

Theoretical Study on Electron Collisions with Methylamine

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Abstract: In this work, we present a theoretical study on electron collisions with methylamine (CH₃NH₂). Elastic differential, integral, and momentum-transfer cross sections, as well as the grand-total and total absorption cross sections were calculated in the 1-500 eV energy range. A complex optical potential derived from a Hartree-Fock molecular wave function was used to represent the collision dynamics and a single-center expansion method combined with the Padé approximant technique was used to solve the scattering equations. For that, the EPolyScat-D package, originally developed by Gianturco *et al.* [1] and further modified by Souza *et al.* [2] to include the absorption potential, was used to perform the calculations. In this framework, the complex optical potential is given by:

$$V_{\rm opt} = V_{\rm st} + V_{\rm ex} + V_{\rm cp} + i V_{\rm abs}, \qquad (1)$$

where V_{st} and V_{ex} are the static and exchange components, respectively, derived exactly from the target wave function, V_{cp} is the correlation-polarization contribution obtained within the framework of free-electron-gas model [3], and V_{abs} is the improved model absorption potential developed by our group [4].

In Fig. 1, we present our calculated results for the in Differential Cross Sections (DCS) for the elastic e^{-} -CH₃NH₂ scattering at 500 eV. Unfortunately, there is no experimental data available in the literature for this molecule. Thus, experimental results for the isoelectronic molecule methanol (CH₃OH) taken from Sugohara *et al.* [5]



are presented for comparison purposes. The computed results of the elastic e^{-} -CH₃NH₂ scattering present similar trend to that observed for the measured e^{-} -CH₃OH DCS. In addition, the DCS magnitudes are practically the same for all the angular region covered by the measurements. The complete results obtained in the 1-500 eV energy range will be presented at the Conference.



Figure 1: Differential cross sections for elastic scattering at 500 eV. Solid line: present results for e^{-} -CH₃NH₂; Circles: experimental data from Sugohara *et al.* [5] for e^{-} -CH₃OH.

Key-words: Electron scattering, methylamine, cross sections.

Support: This work has been supported by FAPESP and CNPq. M. G. P. H. acknowledges FAPESP for the financial support under the grant 2015/08258-2.

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