

Missouri University of Science and Technology Scholars' Mine

Physics Faculty Research & Creative Works

Physics

01 Jul 2014

Dynamical (e,2e) Investigations of Structurally Related Cyclic Ethers

J. D. Builth-Williams

Luca Chiari

Penny A. Thorn

Susan M. Bellm

et. al. For a complete list of authors, see https://scholarsmine.mst.edu/phys_facwork/550

Follow this and additional works at: https://scholarsmine.mst.edu/phys_facwork

Part of the Physics Commons

Recommended Citation

J. D. Builth-Williams and L. Chiari and P. A. Thorn and S. M. Bellm and D. B. Jones and H. Chaluvadi and D. H. Madison and C. Ning and B. Lohmann and O. Ingólfsson and M. J. Brunger, "Dynamical (e,2e) Investigations of Structurally Related Cyclic Ethers," *Journal of Physics: Conference Series*, vol. 488, no. SECTION 5, Institute of Physics - IOP Publishing, Jul 2014. The definitive version is available at https://doi.org/10.1088/1742-6596/488/5/052004

This Article - Conference proceedings is brought to you for free and open access by Scholars' Mine. It has been accepted for inclusion in Physics Faculty Research & Creative Works by an authorized administrator of Scholars' Mine. This work is protected by U. S. Copyright Law. Unauthorized use including reproduction for redistribution requires the permission of the copyright holder. For more information, please contact scholarsmine@mst.edu.

Dynamical (e,2e) investigations of structurally related cyclic ethers

J. Builth-Williams*, L. Chiari*, P.A. Thorn*, S.M. Bellm*, D.B. Jones^{†,1}, H. Chaluvadi[>], D.H. Madison[>], C.G. Ning[&], B. Lohmann[^], O. Ingólfsson⁺, and M. J. Brunger^{*,#}

*ARC Centre of Excellence for Antimatter-Matter Studies, Flinders University, GPO Box 2100, Adelaide, SA 5001, Australia.

[†]School of Chemical and Physical Sciences, Flinders University, GPO Box 2100, Adelaide, SA 5001, Australia.

²Department of Physics, Missouri University of Science and Technology, Rolla, Missouri 65409, USA.

*Department of Physics, State Key Laboratory of Low-Dimensional Quantum Physics, Tsinghua University, Beijing 100084, China.

[^]University of the Sunshine Coast, Maroochydore DC, Queensland 4558, Australia.

⁺Department of Chemistry and Science Institute, University of Iceland, Dunhagi 3, 107 Reykjavik, Iceland.

[#]Institute of Mathematical Sciences, University of Malaya, 50603 Kuala Lumpur, Malaysia.

Synopsis Experimental and theoretical cross sections are presented for electron-impact ionization of a series of cyclic ethers.

Data for positron and electron interactions with biologically relevant compounds is required to accurately simulate charge-particle induced damage in biological systems [1]. Electron scattering is particularly important in this sense as a large number of low-energy secondary electrons (LESEs) are liberated from a single high energy ionizing particle [2]. These LESEs can further efficiently induce DNA damage through single and double strand breakage [3].

It is therefore essential to understand the influence that the structures of biologically relevant species play in the nature of electronimpact ionization in the biological system. With this in mind, we have investigated the role of molecular structure in the dynamics of the electron-impact ionization of some cyclic ethers: tetrahydrofuran (THF), tetrahydropyran (THP) and 1,4-dioxane. Typical (e,2e) binding energy spectra for these cyclic ethers is shown in Figure 1.

Triple differential cross sections have been measured for the ionization of the highest occupied molecular orbitals of each of these targets using an (e,2e) coincident technique [4]. Here, angular distributions of the ejected electron, with energy of 20 eV, are measured when the incident electron has energy of 250 eV and the scattered electron is detected at -5°. These measurements are compared against theoretically calculated cross sections obtained within a molecular 3-body distorted wave model [5].

By comparing the TDCS results for each species, we can gain insights into how the dynamics of the ionization process is influenced by molecular structure.

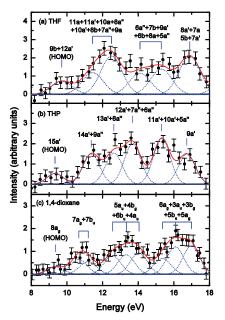


Figure 1. Measured binding energy spectra for the cyclic ethers. (a) THF, (b) THP, and (c) 1,4-dioxane. Here the incident electron energy was 250eV, the scattered electron was detected at -10°, the ejected electron was detected at 75° with 20eV of energy.

References

[1] I. Baccarelli et al 2011 Phys. Rep. 508 1.

[2] S.M. Pimblott and J.A. LaVerne 2007 Radiat. Phys. Chem. 76 1244.

[3] B. Boudaiffa et al 2000 Science 287 1658.

[4] S.J. Cavanagh and B. Lohmann 1999 J. Phys. B: At. Mol. Opt. Phys. 32 L261.

[5] D.H. Madison and O. Al-Hagan 2010 Journal of Atomic, Molecular, and Optical Physics 2010 367180.

¹E-mail: <u>darryl.jones@flinders.edu.au</u>



Content from this work may be used under the terms of the Creative Commons Attribution 3.0 licence. Any further distribution $(\mathbf{\hat{t}})$ of this work must maintain attribution to the author(s) and the title of the work, journal citation and DOI. Published under licence by IOP Publishing Ltd