Cross sections calculations for electron scattering from dimethylamine, NH(CH$_3$)$_2$, molecule

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Synopsis The total cross section for single electron-impact ionization and the integral elastic cross section for electron scattering from dimethylamine have been calculated using the binary-encounter-Bethe model and the independent atom method, respectively.

In the present work we have theoretically studied elastic electron scattering from dimethylamine, (NH(CH$_3$)$_2$), and positive ionization of this molecule by electron impact.
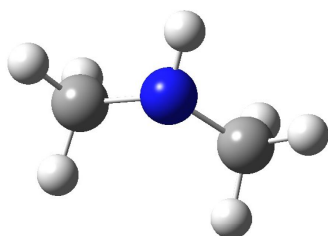

Figure 1. Geometry of the dimethylamine molecule.

The integral elastic cross section has been calculated using the independent atom method [1] for electron energies ranging from 30 eV to 3 keV. The interaction between scattered electron and dimethylamine molecule has been described by a static-polarization model potential. The total cross section for the single electron-impact ionization has been derived using the binary-encounter-Bethe (BEB) model [2] for energies between the ionization threshold up to 3 keV. All physical quantities necessary in the BEB calculations have been obtained for the ground state of the geometrically optimized molecule with the Hartree-Fock method using Gaussian code [3] and Gaussian 6-311G+(d,p) basis set. The valence orbital energies have been calculated with OVGF method implemented in Gaussian.

In figure 2 the calculated elastic and ionization cross sections are shown. Predicted total cross section, estimated as the sum of elastic and ionization cross sections is also shown. Although this approach seems to be rather crude, we expect that the total cross section estimated

this way will be quite satisfactorily to within ±10%. This expectation is justified by the results of our previous calculations which reproduced the experimental intermediate-energy data successfully for a variety of complex molecular targets [4].
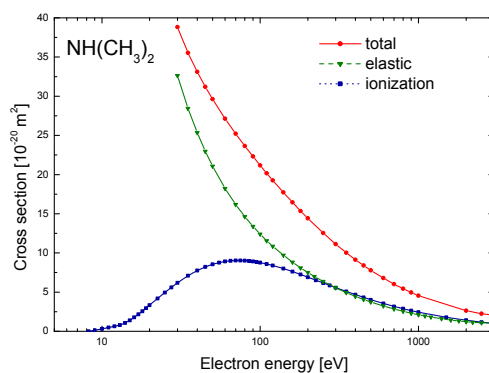
Figure 2. Calculated cross sections for electron impact ionization and elastic scattering for dimethylamine molecule. Total cross section is obtained as the sum of these partial cross sections.

References

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