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 (CH$_3$NH$_2$). 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. \cite{1} and further modified by Souza et al. \cite{2} to include the absorption potential, was used to perform the calculations. In this framework, the complex optical potential is given by:

\begin{equation}
V_{\text{opt}} = V_{\text{st}} + V_{\text{ex}} + V_{\text{cp}} + iV_{\text{abs}},
\end{equation}

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

In Fig. 1, we present our calculated results for the in Differential Cross Sections (DCS) for the elastic $e^{-}$-CH$_3$NH$_2$ 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 (CH$_3$OH) taken from Sugohara et al. \cite{5}
are presented for comparison purposes. The computed results of the elastic $e^-$-CH$_3$NH$_2$ scattering present similar trend to that observed for the measured $e^-$-CH$_3$OH 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 $e^-$-CH$_3$NH$_2$; Circles: experimental data from Sugohara et al. [5] for $e^-$-CH$_3$OH.

**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.

**References:**