

THEORETICAL STUDY ON ELECTRON-NH₂ RADICAL COLLISIONS

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The interaction of electrons with highly reactive radicals has grown recently, in view of their importance in many plasma processes, including anisotropic etching, film deposition and surface modifications. Cross sections for electron scattering from a variety of such molecules are demanded in different fields of pure and applied sciences [1-3]. NH₂ is one of these radicals, also known as an important intermediate species in astrochemistry and various combustion processes.

In view of the above applications, the knowledge of cross sections for e⁻-NH₂ collisions would certainly be of interest. Since the experimental determination of such cross sections is difficult, theoretical calculations are presently an important manner to fulfill the lack of data on this matter. However, except for the calculations of total cross sections by Joshipura *et al.* [7], no theoretical investigation on those collisions has been reported.

In this work we present calculated differential, integral and momentum-transfer cross sections for e⁻-NH₂ elastic scattering at impact energies ranging from 1 to 30 eV. In our study, the electron-molecule scattering dynamics is represented by an interaction potential (V^{SEP}) composed of static, exchange and correlation-polarization contributions:

$$V^{SEP}(\vec{r}) = V_{st}(\vec{r}) + V_{ex}(\vec{r}) + V_{cp}(\vec{r}). \quad (1)$$

The iterative Schwinger variational method [4] is used to solve the scattering equations.

Fig. 1 shows our calculated integral cross sections (ICS's) for elastic e⁻-NH₂ collision, in the (1-30)-eV range. The calculated ICS's for e⁻-NH radical scattering [5] as well as calculated ICS's for e⁻-NH₃ collisions [6] are also shown.

Additional results and discussion will be presented during the Symposium.

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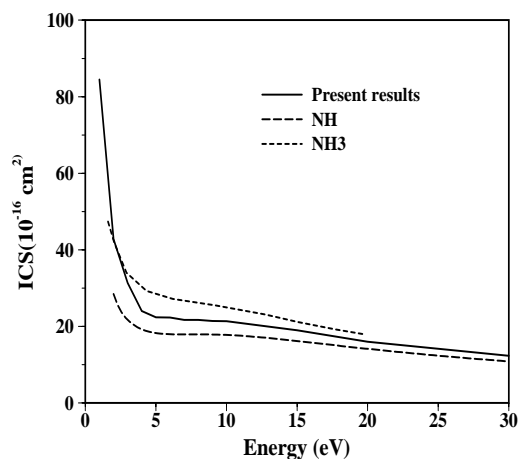


Fig. 1. ICS's for elastic e⁻-NH₂ scattering in the (1-30)-eV energy range. Full curve, present calculated data; long-dashed line, calculated data for e⁻-NH collisions [5]; dashed line, calculated ICS's for e⁻-NH₃ collisions [6].

References

- [1] S. C. Brown, *Electron-molecule scattering*, Wiley, N.York 1979.
- [2] R. K. Janev, in *Atomic and Plasma-Material Interaction Processes in Controlled Thermonuclear Fusion*, edited by R. K. Janev and H. W. Drawin, Elsevier, Ams terdam, 1993.
- [3] J. J. Perry, Y. H. Kim, J. L. Fox and H. S. Porter, *J. Geophys. Res.* **104** (1999) 16541.
- [4] R. R. Lucchese, G. Raseev, and V. McKoy, *Phys. Rev. A* **25**, 2572 (1982).
- [5] N. B. H. Lozano, M.-T. Lee, and A. M. C. Sobrinho, *THEOCHEM* **719**, 57 (2005).
- [6] F. A. Gianturco, *J. Phys. B* **24**, 4627 (1991).
- [7] K. N. Joshipura, M. Vinodkumar, and U. M. Patel, *J. Phys. B* **34**, 509 (2000).