46)		484.92 (17)	
δ_2 (radian)	[0.158]		[0.158]		[0.158]		[0.158]	
ε_2 (radian)	[1.897]		[1.897]		[1.897]		[1.897]	
ν_{RMS} (kHz)	26.7		22.7		25.3		25.9	
Number of Transitions	10		10		22		26	
	$^{13}C_5$		$^{13}C_6$		$^{13}C_7$		$^{13}C_9$	
	Experiment	Theory	Experiment	Theory	Experiment	Theory	Experiment	Theory
A (MHz)	2,202.4230 (11)	2,195.0	2,211.7917 (16)	2,204.4	2,209.1097 (68)	2,201.7	2,212.74758 (27)	2,205.3
B (MHz)	684.29154 (28)	673.5	683.64551 (39)	672.9	674.04712 (43)	663.4	679.1537 (37)	668.5
C (MHz)	554.21170 (36)	549.7	544.18937 (41)	549.6	547.50723 (40)	543.0	551.1774 (39)	546.6
V_{3_1} (cm^{-1})	[539]		[539]		539.12 (83)		539 (1)	
δ_1 (radian)	[1.988]		[1.988]		[1.988]		[1.988]	
ε_1 (radian)	[0.518]		[0.518]		[0.518]		[0.518]	
V_{3_2} (cm^{-1})	[484.85]		[484.85]		486.52 (64)		485 (3)	
δ_2 (radian)	[0.158]		[0.158]		[0.158]		[0.158]	
ε_2 (radian)	[1.897]		[1.897]		[1.897]		[1.897]	
ν_{RMS} (kHz)	24.1		24.5		27.6		25.2	
Number of Transitions	21		11		21		17	
	$^{13}C_{10}$		$^{13}C_{11}$		^{18}O			
	Experiment	Theory	Experiment	Theory	Experiment	Theory		
A (MHz)	2,197.3535 (21)	2,190.0	2,201.7809 (15)	2,194.4	2,148.8408 (21)	2,141.6		
B (MHz)	675.58716 (63)	664.9	675.11857 (43)	664.5	676.68972 (50)	666.0		
C (MHz)	548.22199 (63)	543.7	548.25966 (47)	543.7	545.66703 (49)	541.2		
V_{3_1} (cm^{-1})	[539]		[539]		542 (2)			
δ_1 (radian)	[1.988]		[1.988]		[1.988]			
ε_1 (radian)	[0.518]		[0.518]		[0.518]			
V_{3_2} (cm^{-1})	[484.85]		[484.85]		485.92 (62)			
δ_2 (radian)	[0.158]		[0.158]		[0.158]			
ε_2 (radian)	[1.897]		[1.897]		[1.897]			
ν_{RMS} (kHz)	27.2		29.8		26.8			
Number of Transitions	9		16		14			

Parent XIAM Output

```
   J K- K+  J K- K+    Sym   calc/GHz  diff/MHz     obs/GHz
 1:  5  1  5  4  1  4   S 4   5.8401660    0.0110   5.8401770   Err 0.1D-04          -
 2:  5  1  5  4  1  4   S 2   5.8401719    0.0051   5.8401770   Err 0.1D-04          -
 3:  5  1  5  4  1  4   S 1   5.8401723    0.0047   5.8401770   Err 0.1D-04          -
 4:  4  1  4  3  0  3   S 1   5.9208929    0.0012   5.9208941   Err 0.1D-04          -
 5:  6  0  6  5  1  5   S 1   6.3503895   -0.0434   6.3503461   Err 0.1D-04          -
 6: 16  3 13 16  2 14   S 1   6.8348399   -0.0454   6.8347945   Err 0.1D-04          -
 7: 16  3 13 16  2 14   S 3   6.8347929    0.0025   6.8347954   Err 0.1D-04          -
 8: 16  3 13 16  2 14   S 2   6.8347709    0.0245   6.8347954   Err 0.1D-04          -
 9:  6  2  5  5  2  4   S 2   7.3999897   -0.0235   7.3999663   Err 0.1D-04          -
10:  6  2  5  5  2  4   S 4   7.3999694   -0.0017   7.3999677   Err 0.1D-04          -
```

11: 6 2 5 5 2 4 S 1 7.3999666 0.0011 7.3999677 Err 0.1D-04 -
12: 6 2 5 5 2 4 S 3 7.3999567 0.0110 7.3999677 Err 0.1D-04 -
13: 6 2 5 5 2 4 S 5 7.3999901 -0.0217 7.3999684 Err 0.1D-04 -
14: 6 5 1 5 5 0 S 1 7.4553492 0.0024 7.4553516 Err 0.1D-04 -
15: 6 5 1 5 5 0 S 2 7.4553451 0.0065 7.4553516 Err 0.1D-04 -
16: 6 5 1 5 5 0 S 5 7.4553320 0.0196 7.4553516 Err 0.1D-04 -
17: 6 3 4 6 2 4 S 2 7.5870877 0.0046 7.5870922 Err 0.1D-04 -
18: 7 0 7 6 1 6 S 1 7.6633928 -0.0069 7.6633859 Err 0.1D-04 -
19: 4 3 2 4 2 2 S 2 7.8701364 0.0080 7.8701444 Err 0.1D-04 -
20: 4 3 2 4 2 2 S 4 7.8713085 -0.0221 7.8712864 Err 0.1D-04 -
21: 19 3 16 19 3 17 S 2 8.1387992 0.0270 8.1388262 Err 0.1D-04 -
22: 7 1 6 6 1 5 S 1 9.0056928 0.0464 9.0057392 Err 0.1D-04 -
23: 8 4 5 7 4 3 S 3 9.9653740 -0.0195 9.9653545 Err 0.1D-04 -
24: 12 2 11 12 1 12 S 1 10.0035689 0.0109 10.0035797 Err 0.1D-04 -
25: 13 2 12 13 1 13 S 3 10.8166388 -0.0056 10.8166332 Err 0.1D-04 -
26: 7 4 4 7 3 5 S 4 11.1091145 0.0318 11.1091463 Err 0.1D-04 -
27: 5 4 2 5 3 3 S 1 11.1321936 -0.0110 11.1321826 Err 0.1D-04 -
28: 5 4 1 5 3 3 S 3 11.1339331 0.0116 11.1339447 Err 0.1D-04 -
29: 10 1 10 9 1 9 S 1 11.5256777 -0.0092 11.5256686 Err 0.1D-04 -
30: 10 1 10 9 1 9 S 4 11.5256717 -0.0031 11.5256686 Err 0.1D-04 -
31: 10 1 10 9 1 9 S 5 11.5256637 0.0048 11.5256686 Err 0.1D-04 -
32: 10 1 10 9 1 9 S 2 11.5256738 -0.0060 11.5256678 Err 0.1D-04 -
33: 5 2 3 4 1 4 S 1 11.8878217 0.0475 11.8878691 Err 0.1D-04 -
34: 19 4 15 18 5 14 S 3 12.4538557 0.0055 12.4538611 Err 0.1D-04 -
35: 15 2 14 15 1 15 S 1 12.5327503 0.0029 12.5327531 Err 0.1D-04 -
36: 15 2 14 15 1 15 S 2 12.5325339 -0.0287 12.5325053 Err 0.1D-04 -
37: 15 2 14 15 1 15 S 3 12.5325217 -0.0164 12.5325053 Err 0.1D-04 -
38: 20 4 17 20 3 18 S 1 13.8328062 0.0356 13.8328418 Err 0.1D-04 -
39: 20 4 17 20 3 18 S 3 13.8327269 0.0239 13.8327508 Err 0.1D-04 -
40: 5 3 2 4 2 2 S 3 14.1040561 -0.0263 14.1040298 Err 0.1D-04 -
41: 18 5 14 18 4 15 S 5 14.1855547 0.0011 14.1855558 Err 0.1D-04 -
42: 19 5 15 19 4 16 S 1 14.2966317 0.0158 14.2966475 Err 0.1D-04 -
43: 20 5 16 20 4 17 S 1 14.4616892 0.0085 14.4616977 Err 0.1D-04 -
44: 12 4 8 11 4 7 S 2 15.0716834 -0.0165 15.0716669 Err 0.1D-04 -
45: 14 0 14 13 1 13 S 3 15.9645341 0.0032 15.9645373 Err 0.1D-04 -
46: 12 2 11 11 1 10 S 4 15.9814789 -0.0004 15.9814785 Err 0.1D-04 -
47: 12 2 11 11 1 10 S 5 15.9814739 0.0046 15.9814785 Err 0.1D-04 -
48: 14 1 14 13 0 13 S 1 16.0336569 0.0331 16.0336900 Err 0.1D-04 -
49: 20 6 14 20 5 15 S 3 16.3455141 -0.0240 16.3454900 Err 0.1D-04 -
50: 13 2 12 12 1 11 S 3 16.7932325 -0.0319 16.7932006 Err 0.1D-04 -
51: 13 2 11 12 2 10 S 5 16.8029717 -0.0131 16.8029586 Err 0.1D-04 -
52: 13 2 11 12 2 10 S 3 16.8029833 -0.0247 16.8029586 Err 0.1D-04 -
53: 12 6 7 12 5 7 S 2 17.3866930 -0.0245 17.3866685 Err 0.1D-04 -

```
 54: 12  6  7 12  5  8   S 5  17.4051875    0.0447  17.4052322   Err 0.1D-04          -
 55:  6  4  3  5  3  2   S 5  18.5733459   -0.0015  18.5733444   Err 0.1D-04          -
 56: 12  3  9 12  2 10   S 1   6.0968770   -0.0460   6.0968310   Err 0.1D-04          -
 57: 22  4 18 22  4 19   S 1   6.1723844   -0.0307   6.1723537   Err 0.1D-04          -
 58:  8  6  2  9  5  4   S 4   6.2873121   -0.0103   6.2873018   Err 0.1D-04          -
 59:  8  6  2  9  5  4   S 3   6.2867623   -0.0215   6.2867408   Err 0.1D-04          -
 60:  6  3  3  5  3  2   S 1   7.4877345   -0.0400   7.4876945   Err 0.1D-04          -
 61: 22  5 18 22  4 18   S 3   8.8129751    0.0143   8.8129894   Err 0.1D-04          -
 62: 14  1 13 14  1 14   S 4  11.0750236    0.0079  11.0750315   Err 0.1D-04          -
 63:  9  4  6  9  3  7   S 3  11.1087290    0.0263  11.1087553   Err 0.1D-04          -
 64:  6  4  2  6  3  4   S 2  11.1318760   -0.0373  11.1318387   Err 0.1D-04          -
 65:  3  3  0  2  2  1   S 3  11.6899441   -0.0042  11.6899398   Err 0.1D-04          -
 66:  4  3  1  3  2  2   S 2  12.9495810    0.0143  12.9495953   Err 0.1D-04          -
 67: 15  5 10 15  4 11   S 2  13.5357718    0.0103  13.5357822   Err 0.1D-04          -
 68: 12 10  2 13  9  4   S 4  14.0693322   -0.0206  14.0693116   Err 0.1D-04          -
 69: 18  1 17 18  0 18   S 4  15.1182979   -0.0000  15.1182979   Err 0.1D-04          -
 70: 15  0 15 14  0 14   S 4  17.1129550    0.0115  17.1129665   Err 0.1D-04          -
 71: 16  6 11 16  5 11   S 3  17.1325797    0.0249  17.1326046   Err 0.1D-04          -
Maximum (obs-calc)/err in line  33   0.0000475

 RMS deviations (MHz), B and V sorted
  B  V   n splittings MHz
  B  V   n abs. freq. MHz
  1  1  71         0.021830         0.024290

          Parameters  and  Errors
 BJ          0.619625431 { 0.000000209}
 BK           1.593166149 { 0.000000509}
 B-          0.064894950 { 0.000000059}
\F12         -0.845407858 {     derived}
\F          158.893139628 {     derived}  160.208830266 {     derived}
 V1n         16008.412209 {  141.958211}   14537.151768 {    7.042534}
\rho          0.006596801 {     derived}    0.013849933 {     derived}
\beta         0.622710311 {     derived}    3.101612089 {     derived}
\gamma        0.408083379 {     derived}    1.967654077 {     derived}
 epsil        0.490096478 { 0.040270110}    1.898204000 {     fixed  }
 delta        1.178166745 { 0.021246186}    2.987406149 { 0.014790442}

 Standard Deviation       0.023361 MHz

------------------------------------ B =  1
 Rotational Constants and Errors (in GHz)
    B_z       2.212791580       0.000000584
```

```
    B_x       0.684520381       0.000000221
    B_y       0.554730481       0.000000214
 Ray's kappa   -0.84344
 F0(calc)     158.000000000       0.000000000
 I_alpha        3.198601709       0.000000000
 <(i,x)  <(i,y)  <(i,z)       35.3977       64.2215       67.5040
d<(i,x) d<(i,y) d<(i,z)        2.4566        2.3219        1.2173

 F0(calc)     158.000000000       0.000000000
 I_alpha        3.198601709       0.000000000
 <(i,x)  <(i,y)  <(i,z)       92.8309       81.6385      171.1658
d<(i,x) d<(i,y) d<(i,z)        0.2699        0.8015        0.8474

 V1n_1      6.387858 kj +/- 0.056646 kj         1.525676 kcal +/- 0.013529 kcal
        533.983079 cm +/-   4.7352 cm    s=  44.777577
 V1n_2      5.800779 kj +/- 0.002810 kj         1.385458 kcal +/- 0.000671 kcal
        484.907120 cm +/-   0.2349 cm    s=  40.662274

F(calc)       158.893139628
F(calc)       160.208830266
```

$^{13}C_1$ XIAM Output

```
    J K- K+  J K- K+    Sym   calc/GHz  diff/MHz     obs/GHz
  1:  8  2  7  7  2  6   S 1   9.8023906   -0.0179   9.8023727   Err 0.1D-04          -
  2: 13  1 12 13  1 13   S 1  10.0432839    0.0019  10.0432858   Err 0.1D-04          -
  3:  9 K   1  8 K   1   S 2  10.3756493    0.0167  10.3756660   Err 0.1D-04          -
  4: 16  4 13 16  3 14   S 1  11.8999613   -0.0212  11.8999401   Err 0.1D-04          -
  5: 19 13  7 20 12  9   S 3  14.3587402    0.0065  14.3587467   Err 0.1D-04          -
  6: 13  2 12 12  1 11   S 1  16.6986423   -0.0175  16.6986249   Err 0.1D-04          -
  7: 14  3 12 13  3 11   S 1  17.3588495    0.0253  17.3588748   Err 0.1D-04          -
  8: 14  4 11 13  4 10   S 1  17.5271529    0.0187  17.5271716   Err 0.1D-04          -
  9:  5  2  4  4  2  3   S 1   6.1701027   -0.0385   6.1700642   Err 0.1D-04          -
 10: 13  3 10 13  2 11   S 1   5.9684040   -0.0073   5.9683967   Err 0.2D-04          -
 Maximum (obs-calc)/err in line   9   0.0000385

 RMS deviations (MHz), B and V sorted
  B  V   n splittings MHz
  B  V   n abs. freq. MHz
  1  1  10          0.020697          0.026906

          Parameters  and  Errors
 BJ           0.618830585 { 0.000000455}
```

```
 BK          1.571710529 { 0.000001151}
 B-          0.065576116 { 0.000000198}
\F12        -0.884351568 {     derived}
\F         158.915272309 {     derived}  160.185131624 {     derived}
\rho         0.006778447 {     derived}    0.013703962 {     derived}
\beta        2.548616396 {     derived}    0.041195582 {     derived}
\gamma       0.431314831 {     derived}    1.967133195 {     derived}

 Standard Deviation       0.026720 MHz

------------------------------------ B =  1
 Rotational Constants and Errors (in GHz)
    B_z       2.190541114       0.000001451
    B_x       0.684406700       0.000000514
    B_y       0.553254469       0.000000478
 Ray's kappa   -0.83979
 F0(calc)     158.000000000       0.000000000
 I_alpha        3.198601709       0.000000000
 <(i,x)  <(i,y)  <(i,z)       37.4014       63.1113      113.9194
d<(i,x) d<(i,y) d<(i,z)        0.0000        0.0000        0.0000

 F0(calc)     158.000000000       0.000000000
 I_alpha        3.198601709       0.000000000
 <(i,x)  <(i,y)  <(i,z)       92.8831       81.4493        9.0305
d<(i,x) d<(i,y) d<(i,z)        0.0000        0.0000        0.0000

 V1n_1      6.451030 kj +/- 0.000000 kj         1.540764 kcal +/- 0.000000 kcal
         539.263862 cm +/-   0.0000 cm    s=  45.214104
 V1n_2      5.800159 kj +/- 0.000000 kj         1.385310 kcal +/- 0.000000 kcal
         484.855317 cm +/-   0.0000 cm    s=  40.652267

F(calc)       158.915272309
F(calc)       160.185131624
```

$^{13}C_2$ XIAM Output

```
     J K- K+  J K- K+    Sym   calc/GHz  diff/MHz     obs/GHz
  1: 10  4  6 10  3  7    S 1  10.5154176    0.0211  10.5154388   Err 0.1D-04          -
  2:  3  3  0  2  2  1    S 1  11.5699635   -0.0346  11.5699289   Err 0.1D-04          -
  3: 15  3 13 15  1 14    S 1  11.5852177    0.0022  11.5852199   Err 0.1D-04          -
  4: 10  8  2  9  8  1    S 1  12.3931807    0.0132  12.3931939   Err 0.1D-04          -
  5: 12  1 11 11  2 10    S 1  13.4418838   -0.0072  13.4418766   Err 0.1D-04          -
  6:  5  3  2  4  2  3    S 1  14.0966956    0.0191  14.0967147   Err 0.1D-04          -
  7: 12  2 11 11  2 10    S 1  14.4867058   -0.0202  14.4866855   Err 0.1D-04          -
```

```
  8: 12  8  4 11  8  3   S 1  14.8832504    0.0190  14.8832694   Err 0.1D-04          -
  9: 20  6 14 20  5 15   S 1  16.0507220   -0.0007  16.0507212   Err 0.1D-04          -
 10: 20  6 15 20  5 16   S 1  16.7382123   -0.0080  16.7382043   Err 0.1D-04          -
Maximum (obs-calc)/err in line   2   0.0000346

 RMS deviations (MHz), B and V sorted
  B  V   n splittings MHz
  B  V   n abs. freq. MHz
  1  1  10         0.017613         0.022897

          Parameters  and  Errors
 BJ          0.617896199 { 0.000000484}
 BK           1.571430746 { 0.000001196}
 B-          0.065415607 { 0.000000284}
\F12         -0.883851514 {     derived}
\F         158.914205871 {     derived}  160.183888508 {     derived}
\rho         0.006772552 {     derived}    0.013696345 {     derived}
\beta        2.549085033 {     derived}    0.041159580 {     derived}
\gamma       0.431391285 {     derived}    1.967061514 {     derived}

 Standard Deviation       0.022739 MHz

------------------------------------ B =  1
 Rotational Constants and Errors (in GHz)
     B_z       2.189326945       0.000001256
     B_x       0.683311806       0.000000536
     B_y       0.552480592       0.000000585
 Ray's kappa   -0.84014
 F0(calc)     158.000000000       0.000000000
 I_alpha        3.198601709       0.000000000
 <(i,x)  <(i,y)  <(i,z)       37.4014       63.1113      113.9194
d<(i,x) d<(i,y) d<(i,z)        0.0000        0.0000        0.0000

 F0(calc)     158.000000000       0.000000000
 I_alpha        3.198601709       0.000000000
 <(i,x)  <(i,y)  <(i,z)       92.8831       81.4493        9.0305
d<(i,x) d<(i,y) d<(i,z)        0.0000        0.0000        0.0000

 V1n_1      6.451030 kj +/- 0.000000 kj         1.540764 kcal +/- 0.000000 kcal
         539.263862 cm +/-   0.0000 cm    s=  45.214407
 V1n_2      5.800159 kj +/- 0.000000 kj         1.385310 kcal +/- 0.000000 kcal
         484.855317 cm +/-   0.0000 cm    s=  40.652540
```

F(calc) 158.914205871
F(calc) 160.183888508

$^{13}C_3$ XIAM Output

```
   J K- K+  J K- K+    Sym   calc/GHz  diff/MHz     obs/GHz
  1: 13  3 11 13  1 12   S 1  10.8882862    0.0293  10.8883154   Err 0.1D-04          -
  2: 17  2 15 17  1 16   S 1  10.8795880   -0.0036  10.8795844   Err 0.1D-04          -
  3:  7  4  3  7  3  4   S 5  11.0667559   -0.0106  11.0667453   Err 0.1D-04          -
  4:  9  3  6  8  3  5   S 2  11.2954588   -0.0199  11.2954389   Err 0.1D-04          -
  5:  3  3  1  2  2  0   S 3  11.6647604   -0.0045  11.6647559   Err 0.1D-04          -
  6: 14  5  9 14  4 11   S 1  14.1425038   -0.0094  14.1424944   Err 0.1D-04          -
  7: 17  4 14 17  2 15   S 1  14.2515049   -0.0386  14.2514663   Err 0.1D-04          -
  8: 17  4 14 17  2 15   S 3  14.2514840   -0.0177  14.2514663   Err 0.1D-04          -
  9:  8  5  3  8  4  4   S 1  14.2905157   -0.0379  14.2904777   Err 0.1D-04          -
 10: 10  2  9  9  1  8   S 5  14.4111335    0.0239  14.4111574   Err 0.1D-04          -
 11: 10  2  9  9  1  8   S 2  14.4111405    0.0186  14.4111592   Err 0.1D-04          -
 12: 13  1 12 12  2 11   S 1  14.7915695    0.0115  14.7915810   Err 0.1D-04          -
 13: 13  1 12 12  2 11   S 3  14.7915396    0.0414  14.7915810   Err 0.1D-04          -
 14: 12  5  7 11  5  6   S 5  14.9107014   -0.0185  14.9106829   Err 0.1D-04          -
 15: 12  5  7 11  5  6   S 1  14.9119790    0.0252  14.9120041   Err 0.1D-04          -
 16: 12  5  7 11  5  6   S 3  14.9114546   -0.0021  14.9114525   Err 0.1D-04          -
 17: 16 12  4 17 11  6   S 2  15.5600517    0.0263  15.5600780   Err 0.1D-04          -
 18: 16 12  5 17 11  7   S 5  15.5560982   -0.0146  15.5560835   Err 0.1D-04          -
 19: 14  1 13 13  2 12   S 1  16.1628316   -0.0183  16.1628133   Err 0.1D-04          -
 20:  7  5  2  6  5  1   S 1   8.6612881   -0.0250   8.6612631   Err 0.1D-04          -
 21: 16  3 14 15  4 11   S 5   7.3941184   -0.0064   7.3941119   Err 0.1D-04          -
 22: 13  8  5 14  7  8   S 1   6.4783936    0.0174   6.4784110   Err 0.1D-04          -
Maximum (obs-calc)/err in line  13   0.0000414

 RMS deviations (MHz), B and V sorted
  B  V   n splittings MHz
  B  V   n abs. freq. MHz
  1  1  22         0.021589         0.026495

          Parameters  and  Errors
 BJ          0.616683357 { 0.000000314}
 BK           1.593737342 { 0.000000760}
 B-          0.064379929 { 0.000000136}
\F12         -0.892514277 {     derived}
\F         158.916336923 {     derived}  160.205123651 {     derived}
 V1n         16154.198976 {   47.471796}   14529.193717 {   13.764905}
```

\rho 0.006811714 { derived} 0.013828067 { derived}
\beta 2.554798920 { derived} 0.040736183 { derived}
\gamma 0.432522489 { derived} 1.966003207 { derived}

Standard Deviation 0.025315 MHz

---------- B = 1
Rotational Constants and Errors (in GHz)
B_z 2.210420700 0.000000973
B_x 0.681063286 0.000000358
B_y 0.552303428 0.000000325
Ray's kappa -0.84469
F0(calc) 158.000000000 0.000000000
I_alpha 3.198601709 0.000000000
<(i,x) <(i,y) <(i,z) 37.4014 63.1113 113.9194
d<(i,x) d<(i,y) d<(i,z) 0.0000 0.0000 0.0000

F0(calc) 158.000000000 0.000000000
I_alpha 3.198601709 0.000000000
<(i,x) <(i,y) <(i,z) 92.8831 81.4493 9.0305
d<(i,x) d<(i,y) d<(i,z) 0.0000 0.0000 0.0000

V1n_1 6.446031 kj +/- 0.018943 kj 1.539570 kcal +/- 0.004524 kcal
538.846001 cm +/- 1.5835 cm s= 45.178766
V1n_2 5.797603 kj +/- 0.005493 kj 1.384700 kcal +/- 0.001312 kcal
484.641668 cm +/- 0.4591 cm s= 40.634082

F(calc) 158.916336923
F(calc) 160.205123651

$^{13}C_4$ XIAM Output

	J K- K+	J K- K+	Sym	calc/GHz	diff/MHz	obs/GHz		
1:	18 4 14	17 5 13	S 1	10.4912476	0.0158	10.4912634	Err 0.1D-04	-
2:	9 4 5	9 3 6	S 2	10.8229401	0.0334	10.8229735	Err 0.1D-04	-
3:	7 4 4	7 3 5	S 1	11.0747520	-0.0409	11.0747111	Err 0.1D-04	-
4:	7 4 3	7 3 5	S 3	11.0772786	0.0218	11.0773004	Err 0.1D-04	-
5:	6 4 3	6 3 4	S 4	11.0787654	0.0111	11.0787765	Err 0.1D-04	-
6:	21 3 18	21 2 19	S 1	11.4646460	-0.0152	11.4646308	Err 0.1D-04	-
7:	10 1 10	9 0 9	S 1	11.7215931	-0.0237	11.7215694	Err 0.1D-04	-
8:	10 1 10	9 0 9	S 2	11.7215729	-0.0035	11.7215694	Err 0.1D-04	-
9:	10 1 10	9 0 9	S 4	11.7215901	-0.0205	11.7215697	Err 0.1D-04	-
10:	10 1 10	9 0 9	S 3	11.7215970	-0.0273	11.7215697	Err 0.1D-04	-
11:	16 1 15	16 1 16	S 1	13.1101181	-0.0128	13.1101052	Err 0.1D-04	-

```
 12: 13  5  9 13  4  9   S 2  13.8730312    0.0145  13.8730456   Err 0.1D-04          -
 13: 14  5  9 14  4 11   S 1  14.0863421   -0.0089  14.0863333   Err 0.1D-04          -
 14: 13  5  9 13  4 10   S 2  14.0862294   -0.0016  14.0862278   Err 0.1D-04          -
 15: 13  5  8 13  4 10   S 1  14.1029822    0.0212  14.1030034   Err 0.1D-04          -
 16: 11  5  6 11  4  7   S 1  14.1027037    0.0369  14.1027405   Err 0.1D-04          -
 17: 17  1 16 17  1 17   S 1  14.1032615   -0.0085  14.1032530   Err 0.1D-04          -
 18:  7  5  2  7  4  3   S 3  14.2532195   -0.0403  14.2531792   Err 0.1D-04          -
 19:  7  5  3  7  4  4   S 3  14.2528191    0.0367  14.2528558   Err 0.1D-04          -
 20: 18  5 13 18  4 15   S 2  14.4077896    0.0086  14.4077983   Err 0.1D-04          -
 21: 13  1 12 12  2 11   S 1  14.8402979    0.0294  14.8403272   Err 0.1D-04          -
 22: 13  1 12 12  2 11   S 4  14.8403279   -0.0007  14.8403272   Err 0.1D-04          -
 23: 12  2 11 11  1 10   S 1  15.9323345   -0.0032  15.9323313   Err 0.1D-04          -
 24: 15  4 11 15  3 12   S 4   8.8791523   -0.0254   8.8791269   Err 0.1D-04          -
 25: 15  4 11 15  3 12   S 1   8.8794527   -0.0238   8.8794288   Err 0.1D-04          -
 26: 17  4 13 17  3 14   S 1   8.1848183   -0.0163   8.1848020   Err 0.1D-04          -
Maximum (obs-calc)/err in line   3   0.0000409

RMS deviations (MHz), B and V sorted
 B  V   n splittings MHz
 B  V   n abs. freq. MHz
 1  1  26         0.022699         0.027064

          Parameters  and  Errors
 BJ          0.617981689 { 0.000000386}
 BK           1.587522759 { 0.000000825}
 B-          0.064804897 { 0.000000084}
\F12         -0.890492234 {     derived}
\F         158.916777850 {     derived}  160.200195828 {     derived}
 V1n         16170.124065 {   37.156860}   14537.612956 {    5.234508}
\rho         0.006806160 {     derived}    0.013797403 {     derived}
\beta        2.552681903 {     derived}    0.040897114 {     derived}
\gamma       0.432162188 {     derived}    1.966339828 {     derived}

 Standard Deviation       0.025881 MHz

------------------------------------ B =  1
 Rotational Constants and Errors (in GHz)
     B_z       2.205504448       0.000000970
     B_x       0.682786586       0.000000391
     B_y       0.553176792       0.000000399
 Ray's kappa   -0.84312
 F0(calc)     158.000000000       0.000000000
 I_alpha       3.198601709       0.000000000
```

```
 <(i,x)  <(i,y)  <(i,z)      37.4014      63.1113     113.9194
d<(i,x) d<(i,y) d<(i,z)       0.0000       0.0000       0.0000

 F0(calc)    158.000000000      0.000000000
 I_alpha       3.198601709      0.000000000
 <(i,x)  <(i,y)  <(i,z)      92.8831      81.4493       9.0305
d<(i,x) d<(i,y) d<(i,z)       0.0000       0.0000       0.0000

 V1n_1      6.452386 kj +/- 0.014827 kj        1.541088 kcal +/- 0.003541 kcal
        539.377205 cm +/-   1.2394 cm    s=  45.223178
 V1n_2      5.800963 kj +/- 0.002089 kj        1.385502 kcal +/- 0.000499 kcal
        484.922503 cm +/-   0.1746 cm    s=  40.657515

F(calc)      158.916777850
F(calc)      160.200195828
```

$^{13}C_5$ XIAM Output

```
   J K- K+  J K- K+    Sym   calc/GHz  diff/MHz     obs/GHz
  1:  9  5  5  8  5  4   S 2  11.1992637    0.0108  11.1992745   Err 0.1D-04          -
  2: 15  3 13 15  1 14   S 1  11.6197470   -0.0050  11.6197420   Err 0.1D-04          -
  3: 17  4 14 17  3 15   S 1  12.3010503   -0.0013  12.3010491   Err 0.1D-04          -
  4: 18  3 16 18  1 17   S 1  13.5383174    0.0221  13.5383395   Err 0.1D-04          -
  5: 18  3 16 18  1 17   S 4  13.5381164   -0.0123  13.5381041   Err 0.1D-04          -
  6: 11 10  1 10 10  0   S 1  13.6562193    0.0092  13.6562285   Err 0.1D-04          -
  7: 11 10  1 10 10  0   S 2  13.6562173    0.0112  13.6562285   Err 0.1D-04          -
  8: 11 10  1 10 10  0   S 4  13.6561991    0.0294  13.6562285   Err 0.1D-04          -
  9: 11 10  1 10 10  0   S 3  13.6561975    0.0310  13.6562285   Err 0.1D-04          -
 10: 11 10  1 10 10  0   S 5  13.6561954    0.0331  13.6562285   Err 0.1D-04          -
 11: 11  5  6 10  5  5   S 1  13.7135177   -0.0177  13.7135000   Err 0.1D-04          -
 12:  8  5  3  8  4  4   S 1  14.1938670    0.0225  14.1938895   Err 0.1D-04          -
 13:  8  5  4  8  4  5   S 5  14.1938836    0.0059  14.1938895   Err 0.1D-04          -
 14: 17  3 14 16  4 13   S 3  14.6163241   -0.0317  14.6162923   Err 0.1D-04          -
 15: 17  3 14 16  4 13   S 2  14.6168365   -0.0194  14.6168172   Err 0.1D-04          -
 16: 17  3 14 16  4 13   S 5  14.6167915    0.0257  14.6168172   Err 0.1D-04          -
 17: 13  1 12 12  2 11   S 3  14.8826157   -0.0016  14.8826141   Err 0.1D-04          -
 18: 13  1 12 12  2 11   S 2  14.8827078   -0.0086  14.8826992   Err 0.1D-04          -
 19: 12  2 11 11  1 10   S 1  15.9425125   -0.0492  15.9424634   Err 0.1D-04          -
 20: 15  6  9 15  5 10   S 1  17.1204093   -0.0143  17.1203951   Err 0.1D-04          -
 21: 11  6  6 11  5  7   S 1  17.3284565   -0.0197  17.3284368   Err 0.1D-04          -
Maximum (obs-calc)/err in line  19   0.0000492

RMS deviations (MHz), B and V sorted
 B  V   n splittings MHz
```

```
 B  V   n abs. freq. MHz
 1  1  21         0.021703         0.024804

          Parameters  and  Errors
 BJ          0.619251617 { 0.000000306}
 BK           1.583171340 { 0.000000956}
 B-          0.065039920 { 0.000000105}
\F12         -0.889210912 {     derived}
\F         158.917426136 {     derived}  160.197119279 {     derived}
\rho         0.006804099 {     derived}    0.013778202 {     derived}
\beta        2.551045009 {     derived}    0.041032828 {     derived}
\gamma       0.432035700 {     derived}    1.966458105 {     derived}

 Standard Deviation       0.024122 MHz

------------------------------------ B =  1
 Rotational Constants and Errors (in GHz)
     B_z       2.202422957       0.000001084
     B_x       0.684291537       0.000000279
     B_y       0.554211696       0.000000362
 Ray's kappa   -0.84216
 F0(calc)     158.000000000       0.000000000
 I_alpha        3.198601709       0.000000000
 <(i,x)  <(i,y)  <(i,z)       37.4014       63.1113      113.9194
d<(i,x) d<(i,y) d<(i,z)        0.0000        0.0000       0.0000

 F0(calc)     158.000000000       0.000000000
 I_alpha        3.198601709       0.000000000
 <(i,x)  <(i,y)  <(i,z)       92.8831       81.4493       9.0305
d<(i,x) d<(i,y) d<(i,z)        0.0000        0.0000       0.0000

 V1n_1      6.451030 kj +/- 0.000000 kj         1.540764 kcal +/- 0.000000 kcal
        539.263862 cm +/-   0.0000 cm    s=  45.213491
 V1n_2      5.800159 kj +/- 0.000000 kj         1.385310 kcal +/- 0.000000 kcal
        484.855317 cm +/-   0.0000 cm    s=  40.651716

F(calc)       158.917426136
F(calc)       160.197119279
```

$^{13}C_6$ XIAM Output

```
    J K- K+  J K- K+    Sym   calc/GHz  diff/MHz     obs/GHz
  1:  8  7  1  7  7  0   S 1   9.9272482   -0.0136   9.9272346   Err 0.1D-04          -
  2:  5  3  3  4  2  2   S 1  14.0872932   -0.0007  14.0872925   Err 0.1D-04          -
```

```
  3: 17  1 16 17  0 17   S 1  14.1174514    0.0135  14.1174649   Err 0.1D-04          -
  4: 17  3 14 16  4 13   S 1  14.4865382    0.0039  14.4865421   Err 0.1D-04          -
  5: 13  0 13 12  1 12   S 1  14.8211058   -0.0090  14.8210968   Err 0.1D-04          -
  6: 12  6  6 11  6  5   S 1  14.9350321   -0.0285  14.9350035   Err 0.1D-04          -
  7: 13  1 12 12  1 11   S 1  15.9622550    0.0391  15.9622941   Err 0.1D-04          -
  8: 19  6 13 19  5 14   S 1  16.6299750   -0.0110  16.6299640   Err 0.1D-04          -
  9: 15  1 15 14  0 14   S 1  17.1132470   -0.0002  17.1132468   Err 0.1D-04          -
 10: 19  4 15 19  3 16   S 1   7.9857440    0.0261   7.9857701   Err 0.1D-04          -
 11: 11  1 10 11  0 11   S 1   7.8708840   -0.0240   7.8708599   Err 0.1D-04          -
 Maximum (obs-calc)/err in line   7   0.0000391

 RMS deviations (MHz), B and V sorted
  B  V   n splittings MHz
  B  V   n abs. freq. MHz
  1  1  11         0.019519         0.024842

          Parameters  and  Errors
 BJ          0.618917443 { 0.000000382}
 BK           1.592874267 { 0.000001536}
 B-          0.064728070 { 0.000000123}
\F12         -0.893070740 {     derived}
\F         158.918609735 {     derived}  160.206554155 {     derived}
\rho         0.006822430 {     derived}    0.013836710 {     derived}
\beta        2.553369526 {     derived}    0.040852093 {     derived}
\gamma       0.432379636 {     derived}    1.966136621 {     derived}

 Standard Deviation       0.024468 MHz

------------------------------------ B =  1
 Rotational Constants and Errors (in GHz)
     B_z       2.211791710       0.000001645
     B_x       0.683645513       0.000000388
     B_y       0.554189373       0.000000414
 Ray's kappa   -0.84380
 F0(calc)     158.000000000       0.000000000
 I_alpha        3.198601709       0.000000000
 <(i,x)  <(i,y)  <(i,z)       37.4014       63.1113      113.9194
d<(i,x) d<(i,y) d<(i,z)        0.0000        0.0000        0.0000

 F0(calc)     158.000000000       0.000000000
 I_alpha        3.198601709       0.000000000
 <(i,x)  <(i,y)  <(i,z)       92.8831       81.4493        9.0305
d<(i,x) d<(i,y) d<(i,z)        0.0000        0.0000        0.0000
```

V1n_1 6.451030 kj +/- 0.000000 kj 1.540764 kcal +/- 0.000000 kcal
539.263862 cm +/- 0.0000 cm s= 45.213154
V1n_2 5.800159 kj +/- 0.000000 kj 1.385310 kcal +/- 0.000000 kcal
484.855317 cm +/- 0.0000 cm s= 40.651413

F(calc) 158.918609735
F(calc) 160.206554155

$^{13}C_7$ XIAM Output

	J K- K+	J K- K+	Sym	calc/GHz	diff/MHz	obs/GHz	
1:	15 2	14 15 1	15 S 1	12.3764099	-0.0149	12.3763950	Err 0.1D-04 -
2:	11 8 3	10 8 2	S 1	13.4773641	-0.0341	13.4773300	Err 0.1D-04 -
3:	11 7 4	10 7 3	S 1	13.4856534	0.0063	13.4856597	Err 0.1D-04 -
4:	9 2 8	8 1 7	S 1	13.6001796	-0.0209	13.6001586	Err 0.1D-04 -
5:	9 2 8	8 1 7	S 3	13.6001730	-0.0144	13.6001586	Err 0.1D-04 -
6:	15 5 10	15 4 12	S 1	14.1848021	-0.0391	14.1847630	Err 0.1D-04 -
7:	17 5 12	17 4 14	S 1	14.2967424	0.0064	14.2967488	Err 0.1D-04 -
8:	6 5 1	6 4 2	S 4	14.3639682	0.0300	14.3639982	Err 0.1D-04 -
9:	12 10 3	13 9 4	S 1	14.4018594	-0.0275	14.4018319	Err 0.1D-04 -
10:	12 5 7	11 5 7	S 3	14.7697666	0.0229	14.7697895	Err 0.1D-04 -
11:	22 6 16	22 5 17	S 1	15.7477906	-0.0042	15.7477863	Err 0.1D-04 -
12:	19 1 18	19 1 19	S 5	15.8581740	0.0355	15.8582095	Err 0.1D-04 -
13:	6 4 3	5 3 2	S 1	18.5163031	-0.0024	18.5163007	Err 0.1D-04 -
14:	19 14 6	20 13 8	S 5	18.5739989	0.0334	18.5740323	Err 0.1D-04 -
15:	19 14 6	20 13 8	S 2	18.5744378	-0.0047	18.5744331	Err 0.1D-04 -
16:	19 4 16	18 5 13	S 1	8.9962022	0.0024	8.9962046	Err 0.1D-04 -
17:	7 3 5	7 2 6	S 1	8.2278019	-0.0202	8.2277817	Err 0.1D-04 -
18:	17 3 15	16 4 12	S 4	7.8409336	0.0342	7.8409678	Err 0.1D-04 -
19:	21 6 16	22 3 19	S 1	7.7078484	0.0195	7.7078679	Err 0.1D-04 -
20:	16 9 8	17 8 10	S 2	6.1894195	0.0125	6.1894320	Err 0.1D-04 -
21:	17 5 13	18 2 16	S 4	6.1795658	-0.0330	6.1795329	Err 0.1D-04 -

Maximum (obs-calc)/err in line 6 0.0000391

RMS deviations (MHz), B and V sorted
B V n splittings MHz
B V n abs. freq. MHz
1 1 21 0.023344 0.028902

Parameters and Errors
BJ 0.610777178 { 0.000000399}
BK 1.598332478 { 0.000000724}
B- 0.063269945 { 0.000000118}

\F12 -0.891981916 { derived}
\F 158.910641942 { derived} 160.203676010 { derived}
V1n 16162.508844 { 24.775604} 14585.450079 { 19.176155}
\rho 0.006788057 { derived} 0.013819675 { derived}
\beta 2.559159325 { derived} 0.040397000 { derived}
\gamma 0.433144390 { derived} 1.965423194 { derived}

Standard Deviation 0.027620 MHz

---------- B = 1
Rotational Constants and Errors (in GHz)
B_z 2.209109655 0.000001047
B_x 0.674047123 0.000000434
B_y 0.547507233 0.000000397
Ray's kappa -0.84769
F0(calc) 158.000000000 0.000000000
I_alpha 3.198601709 0.000000000
<(i,x) <(i,y) <(i,z) 37.4014 63.1113 113.9194
d<(i,x) d<(i,y) d<(i,z) 0.0000 0.0000 0.0000

F0(calc) 158.000000000 0.000000000
I_alpha 3.198601709 0.000000000
<(i,x) <(i,y) <(i,z) 92.8831 81.4493 9.0305
d<(i,x) d<(i,y) d<(i,z) 0.0000 0.0000 0.0000

V1n_1 6.449347 kj +/- 0.009886 kj 1.540362 kcal +/- 0.002361 kcal
539.123188 cm +/- 0.8264 cm s= 45.203626
V1n_2 5.820051 kj +/- 0.007652 kj 1.390061 kcal +/- 0.001828 kcal
486.518178 cm +/- 0.6396 cm s= 40.792877

F(calc) 158.910641942
F(calc) 160.203676010

$^{13}C_9$ XIAM Output

	J K- K+	J K- K+	Sym	calc/GHz	diff/MHz	obs/GHz		
1:	11 4 7	11 3 8	S 1	10.4982876	-0.0164	10.4982712	Err 0.1D-04	-
2:	14 3 12	14 1 13	S 1	11.2047881	0.0272	11.2048153	Err 0.1D-04	-
3:	15 3 13	15 1 14	S 5	11.6285425	0.0033	11.6285458	Err 0.1D-04	-
4:	15 3 13	15 1 14	S 4	11.6285581	-0.0122	11.6285458	Err 0.1D-04	-
5:	15 1 14	15 0 15	S 1	12.0355616	0.0134	12.0355750	Err 0.1D-04	-
6:	16 1 15	16 1 16	S 1	13.0331648	-0.0216	13.0331432	Err 0.1D-04	-
7:	18 3 16	18 1 17	S 2	13.4860205	0.0211	13.4860416	Err 0.2D-04	-
8:	18 3 16	18 1 17	S 4	13.4859944	0.0472	13.4860416	Err 0.2D-04	-

```
  9: 15 11  4 16 10  6   S 1  13.7382388    0.0012  13.7382400   Err 0.1D-04          -
 10: 19  2 18 19  1 19   S 1  16.0538152   -0.0201  16.0537951   Err 0.1D-04          -
 11: 18 13  6 19 12  8   S 5  16.4119227   -0.0010  16.4119217   Err 0.1D-04          -
 12:  5  4  2  4  3  1   S 3  17.3346880    0.0020  17.3346900   Err 0.1D-04          -
 13:  5  4  2  4  3  1   S 1  17.3367903   -0.0118  17.3367785   Err 0.1D-04          -
 14: 15  1 14 14  2 13   S 1  17.4228258   -0.0160  17.4228098   Err 0.1D-04          -
 15: 15  1 14 14  2 13   S 3  17.4227939    0.0158  17.4228098   Err 0.1D-04          -
 16:  2  2  0  1  1  1   S 1   7.3251717   -0.0078   7.3251639   Err 0.1D-04          -
 17:  2  2  0  1  1  1   S 3   7.3252387    0.0344   7.3252731   Err 0.1D-04          -
Maximum (obs-calc)/err in line  17   0.0000344

 RMS deviations (MHz), B and V sorted
  B  V   n splittings MHz
  B  V   n abs. freq. MHz
  1  1  17         0.018358         0.025918

          Parameters  and  Errors
 BJ          0.615165587 { 0.000003785}
 BK           1.597580196 { 0.000005190}
 B-          0.063988148 { 0.000000193}
 DJ          0.004125E-6 { 0.008972E-6}
 DJK         -0.029242E-6 { 0.032068E-6}
\F12         -0.893470044 {     derived}
\F         158.915282177 {     derived}  160.207435300 {     derived}
 V1n         16146.382669 {   33.205639}   14526.320868 {   81.984523}
\rho         0.006811118 {     derived}    0.013842539 {     derived}
\beta        2.556514809 {     derived}    0.040605947 {     derived}
\gamma       0.432814424 {     derived}    1.965730776 {     derived}

 Standard Deviation       0.025231 MHz

------------------------------------ B =  1
 Rotational Constants and Errors (in GHz)
     B_z       2.212745783       0.000002739
     B_x       0.679153735       0.000003691
     B_y       0.551177439       0.000003886
 Ray's kappa   -0.84596
 F0(calc)     158.000000000       0.000000000
 I_alpha        3.198601709       0.000000000
 <(i,x)  <(i,y)  <(i,z)       37.4014       63.1113      113.9194
d<(i,x) d<(i,y) d<(i,z)        0.0000        0.0000        0.0000

 F0(calc)     158.000000000       0.000000000
```

```
 I_alpha        3.198601709       0.000000000
 <(i,x)  <(i,y)  <(i,z)       92.8831       81.4493       9.0305
d<(i,x) d<(i,y) d<(i,z)        0.0000        0.0000        0.0000

 V1n_1      6.442912 kj +/- 0.013250 kj        1.538825 kcal +/- 0.003165 kcal
        538.585277 cm +/-   1.1076 cm    s=  45.157206
 V1n_2      5.796457 kj +/- 0.032714 kj        1.384426 kcal +/- 0.007814 kcal
        484.545840 cm +/-   2.7347 cm    s=  40.626317

F(calc)       158.915282177
F(calc)       160.207435300
```

$^{13}C_{10}$ XIAM Output

```
    J K- K+  J K- K+    Sym   calc/GHz  diff/MHz     obs/GHz
  1:  8  4  5  7  4  4   S 1   9.8431248   -0.0220   9.8431028   Err 0.1D-04          -
  2: 14  4 11 14  3 12   S 1  11.4275093   -0.0293  11.4274801   Err 0.1D-04          -
  3: 10  8  3  9  8  1   S 1  12.2712087    0.0163  12.2712250   Err 0.1D-04          -
  4: 17  5 12 17  4 13   S 1  12.8327712   -0.0003  12.8327709   Err 0.1D-04          -
  5: 11  4  8 10  4  7   S 1  13.5772761   -0.0197  13.5772564   Err 0.1D-04          -
  6: 12  9  4 11  9  2   S 1  14.7287188   -0.0022  14.7287166   Err 0.1D-04          -
  7: 12  7  5 11  7  4   S 1  14.7471967   -0.0068  14.7471899   Err 0.1D-04          -
  8:  9  3  7  8  2  6   S 1  18.0543900    0.0326  18.0544226   Err 0.1D-04          -
  9: 10  1  9 10  0 10   S 1   6.7150243    0.0167   6.7150410   Err 0.1D-04          -
 Maximum (obs-calc)/err in line   8   0.0000326

 RMS deviations (MHz), B and V sorted
  B  V   n splittings MHz
  B  V   n abs. freq. MHz
  1  1   9         0.020280         0.027040

          Parameters  and  Errors
 BJ          0.611904574 { 0.000000567}
 BK           1.585448914 { 0.000002106}
 B-          0.063682586 { 0.000000261}
\F12         -0.887125114 {     derived}
\F          158.909764480 {     derived}  160.191854894 {     derived}
\rho          0.006767241 {     derived}    0.013746285 {     derived}
\beta         2.555733880 {     derived}    0.040671728 {     derived}
\gamma        0.432772101 {     derived}    1.965770254 {     derived}

 Standard Deviation       0.027209 MHz

---------------------------------- B =  1
```

Rotational Constants and Errors (in GHz)
B_z 2.197353488 0.000002102
B_x 0.675587160 0.000000624
B_y 0.548221988 0.000000624
Ray's kappa -0.84554
F0(calc) 158.000000000 0.000000000
I_alpha 3.198601709 0.000000000
<(i,x) <(i,y) <(i,z) 37.4014 63.1113 113.9194
d<(i,x) d<(i,y) d<(i,z) 0.0000 0.0000 0.0000

F0(calc) 158.000000000 0.000000000
I_alpha 3.198601709 0.000000000
<(i,x) <(i,y) <(i,z) 92.8831 81.4493 9.0305
d<(i,x) d<(i,y) d<(i,z) 0.0000 0.0000 0.0000

V1n_1 6.451030 kj +/- 0.000000 kj 1.540764 kcal +/- 0.000000 kcal
539.263862 cm +/- 0.0000 cm s= 45.215671
V1n_2 5.800159 kj +/- 0.000000 kj 1.385310 kcal +/- 0.000000 kcal
484.855317 cm +/- 0.0000 cm s= 40.653676

F(calc) 158.909764480
F(calc) 160.191854894

$^{13}C_{11}$ XIAM Output

J K- K+ J K- K+ Sym calc/GHz diff/MHz obs/GHz
1: 8 7 2 9 6 3 S 1 9.5984068 -0.0087 9.5983981 Err 0.1D-04 -
2: 9 4 6 8 4 5 S 1 11.0804093 0.0311 11.0804404 Err 0.1D-04 -
3: 14 3 12 14 1 13 S 1 11.1416431 -0.0134 11.1416297 Err 0.1D-04 -
4: 16 1 15 16 0 16 S 1 12.9494408 0.0139 12.9494547 Err 0.1D-04 -
5: 16 5 12 16 4 13 S 1 14.0663788 -0.0058 14.0663730 Err 0.1D-04 -
6: 6 5 1 6 4 2 S 1 14.2884165 0.0233 14.2884398 Err 0.1D-04 -
7: 12 11 1 11 11 0 S 1 14.7139663 0.0090 14.7139754 Err 0.1D-04 -
8: 12 6 6 11 6 5 S 1 14.7584610 0.0135 14.7584745 Err 0.1D-04 -
9: 19 13 7 20 12 8 S 1 15.1180274 0.0009 15.1180283 Err 0.1D-04 -
10: 15 2 14 14 2 13 S 1 17.7590684 -0.0356 17.7590328 Err 0.1D-04 -
11: 21 6 16 22 3 19 S 1 7.4505143 0.0071 7.4505214 Err 0.1D-04 -
12: 10 2 8 9 3 7 S 1 6.2164022 -0.0294 6.2163728 Err 0.1D-04 -
13: 17 5 13 18 2 16 S 1 6.0044785 -0.0208 6.0044577 Err 0.1D-04 -
Maximum (obs-calc)/err in line 10 0.0000356

RMS deviations (MHz), B and V sorted
B V n splittings MHz
B V n abs. freq. MHz

```
 1  1  13         0.019346         0.023811

          Parameters  and  Errors
 BJ          0.611689192 { 0.000000422}
 BK           1.590092751 { 0.000000842}
 B-          0.063429653 { 0.000000147}
\F12         -0.888938855 {     derived}
\F         158.910229643 {     derived}  160.196314659 {     derived}
\rho         0.006775558 {     derived}    0.013773942 {     derived}
\beta        2.556918541 {     derived}    0.040588221 {     derived}
\gamma       0.433062258 {     derived}    1.965499720 {     derived}

 Standard Deviation       0.023251 MHz

------------------------------------ B =  1
 Rotational Constants and Errors (in GHz)
     B_z      2.201781943       0.000001196
     B_x      0.675118844       0.000000424
     B_y      0.548259539       0.000000468
 Ray's kappa   -0.84656
 F0(calc)    158.000000000       0.000000000
 I_alpha       3.198601709       0.000000000
 <(i,x)  <(i,y)  <(i,z)      37.4014       63.1113      113.9194
d<(i,x) d<(i,y) d<(i,z)       0.0000        0.0000       0.0000

 F0(calc)    158.000000000       0.000000000
 I_alpha       3.198601709       0.000000000
 <(i,x)  <(i,y)  <(i,z)      92.8831       81.4493       9.0305
d<(i,x) d<(i,y) d<(i,z)       0.0000        0.0000       0.0000

 V1n_1      6.451030 kj +/- 0.000000 kj         1.540764 kcal +/- 0.000000 kcal
        539.263862 cm +/-   0.0000 cm    s=  45.215539
 V1n_2      5.800159 kj +/- 0.000000 kj         1.385310 kcal +/- 0.000000 kcal
        484.855317 cm +/-   0.0000 cm    s=  40.653557

F(calc)      158.910229643
F(calc)      160.196314659
```

^{18}O XIAM Output

```
   J K- K+  J K- K+    Sym   calc/GHz  diff/MHz     obs/GHz
  1:  8  4  4  7  4  3   S 3   9.8392742    0.0137   9.8392880   Err 0.1D-04          -
  2: 10  5  6  9  5  5   S 1  12.2956233   -0.0023  12.2956210   Err 0.1D-04          -
  3: 11  2 10 10  2  9   S 1  13.1740399    0.0057  13.1740456   Err 0.1D-04          -
```

```
  4: 11  5  6 10  5  5   S 3  13.5395579    0.0345  13.5395923   Err 0.1D-04          -
  5: 11  5  6 11  4  7   S 1  13.6408963   -0.0260  13.6408703   Err 0.1D-04          -
  6: 19  5 14 19  4 16   S 1  14.3808940    0.0243  14.3809183   Err 0.1D-04          -
  7: 13  1 13 12  1 12   S 1  14.6384785   -0.0117  14.6384667   Err 0.1D-04          -
  8: 12  2 10 11  2  9   S 1  15.3477300    0.0005  15.3477305   Err 0.1D-04          -
  9:  9  2  7  8  1  7   S 1  15.4687482   -0.0001  15.4687480   Err 0.1D-04          -
 10: 21  5 16 21  4 18   S 3  15.5480429   -0.0142  15.5480287   Err 0.1D-04          -
 11: 15  6  9 15  5 10   S 4  16.6090682    0.0000  16.6090682   Err 0.1D-04          -
 12: 15  6  9 15  5 10   S 3  16.6044484    0.0099  16.6044584   Err 0.1D-04          -
 13:  7  6  1  6  6  0   S 1   8.5799615   -0.0510   8.5799106   Err 0.1D-04          -
 14:  6  5  2  7  4  3   S 1   5.2152001    0.0033   5.2152034   Err 0.1D-04          -
Maximum (obs-calc)/err in line  13   0.0000510

RMS deviations (MHz), B and V sorted
 B  V   n splittings MHz
 B  V   n abs. freq. MHz
 1  1  14         0.020224         0.027448

          Parameters  and  Errors
 BJ          0.611178376 { 0.000000450}
 BK           1.537662448 { 0.000002029}
 B-          0.065511345 { 0.000000208}
\F12         -0.867229408 {     derived}
\F         158.901657012 {     derived}  160.142958705 {     derived}
 V1n         16261.572513 {   51.037763}   14567.584012 {   18.730720}
\rho         0.006664977 {     derived}    0.013443218 {     derived}
\beta        2.545159135 {     derived}    0.041434100 {     derived}
\gamma       0.430377677 {     derived}    1.968013429 {     derived}

 Standard Deviation       0.026754 MHz

------------------------------------ B =  1
 Rotational Constants and Errors (in GHz)
     B_z       2.148840825       0.000002074
     B_x       0.676689721       0.000000498
     B_y       0.545667032       0.000000493
 Ray's kappa   -0.83655
 F0(calc)     158.000000000       0.000000000
 I_alpha        3.198601709       0.000000000
 <(i,x)  <(i,y)  <(i,z)       37.4014       63.1113      113.9194
d<(i,x) d<(i,y) d<(i,z)        0.0000        0.0000        0.0000

 F0(calc)     158.000000000       0.000000000
```

```
 I_alpha        3.198601709       0.000000000
 <(i,x)  <(i,y)  <(i,z)       92.8831       81.4493        9.0305
d<(i,x) d<(i,y) d<(i,z)        0.0000        0.0000        0.0000

 V1n_1      6.488877 kj +/- 0.020366 kj         1.549803 kcal +/- 0.004864 kcal
        542.427596 cm +/-   1.7024 cm    s=  45.483261
 V1n_2      5.812922 kj +/- 0.007474 kj         1.388358 kcal +/- 0.001785 kcal
        485.922230 cm +/-   0.6248 cm    s=  40.745213

F(calc)       158.901657012
F(calc)       160.142958705
```

EQ3 Kraitchman Output

```
|                                                                      |
|   KRA  -  SINGLE ISOTOPIC SUBSTITUTION - Various permutations        |
|          of Kraitchman's equations for symmetric/asymmetric tops     |

|______________________________________________________________________
_____|
 version 4a.IV.2017                              Zbigniew KISIEL

 ---------------------------------------------------------------------------
    R-Carvon EQ3
 ---------------------------------------------------------------------------

  parent species
Planar calculation will be made from I.a and I.b

 ---------------------------------------------------------------------------
  C(1)
 ---------------------------------------------------------------------------

 The parent species:

  X,  Y,  Z  =       2212.79190000       684.52040000       554.73050000
 eX, eY, eZ  =          0.00050000         0.00020000         0.00020000
 IX, IY, IZ  =        228.38975906       738.29649036       911.03519439
eIX,eIY,eIZ  =          0.00005161         0.00021571         0.00032846
 PX, PY, PZ  =        710.47096284       200.56423155        27.82552752

 Mass        =        150.10446507

 The isotopic species:
```

```
 X,  Y,  Z  =       2190.54100000       684.40670000       553.25450000
eX, eY, eZ  =          0.00100000         0.00050000         0.00050000
 IX, IY, IZ  =       230.70967807       738.41914303       913.46569960
eIX,eIY,eIZ  =          0.00010532         0.00053946         0.00082554
 PX, PY, PZ  =       710.58758228       202.87811732        27.83156075

 Mass change =          1.00335484
 Total mass  =        151.10781991
 M DM/(M+DM) =          0.99669257
```

KRAITCHMAN RESULTS:

```
                    a                  b

    PLANAR:         0.35000  +- 0.00083    1.52584  +- 0.00004
+Costain err.       0.35000  +- 0.00437    1.52584  +- 0.00098

                    a                  b                  c

 NONPLANAR:         0.34128  +- 0.00078    1.52382  +- 0.00018    0.07833  +- 0.00347
+Costain err.       0.34128  +- 0.00446    1.52382  +- 0.00100    0.07833  +- 0.01946

                                          R=  1.56353  +- 0.00169

DIX,DIY,DIZ  =          2.31991900         0.12265267         2.43050521
DPX,DPY,DPZ  =          0.11661944         2.31388577         0.00603323
IXY,IXZ,IYZ  =       -509.90673130      -682.64543532      -172.73870403
```

C(2)

The parent species:

```
 X,  Y,  Z  =       2212.79190000       684.52040000       554.73050000
eX, eY, eZ  =          0.00050000         0.00020000         0.00020000
 IX, IY, IZ  =       228.38975906       738.29649036       911.03519439
eIX,eIY,eIZ  =          0.00005161         0.00021571         0.00032846
 PX, PY, PZ  =       710.47096284       200.56423155        27.82552752

 Mass        =        150.10446507
```

The isotopic species:

X, Y, Z =	2189.32700000	683.31180000	552.48060000
eX, eY, eZ =	0.00100000	0.00050000	0.00060000
IX, IY, IZ =	230.83760850	739.60234391	914.74525784
eIX,eIY,eIZ =	0.00010544	0.00054119	0.00099342
PX, PY, PZ =	711.75499663	202.99026122	27.84734728

Mass change = 1.00335484
Total mass = 151.10781991
M DM/(M+DM) = 0.99669257

KRAITCHMAN RESULTS:

	a	b	
PLANAR:	1.14188 +- 0.00025	1.56916 +- 0.00004	
+Costain err.	1.14188 +- 0.00134	1.56916 +- 0.00096	

	a	b	c
NONPLANAR:	1.13231 +- 0.00027	1.56202 +- 0.00019	0.14914 +- 0.00206
+Costain err.	1.13231 +- 0.00135	1.56202 +- 0.00098	0.14914 +- 0.01027

R= 1.93501 +- 0.00137

DIX,DIY,DIZ =	2.44784943	1.30585355	3.71006346
DPX,DPY,DPZ =	1.28403378	2.42602967	0.02181976
IXY,IXZ,IYZ =	-509.90673130	-682.64543532	-172.73870403

C(3)

The parent species:

X, Y, Z =	2212.79190000	684.52040000	554.73050000
eX, eY, eZ =	0.00050000	0.00020000	0.00020000
IX, IY, IZ =	228.38975906	738.29649036	911.03519439
eIX,eIY,eIZ =	0.00005161	0.00021571	0.00032846
PX, PY, PZ =	710.47096284	200.56423155	27.82552752

Mass = 150.10446507

The isotopic species:

X, Y, Z =	2210.42100000	681.06330000	552.30340000
eX, eY, eZ =	0.00100000	0.00040000	0.00030000
IX, IY, IZ =	228.63473017	742.04410794	915.03874302
eIX,eIY,eIZ =	0.00010343	0.00043582	0.00049703
PX, PY, PZ =	714.22406039	200.81468262	27.82004755

Mass change = 1.00335484
Total mass = 151.10781991
M DM/(M+DM) = 0.99669257

KRAITCHMAN RESULTS:

	a	b	
PLANAR:	1.93862 +- 0.00013	0.49758 +- 0.00012	
+Costain err.	1.93862 +- 0.00078	0.49758 +- 0.00302	

	a	b	c
NONPLANAR:	1.94003 +- 0.00010	0.50313 +- 0.00039	0.07441*i+- 0.00264
+Costain err.	1.94003 +- 0.00078	0.50313 +- 0.00301	0.07441*i+- 0.02033

R= 2.00283 +- 0.00131

DIX,DIY,DIZ =	0.24497111	3.74761758	4.00354863
DPX,DPY,DPZ =	3.75309755	0.25045108	-0.00547997
IXY,IXZ,IYZ =	-509.90673130	-682.64543532	-172.73870403

C(4)

The parent species:

X, Y, Z =	2212.79190000	684.52040000	554.73050000
eX, eY, eZ =	0.00050000	0.00020000	0.00020000
IX, IY, IZ =	228.38975906	738.29649036	911.03519439
eIX,eIY,eIZ =	0.00005161	0.00021571	0.00032846
PX, PY, PZ =	710.47096284	200.56423155	27.82552752

Mass = 150.10446507

The isotopic species:

X, Y, Z =	2205.50400000	682.78660000	553.17680000
eX, eY, eZ =	0.00100000	0.00040000	0.00040000
IX, IY, IZ =	229.14445356	740.17124662	913.59400629
eIX,eIY,eIZ =	0.00010390	0.00043362	0.00066062
PX, PY, PZ =	712.31039968	201.28360661	27.86084694

Mass change = 1.00335484
Total mass = 151.10781991
M DM/(M+DM) = 0.99669257

KRAITCHMAN RESULTS:

	a	b			
PLANAR:	1.37047	+- 0.00018	0.87177	+- 0.00007	
+Costain err.	1.37047	+- 0.00111	0.87177	+- 0.00172	

	a	b	c			
NONPLANAR:	1.35751	+- 0.00016	0.85101	+- 0.00026	0.18889	+- 0.00119
+Costain err.	1.35751	+- 0.00112	0.85101	+- 0.00178	0.18889	+- 0.00803

R= 1.61330 +- 0.00163

DIX,DIY,DIZ =	0.75469449	1.87475626	2.55881191
DPX,DPY,DPZ =	1.83943684	0.71937507	0.03531943
IXY,IXZ,IYZ =	-509.90673130	-682.64543532	-172.73870403

C(5)

The parent species:

X, Y, Z =	2212.79190000	684.52040000	554.73050000
eX, eY, eZ =	0.00050000	0.00020000	0.00020000
IX, IY, IZ =	228.38975906	738.29649036	911.03519439
eIX,eIY,eIZ =	0.00005161	0.00021571	0.00032846

PX, PY, PZ = 710.47096284 200.56423155 27.82552752

Mass = 150.10446507

The isotopic species:

X, Y, Z = 2202.42300000 684.29150000 554.21170000
eX, eY, eZ = 0.00100000 0.00030000 0.00040000
IX, IY, IZ = 229.46500690 738.54345538 911.88801842
eIX,eIY,eIZ = 0.00010419 0.00032378 0.00065815
PX, PY, PZ = 710.48323345 201.40478497 28.06022193

Mass change = 1.00335484
Total mass = 151.10781991
M DM/(M+DM) = 0.99669257

KRAITCHMAN RESULTS:

a b

PLANAR: 0.49725 +- 0.00039 1.03891 +- 0.00006
+Costain err. 0.49725 +- 0.00304 1.03891 +- 0.00144

a b c

NONPLANAR: 0.11085 +- 0.00190 0.91772 +- 0.00023 0.48644 +- 0.00044
+Costain err. 0.11085 +- 0.01366 0.91772 +- 0.00165 0.48644 +- 0.00311

R= 1.04457 +- 0.00251

DIX,DIY,DIZ = 1.07524784 0.24696502 0.85282404
DPX,DPY,DPZ = 0.01227061 0.84055343 0.23469441
IXY,IXZ,IYZ = -509.90673130 -682.64543532 -172.73870403

C(6)

The parent species:

X, Y, Z = 2212.79190000 684.52040000 554.73050000
eX, eY, eZ = 0.00050000 0.00020000 0.00020000
IX, IY, IZ = 228.38975906 738.29649036 911.03519439

eIX,eIY,eIZ = 0.00005161 0.00021571 0.00032846
PX, PY, PZ = 710.47096284 200.56423155 27.82552752

Mass = 150.10446507

The isotopic species:

X, Y, Z = 2211.79200000 683.64550000 554.18940000
eX, eY, eZ = 0.00200000 0.00040000 0.00040000
IX, IY, IZ = 228.49300879 739.24133034 911.92471184
eIX,eIY,eIZ = 0.00020661 0.00043253 0.00065820
PX, PY, PZ = 711.33651669 200.58819515 27.90481364

Mass change = 1.00335484
Total mass = 151.10781991
M DM/(M+DM) = 0.99669257

KRAITCHMAN RESULTS:

a b

PLANAR: 0.97354 +- 0.00025 0.32216 +- 0.00033
+Costain err. 0.97354 +- 0.00156 0.32216 +- 0.00467

a b c

NONPLANAR: 0.93182 +- 0.00024 0.15515 +- 0.00147 0.28224 +- 0.00081
+Costain err. 0.93182 +- 0.00163 0.15515 +- 0.00978 0.28224 +- 0.00538

R= 0.98591 +- 0.00267

DIX,DIY,DIZ = 0.10324973 0.94483998 0.88951745
DPX,DPY,DPZ = 0.86555385 0.02396360 0.07928613
IXY,IXZ,IYZ = -509.90673130 -682.64543532 -172.73870403

C(7)

The parent species:

X, Y, Z = 2212.79190000 684.52040000 554.73050000
eX, eY, eZ = 0.00050000 0.00020000 0.00020000

IX, IY, IZ = 228.38975906 738.29649036 911.03519439
eIX,eIY,eIZ = 0.00005161 0.00021571 0.00032846
PX, PY, PZ = 710.47096284 200.56423155 27.82552752

Mass = 150.10446507

The isotopic species:

X, Y, Z = 2209.11000000 674.04710000 547.50720000
eX, eY, eZ = 0.00100000 0.00040000 0.00040000
IX, IY, IZ = 228.77041383 749.76809321 923.05454412
eIX,eIY,eIZ = 0.00010356 0.00044494 0.00067437
PX, PY, PZ = 722.02611175 201.02843237 27.74198146

Mass change = 1.00335484
Total mass = 151.10781991
M DM/(M+DM) = 0.99669257

KRAITCHMAN RESULTS:

a b

PLANAR: 3.39132 +- 0.00007 0.62491 +- 0.00009
+Costain err. 3.39132 +- 0.00045 0.62491 +- 0.00240

a b c

NONPLANAR: 3.40358 +- 0.00007 0.69031 +- 0.00034 0.29235*i+- 0.00079
+Costain err. 3.40358 +- 0.00045 0.69031 +- 0.00220 0.29235*i+- 0.00519

R= 3.46055 +- 0.00076

DIX,DIY,DIZ = 0.38065477 11.47160285 12.01934974
DPX,DPY,DPZ = 11.55514891 0.46420083 -0.08354606
IXY,IXZ,IYZ = -509.90673130 -682.64543532 -172.73870403

C(9)

The parent species:

X, Y, Z =	2212.79190000	684.52040000	554.73050000
eX, eY, eZ =	0.00050000	0.00020000	0.00020000
IX, IY, IZ =	228.38975906	738.29649036	911.03519439
eIX,eIY,eIZ =	0.00005161	0.00021571	0.00032846
PX, PY, PZ =	710.47096284	200.56423155	27.82552752

Mass = 150.10446507

The isotopic species:

X, Y, Z =	2212.74270000	679.16000000	551.18420000
eX, eY, eZ =	0.00100000	0.00050000	0.00050000
IX, IY, IZ =	228.39483728	744.12363640	916.89676319
eIX,eIY,eIZ =	0.00010322	0.00054783	0.00083175
PX, PY, PZ =	716.31278116	200.58398203	27.81085525

Mass change = 1.00335484
Total mass = 151.10781991
M DM/(M+DM) = 0.99669257

KRAITCHMAN RESULTS:

	a	b	
PLANAR:	2.41794 +- 0.00012	0.07179 +- 0.00082	
+Costain err.	2.41794 +- 0.00063	0.07179 +- 0.02091	

	a	b	c
NONPLANAR:	2.42097 +- 0.00011	0.14158 +- 0.00193	0.12185*i+- 0.00224
+Costain err.	2.42097 +- 0.00063	0.14158 +- 0.01077	0.12185*i+- 0.01251

R= 2.42204 +- 0.00109

DIX,DIY,DIZ =	0.00507821	5.82714604	5.86156880
DPX,DPY,DPZ =	5.84181832	0.01975048	-0.01467227
IXY,IXZ,IYZ =	-509.90673130	-682.64543532	-172.73870403

C(10)

The parent species:

X, Y, Z =	2212.79190000	684.52040000	554.73050000
eX, eY, eZ =	0.00050000	0.00020000	0.00020000
IX, IY, IZ =	228.38975906	738.29649036	911.03519439
eIX,eIY,eIZ =	0.00005161	0.00021571	0.00032846
PX, PY, PZ =	710.47096284	200.56423155	27.82552752

Mass = 150.10446507

The isotopic species:

X, Y, Z =	2197.35300000	675.58720000	548.22200000
eX, eY, eZ =	0.00200000	0.00060000	0.00060000
IX, IY, IZ =	229.99445647	748.05888699	921.85101820
eIX,eIY,eIZ =	0.00020934	0.00066436	0.00100892
PX, PY, PZ =	719.95772436	201.89329384	28.10116263

Mass change = 1.00335484
Total mass = 151.10781991
M DM/(M+DM) = 0.99669257

KRAITCHMAN RESULTS:

	a	b			
PLANAR:	3.12473	+- 0.00011	1.28096	+- 0.00009	
+Costain err.	3.12473	+- 0.00049	1.28096	+- 0.00117	

	a	b	c			
NONPLANAR:	3.08052	+- 0.00010	1.16452	+- 0.00028	0.53155	+- 0.00062
+Costain err.	3.08052	+- 0.00050	1.16452	+- 0.00132	0.53155	+- 0.00289

R= 3.33591 +- 0.00080

DIX,DIY,DIZ =	1.60469740	9.76239663	10.81582381
DPX,DPY,DPZ =	9.48676152	1.32906229	0.27563511
IXY,IXZ,IYZ =	-509.90673130	-682.64543532	-172.73870403

C(11)

The parent species:

X, Y, Z =	2212.79190000	684.52040000	554.73050000
eX, eY, eZ =	0.00050000	0.00020000	0.00020000
IX, IY, IZ =	228.38975906	738.29649036	911.03519439
eIX,eIY,eIZ =	0.00005161	0.00021571	0.00032846
PX, PY, PZ =	710.47096284	200.56423155	27.82552752

Mass = 150.10446507

The isotopic species:

X, Y, Z =	2201.78100000	675.11860000	548.25900000
eX, eY, eZ =	0.00100000	0.00040000	0.00050000
IX, IY, IZ =	229.53191480	748.57811487	921.78880584
eIX,eIY,eIZ =	0.00010425	0.00044352	0.00084065
PX, PY, PZ =	720.41750295	201.37130289	28.16061191

Mass change = 1.00335484
Total mass = 151.10781991
M DM/(M+DM) = 0.99669257

KRAITCHMAN RESULTS:

	a	b	
PLANAR:	3.20821 +- 0.00008	1.08123 +- 0.00006	
+Costain err.	3.20821 +- 0.00047	1.08123 +- 0.00139	

	a	b	c
NONPLANAR:	3.15577 +- 0.00008	0.90771 +- 0.00029	0.58540 +- 0.00045
+Costain err.	3.15577 +- 0.00048	0.90771 +- 0.00168	0.58540 +- 0.00260

R= 3.33549 +- 0.00079

DIX,DIY,DIZ =	1.14215574	10.28162451	10.75361145
DPX,DPY,DPZ =	9.94654011	0.80707134	0.33508440
IXY,IXZ,IYZ =	-509.90673130	-682.64543532	-172.73870403

Oxygen-18

The parent species:

X, Y, Z =	2212.79190000	684.52040000	554.73050000
eX, eY, eZ =	0.00050000	0.00020000	0.00020000
IX, IY, IZ =	228.38975906	738.29649036	911.03519439
eIX,eIY,eIZ =	0.00005161	0.00021571	0.00032846
PX, PY, PZ =	710.47096284	200.56423155	27.82552752

Mass = 150.10446507

The isotopic species:

X, Y, Z =	2148.84100000	676.68970000	545.66700000
eX, eY, eZ =	0.00200000	0.00050000	0.00050000
IX, IY, IZ =	235.18678623	746.84010840	926.16744077
eIX,eIY,eIZ =	0.00021890	0.00055183	0.00084866
PX, PY, PZ =	718.91038147	207.25705930	27.92972693

Mass change = 2.00424499
Total mass = 152.10871006
M DM/(M+DM) = 1.97783626

KRAITCHMAN RESULTS:

	a	b	
PLANAR:	2.06448 +- 0.00007	1.86927 +- 0.00003	
+Costain err.	2.06448 +- 0.00073	1.86927 +- 0.00080	

	a	b	c
NONPLANAR:	2.05191 +- 0.00007	1.85414 +- 0.00008	0.23537 +- 0.00063
+Costain err.	2.05191 +- 0.00073	1.85414 +- 0.00081	0.23537 +- 0.00640

R= 2.77553 +- 0.00094

DIX,DIY,DIZ =	6.79702716	8.54361804	15.13224638
DPX,DPY,DPZ =	8.43941863	6.69282775	0.10419941
IXY,IXZ,IYZ =	-509.90673130	-682.64543532	-172.73870403

EQ3 EVAL Output

```
_____________________________________________________________________
____
|                                                                   |
|     E V A L   -  Internals and their errors from Cartesians       |
|___________________________________________________________________
_____|
 version 20.V.2020                          Zbigniew KISIEL
```

WARNING:

The EVAL uncertainties are evaluated by assuming that the correlation matrix is a unit matrix.

The EVAL uncertainties may thus differ significantly (but typically by not more than 30% either way) from uncertainties in explicitly fitted internals corresponding to the input Cartesians.

```
!
! EQ3, KRA coordinates
!
```

INPUT CARTESIANS:

C(1)	0.34128	0.00446	1.52382	0.00100	0.07833	0.01946
C(2)	-1.13231	0.00135	1.56202	0.00098	-0.14914	0.01027
C(3)	-1.94003	0.00078	0.50313	0.00301	0.00000	0.00000
C(4)	-1.35751	0.00112	-0.85101	0.00178	0.18889	0.00803
C(5)	0.11085	0.01366	-0.91772	0.00165	0.48644	0.00311
C(6)	0.93182	0.00163	0.15515	0.00978	-0.28224	0.00538
C(7)	-3.40358	0.00045	0.69031	0.00220	0.00000	0.00000
C(9)	2.42097	0.00063	0.14158	0.01077	0.00000	0.00000
C(10)	3.08052	0.00050	-1.16452	0.00132	-0.53155	0.00289
C(11)	3.15577	0.00048	0.90771	0.00168	0.58540	0.00260
Oxygen	-2.05191	0.00073	-1.85414	0.00081	0.23537	0.00640

CALCULATED INTERNALS:

```
!
!  Bond lengths
!
        C(1)  C(2)   =    1.49153 +- 0.00570
        C(2)  C(3)   =    1.34011 +- 0.00290
        C(3)  C(4)   =    1.48617 +- 0.00339
        C(4)  C(5)   =    1.49969 +- 0.01353
        C(5)  C(6)   =    1.55432 +- 0.01044
        C(6)  C(1)   =    1.53363 +- 0.01014
        C(3)  C(7)   =    1.47547 +- 0.00101
        C(6)  C(9)   =    1.51572 +- 0.00199
        C(9)  C(11)  =    1.21226 +- 0.00702
        C(9)  C(10)  =    1.55674 +- 0.00916
        C(4)  Oxygen =    1.22091 +- 0.00182
!
!  Bond angles
!
    C(1)  C(2)  C(3)   =  123.93594 +- 0.29467
    C(2)  C(3)  C(4)   =  119.85809 +- 0.10301
    C(3)  C(4)  C(5)   =  116.71290 +- 0.14109
    C(4)  C(5)  C(6)   =  112.85040 +- 0.44543
    C(5)  C(6)  C(1)   =  107.23860 +- 0.58052
    C(6)  C(1)  C(2)   =  111.55720 +- 0.48791
    C(2)  C(3)  C(7)   =  119.84242 +- 0.21921
    C(4)  C(3)  C(7)   =  120.29049 +- 0.19033
    C(1)  C(6)  C(9)   =  110.03058 +- 0.66943
    C(5)  C(6)  C(9)   =  114.87618 +- 0.69813
    C(6)  C(9)  C(11)  =  132.82609 +- 0.74209
    C(6)  C(9)  C(10)  =  111.11103 +- 0.59933
!
! Dihedral Angles
!
C(1)  C(2)  C(3)  C(4)   =  -10.31757 +- 1.36232
C(2)  C(3)  C(4)  C(5)   =   12.37439 +- 0.85149
C(3)  C(4)  C(5)  C(6)   =  -36.77900 +- 0.70605
C(4)  C(5)  C(6)  C(1)   =   56.54878 +- 0.74010
C(5)  C(6)  C(1)  C(2)   =  -52.75367 +- 1.33860
C(6)  C(1)  C(2)  C(3)   =   32.32692 +- 1.76426
C(1)  C(2)  C(3)  C(7)   =  168.59439 +- 0.99454
C(5)  C(4)  C(3)  C(7)   = -166.53263 +- 0.35686
C(4)  C(5)  C(6)  C(9)   =  179.17690 +- 0.51923
C(2)  C(1)  C(6)  C(9)   = -178.33977 +- 0.91359
```

C(5) C(6) C(9) C(11) = -110.37086 +- 0.86892
C(1) C(6) C(9) C(11) = 10.74277 +- 1.08311
C(1) C(6) C(9) C(10) = -172.42434 +- 0.79001
C(5) C(6) C(9) C(10) = 66.46202 +- 0.48033
C(2) C(3) C(4) Oxygen = -174.79921 +- 0.76425
C(6) C(5) C(4) Oxygen = 150.30335 +- 0.68223

S6. AX3 Assignments and Outputs of Structure Evaluation - Isotopologue Overview

Ground Vibrational State	$^{13}C_1$		$^{13}C_2$		$^{13}C_3$		$^{13}C_4$	
	Experiment	Theory	Experiment	Theory	Experiment	Theory	Experiment	Theory
A (MHz)	1,670.9006 (12)	1712.0	1,672.5283 (12)	1713.5	1,685.0670 (13)	1,726.5	1,684.3820 (12)	1725.8
B (MHz)	876.82358 (45)	837.5	877.87524 (76)	838.3	874.8671 (11)	835.6	875.76813 (75)	836.4
C (MHz)	768.27971 (53)	729.7	768.03158 (60)	729.3	768.30051 (71)	729.7	769.00397 (70)	730.4
D_J (kHz)	0.1728 (10)		0.1786 (15)		0.1868 (18)		0.1881 (15)	
D_{JK} (kHz)	0.1788 (43)		0.1656 (41)		0.1695 (40)		0.1480 (41)	
d_J (kHz)	[-0.0021]		-0.00297 (40)		-0.00332 (96)		-0.00202 (40)	
V_{3_1} (cm^{-1})	512 (2)		513 (2)		511 (3)		515 (2)	
δ_1 (radian)	0.533 (44)		0.502 (46)		0.528 (60)		0.455 (47)	
ε_1 (radian)	0.402 (48)		0.419 (48)		[0.392]		[0.392]	
V_{3_2} (cm^{-1})	503.45 (39)		499.68 (22)		502 (2)		503 (1)	
δ_2 (radian)	2.5492 (58)		2.5428 (32)		2.585 (32)		2.588 (21)	
ε_2 (radian)	[1.398]		[1.398]		[1.398]		[1.398]	
ν_{RMS} (kHz)	21.9		23.5		23.8		22.9	
Number of Transitions	36		33		30		36	
	$^{13}C_5$		$^{13}C_6$		$^{13}C_7$		$^{13}C_9$	
	Experiment	Theory	Experiment	Theory	Experiment	Theory	Experiment	Theory
A (MHz)	1,674.5065 (17)	1712.0	1,683.0704 (11)	1724.5	1,677.5119 (12)	1718.8	1,686.38574 (99)	1727.9
B (MHz)	875.90782 (75)	837.5	875.24309 (50)	835.9	865.70048 (69)	826.8	872.85569 (51)	833.7
C (MHz)	759.98946 (79)	729.7	769.88061 (54)	731.2	762.25039 (57)	724.0	767.10557 (46)	728.6
D_J (kHz)	0.1731 (15)		0.18189 (84)		0.1943 (12)		0.19005 (86)	
D_{JK} (kHz)	0.1800 (62)		0.1517 (34)		0.1635 (41)		0.1477 (35)	
d_J (kHz)	[-0.0021]		-0.00202 (25)		-0.00239 (42)		-0.0012 (32)	
V_{3_1} (cm^{-1})	506 (4)		510.32 (80)		510 (3)		507 (2)	
δ_1 (radian)	0.575 (67)		0.555 (13)		0.504 (57)		0.591 (36)	
ε_1 (radian)	0.349 (62)		[0.392]		[0.392]		[0.392]	
V_{3_2} (cm^{-1})	500.85 (69)		499.77 (33)		499.05 (31)		496 (2)	
δ_2 (radian)	2.5328 (61)		2.5308 (46)		2.5360 (41)		2.485 (28)	
ε_2 (radian)	[1.398]		[1.389]		[1.398]		[1.398]	
ν_{RMS} (kHz)	25.4		25.9		22.5		23.6	
Number of Transitions	19		48		27		48	
	$^{13}C_{10}$		$^{13}C_{11}$					
	Experiment	Theory	Experiment	Theory				
A (MHz)	1,684.7907 (12)	1726.3	1,669.6383 (12)	1710.7				
B (MHz)	863.34592 (69)	824.6	873.07174 (56)	833.9				
C (MHz)	760.06361 (66)	721.9	766.34711 (68)	727.9				
D_J (kHz)	0.1807 (13)		0.1693 (11)					
D_{JK} (kHz)	0.1588 (37)		0.1243 (40)					
d_J (kHz)	[-0.0021]		-0.00119 (44)					
V_{3_1} (cm^{-1})	510.32 (75)		512 (3)					
δ_1 (radian)	[0.542]		0.522 (44)					
ε_1 (radian)	[0.392]		[0.392]					
V_{3_2} (cm^{-1})	499.92 (83)		499 (3)					
δ_2 (radian)	[2.54]		2.541 (43)					
ε_2 (radian)	[1.398]		[1.398]					
ν_{RMS} (kHz)	23.9		25.5					
Number of Transitions	23		36					

Parent XIAM Output

	J	K-	K+	J	K-	K+	Sym	calc/GHz	diff/MHz	obs/GHz			
1:	3	1	3	2	0	2	S 1	5.4948486	-0.0298	5.4948189	Err	0.1D-04	-
2:	3	1	3	2	0	2	S 3	5.4948326	-0.0137	5.4948189	Err	0.1D-04	-
3:	3	1	3	2	0	2	S 2	5.4948254	-0.0065	5.4948189	Err	0.1D-04	-

4:	3	1	3	2	0	2	S 4	5.4948129	0.0059	5.4948189	Err 0.1D-04	-
5:	3	1	3	2	0	2	S 5	5.4948058	0.0131	5.4948189	Err 0.1D-04	-
6:	4	0	4	3	1	3	S 5	5.9186841	-0.0216	5.9186625	Err 0.1D-04	-
7:	4	0	4	3	1	3	S 3	5.9186741	-0.0117	5.9186625	Err 0.1D-04	-
8:	4	0	4	3	1	3	S 1	5.9186677	-0.0052	5.9186625	Err 0.1D-04	-
9:	4	0	4	3	1	3	S 3	5.9186741	-0.0117	5.9186625	Err 0.1D-04	-
10:	3	1	2	2	0	2	S 1	6.1360973	-0.0203	6.1360770	Err 0.1D-04	-
11:	3	1	2	2	0	2	S 3	6.1360775	-0.0005	6.1360770	Err 0.1D-04	-
12:	3	1	2	2	0	2	S 5	6.1360668	0.0102	6.1360770	Err 0.1D-04	-
13:	3	1	2	2	0	2	S 4	6.1360621	0.0149	6.1360770	Err 0.1D-04	-
14:	3	1	2	2	0	2	S 2	6.1360843	-0.0073	6.1360770	Err 0.1D-04	-
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16:	4	1	4	3	1	3	S 3	6.3661401	-0.0092	6.3661308	Err 0.1D-04	-
17:	4	1	4	3	1	3	S 2	6.3661352	-0.0048	6.3661304	Err 0.1D-04	-
18:	4	1	4	3	1	3	S 5	6.3661326	-0.0034	6.3661292	Err 0.1D-04	-
19:	4	0	4	3	0	3	S 1	6.5038846	-0.0261	6.5038585	Err 0.1D-04	-
20:	4	0	4	3	0	3	S 3	6.5038792	-0.0207	6.5038585	Err 0.1D-04	-
21:	4	0	4	3	0	3	S 2	6.5038732	-0.0147	6.5038585	Err 0.1D-04	-
22:	4	0	4	3	0	3	S 5	6.5038687	-0.0102	6.5038585	Err 0.1D-04	-
23:	4	0	4	3	0	3	S 4	6.5038670	-0.0079	6.5038591	Err 0.1D-04	-
24:	4	3	2	3	3	1	S 1	6.6165021	0.0385	6.6165406	Err 0.1D-04	-
25:	4	3	2	3	3	1	S 4	6.6165528	-0.0122	6.6165406	Err 0.1D-04	-
26:	4	3	1	3	3	0	S 1	6.6199472	0.0326	6.6199798	Err 0.1D-04	-
27:	4	2	2	3	2	1	S 4	6.6849446	0.0081	6.6849527	Err 0.1D-04	-
28:	4	2	2	3	2	1	S 1	6.6849534	-0.0007	6.6849527	Err 0.1D-04	-
29:	4	2	2	3	2	1	S 5	6.6847629	0.0089	6.6847718	Err 0.1D-04	-
30:	4	2	2	3	2	1	S 3	6.6849053	0.0485	6.6849538	Err 0.1D-04	-
31:	4	1	3	3	1	2	S 1	6.7905812	-0.0372	6.7905440	Err 0.1D-04	-
32:	4	1	4	3	0	3	S 5	6.9513172	0.0084	6.9513256	Err 0.1D-04	-
33:	4	1	4	3	0	3	S 4	6.9513249	0.0007	6.9513256	Err 0.1D-04	-
34:	4	1	4	3	0	3	S 2	6.9513357	-0.0101	6.9513256	Err 0.1D-04	-
35:	4	1	4	3	0	3	S 3	6.9513451	-0.0195	6.9513256	Err 0.1D-04	-
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37:	5	1	5	4	1	4	S 3	7.9426452	-0.0145	7.9426308	Err 0.1D-04	-
38:	5	1	5	4	1	4	S 4	7.9426375	-0.0068	7.9426308	Err 0.1D-04	-
39:	5	1	5	4	1	4	S 1	7.9426488	-0.0180	7.9426308	Err 0.1D-04	-
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42:	5	2	4	4	2	3	S 5	8.2258540	-0.0324	8.2258217	Err 0.1D-04	-
43:	5	2	4	4	2	3	S 2	8.2258228	-0.0014	8.2258214	Err 0.1D-04	-
44:	5	2	4	4	2	3	S 3	8.2258222	-0.0009	8.2258214	Err 0.1D-04	-
45:	5	2	4	4	2	3	S 1	8.2258170	0.0044	8.2258214	Err 0.1D-04	-
46:	5	2	4	4	2	3	S 4	8.2258019	0.0194	8.2258214	Err 0.1D-04	-

47: 5 3 2 4 3 1 S 1 8.2881735 0.0400 8.2882136 Err 0.1D-04 -
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49: 5 1 5 4 0 4 S 4 8.3900955 0.0035 8.3900990 Err 0.1D-04 -
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51: 5 1 5 4 0 4 S 3 8.3901112 -0.0122 8.3900990 Err 0.1D-04 -
52: 5 1 5 4 0 4 S 1 8.3901240 -0.0250 8.3900990 Err 0.1D-04 -
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54: 5 2 3 4 2 2 S 4 8.4024900 -0.0001 8.4024899 Err 0.1D-04 -
55: 5 2 3 4 2 2 S 2 8.4024836 0.0063 8.4024899 Err 0.1D-04 -
56: 5 2 3 4 2 2 S 3 8.4024800 0.0099 8.4024899 Err 0.1D-04 -
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61: 5 1 4 4 1 3 S 5 8.4655708 -0.0067 8.4655641 Err 0.1D-04 -
62: 4 2 3 3 1 2 S 1 8.8652848 -0.0427 8.8652421 Err 0.1D-04 -
63: 6 0 6 5 1 5 S 4 9.2976433 0.0095 9.2976527 Err 0.1D-04 -
64: 6 0 6 5 1 5 S 2 9.2976566 -0.0039 9.2976527 Err 0.1D-04 -
65: 6 0 6 5 1 5 S 5 9.2976679 -0.0175 9.2976505 Err 0.1D-04 -
66: 6 0 6 5 1 5 S 3 9.2976763 -0.0258 9.2976505 Err 0.1D-04 -
67: 6 0 6 5 1 5 S 1 9.2976773 -0.0268 9.2976505 Err 0.1D-04 -
68: 21 6 16 21 5 17 S 1 9.3474100 -0.0189 9.3473911 Err 0.1D-04 -
69: 6 1 6 5 1 5 S 1 9.5117286 -0.0404 9.5116882 Err 0.1D-04 -
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72: 6 1 6 5 1 5 S 5 9.5117118 -0.0236 9.5116882 Err 0.1D-04 -
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74: 6 0 6 5 0 5 S 3 9.6168572 -0.0125 9.6168447 Err 0.1D-04 -
75: 6 0 6 5 0 5 S 2 9.6168394 0.0112 9.6168506 Err 0.1D-04 -
76: 6 0 6 5 0 5 S 5 9.6168362 0.0125 9.6168487 Err 0.1D-04 -
77: 6 0 6 5 0 5 S 4 9.6168277 0.0210 9.6168487 Err 0.1D-04 -
78: 9 2 8 8 3 5 S 5 9.6498832 -0.0207 9.6498625 Err 0.1D-04 -
79: 6 1 6 5 0 5 S 5 9.8308801 0.0213 9.8309014 Err 0.1D-04 -
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82: 6 1 6 5 0 5 S 1 9.8309159 -0.0146 9.8309014 Err 0.1D-04 -
83: 6 1 6 5 0 5 S 4 9.8309044 -0.0027 9.8309017 Err 0.1D-04 -
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88: 6 3 3 5 3 2 S 1 9.9682422 0.0121 9.9682543 Err 0.1D-04 -
89: 6 3 3 5 3 2 S 4 9.9682262 0.0281 9.9682543 Err 0.1D-04 -

90:	6	1	5	5	1	4	S 1	10.1224778	-0.0439	10.1224339	Err 0.1D-04	-
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92:	6	1	5	5	1	4	S 3	10.1224661	-0.0332	10.1224329	Err 0.1D-04	-
93:	6	1	5	5	1	4	S 5	10.1224561	-0.0232	10.1224329	Err 0.1D-04	-
94:	6	2	4	5	2	3	S 1	10.1325050	-0.0109	10.1324942	Err 0.1D-04	-
95:	6	2	4	5	2	3	S 2	10.1324978	-0.0037	10.1324942	Err 0.1D-04	-
96:	6	2	4	5	2	3	S 4	10.1324933	0.0008	10.1324942	Err 0.1D-04	-
97:	6	2	4	5	2	3	S 3	10.1324908	0.0033	10.1324942	Err 0.1D-04	-
98:	6	2	4	5	2	3	S 5	10.1324739	0.0203	10.1324942	Err 0.1D-04	-
99:	5	2	4	4	1	3	S 3	10.3004670	0.0028	10.3004698	Err 0.1D-04	-
100:	5	2	4	4	1	3	S 2	10.3004512	0.0185	10.3004698	Err 0.1D-04	-
101:	7	0	7	6	1	6	S 1	10.9374554	0.0303	10.9374857	Err 0.1D-04	-
102:	7	0	7	6	1	6	S 3	10.9374499	0.0372	10.9374870	Err 0.1D-04	-
103:	7	0	7	6	1	6	S 5	10.9374266	-0.0196	10.9374070	Err 0.1D-04	-
104:	7	0	7	6	1	6	S 2	10.9374063	0.0007	10.9374070	Err 0.1D-04	-
105:	7	1	7	6	1	6	S 1	11.0739427	0.0033	11.0739461	Err 0.1D-04	-
106:	7	1	7	6	1	6	S 4	11.0739443	0.0018	11.0739461	Err 0.1D-04	-
107:	7	1	7	6	1	6	S 3	11.0739388	0.0073	11.0739461	Err 0.1D-04	-
108:	7	1	7	6	1	6	S 5	11.0739256	0.0204	11.0739461	Err 0.1D-04	-
109:	7	1	7	6	1	6	S 2	11.0739389	0.0075	11.0739464	Err 0.1D-04	-
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111:	7	0	7	6	0	6	S 2	11.1514697	0.0251	11.1514947	Err 0.1D-04	-
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115:	7	1	7	6	0	6	S 5	11.2879695	0.0330	11.2880025	Err 0.1D-04	-
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120:	7	2	6	6	2	5	S 1	11.4708479	0.0067	11.4708546	Err 0.1D-04	-
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124:	7	2	6	6	2	5	S 4	11.4708256	0.0290	11.4708546	Err 0.1D-04	-
125:	7	3	5	6	3	4	S 3	11.5975303	-0.0059	11.5975244	Err 0.1D-04	-
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128:	6	2	5	5	1	4	S 1	11.6879342	0.0002	11.6879344	Err 0.2D-04	-
129:	6	2	5	5	1	4	S 3	11.6878868	0.0477	11.6879344	Err 0.2D-04	-
130:	7	1	6	6	1	5	S 5	11.7553955	0.0018	11.7553973	Err 0.1D-04	-
131:	7	1	6	6	1	5	S 3	11.7554098	-0.0124	11.7553973	Err 0.1D-04	-
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133: 7 1 6 6 1 5 S 2 11.7554086 -0.0108 11.7553978 Err 0.1D-04 -
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139: 8 0 8 7 1 7 S 1 12.5466320 -0.0098 12.5466222 Err 0.1D-04 -
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142: 8 1 8 7 1 7 S 4 12.6303576 -0.0402 12.6303175 Err 0.1D-04 -
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146: 8 1 8 7 1 7 S 5 12.6303169 0.0005 12.6303175 Err 0.1D-04 -
147: 5 3 2 4 2 3 S 1 12.6392664 -0.0433 12.6392232 Err 0.1D-04 -
148: 8 0 8 7 0 7 S 1 12.6831193 -0.0127 12.6831066 Err 0.1D-04 -
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154: 7 2 6 6 1 5 S 1 13.0363043 -0.0071 13.0362972 Err 0.1D-04 -
155: 8 2 7 7 2 6 S 4 13.0784014 0.0391 13.0784405 Err 0.1D-04 -
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174: 13 4 9 12 5 7 S 1 14.4941712 0.0182 14.4941894 Err 0.1D-04 -
175: 9 5 4 8 5 3 S 1 14.9116743 0.0004 14.9116748 Err 0.1D-04 -

176: 9 1 8 8 1 7 S 1 14.9326610 -0.0110 14.9326500 Err 0.1D-04 -
177: 9 1 8 8 1 7 S 3 14.9326446 0.0054 14.9326500 Err 0.1D-04 -
178: 9 1 8 8 1 7 S 2 14.9326332 0.0168 14.9326500 Err 0.1D-04 -
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187: 9 2 7 8 2 6 S 3 15.2842710 -0.0357 15.2842353 Err 0.1D-04 -
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190: 11 2 9 10 3 7 S 1 15.3397698 0.0307 15.3398005 Err 0.1D-04 -
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206: 7 2 5 6 1 6 S 4 16.2272514 -0.0036 16.2272478 Err 0.1D-04 -
207: 10 2 9 9 2 8 S 1 16.2615085 0.0389 16.2615473 Err 0.1D-04 -
208: 10 1 9 9 1 8 S 1 16.4791513 0.0139 16.4791652 Err 0.1D-04 -
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213: 10 3 7 9 3 6 S 4 16.8699069 -0.0083 16.8698985 Err 0.1D-04 -
214: 10 3 7 9 3 6 S 3 16.8699005 -0.0019 16.8698985 Err 0.1D-04 -
215: 10 3 7 9 3 6 S 5 16.8698803 0.0183 16.8698985 Err 0.1D-04 -
216: 10 2 8 9 2 7 S 2 16.9619251 -0.0474 16.9618777 Err 0.1D-04 -
217: 10 2 8 9 2 7 S 3 16.9619190 -0.0414 16.9618777 Err 0.1D-04 -
218: 10 2 8 9 2 7 S 5 16.9619047 -0.0270 16.9618777 Err 0.1D-04 -

219: 10 2 8 9 2 7 S 4 16.9619054 -0.0265 16.9618788 Err 0.1D-04 -
220: 11 0 11 10 1 10 S 1 17.2600824 0.0245 17.2601069 Err 0.1D-04 -
221: 17 6 11 16 7 9 S 1 17.3835747 -0.0209 17.3835537 Err 0.1D-04 -
222: 7 4 4 6 3 3 S 1 17.5599264 0.0099 17.5599363 Err 0.1D-04 -
223: 7 4 3 6 3 4 S 1 17.6114415 0.0063 17.6114478 Err 0.1D-04 -
224: 11 1 10 10 1 9 S 1 18.0078984 0.0474 18.0079458 Err 0.1D-04 -
225: 11 2 9 10 2 8 S 5 18.6109289 0.0011 18.6109300 Err 0.1D-04 -
226: 9 4 5 9 3 6 S 3 5.6250245 -0.0430 5.6249815 Err 0.1D-04 -
227: 11 1 10 11 1 11 S 1 5.8402763 0.0330 5.8403092 Err 0.1D-04 -
228: 2 2 0 1 1 1 S 4 5.9516018 -0.0026 5.9515992 Err 0.1D-04 -
229: 6 4 2 6 3 3 S 4 5.9660848 -0.0072 5.9660776 Err 0.1D-04 -
230: 8 4 5 8 3 6 S 1 6.0170478 0.0122 6.0170600 Err 0.1D-04 -
231: 9 4 6 9 3 7 S 4 6.0425360 0.0090 6.0425450 Err 0.1D-04 -
232: 9 4 6 9 3 7 S 1 6.0427340 -0.0152 6.0427188 Err 0.1D-04 -
233: 11 2 10 11 0 11 S 2 6.2122121 -0.0036 6.2122085 Err 0.1D-04 -
234: 11 2 10 11 0 11 S 4 6.2125435 0.0110 6.2125545 Err 0.1D-04 -
235: 11 2 10 11 0 11 S 1 6.2116237 0.0230 6.2116467 Err 0.1D-04 -
236: 11 2 10 11 0 11 S 3 6.2116041 0.0426 6.2116467 Err 0.1D-04 -
237: 22 17 5 21 18 3 S 5 6.2510408 0.0176 6.2510584 Err 0.1D-04 -
238: 12 1 11 12 0 12 S 1 6.5576323 0.0142 6.5576465 Err 0.1D-04 -
239: 4 2 3 3 2 2 S 4 6.5905546 0.0213 6.5905759 Err 0.1D-04 -
240: 4 2 3 3 2 2 S 1 6.5905661 0.0097 6.5905759 Err 0.1D-04 -
241: 4 2 3 3 2 2 S 3 6.5906028 -0.0270 6.5905759 Err 0.1D-04 -
242: 4 2 3 3 2 2 S 2 6.5906092 -0.0334 6.5905759 Err 0.1D-04 -
243: 12 4 8 12 3 10 S 4 6.6227941 -0.0105 6.6227836 Err 0.1D-04 -
244: 7 2 6 6 3 3 S 4 6.9422694 -0.0458 6.9422236 Err 0.1D-04 -
245: 15 2 13 15 1 14 S 2 6.9523016 0.0247 6.9523263 Err 0.1D-04 -
246: 10 5 6 9 6 4 S 4 7.1449854 0.0085 7.1449939 Err 0.1D-04 -
247: 13 1 12 13 0 13 S 3 7.2395605 -0.0398 7.2395207 Err 0.1D-04 -
248: 8 3 6 7 4 3 S 4 7.2409768 -0.0129 7.2409639 Err 0.1D-04 -
249: 16 4 13 16 3 14 S 1 7.4266094 -0.0126 7.4265968 Err 0.1D-04 -
250: 8 1 8 7 2 5 S 1 7.4769224 0.0180 7.4769405 Err 0.1D-04 -
251: 9 5 4 9 4 5 S 1 7.6534868 0.0355 7.6535223 Err 0.1D-04 -
252: 8 5 4 8 4 5 S 2 7.7043053 -0.0069 7.7042984 Err 0.1D-04 -
253: 3 2 1 2 1 2 S 4 7.7472477 0.0112 7.7472589 Err 0.1D-04 -
254: 14 1 13 14 0 14 S 3 7.9055601 0.0147 7.9055748 Err 0.1D-04 -
255: 19 13 6 18 14 4 S 5 8.2072490 -0.0189 8.2072301 Err 0.1D-04 -
256: 5 4 1 4 4 0 S 1 8.2700565 -0.0045 8.2700520 Err 0.1D-04 -
257: 5 3 3 4 3 2 S 1 8.2762603 0.0487 8.2763091 Err 0.1D-04 -
258: 8 2 7 7 3 4 S 3 8.3558870 0.0125 8.3558995 Err 0.1D-04 -
259: 8 2 7 7 3 4 S 1 8.3558868 0.0120 8.3558988 Err 0.1D-04 -
260: 4 2 3 3 1 2 S 4 8.8651862 -0.0268 8.8651594 Err 0.1D-04 -
261: 15 6 9 15 5 10 S 4 9.0539154 -0.0185 9.0538969 Err 0.1D-04 -

262: 12 6 7 12 5 7 S 1 9.3320644 -0.0161 9.3320483 Err 0.1D-04 -
263: 18 5 14 18 3 15 S 4 9.5881142 -0.0081 9.5881061 Err 0.1D-04 -
264: 17 5 13 17 3 14 S 1 9.8477023 -0.0198 9.8476825 Err 0.1D-04 -
265: 6 3 4 5 3 3 S 3 9.9374535 -0.0401 9.9374133 Err 0.1D-04 -
266: 18 2 17 18 1 18 S 1 10.4910544 0.0199 10.4910743 Err 0.1D-04 -
267: 19 7 12 19 6 13 S 2 10.6023053 0.0496 10.6023549 Err 0.1D-04 -
268: 11 4 7 10 5 5 S 5 10.7620729 0.0299 10.7621029 Err 0.1D-04 -
269: 11 4 7 10 5 6 S 5 10.7806902 -0.0133 10.7806770 Err 0.1D-04 -
270: 10 2 9 9 3 6 S 3 10.7933161 0.0183 10.7933344 Err 0.1D-04 -
271: 4 3 2 3 2 1 S 4 10.8884444 0.0353 10.8884798 Err 0.1D-04 -
272: 17 7 11 17 6 12 S 5 10.9025620 -0.0355 10.9025264 Err 0.1D-04 -
273: 13 7 7 13 6 7 S 2 11.0823530 0.0123 11.0823653 Err 0.1D-04 -
274: 10 7 3 10 6 4 S 4 11.1638493 -0.0103 11.1638390 Err 0.1D-04 -
275: 9 7 3 9 6 4 S 3 11.1760609 0.0128 11.1760736 Err 0.1D-04 -
276: 17 9 9 16 10 7 S 5 11.8725307 0.0397 11.8725704 Err 0.1D-04 -
277: 13 5 9 12 6 6 S 2 12.2476751 -0.0124 12.2476626 Err 0.1D-04 -
278: 12 4 8 11 5 7 S 2 12.6092843 0.0056 12.6092899 Err 0.1D-04 -
279: 4 4 1 3 3 1 S 2 12.6400259 0.0162 12.6400421 Err 0.1D-04 -
280: 17 8 9 17 7 10 S 3 12.7291004 0.0364 12.7291368 Err 0.1D-04 -
281: 10 8 3 10 7 4 S 2 12.9005956 0.0175 12.9006132 Err 0.1D-04 -
282: 20 1 19 19 4 16 S 1 13.0028656 0.0371 13.0029027 Err 0.1D-04 -
283: 22 13 9 21 14 7 S 3 13.2298734 0.0022 13.2298756 Err 0.1D-04 -
284: 8 3 6 7 3 5 S 2 13.2548334 0.0428 13.2548762 Err 0.1D-04 -
285: 8 4 4 7 4 3 S 1 13.2712363 0.0003 13.2712366 Err 0.1D-04 -
286: 12 3 10 11 4 7 S 5 13.4644746 0.0466 13.4645213 Err 0.1D-04 -
287: 12 3 10 11 4 8 S 5 13.6244389 0.0359 13.6244748 Err 0.1D-04 -
288: 12 3 10 11 4 8 S 1 13.6239925 0.0092 13.6240017 Err 0.1D-04 -
289: 6 2 4 5 1 5 S 3 13.8761013 -0.0173 13.8760840 Err 0.1D-04 -
290: 6 2 4 5 1 5 S 5 13.8760946 -0.0106 13.8760840 Err 0.1D-04 -
291: 6 2 4 5 1 5 S 4 13.8760656 0.0184 13.8760840 Err 0.1D-04 -
292: 6 3 4 5 2 3 S 4 14.0144316 0.0407 14.0144723 Err 0.1D-04 -
293: 6 3 4 5 2 3 S 1 14.0146002 0.0177 14.0146179 Err 0.1D-04 -
294: 6 3 3 5 2 3 S 1 14.0615976 -0.0142 14.0615835 Err 0.1D-04 -
295: 9 1 9 8 0 8 S 2 14.2659886 0.0094 14.2659980 Err 0.1D-04 -
296: 5 4 2 4 3 1 S 5 14.2793154 0.0088 14.2793242 Err 0.1D-04 -
297: 20 9 11 20 8 12 S 3 14.3962127 0.0169 14.3962296 Err 0.1D-04 -
298: 12 9 3 12 8 4 S 4 14.6156169 0.0040 14.6156209 Err 0.1D-04 -
299: 20 3 17 19 6 14 S 1 14.6438168 -0.0132 14.6438036 Err 0.1D-04 -
300: 9 4 6 8 4 5 S 3 14.9329962 0.0250 14.9330212 Err 0.1D-04 -
301: 12 3 9 11 4 8 S 5 15.3978349 0.0189 15.3978538 Err 0.1D-04 -
302: 16 6 11 15 7 8 S 3 15.5839020 -0.0161 15.5838859 Err 0.1D-04 -
303: 10 0 10 9 1 9 S 1 15.7015745 -0.0009 15.7015736 Err 0.1D-04 -
304: 5 5 1 4 4 1 S 4 16.0163958 -0.0186 16.0163772 Err 0.1D-04 -

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305:  5  5  0  4  4  0   S 4  16.0165410    0.0270  16.0165680   Err 0.1D-04          -
306:  5  5  0  4  4  1   S 1  16.0167551    0.0018  16.0167569   Err 0.1D-04          -
307: 19 10 10 19  9 11   S 3  16.2264072    0.0115  16.2264187   Err 0.1D-04          -
308: 14 10  4 14  9  5   S 2  16.3302202   -0.0251  16.3301951   Err 0.1D-04          -
309: 10  5  6  9  5  5   S 5  16.5812353   -0.0057  16.5812296   Err 0.1D-04          -
310: 10  5  5  9  5  4   S 1  16.5825473    0.0052  16.5825525   Err 0.1D-04          -
311: 10  4  7  9  4  6   S 3  16.6043463   -0.0133  16.6043330   Err 0.1D-04          -
312: 10  4  6  9  4  5   S 1  16.6473981    0.0237  16.6474218   Err 0.1D-04          -
313: 20  9 12 19 10 10   S 3  16.9598800   -0.0317  16.9598483   Err 0.1D-04          -
314: 11  1 11 10  1 10   S 3  17.2766750    0.0262  17.2767012   Err 0.1D-04          -
315: 11  1 11 10  0 10   S 3  17.3057198   -0.0218  17.3056980   Err 0.1D-04          -
316: 22 11 12 22 10 13   S 5  17.9030900   -0.0050  17.9030850   Err 0.1D-04          -
317: 20  6 15 20  5 15   S 5   7.2132167    0.0112   7.2132280   Err 0.1D-04          -
318: 20  3 17 20  3 18   S 2   8.6600183    0.0234   8.6600417   Err 0.1D-04          -
319:  7  1  6  6  2  4   S 1   9.5903692   -0.0284   9.5903409   Err 0.1D-04          -
320:  7  4  4  6  4  3   S 2  11.5960166    0.0056  11.5960222   Err 0.1D-04          -
321: 14  5  9 13  6  7   S 1  14.0697183   -0.0489  14.0696694   Err 0.1D-04          -
322: 22  9 14 22  8 15   S 5  14.2730675   -0.0004  14.2730672   Err 0.1D-04          -
323: 22  9 13 22  8 14   S 2  14.2742726   -0.0476  14.2742250   Err 0.1D-04          -
324: 19  2 17 18  5 14   S 2  14.2768314   -0.0463  14.2767851   Err 0.1D-04          -
325: 17  9  8 17  8  9   S 3  14.5177046   -0.0207  14.5176839   Err 0.1D-04          -
Maximum (obs-calc)/err in line 267   0.0000496

RMS deviations (MHz), B and V sorted
 B  V   n splittings MHz
 B  V   n abs. freq. MHz
 1  1 325         0.022745         0.023515

          Parameters  and  Errors
BJ          0.824792363 { 0.000000131}
BK          0.863022865 { 0.000000456}
B-          0.053486379 { 0.000000117}
DJ          0.183593E-6 { 0.000417E-6}
DJK         0.158304E-6 { 0.001482E-6}
dj         -0.002112E-6 { 0.000182E-6}
\F12        -1.086426728 {     derived}
\F         159.489108927 {     derived}  159.415643294 {     derived}
V1n         15299.125939 {   39.184627}   14981.748742 {    9.217991}
\rho        0.009574157 {     derived}    0.009236614 {     derived}
\beta       0.299096136 {     derived}    2.836742219 {     derived}
\gamma        0.348372645 {     derived}    1.374495187 {     derived}
epsil       0.392137459 { 0.021307932}    1.397899000 {     fixed  }
delta       0.542411467 { 0.023153474}    2.540629557 { 0.004724045}
```

Standard Deviation 0.023177 MHz

---------- B = 1
Rotational Constants and Errors (in GHz)
B_z 1.687815227 0.000000451
B_x 0.878278742 0.000000191
B_y 0.771305983 0.000000160
Ray's kappa -0.76656
F0(calc) 158.000000000 0.000000000
I_alpha 3.198601709 0.000000000
<(i,x) <(i,y) <(i,z) 61.5090 78.6224 31.0779
d<(i,x) d<(i,y) d<(i,z) 1.4737 1.0321 1.3266

F0(calc) 158.000000000 0.000000000
I_alpha 3.198601709 0.000000000
<(i,x) <(i,y) <(i,z) 84.4177 56.1510 145.5674
d<(i,x) d<(i,y) d<(i,z) 0.0387 0.2648 0.2707

V1n_1 6.104830 kj +/- 0.015636 kj 1.458078 kcal +/- 0.003734 kcal
510.323839 cm +/- 1.3071 cm s= 42.633704
V1n_2 5.978187 kj +/- 0.003678 kj 1.427830 kcal +/- 0.000879 kcal
499.737276 cm +/- 0.3075 cm s= 41.749277

F(calc) 159.489108927
F(calc) 159.415643294

$^{13}C_1$ XIAM Output

	J K- K+	J K- K+	Sym	calc/GHz	diff/MHz	obs/GHz		
1:	18 11 7	17 12 5	S 3	10.2958590	-0.0006	10.2958584	Err 0.1D-04	-
2:	18 2 17	18 1 18	S 3	10.5002286	-0.0010	10.5002276	Err 0.1D-04	-
3:	18 2 17	18 1 18	S 1	10.5016475	0.0064	10.5016538	Err 0.1D-04	-
4:	9 2 7	8 3 5	S 1	11.8057498	0.0109	11.8057607	Err 0.1D-04	-
5:	16 8 9	15 9 6	S 1	12.1457232	-0.0121	12.1457111	Err 0.1D-04	-
6:	13 5 9	12 6 6	S 4	12.3693660	0.0172	12.3693832	Err 0.1D-04	-
7:	9 1 8	8 2 7	S 1	13.9325964	0.0125	13.9326088	Err 0.1D-04	-
8:	9 1 8	8 2 7	S 3	13.9326041	0.0048	13.9326088	Err 0.1D-04	-
9:	9 1 8	8 2 7	S 4	13.9326141	-0.0052	13.9326088	Err 0.1D-04	-
10:	9 4 6	8 4 5	S 4	14.8957379	-0.0257	14.8957122	Err 0.1D-04	-
11:	9 2 7	8 2 6	S 5	15.2495617	0.0343	15.2495961	Err 0.1D-04	-
12:	9 2 7	8 2 6	S 3	15.2495716	0.0245	15.2495961	Err 0.1D-04	-
13:	9 2 7	8 2 6	S 2	15.2495794	0.0167	15.2495961	Err 0.1D-04	-
14:	9 2 7	8 2 6	S 1	15.2495884	0.0076	15.2495961	Err 0.1D-04	-

```
 15:  9  2  7  8  2  6   S 4  15.2495633    0.0330  15.2495963   Err 0.1D-04          -
 16: 19  9 11 18 10  9   S 2  15.4663611    0.0037  15.4663648   Err 0.1D-04          -
 17: 18 10  9 18  9 10   S 2  15.9687354    0.0140  15.9687493   Err 0.1D-04          -
 18: 14 10  4 14  9  5   S 1  16.0474245   -0.0028  16.0474217   Err 0.1D-04          -
 19: 14 10  5 14  9  6   S 3  16.0463098    0.0050  16.0463148   Err 0.1D-04          -
 20: 18 11  7 18 10  8   S 1  17.6967253   -0.0204  17.6967049   Err 0.1D-04          -
 21: 15  6  9 15  5 11   S 5   9.0808631    0.0118   9.0808749   Err 0.1D-04          -
 22: 16  6 11 16  5 12   S 1   9.0229918   -0.0156   9.0229763   Err 0.1D-04          -
 23: 16  6 11 16  5 12   S 5   9.0199709    0.0229   9.0199938   Err 0.1D-04          -
 24: 17  3 15 17  2 16   S 4   8.7324034    0.0017   8.7324050   Err 0.1D-04          -
 25: 21 15  6 20 16  4   S 1   8.4324773   -0.0014   8.4324759   Err 0.1D-04          -
 26:  5  2  3  4  2  2   S 5   8.3861253   -0.0366   8.3860886   Err 0.1D-04          -
 27: 14  1 13 14  0 14   S 1   7.9245216   -0.0230   7.9244987   Err 0.1D-04          -
 28:  7  5  3  7  4  4   S 2   7.5888767   -0.0142   7.5888625   Err 0.1D-04          -
 29:  8  5  4  8  4  5   S 4   7.5731355   -0.0110   7.5731245   Err 0.1D-04          -
 30: 16 11  6 15 12  4   S 3   6.9585706   -0.0001   6.9585705   Err 0.1D-04          -
 31: 17 12  5 16 13  3   S 2   6.9093185   -0.0102   6.9093083   Err 0.1D-04          -
 32:  4  0  4  3  0  3   S 1   6.4818008   -0.0366   6.4817643   Err 0.1D-04          -
 33:  4  0  4  3  0  3   S 3   6.4817957   -0.0314   6.4817643   Err 0.1D-04          -
 34:  4  0  4  3  0  3   S 2   6.4817901   -0.0241   6.4817660   Err 0.1D-04          -
 35:  4  0  4  3  0  3   S 5   6.4817858   -0.0198   6.4817660   Err 0.1D-04          -
 36:  4  0  4  3  0  3   S 4   6.4817841   -0.0181   6.4817660   Err 0.1D-04          -
Maximum (obs-calc)/err in line  26   0.0000366

 RMS deviations (MHz), B and V sorted
  B  V   n splittings MHz
  B  V   n abs. freq. MHz
  1  1  36         0.018281         0.023359

          Parameters  and  Errors
 BJ          0.822551644 { 0.000000460}
 BK          0.848348908 { 0.000001099}
 B-          0.054271933 { 0.000000178}
 DJ          0.172818E-6 { 0.001025E-6}
 DJK         0.178801E-6 { 0.004340E-6}
\F12        -1.090397498 {     derived}
\F         159.482935253 {     derived}  159.410293060 {     derived}
 V1n         15363.424697 {   74.304667}   15093.176542 {   11.826266}
\rho         0.009521302 {     derived}    0.009187351 {     derived}
\beta        0.294929358 {     derived}    2.840209239 {     derived}
\gamma       0.356854773 {     derived}    1.374059898 {     derived}
 epsil       0.402284220 { 0.048082948}    1.397899000 {     fixed  }
 delta       0.532661866 { 0.043782005}    2.549180720 { 0.005799273}
```

Standard Deviation 0.021937 MHz

---------- B = 1
Rotational Constants and Errors (in GHz)
B_z 1.670900552 0.000001231
B_x 0.876823577 0.000000453
B_y 0.768279711 0.000000530
Ray's kappa -0.75949
F0(calc) 158.000000000 0.000000000
I_alpha 3.198601709 0.000000000
<(i,x) <(i,y) <(i,z) 62.1416 78.5317 30.5193
d<(i,x) d<(i,y) d<(i,z) 2.8955 2.1560 2.5085

F0(calc) 158.000000000 0.000000000
I_alpha 3.198601709 0.000000000
<(i,x) <(i,y) <(i,z) 84.4877 56.6303 146.0573
d<(i,x) d<(i,y) d<(i,z) 0.0477 0.3252 0.3323

V1n_1 6.130488 kj +/- 0.029650 kj 1.464206 kcal +/- 0.007082 kcal
512.468614 cm +/- 2.4785 cm s= 42.814542
V1n_2 6.022650 kj +/- 0.004719 kj 1.438450 kcal +/- 0.001127 kcal
503.454107 cm +/- 0.3945 cm s= 42.061418

F(calc) 159.482935253
F(calc) 159.410293060

$^{13}C_2$ XIAM Output

	J K- K+	J K- K+	Sym	calc/GHz	diff/MHz	obs/GHz	
1:	21 7 15	21 6 15	S 1	9.7722228	0.0207	9.7722436	Err 0.1D-04 -
2:	19 3 17	19 1 18	S 4	10.0567217	-0.0015	10.0567201	Err 0.1D-04 -
3:	18 11 8	17 12 6	S 3	10.2882277	0.0046	10.2882324	Err 0.1D-04 -
4:	18 11 8	17 12 6	S 2	10.2883161	0.0056	10.2883217	Err 0.1D-04 -
5:	13 5 9	12 6 6	S 5	12.3612781	0.0042	12.3612823	Err 0.1D-04 -
6:	12 4 9	11 5 7	S 2	12.3942656	0.0115	12.3942771	Err 0.1D-04 -
7:	21 2 20	21 1 21	S 5	12.4792344	0.0098	12.4792442	Err 0.1D-04 -
8:	21 1 20	21 0 21	S 5	12.4798155	-0.0019	12.4798136	Err 0.1D-04 -
9:	4 4 0	3 3 0	S 5	12.5339463	0.0071	12.5339533	Err 0.1D-04 -
10:	8 1 8	7 0 7	S 2	12.7063424	0.0288	12.7063711	Err 0.1D-04 -
11:	8 4 4	7 4 3	S 5	13.2453431	-0.0256	13.2453174	Err 0.1D-04 -
12:	6 3 4	5 2 3	S 5	13.9117321	0.0132	13.9117453	Err 0.1D-04 -
13:	21 9 13	21 8 13	S 2	14.0700287	0.0056	14.0700343	Err 0.1D-04 -
14:	14 5 9	13 6 8	S 4	14.2108694	-0.0045	14.2108649	Err 0.1D-04 -

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 15:  9  2  8  8  2  7   S 1  14.6308124   -0.0011  14.6308113   Err 0.1D-04          -
 16: 13  4  9 12  5  7   S 1  14.6426149    0.0096  14.6426245   Err 0.1D-04          -
 17: 14  5  9 14  2 12   S 1  15.2158926    0.0205  15.2159131   Err 0.1D-04          -
 18:  7  3  5  6  2  4   S 1  15.3639046    0.0153  15.3639200   Err 0.1D-04          -
 19: 17 10  7 17  9  8   S 3  16.0160531   -0.0116  16.0160416   Err 0.1D-04          -
 20: 14 10  5 14  9  6   S 2  16.0679547   -0.0554  16.0678993   Err 0.1D-04          -
 21: 14  1 13 13  2 11   S 1  16.9610177   -0.0079  16.9610098   Err 0.1D-04          -
 22: 16  5 12 15  6  9   S 4  17.5162938   -0.0223  17.5162715   Err 0.1D-04          -
 23: 16  5 12 15  6  9   S 2  17.5144523    0.0047  17.5144570   Err 0.1D-04          -
 24: 21  9 12 20 10 10   S 4  18.8792125    0.0068  18.8792192   Err 0.1D-04          -
 25: 10  6  5 10  5  5   S 3   9.2491582    0.0135   9.2491717   Err 0.1D-04          -
 26: 16 10  6 15 11  4   S 2   8.6651797   -0.0087   8.6651710   Err 0.1D-04          -
 27: 15  1 14 15  0 15   S 2   8.6457059    0.0036   8.6457095   Err 0.1D-04          -
 28: 12  7  6 11  8  3   S 1   7.1498911   -0.0232   7.1498679   Err 0.1D-04          -
 29: 10  4  7 10  3  8   S 1   6.0153626   -0.0286   6.0153340   Err 0.1D-04          -
 30:  4  4  0  4  3  1   S 3   5.9273546    0.0067   5.9273613   Err 0.1D-04          -
 31:  4  4  1  4  3  2   S 3   5.9272552    0.0234   5.9272786   Err 0.1D-04          -
 32:  6  4  3  6  3  3   S 3   5.8612376   -0.0413   5.8611963   Err 0.1D-04          -
 33:  8  4  4  8  3  5   S 1   5.6742284    0.0249   5.6742534   Err 0.1D-04          -
Maximum (obs-calc)/err in line  20   0.0000554

RMS deviations (MHz), B and V sorted
 B  V   n splittings MHz
 B  V   n abs. freq. MHz
 1  1  33         0.018767         0.025022

          Parameters  and  Errors
 BJ          0.822953412 { 0.000000583}
 BK          0.849574898 { 0.000000880}
 B-          0.054921831 { 0.000000361}
 DJ          0.178693E-6 { 0.001088E-6}
 DJK         0.165693E-6 { 0.003300E-6}
 dj         -0.002968E-6 { 0.000439E-6}
\F12         -1.110526209 {     derived}
\F         159.506250382 {     derived}  159.406219622 {     derived}
 V1n         15375.746605 {   72.311162}   14980.177660 {    6.584129}
\rho         0.009643203 {     derived}    0.009166893 {     derived}
\beta        0.275206060 {     derived}    2.836656409 {     derived}
\gamma       0.371220207 {     derived}    1.373767983 {     derived}
 epsil       0.418638521 { 0.048313512}    1.397899000 {     fixed  }
 delta       0.501856050 { 0.046403845}    2.542814686 { 0.003187762}

 Standard Deviation       0.023525 MHz
```

```
------------------------------------ B =  1
 Rotational Constants and Errors (in GHz)
     B_z       1.672528310       0.000001161
     B_x       0.877875243       0.000000762
     B_y       0.768031581       0.000000599
 Ray's kappa   -0.75712
 F0(calc)     158.000000000       0.000000000
 I_alpha        3.198601709       0.000000000
 <(i,x)  <(i,y)  <(i,z)       63.9273       78.7228       28.7542
d<(i,x) d<(i,y) d<(i,z)        2.9978        2.1847        2.6587

 F0(calc)     158.000000000       0.000000000
 I_alpha        3.198601709       0.000000000
 <(i,x)  <(i,y)  <(i,z)       84.4355       56.2734      145.6925
d<(i,x) d<(i,y) d<(i,z)        0.0261        0.1787        0.1826

 V1n_1      6.135404 kj +/- 0.028854 kj         1.465380 kcal +/- 0.006892 kcal
        512.879629 cm +/-   2.4120 cm    s=  42.842617
 V1n_2      5.977560 kj +/- 0.002627 kj         1.427681 kcal +/- 0.000627 kcal
        499.684871 cm +/-   0.2196 cm    s=  41.740413

F(calc)       159.506250382
F(calc)       159.406219622
```

$^{13}C_3$ XIAM Output

```
     J K- K+  J K- K+    Sym   calc/GHz  diff/MHz     obs/GHz
  1:  6  1  6  5  0  5   S 1   9.7956786   -0.0250   9.7956536   Err 0.1D-04          -
  2: 17  2 16 17  0 17   S 1   9.8437125    0.0001   9.8437126   Err 0.1D-04          -
  3: 11  4  7 10  5  6   S 1  10.6939184    0.0074  10.6939258   Err 0.1D-04          -
  4: 16  7 10 16  6 10   S 1  10.9486865   -0.0318  10.9486547   Err 0.1D-04          -
  5: 14  7  7 14  6  9   S 2  11.0782906    0.0100  11.0783006   Err 0.1D-04          -
  6: 18  3 15 17  6 12   S 4  11.1062080    0.0031  11.1062111   Err 0.1D-04          -
  7:  7  0  7  6  0  6   S 1  11.1089682    0.0243  11.1089925   Err 0.2D-04          -
  8:  7  0  7  6  0  6   S 3  11.1089599    0.0326  11.1089925   Err 0.2D-04          -
  9:  9  4  5  9  1  8   S 1  11.8403555    0.0014  11.8403569   Err 0.1D-04          -
 10: 17  8 10 17  7 10   S 1  12.7355282    0.0104  12.7355386   Err 0.1D-04          -
 11: 18  2 16 17  5 13   S 1  13.2310924    0.0149  13.2311073   Err 0.1D-04          -
 12: 21  9 12 21  8 13   S 1  14.3484378    0.0094  14.3484472   Err 0.1D-04          -
 13: 17  9  8 17  8  9   S 2  14.5267969   -0.0182  14.5267787   Err 0.1D-04          -
 14: 15  9  7 15  8  8   S 3  14.5762767   -0.0112  14.5762655   Err 0.1D-04          -
 15: 13  3 11 12  4  8   S 5  14.7212362   -0.0049  14.7212312   Err 0.1D-04          -
```

```
 16: 13  3 11 12  4  9   S 1  15.0187554    0.0163  15.0187717   Err 0.1D-04          -
 17: 17  7 11 16  8  9   S 4  15.3492480   -0.0090  15.3492390   Err 0.1D-04          -
 18: 17  7 10 16  8  8   S 2  15.3494270   -0.0104  15.3494166   Err 0.1D-04          -
 19: 14  4 11 13  5  9   S 2  15.5498670   -0.0194  15.5498476   Err 0.1D-04          -
 20: 15  4 11 15  1 14   S 1  15.9698807    0.0176  15.9698983   Err 0.1D-04          -
 21:  7  4  4  6  3  3   S 3  17.5163740    0.0211  17.5163950   Err 0.1D-04          -
 22:  7  4  4  6  3  3   S 2  17.5160746    0.0064  17.5160810   Err 0.1D-04          -
 23:  7  4  4  6  3  3   S 4  17.5183167   -0.0178  17.5182989   Err 0.1D-04          -
 24: 11  5  6 10  5  5   S 3  18.1859979   -0.0373  18.1859606   Err 0.1D-04          -
 25: 11  5  6 10  5  5   S 2  18.1859145    0.0461  18.1859606   Err 0.1D-04          -
 26: 17  6 11 17  5 12   S 1   8.6620467    0.0267   8.6620734   Err 0.1D-04          -
 27:  5  3  3  4  3  2   S 1   8.2439634   -0.0201   8.2439432   Err 0.1D-04          -
 28: 16  3 14 16  2 15   S 5   8.1063230    0.0052   8.1063282   Err 0.1D-04          -
 29: 13  2 12 13  0 13   S 1   7.3707800   -0.0351   7.3707449   Err 0.1D-04          -
 30: 17  3 14 17  2 15   S 3   6.2120254    0.0103   6.2120357   Err 0.1D-04          -
Maximum (obs-calc)/err in line  25   0.0000461

RMS deviations (MHz), B and V sorted
 B  V   n splittings MHz
 B  V   n abs. freq. MHz
 1  1  30         0.018920         0.025226

          Parameters  and  Errors
 BJ          0.821583787 { 0.000000769}
 BK          0.863483221 { 0.000001243}
 B-          0.053283276 { 0.000000529}
 DJ          0.186805E-6 { 0.001757E-6}
 DJK         0.169505E-6 { 0.004019E-6}
 dj         -0.003318E-6 { 0.000956E-6}
\F12         -1.142955077 {     derived}
\F          159.497311179 {     derived}  159.451702370 {     derived}
 V1n         15328.865872 {   98.049454}   15055.894959 {   55.132871}
\rho         0.009610816 {     derived}    0.009417528 {     derived}
\beta        0.289574616 {     derived}    2.864270290 {     derived}
\gamma       0.348368748 {     derived}    1.374492864 {     derived}
 delta       0.528355786 { 0.059923757}    2.585442538 { 0.031809819}

 Standard Deviation       0.023774 MHz

------------------------------------ B =  1
 Rotational Constants and Errors (in GHz)
    B_z       1.685067009       0.000001294
    B_x       0.874867064       0.000001115
```

```
    B_y       0.768300511       0.000000707
 Ray's kappa   -0.76752
 F0(calc)     158.000000000       0.000000000
 I_alpha       3.198601709       0.000000000
 <(i,x)  <(i,y)  <(i,z)       62.2348       78.8923       30.2726
d<(i,x) d<(i,y) d<(i,z)        3.0859        1.1362        3.4334

 F0(calc)     158.000000000       0.000000000
 I_alpha       3.198601709       0.000000000
 <(i,x)  <(i,y)  <(i,z)       84.7891       58.6644      148.1349
d<(i,x) d<(i,y) d<(i,z)        0.2699        1.7859        1.8226

 V1n_1      6.116698 kj +/- 0.039125 kj         1.460912 kcal +/- 0.009345 kcal
        511.315856 cm +/-   3.2706 cm    s=  42.714383
 V1n_2      6.007774 kj +/- 0.022000 kj         1.434897 kcal +/- 0.005254 kcal
        502.210528 cm +/-   1.8390 cm    s=  41.953741

F(calc)       159.497311179
F(calc)       159.451702370
```

$^{13}C_4$ XIAM Output

```
    J K- K+  J K- K+    Sym   calc/GHz  diff/MHz     obs/GHz
  1: 21  4 18 21  2 19   S 1  10.0047156    0.0364  10.0047520   Err 0.1D-04          -
  2: 17  7 11 17  6 12   S 1  10.8995423   -0.0045  10.8995378   Err 0.1D-04          -
  3: 12  7  6 12  6  6   S 4  11.1095801    0.0008  11.1095808   Err 0.1D-04          -
  4: 19 11  8 18 12  6   S 4  11.6400839    0.0266  11.6401105   Err 0.1D-04          -
  5: 19 11  9 18 12  7   S 4  11.6402266    0.0071  11.6402337   Err 0.1D-04          -
  6: 18 10  9 17 11  6   S 1  11.7220014   -0.0151  11.7219863   Err 0.1D-04          -
  7: 16  8  9 15  9  7   S 3  11.8972454   -0.0070  11.8972384   Err 0.1D-04          -
  8: 15  7  8 14  8  7   S 4  11.9929338    0.0013  11.9929352   Err 0.1D-04          -
  9:  4  4  0  3  3  1   S 1  12.6149430    0.0138  12.6149568   Err 0.1D-04          -
 10: 16  8  9 16  7 10   S 5  12.7539837   -0.0309  12.7539528   Err 0.1D-04          -
 11: 16  8  9 16  7 10   S 1  12.7570240   -0.0092  12.7570148   Err 0.1D-04          -
 12: 14  2 13 13  3 10   S 3  13.5046494   -0.0116  13.5046378   Err 0.1D-04          -
 13: 14  2 13 13  3 10   S 4  13.5047139    0.0174  13.5047313   Err 0.1D-04          -
 14: 14  5 10 13  6  7   S 3  13.9102716    0.0034  13.9102750   Err 0.1D-04          -
 15:  9  3  6  8  3  5   S 1  15.0740684   -0.0031  15.0740653   Err 0.1D-04          -
 16:  9  3  6  8  3  5   S 4  15.0740612    0.0028  15.0740640   Err 0.1D-04          -
 17:  9  3  6  8  3  5   S 2  15.0740531    0.0109  15.0740640   Err 0.1D-04          -
 18:  9  3  6  8  3  5   S 3  15.0740477    0.0163  15.0740640   Err 0.1D-04          -
 19: 16  6 10 15  7  9   S 1  15.5546180   -0.0180  15.5546000   Err 0.1D-04          -
 20:  5  5  1  4  4  1   S 5  15.9813229    0.0143  15.9813372   Err 0.1D-04          -
 21: 16 10  7 16  9  8   S 2  16.2789342   -0.0516  16.2788826   Err 0.1D-04          -
```

```
 22: 16 10  7 16  9  8   S 3  16.2790114    0.0085  16.2790199   Err 0.1D-04          -
 23: 16 10  7 16  9  8   S 5  16.2777694    0.0197  16.2777891   Err 0.1D-04          -
 24: 16 10  7 16  9  8   S 4  16.2795358    0.0360  16.2795718   Err 0.1D-04          -
 25: 13 10  3 13  9  4   S 4  16.3207984   -0.0129  16.3207855   Err 0.1D-04          -
 26:  8  3  6  7  2  5   S 3  16.8292326    0.0098  16.8292424   Err 0.1D-04          -
 27: 19  6 13 19  4 16   S 4  17.7704592   -0.0389  17.7704203   Err 0.1D-04          -
 28: 15  1 14 14  2 12   S 5  17.8731314   -0.0209  17.8731105   Err 0.1D-04          -
 29: 17 11  7 17 10  8   S 5  18.0041415    0.0216  18.0041630   Err 0.1D-04          -
 30: 11  5  7 10  5  6   S 4  18.1998399   -0.0162  18.1998237   Err 0.1D-04          -
 31: 18  6 13 18  5 13   S 5   8.2266476    0.0070   8.2266546   Err 0.1D-04          -
 32: 10  5  6 10  4  6   S 2   7.5728367    0.0002   7.5728369   Err 0.1D-04          -
 33: 20  6 15 20  5 15   S 1   7.2101942    0.0106   7.2102048   Err 0.1D-04          -
 34: 21  6 15 21  5 16   S 1   7.1380471    0.0144   7.1380615   Err 0.1D-04          -
 35:  6  4  2  6  3  4   S 2   6.0094018    0.0042   6.0094060   Err 0.1D-04          -
 36: 10  3  8 10  1  9   S 2   5.8232592    0.0098   5.8232691   Err 0.1D-04          -
Maximum (obs-calc)/err in line  21   0.0000516

 RMS deviations (MHz), B and V sorted
  B  V   n splittings MHz
  B  V   n abs. freq. MHz
  1  1  36         0.019109         0.024417

          Parameters  and  Errors
 BJ          0.822386050 { 0.000000682}
 BK          0.861995909 { 0.000001181}
 B-          0.053382077 { 0.000000250}
 DJ          0.188091E-6 { 0.001472E-6}
 DJK         0.148037E-6 { 0.004062E-6}
 dj         -0.002017E-6 { 0.000398E-6}
\F12         -1.211111140 {     derived}
\F          159.549600509 {     derived}  159.454606481 {     derived}
 V1n         15434.934725 {   66.337740}   15079.635122 {   38.390962}
\rho         0.009872617 {     derived}    0.009425934 {     derived}
\beta        0.244759295 {     derived}    2.865476018 {     derived}
\gamma       0.348332100 {     derived}    1.374471012 {     derived}
 delta       0.454502707 { 0.047288808}    2.588090673 { 0.021331494}

 Standard Deviation       0.022931 MHz

------------------------------------ B =  1
 Rotational Constants and Errors (in GHz)
    B_z       1.684381959       0.000001184
    B_x       0.875768127       0.000000749
```

```
    B_y       0.769003972       0.000000703
 Ray's kappa   -0.76673
 F0(calc)     158.000000000       0.000000000
 I_alpha       3.198601709       0.000000000
 <(i,x)  <(i,y)  <(i,z)       66.0655       80.3415       26.0411
d<(i,x) d<(i,y) d<(i,z)        2.4560        0.9338        2.7094

 F0(calc)     158.000000000       0.000000000
 I_alpha       3.198601709       0.000000000
 <(i,x)  <(i,y)  <(i,z)       84.8114       58.8131      148.2867
d<(i,x) d<(i,y) d<(i,z)        0.1808        1.1975        1.2222

 V1n_1      6.159022 kj +/- 0.026471 kj        1.471021 kcal +/- 0.006322 kcal
        514.853931 cm +/-   2.2128 cm    s=  42.995852
 V1n_2      6.017247 kj +/- 0.015319 kj        1.437159 kcal +/- 0.003659 kcal
        503.002414 cm +/-   1.2806 cm    s=  42.006122

F(calc)       159.549600509
F(calc)       159.454606481
```

$^{13}C_5$ XIAM Output

```
   J K- K+  J K- K+    Sym   calc/GHz  diff/MHz     obs/GHz
  1: 18  3 16 18  2 17   S 4   9.7662242   -0.0001   9.7662241   Err 0.1D-04          -
  2:  7  6  1  6  6  0   S 1  11.4839672    0.0230  11.4839901   Err 0.1D-04          -
  3: 14  6  8 13  7  6   S 5  12.0966873   -0.0040  12.0966834   Err 0.1D-04          -
  4: 14  8  6 14  7  7   S 1  12.7172474   -0.0032  12.7172441   Err 0.1D-04          -
  5: 16  2 15 15  3 12   S 1  12.7272823   -0.0007  12.7272816   Err 0.1D-04          -
  6:  8  7  1  7  7  0   S 3  13.1233527   -0.0326  13.1233201   Err 0.1D-04          -
  7:  8  7  1  7  7  0   S 4  13.1233466   -0.0265  13.1233201   Err 0.1D-04          -
  8:  8  7  1  7  7  0   S 5  13.1233382   -0.0181  13.1233201   Err 0.1D-04          -
  9: 19  9 10 19  8 12   S 1  14.2912262    0.0151  14.2912412   Err 0.1D-04          -
 10: 18  9 10 18  8 11   S 2  14.3370595    0.0065  14.3370660   Err 0.1D-04          -
 11: 13  2 12 12  3 10   S 1  14.4561011   -0.0353  14.4560658   Err 0.1D-04          -
 12: 12  9  4 12  8  4   S 1  14.4959895    0.0101  14.4959996   Err 0.1D-04          -
 13:  9  4  5  8  4  4   S 5  14.8508592    0.0268  14.8508860   Err 0.1D-04          -
 14:  9  4  5  8  4  4   S 1  14.8522893    0.0341  14.8523234   Err 0.1D-04          -
 15: 12  1 11 11  2  9   S 5  15.0384767    0.0300  15.0385066   Err 0.1D-04          -
 16:  7  2  6  6  1  6   S 3  15.2082536    0.0234  15.2082770   Err 0.1D-04          -
 17:  7  2  6  6  1  6   S 2  15.2082683    0.0088  15.2082770   Err 0.1D-04          -
 18: 14  4 11 13  5  8   S 1  15.4410079    0.0039  15.4410118   Err 0.1D-04          -
 19: 12  3  9 11  4  8   S 1  15.5472458   -0.0334  15.5472124   Err 0.1D-04          -
 20: 17 10  8 17  9  9   S 3  16.1337737   -0.0005  16.1337732   Err 0.1D-04          -
```

```
 21: 17 10  7 17  9  8   S 4  16.1344457   -0.0176  16.1344281   Err 0.1D-04          -
 22: 16 10  7 16  9  8   S 5  16.1562001   -0.0072  16.1561928   Err 0.1D-04          -
 23: 19  7 13 18  8 11   S 3  18.8682216   -0.0007  18.8682209   Err 0.1D-04          -
 24: 15  2 14 15  0 15   S 2   8.9962029    0.0016   8.9962046   Err 0.1D-04          -
 25:  5  3  2  4  3  1   S 1   8.2277903   -0.0086   8.2277817   Err 0.1D-04          -
 26: 15 10  6 14 11  4   S 2   6.7151709    0.0267   6.7151976   Err 0.1D-04          -
Maximum (obs-calc)/err in line  11   0.0000353

RMS deviations (MHz), B and V sorted
 B  V   n splittings MHz
 B  V   n abs. freq. MHz
 1  1  26         0.019352         0.026795

          Parameters  and  Errors
 BJ          0.817948641 { 0.000000743}
 BK          0.856557840 { 0.000001674}
 B-          0.057959178 { 0.000000198}
 DJ          0.173064E-6 { 0.002291E-6}
 DJK         0.150031E-6 { 0.005988E-6}
\F12        -1.047465140 {     derived}
\F         159.454093550 {     derived}  159.395582926 {     derived}
 V1n         15192.674193 {  133.513803}   15015.152420 {   20.577299}
\rho         0.009375728 {     derived}    0.009123217 {     derived}
\beta        0.322596333 {     derived}    2.833813632 {     derived}
\gamma       0.305898584 {     derived}    1.372171881 {     derived}
 epsil       0.349075046 { 0.061792640}    1.397899000 {     fixed  }
 delta       0.575311067 { 0.066998772}    2.532871791 { 0.006149542}

 Standard Deviation       0.025478 MHz

------------------------------------ B =  1
 Rotational Constants and Errors (in GHz)
     B_z       1.674506480       0.000001773
     B_x       0.875907819       0.000000752
     B_y       0.759989463       0.000000785
 Ray's kappa   -0.74649
 F0(calc)     158.000000000       0.000000000
 I_alpha        3.198601709       0.000000000
 <(i,x)  <(i,y)  <(i,z)       59.2508       79.2749       32.9629
d<(i,x) d<(i,y) d<(i,z)        4.3363        2.9244        3.8387

 F0(calc)     158.000000000       0.000000000
 I_alpha        3.198601709       0.000000000
```

```
 <(i,x)  <(i,y)  <(i,z)      84.3545      55.7162     145.1229
d<(i,x) d<(i,y) d<(i,z)       0.0501       0.3447       0.3523

 V1n_1      6.062353 kj +/- 0.053276 kj        1.447932 kcal +/- 0.012724 kcal
        506.772991 cm +/-   4.4535 cm    s=  42.346355
 V1n_2      5.991516 kj +/- 0.008211 kj        1.431014 kcal +/- 0.001961 kcal
        500.851503 cm +/-   0.6864 cm    s=  41.851551

F(calc)      159.454093550
F(calc)      159.395582926
```

$^{13}C_6$ XIAM Output

```
    J K- K+  J K- K+    Sym   calc/GHz  diff/MHz     obs/GHz
 1:  6  2  5  5  2  4   S 1   9.8274279   -0.0139   9.8274140   Err 0.1D-04          -
 2:  6  2  5  5  2  4   S 4   9.8274087    0.0086   9.8274173   Err 0.1D-04          -
 3:  6  2  5  5  2  4   S 2   9.8274223   -0.0050   9.8274173   Err 0.1D-04          -
 4:  6  2  5  5  2  4   S 3   9.8274240   -0.0067   9.8274173   Err 0.1D-04          -
 5:  6  2  5  5  2  4   S 5   9.8274281   -0.0108   9.8274173   Err 0.1D-04          -
 6: 19  3 17 19  2 18   S 3   9.8389912   -0.0174   9.8389738   Err 0.1D-04          -
 7:  5  1  4  4  0  4   S 1   9.9403034   -0.0194   9.9402840   Err 0.1D-04          -
 8: 17  7 10 17  6 12   S 1  10.8902287    0.0200  10.8902487   Err 0.1D-04          -
 9: 14  7  8 14  6  9   S 1  11.0325859   -0.0007  11.0325852   Err 0.1D-04          -
10: 18  3 15 17  6 12   S 4  11.1855406    0.0344  11.1855750   Err 0.1D-04          -
11:  7  6  1  6  6  0   S 1  11.5426731    0.0223  11.5426954   Err 0.1D-04          -
12: 20 12  9 19 13  7   S 3  11.5990881    0.0136  11.5991017   Err 0.1D-04          -
13: 22  3 20 22  1 21   S 5  11.7177055   -0.0021  11.7177034   Err 0.1D-04          -
14: 14  6  9 13  7  7   S 4  12.1131840    0.0136  12.1131975   Err 0.1D-04          -
15: 22  5 17 22  4 19   S 1  13.0353238    0.0148  13.0353386   Err 0.1D-04          -
16: 22 13 10 21 14  8   S 2  13.1947700   -0.0228  13.1947472   Err 0.1D-04          -
17: 19 10 10 18 11  7   S 1  13.4341497   -0.0258  13.4341239   Err 0.1D-04          -
18:  7  1  6  6  0  6   S 1  14.1078249    0.0267  14.1078516   Err 0.1D-04          -
19: 20  9 12 20  8 12   S 1  14.3595563   -0.0318  14.3595245   Err 0.1D-04          -
20: 17  6 12 17  4 13   S 1  14.4608975    0.0588  14.4609564   Err 0.1D-04          -
21: 14  9  5 14  8  6   S 1  14.5475353   -0.0284  14.5475068   Err 0.1D-04          -
22:  9  6  3  8  6  2   S 1  14.8537047   -0.0038  14.8537009   Err 0.1D-04          -
23:  9  5  4  8  5  3   S 1  14.8697264   -0.0054  14.8697209   Err 0.1D-04          -
24:  7  3  4  6  2  4   S 1  15.5549093   -0.0086  15.5549007   Err 0.1D-04          -
25:  5  5  0  4  4  1   S 1  15.9717774    0.0105  15.9717879   Err 0.1D-04          -
26: 17  6 11 16  7 10   S 1  17.3248253   -0.0319  17.3247935   Err 0.1D-04          -
27: 17  6 11 16  7 10   S 3  17.3308298    0.0307  17.3308606   Err 0.1D-04          -
28: 20 11 10 20 10 11   S 3  17.9161867    0.0094  17.9161962   Err 0.1D-04          -
29: 19  7 13 18  8 10   S 4  18.8659675   -0.0115  18.8659561   Err 0.1D-04          -
```

```
 30: 12  6  7 12  5  8   S 1   9.3299564   -0.0247   9.3299317   Err 0.1D-04          -
 31:  9  3  6  8  4  5   S 1   9.3030694   -0.0237   9.3030457   Err 0.1D-04          -
 32: 13  6  7 13  5  8   S 1   9.2484310    0.0154   9.2484464   Err 0.1D-04          -
 33: 14  6  9 14  5 10   S 1   9.2490963    0.0154   9.2491117   Err 0.1D-04          -
 34: 15  6  9 15  5 11   S 1   9.2181921   -0.0281   9.2181640   Err 0.1D-04          -
 35:  4  2  2  3  1  2   S 1   8.9844157   -0.0478   8.9843679   Err 0.1D-04          -
 36:  7  3  4  7  0  7   S 3   8.9675112   -0.0000   8.9675112   Err 0.1D-04          -
 37: 11  5  6 10  6  5   S 1   8.8206251   -0.0024   8.8206227   Err 0.1D-04          -
 38:  5  3  3  4  3  1   S 5   8.2437570    0.0309   8.2437879   Err 0.1D-04          -
 39:  5  3  2  4  3  2   S 2   8.2705822   -0.0406   8.2705416   Err 0.1D-04          -
 40: 17  4 14 17  2 15   S 5   8.0844577   -0.0300   8.0844278   Err 0.1D-04          -
 41: 10  5  5 10  4  6   S 2   7.5747362    0.0217   7.5747579   Err 0.1D-04          -
 42: 12  1 11 11  4  8   S 4   7.3513304    0.0162   7.3513466   Err 0.1D-04          -
 43: 12  1 11 12  1 12   S 1   6.4751842    0.0307   6.4752150   Err 0.1D-04          -
 44:  5  1  4  4  2  3   S 4   6.3661091    0.0201   6.3661292   Err 0.1D-04          -
 45: 21 16  6 20 17  4   S 5   6.3110943    0.0163   6.3111106   Err 0.1D-04          -
 46: 16  5 11 16  4 12   S 3   6.2116506   -0.0039   6.2116467   Err 0.1D-04          -
 47:  8  4  4  8  3  6   S 1   6.0118046    0.0201   6.0118247   Err 0.1D-04          -
 48: 11  1 10 11  0 11   S 2   5.7898143    0.0244   5.7898387   Err 0.1D-04          -
Maximum (obs-calc)/err in line  20   0.0000588

 RMS deviations (MHz), B and V sorted
  B  V   n splittings MHz
  B  V   n abs. freq. MHz
  1  1  48         0.022815         0.027569

          Parameters  and  Errors
 BJ          0.822561853 { 0.000000471}
 BK          0.860508560 { 0.000000996}
 B-          0.052681239 { 0.000000225}
 DJ          0.181889E-6 { 0.000839E-6}
 DJK         0.151705E-6 { 0.003424E-6}
 dj         -0.002015E-6 { 0.000254E-6}
\F12         -1.061064272 {     derived}
\F          159.474928962 {     derived}  159.403054203 {     derived}
 V1n         15298.931775 {   23.910601}   14982.756131 {    9.956051}
\rho         0.009496842 {     derived}    0.009166786 {     derived}
\beta        0.307139893 {     derived}    2.830443854 {     derived}
\gamma       0.348890403 {     derived}    1.374803452 {     derived}
 delta       0.555181945 { 0.013176368}    2.530846908 { 0.004648857}

 Standard Deviation       0.025987 MHz
```

```
------------------------------------ B =  1
 Rotational Constants and Errors (in GHz)
    B_z      1.683070412      0.000001126
    B_x      0.875243091      0.000000501
    B_y      0.769880614      0.000000541
 Ray's kappa   -0.76924
 F0(calc)    158.000000000      0.000000000
 I_alpha      3.198601709      0.000000000
 <(i,x)  <(i,y)  <(i,z)      60.8506      78.3789      31.8096
d<(i,x) d<(i,y) d<(i,z)       0.6783       0.2494       0.7550

 F0(calc)    158.000000000      0.000000000
 I_alpha      3.198601709      0.000000000
 <(i,x)  <(i,y)  <(i,z)      84.3380      55.6027     145.0068
d<(i,x) d<(i,y) d<(i,z)       0.0378       0.2605       0.2664

 V1n_1     6.104753 kj +/- 0.009541 kj        1.458059 kcal +/- 0.002279 kcal
       510.317362 cm +/-   0.7976 cm    s=  42.636954
 V1n_2     5.978589 kj +/- 0.003973 kj        1.427926 kcal +/- 0.000949 kcal
       499.770879 cm +/-   0.3321 cm    s=  41.755797

F(calc)      159.474928962
F(calc)      159.403054203
```

$^{13}C_7$ XIAM Output

```
  J K- K+  J K- K+    Sym   calc/GHz  diff/MHz     obs/GHz
  1: 18  7 11 18  6 13   S 2  10.8880072   -0.0236  10.8879836   Err 0.1D-04          -
  2: 14  7  7 14  6  9   S 1  11.0780920    0.0310  11.0781230   Err 0.1D-04          -
  3: 12  7  6 12  6  7   S 4  11.1367993   -0.0127  11.1367867   Err 0.1D-04          -
  4: 20  2 19 20  1 20   S 1  11.5310897    0.0124  11.5311021   Err 0.1D-04          -
  5: 11  2 10 10  3  7   S 1  11.6558098   -0.0190  11.6557908   Err 0.1D-04          -
  6: 12  4  8 11  5  6   S 2  12.2859645   -0.0273  12.2859371   Err 0.1D-04          -
  7:  5  3  2  4  2  2   S 1  12.3940518   -0.0208  12.3940310   Err 0.1D-04          -
  8:  5  3  2  4  2  2   S 4  12.3938914    0.0012  12.3938926   Err 0.1D-04          -
  9:  5  3  2  4  2  2   S 3  12.3944415   -0.0152  12.3944263   Err 0.1D-04          -
 10:  5  3  2  4  2  2   S 2  12.3944899    0.0195  12.3945094   Err 0.1D-04          -
 11: 12  2 11 11  3  8   S 2  12.4636536    0.0083  12.4636619   Err 0.1D-04          -
 12: 19 10 10 18 11  8   S 5  13.0364336   -0.0028  13.0364308   Err 0.1D-04          -
 13: 18  2 16 17  5 13   S 3  13.1120351   -0.0167  13.1120184   Err 0.1D-04          -
 14: 20  3 17 19  6 14   S 1  14.2235068    0.0024  14.2235092   Err 0.1D-04          -
 15: 20  9 12 20  8 12   S 1  14.4219349   -0.0046  14.4219303   Err 0.1D-04          -
 16: 17  9  9 17  8 10   S 1  14.5359746    0.0110  14.5359856   Err 0.1D-04          -
```

```
 17: 10  3  7  9  3  6   S 1  16.6294981    0.0035  16.6295017   Err 0.1D-04          -
 18: 10  3  7  9  3  6   S 2  16.6294901    0.0116  16.6295017   Err 0.1D-04          -
 19: 10  3  7  9  3  6   S 4  16.6294866    0.0151  16.6295017   Err 0.1D-04          -
 20: 10  3  7  9  3  6   S 3  16.6294795    0.0221  16.6295017   Err 0.1D-04          -
 21: 12  0 12 11  1 11   S 2  18.5859085    0.0008  18.5859093   Err 0.1D-04          -
 22: 16  1 15 16  1 16   S 1   9.0246291   -0.0245   9.0246046   Err 0.1D-04          -
 23: 19  4 16 19  3 17   S 4   8.6711435   -0.0221   8.6711214   Err 0.1D-04          -
 24:  5  2  3  4  2  2   S 1   8.2853629   -0.0003   8.2853626   Err 0.1D-04          -
 25: 19 13  6 18 14  4   S 3   7.7713140   -0.0189   7.7712951   Err 0.1D-04          -
 26: 19 13  7 18 14  5   S 3   7.7731002    0.0341   7.7731343   Err 0.1D-04          -
 27: 16  4 13 16  3 14   S 3   7.3249812    0.0124   7.3249936   Err 0.1D-04          -
 Maximum (obs-calc)/err in line  26   0.0000341

 RMS deviations (MHz), B and V sorted
  B  V   n splittings MHz
  B  V   n abs. freq. MHz
  1  1  27         0.017333         0.023752

           Parameters  and  Errors
 BJ          0.813975431 { 0.000000567}
 BK           0.863536484 { 0.000001120}
 B-          0.051725046 { 0.000000273}
 DJ          0.194296E-6 { 0.001217E-6}
 DJK           0.163472E-6 { 0.004092E-6}
 dj          -0.002394E-6 { 0.000418E-6}
\F12          -1.110827961 {     derived}
\F          159.506247559 {     derived}  159.401867138 {     derived}
 V1n          15279.315599 {   86.872532}   14961.018433 {    9.234069}
\rho          0.009653136 {     derived}    0.009154510 {     derived}
\beta         0.273117739 {     derived}    2.835573537 {     derived}
\gamma          0.349212532 {     derived}    1.374994819 {     derived}
 delta        0.504324415 { 0.057059733}    2.536022533 { 0.004093387}

 Standard Deviation       0.022516 MHz

------------------------------------ B =  1
 Rotational Constants and Errors (in GHz)
     B_z       1.677511915       0.000001198
     B_x       0.865700477       0.000000685
     B_y       0.762250385       0.000000568
 Ray's kappa   -0.77394
 F0(calc)     158.000000000       0.000000000
 I_alpha       3.198601709       0.000000000
```

```
 <(i,x)  <(i,y)  <(i,z)      63.4783      79.3582      28.8957
d<(i,x) d<(i,y) d<(i,z)       2.9471       1.0969       3.2693

 F0(calc)    158.000000000      0.000000000
 I_alpha       3.198601709      0.000000000
 <(i,x)  <(i,y)  <(i,z)      84.3801      55.8927     145.3034
d<(i,x) d<(i,y) d<(i,z)       0.0334       0.2294       0.2345

 V1n_1      6.096925 kj +/- 0.034665 kj        1.456190 kcal +/- 0.008279 kcal
        509.663037 cm +/-   2.8978 cm    s=  42.573924
 V1n_2      5.969915 kj +/- 0.003685 kj        1.425855 kcal +/- 0.000880 kcal
        499.045788 cm +/-   0.3080 cm    s=  41.687029

F(calc)      159.506247559
F(calc)      159.401867138
```

$^{13}C_9$ XIAM Output

```
    J K- K+  J K- K+    Sym   calc/GHz  diff/MHz     obs/GHz
 1: 18 11  8 17 12  6   S 4   9.7745544    0.0062   9.7745606   Err 0.1D-04          -
 2:  5  1  4  4  0  4   S 1   9.9233826   -0.0299   9.9233527   Err 0.1D-04          -
 3:  5  1  4  4  0  4   S 5   9.9233465    0.0062   9.9233527   Err 0.1D-04          -
 4:  5  1  4  4  0  4   S 4   9.9233477    0.0099   9.9233575   Err 0.1D-04          -
 5:  5  1  4  4  0  4   S 3   9.9233517    0.0058   9.9233575   Err 0.1D-04          -
 6: 14  7  7 14  6  8   S 3  11.1066622   -0.0236  11.1066386   Err 0.1D-04          -
 7: 12  7  5 12  6  6   S 3  11.1713580    0.0165  11.1713745   Err 0.1D-04          -
 8:  7  1  7  6  0  6   S 1  11.2325752   -0.0150  11.2325602   Err 0.1D-04          -
 9:  8  7  1  8  6  2   S 3  11.2321217    0.0190  11.2321407   Err 0.1D-04          -
10:  7  7  0  7  6  1   S 3  11.2385618   -0.0161  11.2385456   Err 0.1D-04          -
11: 14  5 10 14  3 11   S 3  11.2694479    0.0155  11.2694634   Err 0.1D-04          -
12: 13  5  9 12  6  6   S 3  12.0783860    0.0202  12.0784062   Err 0.1D-04          -
13: 15  8  8 15  7  9   S 1  12.8609846   -0.0205  12.8609642   Err 0.1D-04          -
14: 14  8  6 14  7  7   S 2  12.8893051   -0.0184  12.8892867   Err 0.1D-04          -
15: 12  4  8 12  1 11   S 1  12.9007882   -0.0157  12.9007725   Err 0.1D-04          -
16: 12  3 10 11  4  7   S 2  13.3445462    0.0230  13.3445692   Err 0.1D-04          -
17: 10  1  9  9  2  7   S 1  13.5620064   -0.0000  13.5620064   Err 0.1D-04          -
18: 14  5 10 13  6  7   S 1  13.7911844   -0.0226  13.7911618   Err 0.1D-04          -
19: 10  2  8  9  3  7   S 1  13.9112224    0.0139  13.9112363   Err 0.1D-04          -
20:  6  3  4  5  2  4   S 4  14.2907711    0.0271  14.2907982   Err 0.1D-04          -
21: 19  9 10 19  8 11   S 1  14.5063698    0.0016  14.5063714   Err 0.1D-04          -
22: 19  9 10 19  8 11   S 5  14.5081806    0.0083  14.5081889   Err 0.1D-04          -
23:  9  6  3  8  6  2   S 5  14.8071970    0.0084  14.8072054   Err 0.1D-04          -
24: 20 10 11 19 11  8   S 1  14.8916957    0.0102  14.8917060   Err 0.1D-04          -
```

```
 25: 14  4 11 13  5  9   S 1  15.4776244    0.0255  15.4776499   Err 0.1D-04          -
 26: 15  5 11 14  6  9   S 3  15.5100056    0.0091  15.5100147   Err 0.1D-04          -
 27: 10  1 10  9  1  9   S 1  15.6448716    0.0122  15.6448838   Err 0.1D-04          -
 28: 21  2 19 20  5 16   S 1  15.6644801   -0.0099  15.6644702   Err 0.1D-04          -
 29: 18 10  8 18  9  9   S 2  16.3244524    0.0227  16.3244752   Err 0.1D-04          -
 30: 12 10  3 12  9  4   S 2  16.4137865   -0.0195  16.4137670   Err 0.1D-04          -
 31: 10  8  2  9  8  1   S 1  16.4404756   -0.0475  16.4404280   Err 0.1D-04          -
 32: 18  7 12 17  8  9   S 3  16.9456151   -0.0175  16.9455976   Err 0.1D-04          -
 33:  8  3  6  7  2  6   S 4  17.7949981   -0.0271  17.7949711   Err 0.1D-04          -
 34: 19  5 14 19  2 17   S 1  18.6543021   -0.0133  18.6542888   Err 0.1D-04          -
 35: 11  6  6 11  5  6   S 5   9.4019345    0.0074   9.4019418   Err 0.1D-04          -
 36: 12  6  6 12  5  7   S 1   9.3749815    0.0100   9.3749915   Err 0.1D-04          -
 37:  9  3  7  8  4  4   S 1   8.7669435   -0.0142   8.7669293   Err 0.1D-04          -
 38: 15  4 11 15  3 13   S 3   8.3322167    0.0461   8.3322628   Err 0.1D-04          -
 39: 15  4 11 15  3 13   S 4   8.3322528    0.0100   8.3322628   Err 0.1D-04          -
 40: 15  4 11 15  3 13   S 5   8.3323077   -0.0448   8.3322628   Err 0.1D-04          -
 41: 13  1 12 12  4  9   S 1   8.3250327    0.0103   8.3250430   Err 0.1D-04          -
 42: 13  1 12 12  4  9   S 2   8.3250573   -0.0143   8.3250430   Err 0.1D-04          -
 43: 10  5  6 10  4  7   S 4   7.6945341    0.0185   7.6945526   Err 0.1D-04          -
 44: 10  5  6 10  4  7   S 1   7.6948178    0.0454   7.6948632   Err 0.1D-04          -
 45:  5  4  1  5  3  3   S 1   6.0428341    0.0179   6.0428520   Err 0.1D-04          -
 46:  5  4  1  5  3  3   S 4   6.0428350    0.0170   6.0428520   Err 0.1D-04          -
 47: 14  2 12 14  2 13   S 1   6.0149564    0.0238   6.0149802   Err 0.1D-04          -
 48:  8  3  6  8  1  7   S 3   5.8121468   -0.0356   5.8121112   Err 0.1D-04          -
Maximum (obs-calc)/err in line  31   0.0000475

 RMS deviations (MHz), B and V sorted
  B  V   n splittings MHz
  B  V   n abs. freq. MHz
  1  1  48         0.020733         0.025052

          Parameters  and  Errors
 BJ          0.819980631 { 0.000000441}
 BK          0.866405105 { 0.000000804}
 B-          0.052875058 { 0.000000193}
 DJ          0.190054E-6 { 0.000859E-6}
 DJK         0.147731E-6 { 0.003467E-6}
 dj         -0.001203E-6 { 0.000321E-6}
\F12         -0.981409503 {     derived}
\F          159.448322216 {     derived}  159.362766124 {     derived}
 V1n         15207.967561 {   66.882718}   14870.078798 {   60.341125}
\rho          0.009366623 {     derived}    0.008963666 {     derived}
\beta         0.328884973 {     derived}    2.803179022 {     derived}
```

\gamma 0.348607921 { derived} 1.374635371 { derived}
delta 0.590723909 { 0.036232117} 2.485180346 { 0.028233102}

Standard Deviation 0.023615 MHz

---------- B = 1
Rotational Constants and Errors (in GHz)
B_z 1.686385736 0.000000991
B_x 0.872855689 0.000000505
B_y 0.767105574 0.000000457
Ray's kappa -0.76993
F0(calc) 158.000000000 0.000000000
I_alpha 3.198601709 0.000000000
<(i,x) <(i,y) <(i,z) 59.0235 77.7105 33.8460
d<(i,x) d<(i,y) d<(i,z) 1.8537 0.6669 2.0759

F0(calc) 158.000000000 0.000000000
I_alpha 3.198601709 0.000000000
<(i,x) <(i,y) <(i,z) 83.9734 53.0456 142.3903
d<(i,x) d<(i,y) d<(i,z) 0.2240 1.5805 1.6176

V1n_1 6.068455 kj +/- 0.026688 kj 1.449390 kcal +/- 0.006374 kcal
507.283123 cm +/- 2.2310 cm s= 42.390516
V1n_2 5.933627 kj +/- 0.024078 kj 1.417188 kcal +/- 0.005751 kcal
496.012369 cm +/- 2.0128 cm s= 41.448689

F(calc) 159.448322216
F(calc) 159.362766124

$^{13}C_{10}$ XIAM Output

	J K- K+	J K- K+	Sym	calc/GHz	diff/MHz	obs/GHz	
1:	6 2 4	5 2 3	S 1	9.9610933	0.0074	9.9611007	Err 0.1D-04 -
2:	10 3 8	9 4 5	S 4	10.1541278	-0.0027	10.1541250	Err 0.1D-04 -
3:	14 7 8	14 6 9	S 1	11.2041268	0.0230	11.2041498	Err 0.1D-04 -
4:	8 7 2	8 6 3	S 1	11.3199709	0.0227	11.3199936	Err 0.1D-04 -
5:	8 7 1	8 6 2	S 3	11.3206720	-0.0340	11.3206381	Err 0.1D-04 -
6:	7 7 0	7 6 1	S 3	11.3267709	0.0068	11.3267777	Err 0.1D-04 -
7:	15 7 9	14 8 7	S 2	11.4865562	0.0055	11.4865617	Err 0.1D-04 -
8:	15 7 9	14 8 7	S 3	11.4864654	0.0192	11.4864846	Err 0.1D-04 -
9:	15 7 8	14 8 6	S 4	11.4857336	-0.0229	11.4857107	Err 0.1D-04 -
10:	21 6 16	21 4 17	S 2	12.3854797	0.0209	12.3855006	Err 0.1D-04 -
11:	21 6 16	21 4 17	S 1	12.3859096	-0.0227	12.3858869	Err 0.1D-04 -

```
 12: 12  8  5 12  7  6   S 5  13.0304142    0.0320  13.0304462   Err 0.1D-04          -
 13: 12  8  5 12  7  6   S 3  13.0315933   -0.0246  13.0315687   Err 0.1D-04          -
 14:  8  4  5  7  4  4   S 3  13.0491743    0.0124  13.0491867   Err 0.1D-04          -
 15: 12  3 10 11  4  8   S 3  13.2709452    0.0168  13.2709620   Err 0.1D-04          -
 16:  9  4  6  8  4  5   S 3  14.6913436    0.0037  14.6913473   Err 0.1D-04          -
 17: 16  9  8 16  8  9   S 2  14.7251497    0.0095  14.7251592   Err 0.1D-04          -
 18: 16  9  8 16  8  9   S 1  14.7263833    0.0006  14.7263839   Err 0.1D-04          -
 19: 15  9  7 15  8  8   S 5  14.7456011   -0.0186  14.7455826   Err 0.1D-04          -
 20: 12  3  9 11  4  8   S 1  14.8918994    0.0061  14.8919055   Err 0.1D-04          -
 21: 11  4  8 10  4  7   S 1  17.9798404   -0.0428  17.9797976   Err 0.1D-04          -
 22: 20  8 13 19  9 11   S 5  18.0603950    0.0002  18.0603953   Err 0.1D-04          -
 23: 10  1 10  9  2  7   S 1   8.4642653    0.0014   8.4642667   Err 0.1D-04          -
Maximum (obs-calc)/err in line  21   0.0000428

 RMS deviations (MHz), B and V sorted
  B  V   n splittings MHz
  B  V   n abs. freq. MHz
  1  1  23         0.019303         0.025177

          Parameters  and  Errors
 BJ          0.811704764 { 0.000000657}
 BK          0.873085915 { 0.000000911}
 B-          0.051641153 { 0.000000168}
 DJ          0.180676E-6 { 0.001333E-6}
 DJK         0.158811E-6 { 0.003686E-6}
\F12        -1.086133128 {     derived}
\F         159.482937282 {     derived}  159.409851100 {     derived}
 V1n         15299.110194 {   22.555571}   14987.313823 {   24.843580}
\rho         0.009544676 {     derived}    0.009209411 {     derived}
\beta        0.294879991 {     derived}    2.840439651 {     derived}
\gamma       0.349164494 {     derived}    1.374966301 {     derived}

 Standard Deviation       0.023902 MHz

------------------------------------ B =  1
 Rotational Constants and Errors (in GHz)
     B_z       1.684790678       0.000001237
     B_x       0.863345916       0.000000694
     B_y       0.760063611       0.000000662
 Ray's kappa   -0.77662
 F0(calc)     158.000000000       0.000000000
 I_alpha        3.198601709       0.000000000
 <(i,x)  <(i,y)  <(i,z)       61.5090       78.6224       31.0779
```

d<(i,x) d<(i,y) d<(i,z) 0.0000 0.0000 0.0000

F0(calc) 158.000000000 0.000000000
I_alpha 3.198601709 0.000000000
<(i,x) <(i,y) <(i,z) 84.4177 56.1510 145.5674
d<(i,x) d<(i,y) d<(i,z) 0.0000 0.0000 0.0000

V1n_1 6.104824 kj +/- 0.009000 kj 1.458076 kcal +/- 0.002150 kcal
  510.323313 cm +/- 0.7524 cm s= 42.635310
V1n_2 5.980408 kj +/- 0.009913 kj 1.428361 kcal +/- 0.002368 kcal
  499.922907 cm +/- 0.8287 cm s= 41.766401

F(calc) 159.482937282
F(calc) 159.409851100

$^{13}C_{11}$ XIAM Output

	J K- K+	J K- K+	Sym	calc/GHz	diff/MHz	obs/GHz		
1:	19 2 17	19 1 18	S 1	9.7680890	0.0014	9.7680904	Err 0.1D-04	-
2:	18 3 15	17 6 12	S 1	11.3678002	0.0291	11.3678293	Err 0.1D-04	-
3:	18 3 15	17 6 12	S 4	11.3684203	-0.0103	11.3684100	Err 0.1D-04	-
4:	18 3 15	17 6 12	S 3	11.3684954	-0.0104	11.3684850	Err 0.1D-04	-
5:	7 3 4	6 3 3	S 2	11.5950996	-0.0013	11.5950984	Err 0.1D-04	-
6:	7 3 4	6 3 3	S 3	11.5951112	-0.0129	11.5950984	Err 0.1D-04	-
7:	5 2 3	4 1 4	S 1	11.5976730	0.0025	11.5976755	Err 0.1D-04	-
8:	4 4 1	3 3 0	S 1	12.5084725	-0.0468	12.5084257	Err 0.1D-04	-
9:	8 4 5	7 4 4	S 1	13.1817080	0.0262	13.1817342	Err 0.1D-04	-
10:	8 4 5	7 4 4	S 4	13.1817026	0.0316	13.1817342	Err 0.1D-04	-
11:	10 2 8	9 3 6	S 4	13.5536358	-0.0243	13.5536116	Err 0.1D-04	-
12:	11 1 10	10 2 8	S 5	14.5724959	-0.0090	14.5724869	Err 0.2D-04	-
13:	11 1 10	10 2 8	S 4	14.5724779	0.0090	14.5724869	Err 0.2D-04	-
14:	11 1 10	10 2 8	S 2	14.5724726	0.0143	14.5724869	Err 0.2D-04	-
15:	20 3 17	19 6 14	S 3	14.7047869	-0.0141	14.7047728	Err 0.1D-04	-
16:	20 3 17	19 6 14	S 2	14.7047647	0.0081	14.7047728	Err 0.1D-04	-
17:	9 5 4	8 5 3	S 4	14.8208050	0.0115	14.8208165	Err 0.1D-04	-
18:	9 5 4	8 5 3	S 1	14.8209698	-0.0043	14.8209655	Err 0.1D-04	-
19:	9 4 6	8 4 5	S 1	14.8417721	0.0118	14.8417839	Err 0.1D-04	-
20:	9 4 6	8 4 5	S 4	14.8417545	0.0295	14.8417839	Err 0.1D-04	-
21:	13 5 8	13 2 11	S 3	15.2063119	-0.0462	15.2062658	Err 0.1D-04	-
22:	13 5 8	13 2 11	S 5	15.2071931	0.0010	15.2071941	Err 0.1D-04	-
23:	16 6 10	15 7 8	S 4	15.6327021	0.0021	15.6327043	Err 0.1D-04	-
24:	21 2 19	20 5 16	S 3	15.7168096	0.0105	15.7168201	Err 0.1D-04	-
25:	12 10 2	12 9 3	S 2	16.1009238	0.0011	16.1009248	Err 0.1D-04	-
26:	8 1 7	7 0 7	S 3	16.2763899	0.0209	16.2764108	Err 0.1D-04	-

```
 27:  8  1  7  7  0  7   S 1  16.2764332   -0.0224  16.2764108   Err 0.1D-04          -
 28: 16  5 12 15  6 10   S 1  17.4036722   -0.0331  17.4036392   Err 0.1D-04          -
 29: 12 11  1 12 10  2   S 1  17.8040447    0.0431  17.8040878   Err 0.1D-04          -
 30: 19  7 13 19  5 14   S 1  18.2095411   -0.0086  18.2095325   Err 0.1D-04          -
 31:  4  2  3  3  1  3   S 1   9.4258257   -0.0240   9.4258017   Err 0.1D-04          -
 32: 11  6  6 11  5  7   S 1   9.2425981    0.0222   9.2426203   Err 0.1D-04          -
 33: 20  5 16 20  4 17   S 1   8.6585332    0.0177   8.6585509   Err 0.1D-04          -
 34: 14  8  6 13  9  4   S 5   8.6647958   -0.0088   8.6647870   Err 0.1D-04          -
 35:  5  5  1  5  4  2   S 5   7.6266467   -0.0128   7.6266339   Err 0.1D-04          -
 36:  8  4  5  8  3  5   S 1   5.6805233   -0.0085   5.6805148   Err 0.1D-04          -
Maximum (obs-calc)/err in line   8   0.0000468

RMS deviations (MHz), B and V sorted
 B  V   n splittings MHz
 B  V   n abs. freq. MHz
 1  1  36         0.021245         0.027147

          Parameters  and  Errors
 BJ          0.819709427 { 0.000000529}
 BK          0.849928849 { 0.000000986}
 B-          0.053362313 { 0.000000326}
 DJ          0.169319E-6 { 0.001122E-6}
 DJK         0.124294E-6 { 0.003977E-6}
 dj         -0.001187E-6 { 0.000442E-6}
\F12         -1.093365639 {     derived}
\F          159.488813904 {     derived}  159.402106078 {     derived}
 V1n         15340.514124 {   75.246007}   14966.888603 {   79.665106}
\rho         0.009551212 {     derived}    0.009143766 {     derived}
\beta        0.287661510 {     derived}    2.835891782 {     derived}
\gamma       0.348211072 {     derived}    1.374398817 {     derived}
 delta       0.522239157 { 0.043774429}    2.541296495 { 0.043285798}

 Standard Deviation       0.025494 MHz

------------------------------------ B =  1
 Rotational Constants and Errors (in GHz)
     B_z       1.669638276       0.000001182
     B_x       0.873071740       0.000000563
     B_y       0.766347114       0.000000675
 Ray's kappa   -0.76370
 F0(calc)     158.000000000       0.000000000
 I_alpha        3.198601709       0.000000000
 <(i,x)  <(i,y)  <(i,z)       62.5510       79.0103       29.9221
```

d<(i,x) d<(i,y) d<(i,z) 2.2581 0.8365 2.5081

F0(calc) 158.000000000 0.000000000
I_alpha 3.198601709 0.000000000
<(i,x) <(i,y) <(i,z) 84.4231 56.1883 145.6056
d<(i,x) d<(i,y) d<(i,z) 0.3588 2.4278 2.4801

V1n_1 6.121346 kj +/- 0.030026 kj 1.462022 kcal +/- 0.007171 kcal
  511.704400 cm +/- 2.5099 cm s= 42.749119
V1n_2 5.972257 kj +/- 0.031789 kj 1.426414 kcal +/- 0.007592 kcal
  499.241596 cm +/- 2.6573 cm s= 41.707944

F(calc) 159.488813904
F(calc) 159.402106078

AX3 Kraitchman Output

| KRA - SINGLE ISOTOPIC SUBSTITUTION - Various permutations |
| of Kraitchman's equations for symmetric/asymmetric tops |

version 4a.IV.2017 Zbigniew KISIEL

R-Carvon AX3
---

parent species
Planar calculation will be made from I.a and I.b

C(1)

The parent species:

X, Y, Z = 1687.81520000 878.27870000 771.30600000
eX, eY, eZ = 0.00050000 0.00020000 0.00020000
IX, IY, IZ = 299.42792842 575.41986262 655.22504544
eIX,eIY,eIZ = 0.00008870 0.00013103 0.00016990
PX, PY, PZ = 465.60848982 189.61655562 109.81137280

Mass = 150.10446507

The isotopic species:

X, Y, Z =	1670.90100000	876.82360000	768.27970000
eX, eY, eZ =	0.00100000	0.00050000	0.00050000
IX, IY, IZ =	302.45897806	576.37477926	657.80601635
eIX,eIY,eIZ =	0.00018102	0.00032867	0.00042810
PX, PY, PZ =	465.86090878	191.94510758	110.51387048

Mass change = 1.00335484
Total mass = 151.10781991
M DM/(M+DM) = 0.99669257

KRAITCHMAN RESULTS:

	a	b			
PLANAR:	0.97343	+- 0.00018	1.74689	+- 0.00006	
+Costain err.	0.97343	+- 0.00155	1.74689	+- 0.00086	

	a	b	c			
NONPLANAR:	0.50062	+- 0.00030	1.52244	+- 0.00010	0.85200	+- 0.00019
+Costain err.	0.50062	+- 0.00301	1.52244	+- 0.00099	0.85200	+- 0.00177

R= 1.81504 +- 0.00144

DIX,DIY,DIZ =	3.03104964	0.95491664	2.58097091
DPX,DPY,DPZ =	0.25241895	2.32855195	0.70249768
IXY,IXZ,IYZ =	-275.99193420	-355.79711702	-79.80518282

C(2)

The parent species:

X, Y, Z =	1687.81520000	878.27870000	771.30600000
eX, eY, eZ =	0.00050000	0.00020000	0.00020000
IX, IY, IZ =	299.42792842	575.41986262	655.22504544
eIX,eIY,eIZ =	0.00008870	0.00013103	0.00016990

PX, PY, PZ = 465.60848982 189.61655562 109.81137280

Mass = 150.10446507

The isotopic species:

X, Y, Z = 1672.31200000 877.66200000 767.82100000
eX, eY, eZ = 0.00300000 0.00200000 0.00200000
IX, IY, IZ = 302.20378069 575.82418847 658.19899286
eIX,eIY,eIZ = 0.00054213 0.00131218 0.00171446
PX, PY, PZ = 465.90970032 192.28929254 109.91448815

Mass change = 1.00335484
Total mass = 151.10781991
M DM/(M+DM) = 0.99669257

KRAITCHMAN RESULTS:

a b

PLANAR: 0.63371 +- 0.00103 1.67007 +- 0.00017
+Costain err. 0.63371 +- 0.00258 1.67007 +- 0.00091

a b c

NONPLANAR: 0.54699 +- 0.00102 1.63740 +- 0.00034 0.32713 +- 0.00178
+Costain err. 0.54699 +- 0.00292 1.63740 +- 0.00098 0.32713 +- 0.00492

R= 1.75706 +- 0.00158

DIX,DIY,DIZ = 2.77585227 0.40432584 2.97394742
DPX,DPY,DPZ = 0.30121050 2.67273692 0.10311535
IXY,IXZ,IYZ = -275.99193420 -355.79711702 -79.80518282

C(3)

The parent species:

X, Y, Z = 1687.81520000 878.27870000 771.30600000
eX, eY, eZ = 0.00050000 0.00020000 0.00020000
IX, IY, IZ = 299.42792842 575.41986262 655.22504544

eIX,eIY,eIZ = 0.00008870 0.00013103 0.00016990
PX, PY, PZ = 465.60848982 189.61655562 109.81137280

Mass = 150.10446507

The isotopic species:

X, Y, Z = 1685.06700000 874.86700000 768.30050000
eX, eY, eZ = 0.00100000 0.00100000 0.00070000
IX, IY, IZ = 299.91626974 577.66381507 657.78820774
eIX,eIY,eIZ = 0.00017798 0.00066029 0.00059931
PX, PY, PZ = 467.76787654 190.02033120 109.89593854

Mass change = 1.00335484
Total mass = 151.10781991
M DM/(M+DM) = 0.99669257

KRAITCHMAN RESULTS:

a b

PLANAR: 1.49914 +- 0.00022 0.70281 +- 0.00014
+Costain err. 1.49914 +- 0.00103 0.70281 +- 0.00214

a b c

NONPLANAR: 1.47067 +- 0.00016 0.63863 +- 0.00037 0.29290 +- 0.00081
+Costain err. 1.47067 +- 0.00103 0.63863 +- 0.00238 0.29290 +- 0.00519

R= 1.62988 +- 0.00161

DIX,DIY,DIZ = 0.48834131 2.24395245 2.56316230
DPX,DPY,DPZ = 2.15938671 0.40377558 0.08456573
IXY,IXZ,IYZ = -275.99193420 -355.79711702 -79.80518282

C(4)

The parent species:

X, Y, Z = 1687.81520000 878.27870000 771.30600000
eX, eY, eZ = 0.00050000 0.00020000 0.00020000

```
 IX, IY, IZ  =       299.42792842       575.41986262       655.22504544
eIX,eIY,eIZ  =         0.00008870         0.00013103         0.00016990
 PX, PY, PZ  =       465.60848982       189.61655562       109.81137280

 Mass        =       150.10446507
```

The isotopic species:

```
  X,  Y,  Z  =      1684.38200000       875.76810000       769.00390000
 eX, eY, eZ  =         0.00100000         0.00070000         0.00070000
 IX, IY, IZ  =       300.03823889       577.06944213       657.18653559
eIX,eIY,eIZ  =         0.00017813         0.00046125         0.00059822
 PX, PY, PZ  =       467.10886942       190.07766618       109.96057271

 Mass change =         1.00335484
 Total mass  =       151.10781991
 M DM/(M+DM) =         0.99669257
```

KRAITCHMAN RESULTS:

```
                    a                  b

    PLANAR:       1.28507  +- 0.00019    0.78485  +- 0.00013
+Costain err.     1.28507  +- 0.00118    0.78485  +- 0.00192

                    a                  b                  c

  NONPLANAR:      1.22565  +- 0.00017    0.68139  +- 0.00030    0.38884  +- 0.00053
+Costain err.     1.22565  +- 0.00123    0.68139  +- 0.00222    0.38884  +- 0.00389

                                        R=  1.45523  +- 0.00180

DIX,DIY,DIZ  =        0.61031047         1.64957950         1.96149015
DPX,DPY,DPZ  =        1.50037959         0.46111056         0.14919991
IXY,IXZ,IYZ  =     -275.99193420      -355.79711702       -79.80518282
```

C(5)

The parent species:

```
  X,  Y,  Z  =      1687.81520000       878.27870000       771.30600000
```

```
 eX, eY, eZ  =         0.00050000        0.00020000        0.00020000
 IX, IY, IZ  =       299.42792842      575.41986262      655.22504544
eIX,eIY,eIZ  =         0.00008870        0.00013103        0.00016990
 PX, PY, PZ  =       465.60848982      189.61655562      109.81137280

 Mass        =       150.10446507
```

The isotopic species:

```
  X,  Y,  Z  =      1674.50800000      875.90800000      770.51890000
 eX, eY, eZ  =         0.00200000        0.00090000        0.00090000
 IX, IY, IZ  =       301.80746159      576.97727261      655.89437053
eIX,eIY,eIZ  =         0.00036047        0.00059285        0.00076611
 PX, PY, PZ  =       465.53209078      190.36227976      111.44518184

 Mass change =         1.00335484
 Total mass  =       151.10781991
 M DM/(M+DM) =         0.99669257
```

KRAITCHMAN RESULTS:

```
                    a                 b

    PLANAR:       1.24463  +- 0.00024    1.54948  +- 0.00012
+Costain err.     1.24463  +- 0.00123    1.54948  +- 0.00098

                    a                 b                 c

  NONPLANAR:      0.27585*i+- 0.00096    0.85597  +- 0.00030    1.28615  +-
0.00021
 +Costain err.    0.27585*i+- 0.00552    0.85597  +- 0.00178    1.28615  +- 0.00118

                                        R=  1.52012  +- 0.00174

DIX,DIY,DIZ  =        2.37953317        1.55740999        0.66932509
DPX,DPY,DPZ  =       -0.07639904        0.74572414        1.63380903
IXY,IXZ,IYZ  =     -275.99193420     -355.79711702      -79.80518282
```

C(6)

The parent species:

X, Y, Z =	1687.81520000	878.27870000	771.30600000
eX, eY, eZ =	0.00050000	0.00020000	0.00020000
IX, IY, IZ =	299.42792842	575.41986262	655.22504544
eIX,eIY,eIZ =	0.00008870	0.00013103	0.00016990
PX, PY, PZ =	465.60848982	189.61655562	109.81137280

Mass = 150.10446507

The isotopic species:

X, Y, Z =	1683.07000000	875.24310000	769.88060000
eX, eY, eZ =	0.00100000	0.00050000	0.00050000
IX, IY, IZ =	300.27212707	577.41558762	656.43816574
eIX,eIY,eIZ =	0.00017841	0.00032986	0.00042632
PX, PY, PZ =	466.79081315	189.64735259	110.62477448

Mass change = 1.00335484
Total mass = 151.10781991
M DM/(M+DM) = 0.99669257

KRAITCHMAN RESULTS:

	a	b	
PLANAR:	1.41288 +- 0.00013	0.92365 +- 0.00011	
+Costain err.	1.41288 +- 0.00107	0.92365 +- 0.00163	

	a	b	c
NONPLANAR:	1.08784 +- 0.00014	0.17526 +- 0.00087	0.90506 +- 0.00017
+Costain err.	1.08784 +- 0.00139	0.17526 +- 0.00860	0.90506 +- 0.00167

R= 1.42592 +- 0.00183

DIX,DIY,DIZ =	0.84419864	1.99572500	1.21312029
DPX,DPY,DPZ =	1.18232333	0.03079697	0.81340167
IXY,IXZ,IYZ =	-275.99193420	-355.79711702	-79.80518282

C(7)

The parent species:

X, Y, Z =	1687.81520000	878.27870000	771.30600000
eX, eY, eZ =	0.00050000	0.00020000	0.00020000
IX, IY, IZ =	299.42792842	575.41986262	655.22504544
eIX,eIY,eIZ =	0.00008870	0.00013103	0.00016990
PX, PY, PZ =	465.60848982	189.61655562	109.81137280

Mass = 150.10446507

The isotopic species:

X, Y, Z =	1677.51200000	865.70050000	762.25040000
eX, eY, eZ =	0.00200000	0.00070000	0.00060000
IX, IY, IZ =	301.26700071	583.78042857	663.00917507
eIX,eIY,eIZ =	0.00035918	0.00047204	0.00052188
PX, PY, PZ =	472.76130146	190.24787361	111.01912711

Mass change = 1.00335484
Total mass = 151.10781991
M DM/(M+DM) = 0.99669257

KRAITCHMAN RESULTS:

	a	b			
PLANAR:	2.88659	+- 0.00008	1.37879	+- 0.00014	
+Costain err.	2.88659	+- 0.00053	1.37879	+- 0.00110	

	a	b	c			
NONPLANAR:	2.67130	+- 0.00008	0.80000	+- 0.00026	1.11620	+- 0.00019
+Costain err.	2.67130	+- 0.00057	0.80000	+- 0.00189	1.11620	+- 0.00136

R= 3.00362 +- 0.00087

DIX,DIY,DIZ =	1.83907229	8.36056594	7.78412963
DPX,DPY,DPZ =	7.15281164	0.63131799	1.20775430
IXY,IXZ,IYZ =	-275.99193420	-355.79711702	-79.80518282

C(9)

The parent species:

X, Y, Z =	1687.81520000	878.27870000	771.30600000
eX, eY, eZ =	0.00050000	0.00020000	0.00020000
IX, IY, IZ =	299.42792842	575.41986262	655.22504544
eIX,eIY,eIZ =	0.00008870	0.00013103	0.00016990
PX, PY, PZ =	465.60848982	189.61655562	109.81137280

Mass = 150.10446507

The isotopic species:

X, Y, Z =	1686.38600000	872.85570000	767.10560000
eX, eY, eZ =	0.00100000	0.00050000	0.00050000
IX, IY, IZ =	299.68169144	578.99491164	658.81282694
eIX,eIY,eIZ =	0.00017771	0.00033167	0.00042941
PX, PY, PZ =	469.06302357	189.74980337	109.93188807

Mass change = 1.00335484
Total mass = 151.10781991
M DM/(M+DM) = 0.99669257

KRAITCHMAN RESULTS:

	a	b	
PLANAR:	1.89304 +- 0.00009	0.50784 +- 0.00020	
+Costain err.	1.89304 +- 0.00080	0.50784 +- 0.00296	
	a	b	c
NONPLANAR:	1.86095 +- 0.00008	0.36764 +- 0.00043	0.34970 +- 0.00045
+Costain err.	1.86095 +- 0.00081	0.36764 +- 0.00410	0.34970 +- 0.00431

R= 1.92889 +- 0.00135

DIX,DIY,DIZ =	0.25376301	3.57504902	3.58778150
DPX,DPY,DPZ =	3.45453375	0.13324775	0.12051527
IXY,IXZ,IYZ =	-275.99193420	-355.79711702	-79.80518282

C(10)

The parent species:

X, Y, Z =	1687.81520000	878.27870000	771.30600000
eX, eY, eZ =	0.00050000	0.00020000	0.00020000
IX, IY, IZ =	299.42792842	575.41986262	655.22504544
eIX,eIY,eIZ =	0.00008870	0.00013103	0.00016990
PX, PY, PZ =	465.60848982	189.61655562	109.81137280

Mass = 150.10446507

The isotopic species:

X, Y, Z =	1684.79100000	863.34590000	760.06360000
eX, eY, eZ =	0.00100000	0.00070000	0.00070000
IX, IY, IZ =	299.96540158	585.37257072	664.91673710
eIX,eIY,eIZ =	0.00017804	0.00047462	0.00061237
PX, PY, PZ =	475.16195312	189.75478398	110.21061760

Mass change = 1.00335484
Total mass = 151.10781991
M DM/(M+DM) = 0.99669257

KRAITCHMAN RESULTS:

	a	b	
PLANAR:	3.15694 +- 0.00008	0.74746 +- 0.00014	
+Costain err.	3.15694 +- 0.00048	0.74746 +- 0.00201	

	a	b	c
NONPLANAR:	3.09348 +- 0.00007	0.37785 +- 0.00057	0.64190 +- 0.00033
+Costain err.	3.09348 +- 0.00049	0.37785 +- 0.00401	0.64190 +- 0.00236

R= 3.18189 +- 0.00082

DIX,DIY,DIZ =	0.53747316	9.95270809	9.69169166
DPX,DPY,DPZ =	9.55346329	0.13822836	0.39924480
IXY,IXZ,IYZ =	-275.99193420	-355.79711702	-79.80518282

C(11)

The parent species:

X, Y, Z =	1687.81520000	878.27870000	771.30600000
eX, eY, eZ =	0.00050000	0.00020000	0.00020000
IX, IY, IZ =	299.42792842	575.41986262	655.22504544
eIX,eIY,eIZ =	0.00008870	0.00013103	0.00016990
PX, PY, PZ =	465.60848982	189.61655562	109.81137280

Mass = 150.10446507

The isotopic species:

X, Y, Z =	1669.63800000	873.07170000	766.34710000
eX, eY, eZ =	0.00100000	0.00060000	0.00070000
IX, IY, IZ =	302.68777358	578.85166694	659.46489378
eIX,eIY,eIZ =	0.00018129	0.00039780	0.00060237
PX, PY, PZ =	467.81439357	191.65050021	111.03727337

Mass change = 1.00335484
Total mass = 151.10781991
M DM/(M+DM) = 0.99669257

KRAITCHMAN RESULTS:

	a	b	
PLANAR:	1.84459 +- 0.00011	1.81971 +- 0.00006	
+Costain err.	1.84459 +- 0.00082	1.81971 +- 0.00083	

	a	b	c
NONPLANAR:	1.47964 +- 0.00013	1.42317 +- 0.00014	1.12656 +- 0.00018
+Costain err.	1.47964 +- 0.00102	1.42317 +- 0.00106	1.12656 +- 0.00134

R= 2.34177 +- 0.00112

DIX,DIY,DIZ =	3.25984515	3.43180431	4.23984834
DPX,DPY,DPZ =	2.20590375	2.03394459	1.22590056
IXY,IXZ,IYZ =	-275.99193420	-355.79711702	-79.80518282

AX3 EVAL Output

```
|                                                                      |
|     E V A L   -  Internals and their errors from Cartesians          |

|______________________________________________________________________
_____|
 version 20.V.2020                          Zbigniew KISIEL
```

WARNING:

The EVAL uncertainties are evaluated by assuming that the correlation matrix is a unit matrix.

The EVAL uncertainties may thus differ significantly (but typically by not more than 30% either way) from uncertainties in explicitly fitted internals corresponding to the input Cartesians.

```
!
! AX3, KRA coordinates
!
```

INPUT CARTESIANS:

C(1)	-0.50062	0.00301	-1.52244	0.00099	-0.85200	0.00177
C(2)	0.54699	0.00292	-1.63740	0.00098	0.32713	0.00492
C(3)	1.47067	0.00103	-0.63863	0.00238	0.29290	0.00519
C(4)	1.22565	0.00123	0.68139	0.00222	-0.38884	0.00389
C(5)	0.00000	0.00000	0.85597	0.00178	-1.28615	0.00118
C(6)	-1.08784	0.00139	-0.17526	0.00860	-0.90506	0.00167
C(7)	2.67130	0.00057	-0.80000	0.00189	1.11620	0.00136
C(9)	-1.86095	0.00081	0.36764	0.00410	0.34970	0.00431
C(10)	-3.09348	0.00049	-0.37785	0.00401	0.64190	0.00236
C(11)	-1.47964	0.00102	1.42317	0.00106	1.12656	0.00134

CALCULATED INTERNALS:

```
!
!  Bond lengths
```

```
!
        C(1)  C(2)   =   1.58147 +- 0.00479
        C(2)  C(3)   =   1.36084 +- 0.00283
        C(3)  C(4)   =   1.50574 +- 0.00410
        C(4)  C(5)   =   1.52901 +- 0.00260
        C(5)  C(6)   =   1.54663 +- 0.00596
        C(6)  C(1)   =   1.47056 +- 0.00804
        C(3)  C(7)   =   1.46471 +- 0.00318
        C(6)  C(9)   =   1.57062 +- 0.00501
        C(9)  C(11)  =   1.36494 +- 0.00418
        C(9)  C(10)  =   1.46978 +- 0.00317
!
!  Bond angles
!
    C(1)  C(2)  C(3)   =  112.18020 +- 0.30235
    C(2)  C(3)  C(4)   =  122.98011 +- 0.23464
    C(3)  C(4)  C(5)   =  119.75162 +- 0.16998
    C(4)  C(5)  C(6)   =  110.06478 +- 0.18400
    C(5)  C(6)  C(1)   =  109.80654 +- 0.18033
    C(6)  C(1)  C(2)   =  110.97832 +- 0.15606
    C(2)  C(3)  C(7)   =  117.47627 +- 0.29718
    C(4)  C(3)  C(7)   =  118.97717 +- 0.16877
    C(1)  C(6)  C(9)   =  118.97252 +- 0.36039
    C(5)  C(6)  C(9)   =  108.21554 +- 0.46411
    C(6)  C(9)  C(11)  =  125.76677 +- 0.27956
    C(6)  C(9)  C(10)  =  113.34559 +- 0.35644
!
! Dihedral Angles
!
C(1)  C(2)  C(3)  C(4)   =   23.08275 +- 0.52178
C(2)  C(3)  C(4)  C(5)   =  -10.68582 +- 0.56585
C(3)  C(4)  C(5)  C(6)   =   22.78048 +- 0.39423
C(4)  C(5)  C(6)  C(1)   =  -50.50063 +- 0.23840
C(5)  C(6)  C(1)  C(2)   =   66.16079 +- 0.22974
C(6)  C(1)  C(2)  C(3)   =  -51.57237 +- 0.36032
C(1)  C(2)  C(3)  C(7)   = -165.64857 +- 0.26145
C(5)  C(4)  C(3)  C(7)   =  178.17014 +- 0.24630
C(4)  C(5)  C(6)  C(9)   =   80.83959 +- 0.34218
C(2)  C(1)  C(6)  C(9)   =  -59.23246 +- 0.36379
C(5)  C(6)  C(9)  C(11)  =  -11.75557 +- 0.48647
C(1)  C(6)  C(9)  C(11)  =  114.39851 +- 0.47734
C(1)  C(6)  C(9)  C(10)  =  -65.82658 +- 0.32141
C(5)  C(6)  C(9)  C(10)  =  168.01934 +- 0.25100
```

S7. AX2 Assignments and Outputs of Structure Evaluation

Parent XIAM Output

	J	K-	K+	J	K-	K+	Sym	calc/GHz	diff/MHz	obs/GHz		
1:	4	0	4	3	1	3	S 1	6.1344233	-0.0125	6.1344109	Err 0.2D-04	-
2:	4	0	4	3	1	3	S 2	6.1344230	-0.0121	6.1344109	Err 0.2D-04	-
3:	4	0	4	3	1	3	S 4	6.1344137	-0.0029	6.1344109	Err 0.2D-04	-
4:	4	0	4	3	1	3	S 3	6.1344144	-0.0036	6.1344109	Err 0.2D-04	-
5:	3	1	2	2	0	2	S 1	6.2136335	-0.0281	6.2136054	Err 0.1D-04	-
6:	4	1	4	3	1	3	S 1	6.4659222	-0.0016	6.4659205	Err 0.2D-04	-
7:	4	1	4	3	1	3	S 3	6.4659182	0.0023	6.4659205	Err 0.2D-04	-
8:	4	1	4	3	1	3	S 2	6.4659147	0.0058	6.4659205	Err 0.2D-04	-
9:	4	1	4	3	1	3	S 4	6.4659105	0.0100	6.4659205	Err 0.2D-04	-
10:	4	1	4	3	1	3	S 5	6.4659110	0.0093	6.4659203	Err 0.1D-04	-
11:	4	2	3	3	2	2	S 2	6.7299372	-0.0191	6.7299181	Err 0.2D-04	-
12:	4	2	3	3	2	2	S 5	6.7299520	-0.0339	6.7299181	Err 0.2D-04	-
13:	4	2	3	3	2	2	S 4	6.7299089	0.0092	6.7299181	Err 0.2D-04	-
14:	4	2	3	3	2	2	S 3	6.7298947	0.0234	6.7299181	Err 0.2D-04	-
15:	4	2	3	3	2	2	S 1	6.7299015	0.0166	6.7299181	Err 0.2D-04	-
16:	4	2	2	3	2	1	S 2	6.8670282	0.0333	6.8670614	Err 0.1D-04	-
17:	4	1	3	3	1	2	S 1	6.9571684	0.0277	6.9571961	Err 0.1D-04	-
18:	5	0	5	4	1	4	S 1	7.8463426	-0.0143	7.8463283	Err 0.1D-04	-
19:	5	0	5	4	1	4	S 3	7.8463335	-0.0018	7.8463317	Err 0.2D-04	-
20:	5	0	5	4	1	4	S 2	7.8463275	0.0043	7.8463317	Err 0.2D-04	-
21:	5	0	5	4	1	4	S 4	7.8463181	0.0136	7.8463317	Err 0.2D-04	-
22:	5	0	5	4	1	4	S 5	7.8463185	0.0139	7.8463324	Err 0.1D-04	-
23:	3	1	3	2	0	2	S 1	5.4679331	-0.0334	5.4678997	Err 0.1D-04	-
24:	9	2	8	8	2	7	S 1	14.9197074	0.0070	14.9197145	Err 0.1D-04	-
25:	9	2	8	8	2	7	S 3	14.9196941	0.0210	14.9197152	Err 0.1D-04	-
26:	9	2	8	8	2	7	S 2	14.9196878	0.0274	14.9197152	Err 0.1D-04	-
27:	9	2	8	8	2	7	S 5	14.9196746	0.0406	14.9197152	Err 0.1D-04	-
28:	13	2	12	12	3	10	S 1	15.0649498	-0.0351	15.0649147	Err 0.1D-04	-
29:	9	1	8	8	1	7	S 1	15.1331044	0.0056	15.1331100	Err 0.1D-04	-
30:	9	1	8	8	1	7	S 3	15.1330932	0.0167	15.1331100	Err 0.1D-04	-
31:	9	1	8	8	1	7	S 2	15.1330651	0.0448	15.1331100	Err 0.1D-04	-
32:	9	3	7	8	3	6	S 2	15.2302570	0.0060	15.2302631	Err 0.1D-04	-
33:	9	3	7	8	3	6	S 1	15.2302661	-0.0010	15.2302651	Err 0.1D-04	-
34:	9	3	7	8	3	6	S 5	15.2302406	0.0245	15.2302651	Err 0.1D-04	-
35:	9	3	7	8	3	6	S 3	15.2302444	0.0207	15.2302651	Err 0.1D-04	-
36:	9	3	7	8	3	6	S 4	15.2302301	0.0350	15.2302651	Err 0.1D-04	-
37:	14	2	13	13	3	11	S 1	16.0848421	-0.0328	16.0848093	Err 0.1D-04	-
38:	7	3	4	6	2	5	S 1	16.2103713	-0.0158	16.2103556	Err 0.1D-04	-

39: 7 3 4 6 2 5 S 2 16.2103466 0.0090 16.2103556 Err 0.1D-04 -
40: 7 3 4 6 2 5 S 5 16.2103321 0.0235 16.2103556 Err 0.1D-04 -
41: 10 3 8 9 3 7 S 1 16.8959194 -0.0125 16.8959069 Err 0.1D-04 -
42: 10 3 8 9 3 7 S 2 16.8959010 0.0047 16.8959057 Err 0.1D-04 -
43: 10 3 8 9 3 7 S 3 16.8958965 0.0092 16.8959057 Err 0.1D-04 -
44: 10 3 8 9 3 7 S 5 16.8958804 0.0252 16.8959057 Err 0.1D-04 -
45: 10 3 8 9 3 7 S 4 16.8958757 0.0312 16.8959069 Err 0.1D-04 -
46: 6 1 6 5 0 5 S 1 9.8621384 0.0278 9.8621662 Err 0.1D-04 -
47: 6 1 6 5 0 5 S 2 9.8621442 0.0257 9.8621699 Err 0.1D-04 -
48: 6 1 6 5 0 5 S 3 9.8621389 0.0309 9.8621699 Err 0.1D-04 -
49: 6 1 6 5 0 5 S 4 9.8621450 0.0249 9.8621699 Err 0.1D-04 -
50: 6 1 6 5 0 5 S 5 9.8621445 0.0254 9.8621699 Err 0.1D-04 -
51: 7 1 6 6 2 4 S 1 9.9471685 -0.0262 9.9471423 Err 0.1D-04 -
52: 7 1 6 6 2 4 S 3 9.9471636 -0.0197 9.9471439 Err 0.1D-04 -
53: 7 1 6 6 2 4 S 5 9.9471606 -0.0167 9.9471439 Err 0.1D-04 -
54: 7 1 6 6 2 4 S 2 9.9471693 -0.0254 9.9471439 Err 0.1D-04 -
55: 7 1 6 6 2 4 S 4 9.9471681 -0.0234 9.9471447 Err 0.1D-04 -
56: 6 2 5 5 2 4 S 4 10.0459875 0.0139 10.0460014 Err 0.1D-04 -
57: 6 2 5 5 2 4 S 5 10.0459920 0.0113 10.0460033 Err 0.1D-04 -
58: 6 2 5 5 2 4 S 3 10.0459993 0.0040 10.0460033 Err 0.1D-04 -
59: 6 2 5 5 2 4 S 2 10.0460018 0.0015 10.0460033 Err 0.1D-04 -
60: 6 2 5 5 2 4 S 1 10.0460113 -0.0080 10.0460033 Err 0.1D-04 -
61: 6 1 5 5 1 4 S 1 10.3356203 -0.0400 10.3355803 Err 0.1D-04 -
62: 6 1 5 5 1 4 S 2 10.3356030 -0.0228 10.3355803 Err 0.1D-04 -
63: 6 1 5 5 1 4 S 3 10.3356042 -0.0239 10.3355803 Err 0.1D-04 -
64: 6 1 5 5 1 4 S 4 10.3355873 -0.0071 10.3355803 Err 0.1D-04 -
65: 6 1 5 5 1 4 S 5 10.3355864 -0.0057 10.3355807 Err 0.1D-04 -
66: 6 2 4 5 2 3 S 1 10.4236052 -0.0483 10.4235569 Err 0.1D-04 -
67: 6 2 4 5 2 3 S 2 10.4235923 -0.0391 10.4235532 Err 0.1D-04 -
68: 6 2 4 5 2 3 S 4 10.4235710 -0.0178 10.4235532 Err 0.1D-04 -
69: 6 2 4 5 2 3 S 3 10.4235817 -0.0244 10.4235573 Err 0.1D-04 -
70: 7 0 7 6 1 6 S 1 11.1503995 -0.0190 11.1503804 Err 0.1D-04 -
71: 7 0 7 6 1 6 S 3 11.1503923 -0.0119 11.1503804 Err 0.1D-04 -
72: 7 1 7 6 1 6 S 2 11.2250799 0.0237 11.2251036 Err 0.1D-04 -
73: 7 1 7 6 1 6 S 5 11.2250753 0.0294 11.2251047 Err 0.1D-04 -
74: 7 1 7 6 0 6 S 5 11.3551615 -0.0038 11.3551578 Err 0.1D-04 -
75: 7 1 7 6 0 6 S 4 11.3551629 -0.0060 11.3551570 Err 0.1D-04 -
76: 7 1 7 6 0 6 S 2 11.3551625 -0.0056 11.3551570 Err 0.1D-04 -
77: 10 2 9 9 3 7 S 1 11.6505164 0.0447 11.6505610 Err 0.1D-04 -
78: 10 2 9 9 3 7 S 3 11.6505404 0.0149 11.6505554 Err 0.1D-04 -
79: 10 2 9 9 3 7 S 2 11.6505781 -0.0227 11.6505554 Err 0.1D-04 -
80: 7 2 6 6 2 5 S 1 11.6847309 0.0177 11.6847486 Err 0.1D-04 -
81: 7 6 1 6 6 0 S 1 11.8392199 -0.0432 11.8391767 Err 0.1D-04 -

```
 82:  7  6  1  6  6  0   S 2  11.8391980   -0.0201  11.8391779   Err 0.1D-04          -
 83:  7  6  1  6  6  0   S 3  11.8391978   -0.0199  11.8391779   Err 0.1D-04          -
 84:  7  6  1  6  6  0   S 4  11.8391814   -0.0035  11.8391779   Err 0.1D-04          -
 85:  7  6  1  6  6  0   S 5  11.8391772    0.0007  11.8391779   Err 0.1D-04          -
 86:  7  1  6  6  1  5   S 4  11.9732540    0.0045  11.9732585   Err 0.1D-04          -
 87:  7  1  6  6  1  5   S 2  11.9732690   -0.0088  11.9732601   Err 0.1D-04          -
 88:  7  1  6  6  1  5   S 3  11.9732770   -0.0168  11.9732601   Err 0.1D-04          -
 89:  7  1  6  6  1  5   S 1  11.9732923   -0.0321  11.9732601   Err 0.1D-04          -
 90:  7  3  4  6  3  3   S 1  11.9851597   -0.0136  11.9851461   Err 0.1D-04          -
 91:  4  4  1  3  3  0   S 1  12.1972038   -0.0479  12.1971559   Err 0.2D-04          -
 92:  8  0  8  7  1  7   S 1  12.7554983   -0.0047  12.7554936   Err 0.2D-04          -
 93:  8  0  8  7  1  7   S 3  12.7554923    0.0024  12.7554947   Err 0.2D-04          -
 94:  8  2  7  7  2  6   S 1  13.3092464    0.0053  13.3092517   Err 0.1D-04          -
 95:  8  3  6  7  3  5   S 1  13.5514445    0.0117  13.5514562   Err 0.1D-04          -
 96:  8  3  6  7  3  5   S 2  13.5514539    0.0032  13.5514571   Err 0.1D-04          -
 97:  8  3  6  7  3  5   S 5  13.5514473    0.0098  13.5514571   Err 0.1D-04          -
 98:  8  1  7  7  1  6   S 3  13.5705114   -0.0170  13.5704944   Err 0.1D-04          -
 99:  8  1  7  7  1  6   S 1  13.5705247   -0.0303  13.5704944   Err 0.1D-04          -
100:  8  1  7  7  1  6   S 2  13.5704940   -0.0011  13.5704929   Err 0.1D-04          -
101:  8  1  7  7  1  6   S 5  13.5704806    0.0123  13.5704929   Err 0.1D-04          -
102:  8  3  5  7  3  4   S 5  13.7725088    0.0198  13.7725286   Err 0.1D-04          -
103:  8  3  5  7  3  4   S 4  13.7725337   -0.0051  13.7725286   Err 0.1D-04          -
104:  8  3  5  7  3  4   S 2  13.7725537   -0.0251  13.7725286   Err 0.1D-04          -
105: 14 11  3 13 12  1   S 2   5.8346726   -0.0341   5.8346386   Err 0.1D-04          -
106: 14 11  3 13 12  1   S 4   5.8349369    0.0230   5.8349599   Err 0.1D-04          -
107: 11  1 10 11  0 11   S 1   6.2878171   -0.0119   6.2878052   Err 0.1D-04          -
108: 19 16  3 18 17  1   S 1   6.5142262    0.0154   6.5142416   Err 0.1D-04          -
109: 21 18  3 20 19  1   S 1   6.7858042   -0.0222   6.7857820   Err 0.1D-04          -
110:  5  1  4  4  2  3   S 1   6.9142185   -0.0255   6.9141930   Err 0.1D-04          -
111:  4  1  4  3  0  3   S 1   6.9357424   -0.0069   6.9357355   Err 0.1D-04          -
112:  4  1  4  3  0  3   S 3   6.9357424   -0.0069   6.9357355   Err 0.1D-04          -
113:  4  1  4  3  0  3   S 4   6.9357208    0.0147   6.9357355   Err 0.1D-04          -
114:  4  1  4  3  0  3   S 5   6.9357204    0.0151   6.9357355   Err 0.1D-04          -
115:  4  1  4  3  0  3   S 2   6.9357207    0.0144   6.9357351   Err 0.1D-04          -
116: 17  3 14 17  2 15   S 2   7.3989160    0.0169   7.3989329   Err 0.1D-04          -
117:  5  0  5  4  0  4   S 1   8.1778415    0.0023   8.1778438   Err 0.1D-04          -
118: 13  2 11 12  5  8   S 1   8.2746154   -0.0352   8.2745802   Err 0.1D-04          -
119:  5  2  4  4  2  3   S 5   8.3938802    0.0143   8.3938945   Err 0.1D-04          -
120:  5  2  4  4  2  3   S 2   8.3938843    0.0101   8.3938944   Err 0.1D-04          -
121:  5  2  4  4  2  3   S 1   8.3938830    0.0114   8.3938944   Err 0.1D-04          -
122:  5  2  4  4  2  3   S 3   8.3938728    0.0217   8.3938944   Err 0.1D-04          -
123:  5  2  4  4  2  3   S 4   8.3938679    0.0265   8.3938944   Err 0.1D-04          -
124:  5  3  3  4  3  1   S 5   8.4570725    0.0055   8.4570780   Err 0.1D-04          -
```

125: 10 6 4 10 5 6 S 2 8.4636144 0.0213 8.4636357 Err 0.1D-04 -
126: 8 6 3 8 5 4 S 4 8.5065000 -0.0040 8.5064960 Err 0.1D-04 -
127: 17 5 13 17 3 14 S 2 8.5183408 0.0163 8.5183571 Err 0.1D-04 -
128: 18 5 14 18 3 15 S 5 8.5937266 0.0154 8.5937420 Err 0.1D-04 -
129: 18 5 14 18 3 15 S 4 8.5937332 0.0087 8.5937420 Err 0.1D-04 -
130: 18 5 14 18 3 15 S 2 8.5937675 -0.0256 8.5937420 Err 0.1D-04 -
131: 12 7 6 11 8 4 S 4 8.7392804 -0.0052 8.7392752 Err 0.1D-04 -
132: 18 7 12 18 6 12 S 1 9.2484242 0.0222 9.2484464 Err 0.1D-04 -
133: 6 0 6 5 1 5 S 5 9.5171024 0.0372 9.5171396 Err 0.1D-04 -
134: 6 0 6 5 1 5 S 2 9.5171104 0.0292 9.5171396 Err 0.1D-04 -
135: 6 0 6 5 1 5 S 1 9.5171526 -0.0130 9.5171396 Err 0.1D-04 -
136: 6 0 6 5 1 5 S 3 9.5171443 -0.0068 9.5171375 Err 0.1D-04 -
137: 18 7 11 18 6 13 S 4 9.6828159 -0.0242 9.6827917 Err 0.1D-04 -
138: 6 0 6 5 0 5 S 1 9.7320959 -0.0085 9.7320874 Err 0.1D-04 -
139: 6 0 6 5 0 5 S 3 9.7320924 -0.0050 9.7320874 Err 0.1D-04 -
140: 6 3 3 5 3 2 S 1 10.2246969 0.0281 10.2247250 Err 0.1D-04 -
141: 19 2 17 19 2 18 S 2 10.4718910 0.0040 10.4718950 Err 0.1D-04 -
142: 19 2 17 19 2 18 S 4 10.4717230 -0.0015 10.4717215 Err 0.1D-04 -
143: 4 3 2 3 2 1 S 1 10.5997739 -0.0252 10.5997487 Err 0.1D-04 -
144: 4 3 2 3 2 1 S 5 10.5977681 0.0148 10.5977828 Err 0.1D-04 -
145: 4 3 2 3 2 1 S 4 10.5988800 0.0126 10.5988926 Err 0.1D-04 -
146: 7 0 7 6 0 6 S 1 11.2804420 0.0396 11.2804816 Err 0.1D-04 -
147: 10 3 8 9 4 5 S 4 11.3024164 0.0073 11.3024238 Err 0.1D-04 -
148: 8 1 7 7 2 5 S 2 11.3239943 -0.0317 11.3239626 Err 0.1D-04 -
149: 16 8 8 16 7 10 S 2 11.4398128 -0.0075 11.4398053 Err 0.1D-04 -
150: 6 2 5 5 1 4 S 1 11.5256758 -0.0143 11.5256615 Err 0.1D-04 -
151: 13 8 6 13 7 7 S 5 11.5538309 0.0138 11.5538447 Err 0.1D-04 -
152: 11 1 11 10 2 9 S 1 11.6598184 -0.0114 11.6598070 Err 0.1D-04 -
153: 11 4 8 10 5 6 S 1 11.8286793 0.0352 11.8287146 Err 0.2D-04 -
154: 7 2 5 6 2 4 S 5 12.1936414 -0.0396 12.1936018 Err 0.1D-04 -
155: 7 2 5 6 2 4 S 5 12.1936414 -0.0393 12.1936021 Err 0.1D-04 -
156: 4 4 1 3 3 1 S 3 12.1976801 0.0340 12.1977141 Err 0.1D-04 -
157: 20 2 19 20 0 20 S 1 12.2538501 0.0148 12.2538649 Err 0.1D-04 -
158: 5 3 2 4 2 3 S 3 12.4404085 -0.0157 12.4403928 Err 0.1D-04 -
159: 17 2 16 16 3 13 S 3 12.5620242 0.0045 12.5620287 Err 0.1D-04 -
160: 12 1 12 11 2 10 S 1 12.6091022 0.0395 12.6091417 Err 0.1D-04 -
161: 8 1 8 7 1 7 S 5 12.7968078 -0.0015 12.7968063 Err 0.1D-04 -
162: 8 1 8 7 1 7 S 2 12.7968127 -0.0044 12.7968083 Err 0.1D-04 -
163: 8 1 8 7 1 7 S 4 12.7968093 -0.0006 12.7968087 Err 0.1D-04 -
164: 9 9 0 9 8 1 S 2 13.1974738 -0.0244 13.1974494 Err 0.1D-04 -
165: 8 7 1 7 7 0 S 1 13.5290959 0.0136 13.5291095 Err 0.1D-04 -
166: 8 4 4 7 4 3 S 2 13.5989365 -0.0418 13.5988948 Err 0.1D-04 -
167: 8 4 4 7 4 3 S 3 13.5998194 0.0286 13.5998480 Err 0.1D-04 -

168: 16 8 9 15 9 6 S 1 14.0753402 0.0165 14.0753566 Err 0.1D-04 -
169: 6 2 4 5 1 5 S 5 14.1981912 -0.0263 14.1981649 Err 0.1D-04 -
170: 6 2 4 5 1 5 S 4 14.1981838 -0.0188 14.1981649 Err 0.1D-04 -
171: 6 3 3 5 2 4 S 1 14.2712230 -0.0126 14.2712104 Err 0.1D-04 -
172: 6 3 3 5 2 4 S 3 14.2711992 0.0116 14.2712108 Err 0.1D-04 -
173: 6 3 3 5 2 4 S 4 14.2711820 0.0288 14.2712108 Err 0.1D-04 -
174: 22 10 13 22 9 13 S 3 14.3626455 -0.0050 14.3626405 Err 0.1D-04 -
175: 20 10 10 20 9 11 S 3 14.4972317 0.0046 14.4972363 Err 0.1D-04 -
176: 15 5 11 15 2 13 S 1 14.5349529 -0.0127 14.5349402 Err 0.1D-04 -
177: 15 5 11 15 2 13 S 5 14.5346361 0.0185 14.5346546 Err 0.1D-04 -
178: 19 10 10 19 9 11 S 3 14.5471784 0.0104 14.5471887 Err 0.1D-04 -
179: 19 10 9 19 9 10 S 3 14.5477320 -0.0016 14.5477304 Err 0.1D-04 -
180: 16 10 6 16 9 8 S 1 14.6564082 -0.0250 14.6563832 Err 0.1D-04 -
181: 15 10 6 15 9 7 S 2 14.6799357 0.0150 14.6799508 Err 0.1D-04 -
182: 15 10 5 15 9 6 S 1 14.6813620 -0.0228 14.6813392 Err 0.1D-04 -
183: 7 2 6 6 1 6 S 5 15.3996319 -0.0289 15.3996030 Err 0.1D-04 -
184: 5 5 0 4 4 1 S 1 15.4415552 -0.0030 15.4415522 Err 0.1D-04 -
185: 5 5 0 4 4 0 S 3 15.4417649 0.0189 15.4417838 Err 0.1D-04 -
186: 6 4 3 5 3 2 S 1 15.5541182 -0.0274 15.5540908 Err 0.1D-04 -
187: 6 4 2 5 3 3 S 3 15.5880215 0.0094 15.5880309 Err 0.1D-04 -
188: 6 4 2 5 3 3 S 1 15.5876865 -0.0187 15.5876678 Err 0.1D-04 -
189: 17 8 10 16 9 7 S 1 15.8313834 0.0236 15.8314070 Err 0.1D-04 -
190: 16 5 11 16 2 14 S 2 16.0374100 0.0045 16.0374145 Err 0.1D-04 -
191: 10 1 9 9 2 8 S 4 16.2480782 -0.0475 16.2480306 Err 0.1D-04 -
192: 16 0 16 15 1 14 S 1 16.3082307 0.0069 16.3082376 Err 0.1D-04 -
193: 21 9 13 21 8 14 S 4 12.7438736 -0.0093 12.7438643 Err 0.1D-04 -
194: 21 2 20 20 3 17 S 3 12.8143529 -0.0069 12.8143460 Err 0.1D-04 -
195: 6 3 4 5 2 4 S 5 14.1820970 0.0397 14.1821367 Err 0.1D-04 -
196: 6 3 4 5 2 4 S 2 14.1821836 -0.0469 14.1821367 Err 0.1D-04 -
197: 18 10 8 17 11 6 S 2 14.3053202 0.0254 14.3053455 Err 0.1D-04 -
198: 21 4 17 20 7 14 S 4 16.2669573 -0.0105 16.2669467 Err 0.1D-04 -
Maximum (obs-calc)/err in line 66 0.0000483

RMS deviations (MHz), B and V sorted
B V n splittings MHz
B V n abs. freq. MHz
1 1 198 0.021605 0.022806

Parameters and Errors
BJ 0.842690393 { 0.000000159}
BK 0.779138621 { 0.000000431}
B- 0.062234644 { 0.000000063}
DJ 0.178830E-6 { 0.000498E-6}

```
 DJK          0.108880E-6 { 0.001485E-6}
\F12         -0.909086541 {     derived}
\F          159.088466291 {     derived}  159.372406307 {     derived}
 V1n         16849.242793 {  133.243544}   14456.546962 {   26.936051}
\rho          0.007078753 {     derived}    0.008909387 {     derived}
\beta         0.783893673 {     derived}    2.799662929 {     derived}
\gamma       -0.005699674 {     derived}   -2.221876285 {     derived}
 epsil        6.276576658 { 0.006301018}    4.131030469 { 0.047035467}
 delta        1.060579015 { 0.026474308}    2.528223834 { 0.014278367}

 Standard Deviation       0.022291 MHz

------------------------------------ B =  1
 Rotational Constants and Errors (in GHz)
     B_z       1.621829014       0.000000444
     B_x       0.904925038       0.000000170
     B_y       0.780455749       0.000000171
 Ray's kappa   -0.70413
 F0(calc)     158.000000000       0.000000000
 I_alpha        3.198601709       0.000000000
 <(i,x)  <(i,y)  <(i,z)       29.2355       90.3304       60.7667
d<(i,x) d<(i,y) d<(i,z)        1.5190        0.3198        1.5169

 F0(calc)     158.000000000       0.000000000
 I_alpha        3.198601709       0.000000000
 <(i,x)  <(i,y)  <(i,z)      108.4279      118.7547      144.8566
d<(i,x) d<(i,y) d<(i,z)        1.7704        1.5798        0.8181

 V1n_1      6.723376 kj +/- 0.053168 kj         1.605811 kcal +/- 0.012699 kcal
         562.030164 cm +/-   4.4445 cm    s=  47.071623
 V1n_2      5.768615 kj +/- 0.010748 kj         1.377776 kcal +/- 0.002567 kcal
         482.218433 cm +/-   0.8985 cm    s=  40.387164

F(calc)       159.088466291
F(calc)       159.372406307
```

S8. AX1 Assignments and Outputs of Structure Evaluation

Parent XIAM Output

```
   J K- K+  J K- K+    Sym   calc/GHz  diff/MHz     obs/GHz
  1: 10  5  5  9  5  4   S 1  15.4605699    0.0093  15.4605792   Err 0.1D-04          -
  2: 10  5  5  9  5  4   S 3  15.4605637    0.0155  15.4605792   Err 0.1D-04          -
  3: 10  5  6  9  5  5   S 3  15.4604782   -0.0463  15.4604319   Err 0.1D-04          -
```

```
 4:  7  2  5  6  2  4   S 3  10.9335389    0.0121  10.9335510   Err 0.1D-04          -
 5:  7  2  5  6  2  4   S 2  10.9335234    0.0277  10.9335510   Err 0.1D-04          -
 6: 12  3  9 11  4  8   S 3  11.6975200    0.0077  11.6975277   Err 0.1D-04          -
 7:  5  1  5  4  1  4   S 4   7.5408388   -0.0040   7.5408348   Err 0.1D-04          -
 8:  5  1  5  4  1  4   S 3   7.5408484   -0.0136   7.5408348   Err 0.1D-04          -
 9: 16  4 13 15  5 10   S 3  15.5538211   -0.0201  15.5538010   Err 0.1D-04          -
10: 15  2 14 14  3 11   S 3  15.6624325   -0.0093  15.6624232   Err 0.1D-04          -
11: 15  2 14 14  3 11   S 1  15.6624351   -0.0145  15.6624205   Err 0.1D-04          -
12: 15  2 14 14  3 11   S 2  15.6623867    0.0365  15.6624232   Err 0.1D-04          -
13: 15  2 14 14  3 11   S 4  15.6623847    0.0385  15.6624232   Err 0.1D-04          -
14: 11  9  2 11  8  3   S 3  17.6829712    0.0045  17.6829757   Err 0.1D-04          -
15: 10  9  1 10  8  2   S 3  17.6852927    0.0207  17.6853134   Err 0.1D-04          -
16: 10  9  1 10  8  2   S 1  17.6852884    0.0250  17.6853134   Err 0.1D-04          -
17: 14  6  8 14  5 10   S 3  11.3737719   -0.0036  11.3737683   Err 0.1D-04          -
18: 14  6  8 14  5 10   S 1  11.3737661    0.0022  11.3737683   Err 0.1D-04          -
19:  4  3  1  3  2  1   S 4  11.3744708   -0.0206  11.3744502   Err 0.1D-04          -
20:  4  3  1  3  2  1   S 2  11.3744596   -0.0094  11.3744502   Err 0.1D-04          -
21:  9  0  9  8  0  8   S 3  13.6063053   -0.0005  13.6063048   Err 0.1D-04          -
22:  9  0  9  8  0  8   S 1  13.6063058   -0.0010  13.6063048   Err 0.1D-04          -
23:  9  4  5  8  4  4   S 4  13.9204301    0.0123  13.9204424   Err 0.1D-04          -
24:  9  3  7  8  3  6   S 2  13.9232342    0.0155  13.9232497   Err 0.1D-04          -
25:  9  3  7  8  3  6   S 4  13.9232351    0.0190  13.9232541   Err 0.1D-04          -
26: 11  4  7 11  1 10   S 3  14.2978152   -0.0020  14.2978133   Err 0.1D-04          -
27: 11  4  7 11  1 10   S 4  14.2989659   -0.0069  14.2989590   Err 0.1D-04          -
28: 11  4  7 11  1 10   S 2  14.2989558    0.0032  14.2989590   Err 0.1D-04          -
29:  8  1  7  7  0  7   S 3  14.7566569    0.0141  14.7566710   Err 0.1D-04          -
30:  8  1  7  7  0  7   S 1  14.7566564    0.0146  14.7566710   Err 0.1D-04          -
31:  5  4  2  4  3  2   S 2  15.0038875   -0.0133  15.0038742   Err 0.1D-04          -
32:  5  4  2  4  3  2   S 4  15.0038824   -0.0081  15.0038742   Err 0.1D-04          -
33: 17  8 10 17  7 11   S 2  15.5476396    0.0120  15.5476516   Err 0.1D-04          -
34: 17  8 10 17  7 11   S 4  15.5476343    0.0193  15.5476536   Err 0.1D-04          -
35: 17  8  9 17  7 10   S 4  15.5500027   -0.0063  15.5499964   Err 0.1D-04          -
36: 17  8  9 17  7 10   S 2  15.5499983   -0.0041  15.5499943   Err 0.1D-04          -
37: 14  8  6 14  7  7   S 4  15.5819390   -0.0113  15.5819277   Err 0.1D-04          -
38: 14  8  6 14  7  7   S 2  15.5819346   -0.0069  15.5819277   Err 0.1D-04          -
39: 11  8  4 11  7  5   S 2  15.5967036    0.0056  15.5967092   Err 0.1D-04          -
40: 11  8  4 11  7  5   S 4  15.5966984    0.0108  15.5967092   Err 0.1D-04          -
41: 19  6 14 18  7 11   S 1  16.0241985   -0.0009  16.0241976   Err 0.1D-04          -
42: 19  6 14 18  7 11   S 3  16.0241873    0.0134  16.0242006   Err 0.1D-04          -
43: 19  6 13 18  7 12   S 3  16.0292948    0.0169  16.0293118   Err 0.1D-04          -
44: 19  6 13 18  7 12   S 1  16.0292836    0.0116  16.0292952   Err 0.1D-04          -
45: 18  2 17 17  3 14   S 4  17.9120678   -0.0112  17.9120566   Err 0.1D-04          -
46: 18  2 17 17  3 14   S 4  17.9120678   -0.0112  17.9120566   Err 0.1D-04          -
```

```
 47: 18  2 17 17  3 14   S 2  17.9120697   -0.0131  17.9120566   Err 0.1D-04          -
 48: 19  5 15 18  6 12   S 2  18.1957380   -0.0371  18.1957009   Err 0.1D-04          -
 49: 19  5 15 18  6 12   S 4  18.1957073    0.0060  18.1957133   Err 0.1D-04          -
 50: 12  4  9 11  4  8   S 2  18.5810175   -0.0385  18.5809790   Err 0.1D-04          -
 51: 12  4  9 11  4  8   S 4  18.5810217   -0.0427  18.5809790   Err 0.1D-04          -
 52: 10  3  8  9  4  5   S 2   8.2046159   -0.0155   8.2046004   Err 0.1D-04          -
 53: 10  3  8  9  4  5   S 4   8.2045970    0.0034   8.2046004   Err 0.1D-04          -
 54:  7  4  4  7  3  4   S 3   7.2510046   -0.0046   7.2510000   Err 0.1D-04          -
 55:  9  4  5  9  3  6   S 4   7.1864304   -0.0224   7.1864080   Err 0.1D-04          -
 56: 12  5  8 11  6  6   S 4   7.1480819    0.0304   7.1481123   Err 0.1D-04          -
 57: 15  1 14 15  0 15   S 4   6.6334064    0.0045   6.6334109   Err 0.1D-04          -
 58:  8  1  8  7  2  5   S 1   7.6045667   -0.0155   7.6045512   Err 0.1D-04          -
 59: 17  0 17 16  3 14   S 1  10.8257426    0.0223  10.8257649   Err 0.1D-04          -
 60: 15  4 11 15  1 14   S 1  14.7228199   -0.0038  14.7228161   Err 0.1D-04          -
Maximum (obs-calc)/err in line   3   0.0000463

 RMS deviations (MHz), B and V sorted
  B  V   n splittings MHz
  B  V   n abs. freq. MHz
  1  1  60         0.017950         0.020642

          Parameters  and  Errors
 BJ          0.771699139 { 0.000000321}
 BK           1.040995699 { 0.000000748}
 B-          0.032715640 { 0.000000199}
 DJ          0.017744E-6 { 0.000707E-6}
 DJK          0.030749E-6 { 0.003781E-6}
 dj          0.002566E-6 { 0.000324E-6}
\F12          1.010237237 {     derived}
\F          158.948671050 {     derived}  159.505388379 {     derived}
 V1n         29542.170000 {     fixed  }   14667.421211 {   42.492173}
\rho         0.006485608 {     derived}    0.009903045 {     derived}
\beta        2.431189882 {     derived}    2.875668282 {     derived}
\gamma        1.676585395 {     derived}    1.308610184 {     derived}
 epsil       1.668037000 {     fixed  }    1.329081499 { 0.178814140}
 delta       2.013692000 {     fixed  }    2.555013094 { 0.023952111}

 Standard Deviation       0.019663 MHz

------------------------------------ B =  1
 Rotational Constants and Errors (in GHz)
     B_z       1.812694837       0.000000886
     B_x       0.804414778       0.000000376
```

B_y 0.738983499 0.000000380
Ray's kappa -0.87812
F0(calc) 158.000000000 0.000000000
I_alpha 3.198601709 0.000000000
<(i,x) <(i,y) <(i,z) 95.0325 25.9408 115.3761
d<(i,x) d<(i,y) d<(i,z) 0.0000 0.0000 0.0000

F0(calc) 158.000000000 0.000000000
I_alpha 3.198601709 0.000000000
<(i,x) <(i,y) <(i,z) 82.3863 57.4915 146.3915
d<(i,x) d<(i,y) d<(i,z) 5.8979 2.3415 1.3724

V1n_1 11.788251 kj +/- 0.000000 kj 2.815506 kcal +/- 0.000000 kcal
985.420583 cm +/- 0.0000 cm s= 82.604361
V1n_2 5.852760 kj +/- 0.016956 kj 1.397873 kcal +/- 0.004050 kcal
489.252440 cm +/- 1.4174 cm s= 41.012321

F(calc) 158.948671050
F(calc) 159.505388379

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VITA

Nicole Taylor Moon was born and raised in St. Charles, Missouri. As a true St. Louisan, she knows the most important question is "Where did you go to high school?" From 2011-2015, she attended Incarnate Word Academy in St. Louis, Missouri, and graduated as valedictorian. From 2015-2019, Nicole attended Missouri University of Science and Technology where she earned a Bachelor of Science in chemistry and a minor in mathematics. She graduated as Summa Cum Laude and as an Honors Academy Fellow. During her undergraduate career, she served as the science team lead for the Mars Rover Design Team, president of the W.T. Schrenk Society, and was initiated into Alpha Chi Sigma – Beta Delta chapter.

Having fallen in love with microwave spectroscopy during her undergraduate research, Nicole continued her graduate education with Dr. Garry S. Grubbs II from 2019-2023, with a research emphasis in microwave three-wave mixing spectroscopy. While attending graduate school, she served as the Master of Ceremonies and Vice Master Alchemist for Alpha Chi Sigma – Beta Delta Chapter. She received her Ph.D. in Chemistry from Missouri University of Science and Technology in December 2023.

After defending, Nicole moved to Laurel, Maryland with her amazing husband, Ed Koharik, and dog, Dave, to begin working as a Post Doctoral Fellow at the Johns Hopkins University Applied Physics Laboratory.