Probing Cross Sections for Electron-Methyl Formate Collisions with EPolyScatD

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INTRODUCTION

EPolyScatD is a series of programs for computing electron-molecule (e^--molecule) scattering and molecular photoionization cross sections. It was originally developed by Lucchese *et al.*[1] and later modified by de Souza *et al.*[2] and by Lee *et al.*[3] Since then, the suite of codes have become a tool capable to calculate cross sections for elastic scattering of molecules of any symmetry, at intermediate energies, with absorption effects included. During the last years, EPolyScatD has been applied to probe e^--molecule cross sections for a variety of molecular targets.[2,3] In the present work, as a new application, we present results of e^--molecule cross sections computed for methyl formate ($HCOOCH_3$).

METHODS

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

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

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[4] is used to account for correlation-polarization (U_{cp}) contributions while the model potential developed by Lee *et al.*[5] is used for describing the absorption effects (U_{cbs}).

Using the referred interaction potential, the scattering equations are solved iteratively using the Padé´s approximant method, as in the manner described by Lee *et al.*[3]

RESULTS AND DISCUSSION

In Fig. 1 we show our calculated Differential Cross Sections (DCS) for elastic e^--$HCOOCH_3$ scattering at 100 eV along with experimental data from Homem and Iga.[6]

DCS computed results are in good qualitative as well as quantitative agreement with the experimental data from Homem and Iga.[6] This can be seen in the whole angular region covered by the experimental measurements.

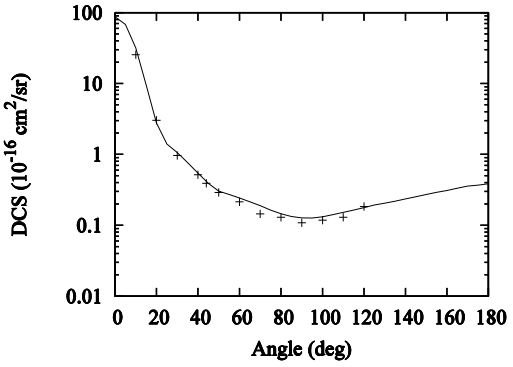

Figure 1. DCS for elastic e^--$HCOOCH_3$ at 100 eV. Solid line: Present results; Crosses: Experimental data of Homem and Iga.[6]

CONCLUSIONS

The agreement between present computed results and experimental data indicates EPolyScatD can be successfully applied for probing e^--molecule cross sections of targets belonging to the class of the esters. More results will be presented during the conference.

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