

Elastic scattering of low-energy electrons with tetrahydropyran.

Alessandra Souza Barbosa¹, Márcio H. F. Betttega²

Departamento de Física, Universidade Federal do Paraná, Curitiba, Brazil

Synopsis In this work we present calculated cross sections for low-energy electron scattering by tetrahydropyran. We compare our cross sections with previous results for the close-related molecules cyclohexane [1] and 1,4-dioxane [2]. We also compare our calculated integral cross sections with experimental total cross sections available in the literature for this molecule [3].

In this work we report calculated cross sections for elastic scattering of low-energy electrons with tetrahydropyran ($C_5H_{10}O$) molecule. We employed the well-established Schwinger multichannel method (SMC) [4] implemented with pseudopotentials (SMCPP) [5] in the static-exchange (SE) and static-exchange-polarization (SEP) approximations for energies up to 30 eV. We compare our calculated cross sections with previous results obtained for cyclohexane [1] and 1,4-dioxane [2] molecules, since their geometrical structure are similar. In figure 1 we present the geometrical structures of the molecules. We also compare our calculated integral cross sections with experimental total cross sections available in the literature for this molecule [3].

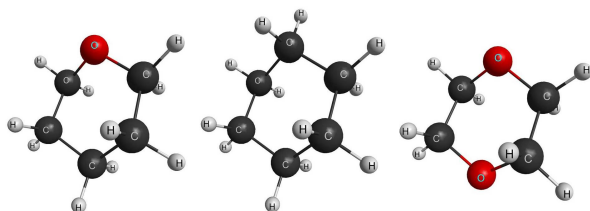


Figure 1. Geometrical structures of tetrahydropyran, cyclohexane and 1,4-dioxane molecules.

Recently we showed that calculated cross sections for elastic electron collisions with cyclohexane and 1,4-dioxane present some similarities among them [1]. These similarities were attributed to the geometrical structure of the molecules. In order to continue this study, we now compare tetrahydropyran cross sections with those obtained for the other close-related molecules. Tetrahydropyran and 1,4-dioxane can be seen as cyclohexane derivatives, with 1 ou 2 oxygen atoms replacing the CH_2 groups. Although the three molecules present similar geometrical structure in the ground state, one should note that while 1,4-dioxane and cyclohexane do not have permanent dipole moment, tetrahydropyran has.

In figure 2 we present a comparison between calculated differential cross sections (DCS) for elastic scattering of electrons by tetrahydropyran, cyclohexane [1] and 1,4-dioxane [2]. The results are presented in the SE approximation at energies between 15 and 30 eV. One can note that the DCSs are, in general, very similar in the oscillatory behavior and magnitude, presenting big discrepancies at lower angles where the dipole moment of the tetrahydropyran molecule increases the cross section abruptly.

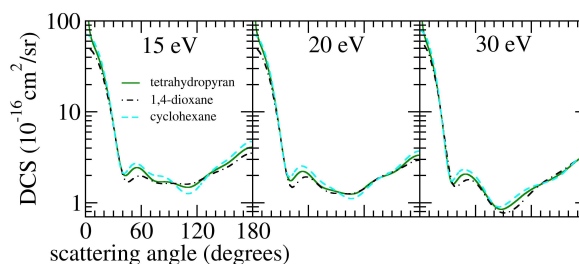


Figure 2. Calculated DCSs, in the SE approximation, for elastic scattering of electrons by tetrahydropyran, cyclohexane [1] and 1,4-dioxane [2] at energies 15 eV, 20 eV and 30 eV.

Acknowledgments: The authors acknowledge financial support from CNPq, CAPES and Finep (CT-Infra) and computational support Prof. Carlos de Carvalho at LFTC-DFis-UFPR and LCPAD-UFPR and from CENAPAD-SP.

References

- [1] A. S. Barbosa and M. H. F. Betttega 2014 *J. Chem. Phys.* **141**, 244307.
- [2] A. S. Barbosa and M. H. F. Betttega 2014 *J. Chem. Phys.* **140**, 184303.
- [3] C. Szmytkowski, E. Ptasinska-Denga 2011 *J. Phys. B: At. Mol. Opt. Phys.* **44**, 015203.
- [4] K. Takatsuka and V. McKoy 1981 *Phys. Rev. A* **24**, 2473; 1984 *Phys. Rev. A* **30**, 1734.
- [5] M. H. F. Betttega, L. G. Ferreira, and M. A. P. Lima 1993 *Phys. Rev. A* **47**, 1111.

¹E-mail: asb07@fisica.ufpr.br

²E-mail: betttega@fisica.ufpr.br

