Dissociative electron attachment studies of di & tri atomic molecules

Minaxi Vinodkumar [*1], **Hitesh Yadav** [†2], **P. C. Vinodkumar** [†3]

[*] *Electronics Department, V. P. & R. P. T. P. Science College, Vallabh Vidyanagar, India*

[†] *Department of Physics, Sardar Patel University, Vallabh Vidyanagar , India*

Dissociative electron attachment (DEA) is a resonant process in which an electron is temporally captured by the molecule to form a transient negative ion (TNI) or a resonant state [1, 2]. This can be understood as vertical transition from the ground state of the neutral molecule to the ground (or any accessible excited state) of the anion, as shown in the Figure 1. Dissociative electron attachment process is active below the ionization threshold of the molecule and generally most efficient at very low incident energies leading to the fragmentation of target to produce neutral and anionic fragments through vibronic excitations. DEA processes are very important in understanding the local chemistry induced by the electron target interactions. This phenomenon is simply expressed as,

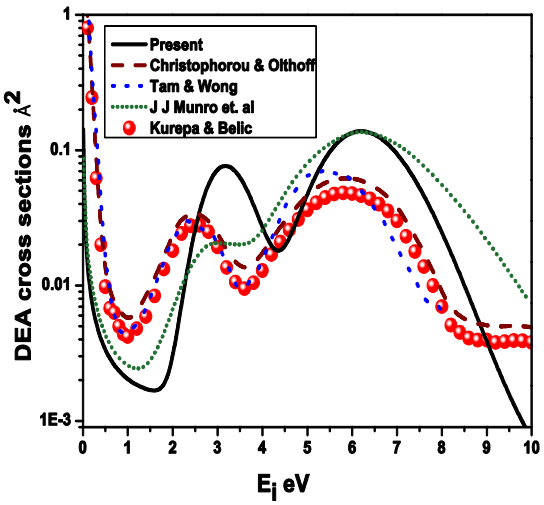

Figure 1 Dissociative electron attachment cross sections. solid line represents the present calculations, dash line represent recommended data by Christophorou & Olthoff,dot represents Tam & Wong, short-dot represents Munro et al. and solid circle represent the Kurapa & Belic experimental result.

$$e^- + Cl_2(\Sigma_g^+) = Cl\left(P_{\frac{3}{2},\frac{1}{2}}\right) + Cl^-(^1S_0) \qquad (1)$$

Dissociative electron attachment (DEA) process, despite being an important phenomenon in the field of plasma physics [3], environmental science [4] and radiation damage [5], finds sparse attention by theoretical groups. On the contrary, substantial progress has been made in experimental studies of this process, largely because of new experimental techniques involving electron beams with high energy resolution.

We have used R-matrix [4] method for low energy computation of eigenphases through which resonance width and resonant energy are computed which are important inputs for computing the DEA cross sections via. Quantemol-N software [6,7].

Acknowledgement

Minaxi Vinodkumar acknowledge DST-SERB, New Delhi for the Major research project [EMR/2016/000470] for _nancial support under which part of this work is carried out

.

[1] Thorman R M, et. al, *Beilstein J. Nanotechnol.* **6**, 1904 (2015).
[2] Christophorou L. G, *Environmental Health Prespectives*, **36**, 3 (1980).
[3] Chutjian et al., Phys. Rep. **264**, 393 (1996).
[4] Q-B. Lu and L. Sanche, Phys. Rev. Lett. **87**, 078501 (2001)
[5] L. Sanche, Eur. Phys. J. D. **35**, 367, (2005)
[6] M. Vinodkumar et al. Phys. Rev. A **93**, 012702, (2016).
[7] J. J. Munro et al. J. Phys. Conf. Ser. **388**, 012013, (2012)
[8] H. Yadav et. al, Molecular Physics, **115**, 952, (2017)