Topic 1

Comparisons and scaling rules between $N+N_2$ and N_2+N_2 collision induced dissociation cross sections from atomistic studies

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Accurate modeling of air plasma chemistry, as in the case of aerothermodynamics or electrical discharges in air, needs elementary processes data with at least the specification of molecular vibration. Although this is presently well recognized in the literature, the associated heavy load of input data to handle can become an issue for both the dynamical and kinetic treatments. For this purpose we are developing some relationships between vibrationally dependent atom–diatom and diatom–diatom collision induced dissociation cross sections, and we show their successful application to the collisions of $N+N_2$ and N_2+N_2.

1. Scaling laws for collision induced dissociation

Quantitative knowledge of elementary processes involved in plasmas are key to successfully perform accurate kinetic simulations. The issue is the huge amount of data to treat, both in dynamical calculations and in kinetic simulations. The aim of this work [1] is to study collision induced dissociation detailed data in atom–molecule (AM) and molecule–molecule (MM) collisions involving nitrogen, obtained by molecular dynamics calculations, considering vibrational states in the range 10–50 and collision energy up to 10 eV, in order to formulate suitable scaling laws resulting in less expensive computational procedures and easier to handle treatments in kinetic simulations. It is shown that, while a direct substitution of MM dissociation cross sections with AM ones might be acceptable only at very high collision energy, scaling laws application allows to obtain quite good results on almost the whole energy range of interest. Two relations are developed in this work. The first one allows to obtain dissociation cross sections of $MM(v_1,v_2)$ collisions, being v_1, v_2 respectively the initial vibrational states of the two molecules, from the corresponding $MM(v_1,0)$, $MM(v_2,0)$ dissociation cross sections. The second relation links the $AM(v)$ cross section with the $MM(v,0)$ one, as in fig.1. As a consequence, using both relations allows in principle to obtain any $MM(v_1,v_2)$ dissociation cross section, provided $AM(v_1)$, $AM(v_2)$ cross sections are known. The advantage is clear, being a three-body dynamical calculation significantly less expensive than a four-body one. The possibility of a compact expression of the MM dissociation cross sections, expressed as a function of the AM ones, is also an advantage for the kinetic codes where those data are used. Rotation of the vibrationally more excited molecule can be included in the scaling. Work is in progress to extend these scaling laws to other collisional systems.

2. References

[1] F.Esposito, E.Garcia, and A.Laganà, Plasma Sources Science and Technology, **26** (2017) 45005 (doi:10.1088/1361-6595/aa5d27).

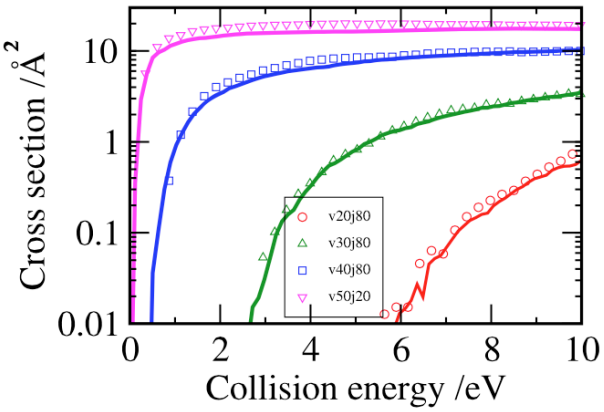

Fig.1. Comparison of computed molecule-molecule collision induced dissociation cross sections from the shown rovibrational states with corresponding values derived from atom-molecule ones.