

Dissociative excitation and vibrational excitation of Cl_2^+

Mingwu Zhang*¹, Åsa Larson†², Ann E Orel††, Xiaohong Cai*

* Institute of Modern Physics, Chinese Academy of Sciences, Lanzhou, 730000, Gansu, China

† Department of Physics, Stockholm University, S-106 91 Stockholm, Sweden

†† Department of Chemical Engineering and Materials Science, University of California at Davis, Davis, California 95616, USA

Synopsis The cross sections for resonant dissociative excitation and vibrational excitation of Cl_2^+ molecular ion in the 0-10 eV region are calculated by solving a driven Schrödinger equation for the four lowest resonant states of all symmetries.

Molecular chlorine has attracted substantial attention for plasma processing and excimer lasers. It is also of atmospheric and environmental interest. In these media, electron collisions with chlorine molecules and molecular ions play a central role [1]. In our previous work [2], we have studied dissociative recombination (DR) of Cl_2^+ , which is the process where an electron is captured by the molecular ion to form a doubly excited neutral state that dissociates to products. In addition, there are other competing processes occurring along with DR. After the formation of chlorine molecule in a resonant state, the incoming electron can auto-ionize, returning the target ion to its initial electronic state, either in a bound vibrational state or to the dissociation continuum. When a bound vibrational state is formed the process is resonant vibrational excitation (VE) (or de-excitation), and dissociation of the molecular ion results in resonant dissociative excitation – (DE).

With the potential energy curves and auto-ionization widths that have been computed by combining electron scattering calculations and *ab initio* structure calculations in our previous study [2], the reaction dynamics of DE and VE for collisions between electrons and chlorine molecular ions is investigated by solving driven time-independent Schrödinger equation. Cross sections for VE from initial $v_i=0$ vibrational state of Cl_2^+ to $v_f=1, 2, \dots, 19$ are computed. In Fig. 1, the sum of these cross sections is presented. Also the cross section for DE for ions in the $v_i=0$ is calculated.

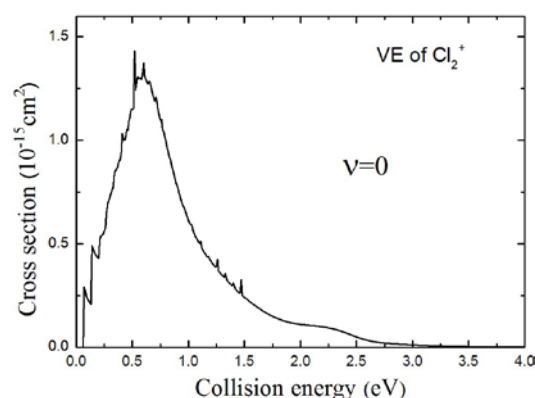


Figure 1. The vibrational excitation cross section of Cl_2^+ for the $v_i=0$ initial vibrational state of the target ion. This is the total cross section for excitation into all vibrational final states from $v_f=1$ up to $v_f=19$.

References

- [1] E G Thorsteinsson *et al* 2010 *Plasma Sources Sci. Technol.* **19** 015001
- [2] M Zhang *et al* 2011 *Phys. Rev. A.* **84** 052707

¹ E-mail: zhangmingwu@impcas.ac.cn

² E-mail: aasal@fysik.su.se