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

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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 electron-impact 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.

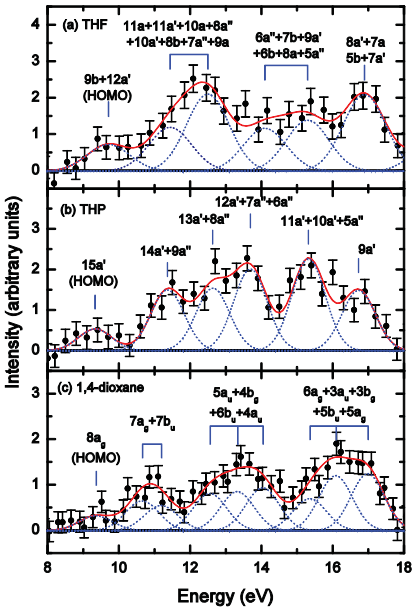

Figure 1. Measured binding energy spectra for the cyclic ethers. (a) THF, (b) THP, and (c) 1,4-dioxane. Here the incident electron energy was 250eV, the scattered electron was detected at -10°, the ejected electron was detected at 75° with 20eV of energy.

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