XVIII Simpósio Brasileiro de Química Teórica (SBQT 2015)
Pirenópolis/GO, 22-25 de Novembro de 2015

Theoretical Study on Electron Collisions with Dimethyl Disulfide

Victor A. S. da Mata[a] (PG) and Gabriel L. C. de Souza[a] (PQ)

[a] *Federal University of Mato Grosso, Department of Chemistry, 78060-900 Cuiabá-MT, Brazil*
E-mail: victorssantana.93@hotmail.com

Keywords: Electron Scattering, dimethyl disulfide, Cross Sections

INTRODUCTION

Disulfide bridges (*R*S–S*R*) can be formed in some metabolic processes. It is known that the cleavage of a given bond can be induced by electron interaction via different mechanisms.[1] In order to understand the physical phenomena that occurs in electron-biomolecules interactions, one needs to know the quantities associated to the cleavage process initiated by the electrons interacting with building blocks, e.g., the electron-molecule (e^--molecule) cross sections for a wide energy range.

In this work, we computed several e^--molecule cross sections, in the 1-300 eV energy range, for a molecule that can be a good prototype for studying large biochemistry systems: the dimethyl disulfide (DMDS). More specifically, Differential and Integral cross sections (DCS and ICS, respectively) for elastic scattering, as well as Momentum Transfer and Total Absorption cross sections (MTCS and TACS, respectively) were probed.

METHODS

The present study made use of a complex optical potential given by:

$$U_{\text{int}} = U_{\text{st}} + U_{\text{ex}} + U_{\text{cp}} + iU_{\text{ab}}$$

In our calculation, static (U_{st}) and exchange (U_{ex}) potentials are derived directly from a Hartree-Fock SCF target wavefunction. The parameter-free model potential introduced by Padial and Norcross[2] is used to account for correlation-polarization (U_{cp}) contributions while the model potential developed by Lee *et al.*[3] is used for describing the absorption effects (U_{ab}). With the referred interaction potential, the scattering equations are solved iteratively using the Padé´s approximant method, as in the manner described by Lucchese *et al.*[4]

RESULTS AND DISCUSSION

In Fig. 1 we show our calculated Differential Cross Sections (DCS) for elastic e^--DMDS scattering at 100 eV along with experimental data taken from Sugohara *et al.*[5] Unfortunately, there is no experimental data available in the literature for the molecule of interest. Thus, experimental results for the isoelectronic molecule, tetramethylsilane (TMS), are presented for comparison purposes.

Computed results of e^--DMDS DCS present similar trend to what is observed in the case of the measured e^--TMS DCS. In addition, the DCS magnitudes are practically the same for all the angular region covered by the measurements.

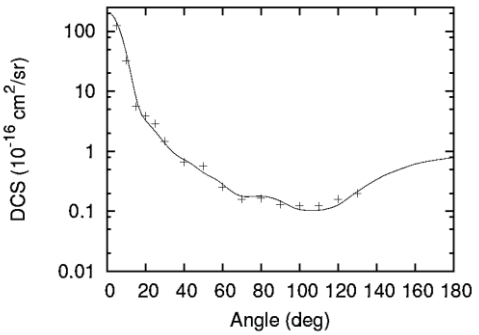

Figure 1. DCS for elastic scattering at 100 eV. Solid line: Present results for e^--DMDS; Crosses: Experimental data from Sugohara *et al.*[5] for e^--TMS.

CONCLUSIONS

This work can aid to fulfil the existent lacuna on e^--DMDS collisions. Up to our knowledge, there are no experimental or theoretical study on e^--DMDS scattering in a wide energy range available in the literature. Provided results can be useful for basic and/or applied issues in the future. Additional results will be presented at the Conference.

ACKNOWLEDGMENTS

The authors thank CAPES and CNPq.

[1] L. Sanche *et al*. Science, 287, 1658 (2000).
[2] N. T. Padial and D. W. Norcross. Phys. Rev. A, 29, 1742 (1984).
[3] M.-T. Lee *et al*. J. Elec. Spec. Rel. Phenom., 155, 14 (2007).
[4] R. R. Lucchese and F. Gianturco. J. Chem. Phys., 102, 5743 (1995).
[5] R. T. Sugohara *et al*. Phys. Rev. A, 84, 062709 (2011).