§8. Electron and Positron Scattering from Excited Molecules in the Energy Region from 0.8 eV to 600 eV

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Almost all theoretical and experimental studies so far carried out have been concerned with ground state targets. However, under normal experimental conditions and in practice, technological environment, almost all molecules are ro-vibrationally in highly excited state, while they may be electronically in the ground state. No systematic study for electron scattering from excited molecules has been reported. Therefore, we conducted an exploratory study from vibrationally excited chlorine molecules. These ro-vibrationally excited chlorine molecules are known to be effective etching gases and widely used for semiconductor, thin-film and other industrial applications [1]. By using electrons from a discharge, electron impact ionization, electronic excitation, or dissociation of chlorine molecules are induced, and these ionized, or excited species are often unstable and eventually dissociate. These fragmented chlorine atoms and ions are then introduced to surfaces and undergo etching processes. Furthermore, chlorine molecules possess some astrophysical and atmospheric significance as chlorine chemistry in interstellar clouds.

Hence, complete, comprehensive and systematic data for electron impact total cross sections (TCSs) on chlorine molecules are undoubtedly needed, but these scattering cross section data are not simply available for a variety of processes and a wide range of collision energies. As described, even TCS in a wide energy range is not known, and above 20 eV, absolutely no data for electron scattering exists todate. Therefore, we have undertaken this project to determine TCS from vibrationally excited chroline molecule experimentally in a wide range of impact energies and calculate elastic cross sections theoretically. In addition, a small scale investigation for determination of total and positronium formation cross sections by positron impact was carried out for a comparative study with that of the electron case so that a combined effort can provide better understanding of collision dynamics and interaction schemes of electron impact [2].

As for our TCSs, the general shape and magnitude of them are found to agree well with those of Cooper et al. [6] below 10 eV. They have two strong peaks due to shape resonances at 7.8 and 12 eV which are associated with dissociative attachment and ion-pair formations, respectively, followed by a sharp decrease beyond this energy. Several weaker structures are also seen at various energies, in which they are also attributed to dissociative attachment and ion-pair formations. Elastic cross sections are found to be smaller by only a few percent than present measured TCSs, and we consider this as being likely to be from overestimation in the present theory although the general shape is in good harmony with the TCS. These cross sections provided should be of good use for applications.

A small-scale study for positron scattering from this molecule is performed to obtain positron-TCSs and Ps formation cross sections. The present positron-TCSs are much smaller than the electron counterparts in the entire energy studied. The ratio of Ps formation to positron-TCS at 2-eV above threshold amounts to approximately 5 %. This value belongs to a group with the smallest numbers among the variety of molecules we have investigated. It is urgently needed to provide a rational to this finding of Ps formation.

References

[1] See for example, Adv. At. Mol. Opt. Phys., vol.44, eds. M. Kimura and Y. Itikawa (Academic Press, NY, 2000).
[2] M. Kimura, O. Sueoka, A. Hamada and Y. Itikawa, Adv. Chem. Phys. 111,