Electron induced processes in molecules and molecular ions relevant in industrial, fusion and astrophysical plasmas

K. Chakrabarti[1], **V. Laporta**[2], **J. Zs. Mezei**[3], **I. F. Schneider**[2] and **J. Tennyson**[4]

[1] *Department of Mathematics, Scottish Church College, 1 & 3 Urquhart Square, Kolkata 700 006, India*

[2] *Laboratoire Ondes et Milieux Complexes, CNRS-Université du Havre-Université Normandie, 76058 Le Havre, France*

[3] *Laboratoire des Sciences des Procédés et des Matériaux, CNRS-Université Paris 13-USPC, 93430 Villetaneuse, France*

[4] *Department of Physics and Astronomy, University College London, London WC1E 6BT, UK*

Collision induced processes such as electronic excitation and dissociation of major diatomic molecular ions, occurring in industrial, fusion and astrophysical plasmas, are studied in the framework of the R-matrix method. The ions chosen and the processes are of great interest in the relevant areas.

The R-matrix method has now become a standard state-of-the-art method for electron-molecule collision calculations, and has been reviewed comprehensively by Tennyson [1]. Here we highlight some of our recent works on electron collision with BF^+, BeH^+ and CH^+ ions.

BF/BF$^+$: We calculated [2] the electronic excitation cross sections from the BF^+ ground $X^2\Sigma^+$ state to the four low lying excited states, namely the $A^2\Pi$, $a^4\Sigma^+$, $C^2\Sigma^+$ and $D^2\Delta$ states. We also estimated the electron impact dissociation cross section for the ion and cross sections for rotational excitation of BF^+ from the $j = 0$ rotational state to the states with $j = 1, 2, 3$ at its equilibrium bond length. The BF neutral and BF^+ potential energy curves (PEC) have been subsequently used for calculation of dissociative recombination of the BF^+ ion by Mezei *et al* [3] . More work is being undertaken on electron collision with BF and estimation of dissociative electron attachment (DEA) cross sections [4].

BeH/BeH$^+$: Electronic excitation from the $X^1\Sigma^+$ ground state of BeH^+ to its $a^3\Sigma^+$, $A^1\Sigma^+$, $b^3\Pi$ and $B^1\Pi$ excited states and the rotational excitation cross sections from $j = 0$ rotational state to the states with $j = 1, 2, 3$ at its equilibrium bond length have been obtained [5]. The BeH^+ and BeH neutral curves have been used for calculation of dissociative recombination, dissociative excitation and vibrational excitation of the BeH^+ ion by Laporta *et al* [6].

CH/CH$^+$: These species are relevant both in fusion plasmas and in astrophysical plasmas. We have obtained the PECs of the low lying states of CH^+ and have calculated vibrationally resolved electronic excitation cross sections from its $X^1\Sigma^+$ ground state to the $A^3\Pi$, $a^1\Pi$ and $b^3\Sigma^-$ excited states. We have also calculated the electron impact dissociation cross section of CH^+ at its equilibrium bond length and obtained reasonably good agreement with experiments between $10 - 18$ eV [7].

[1] J. Tennyson **13**, 491 (2010).
[2] K. Chakrabarti, J. Tennyson, J. Phys. B: At. Mol. Opt. Phys. **42**, 105204 (2009).
[3] J. Zs. Mezei, *et al*, Plasma Sources Sci. Technol. **25**, 055022 (2016).
[4] D. Gupta, K. Chakrabarti, *et al* (in preparation).
[5] K. Chakrabarti, J. Tennyson, Euro. Phys. J. D **66:31**, 1 (2012).
[6] V. Laporta, K. Chakrabarti, *et al* Plasma Phys. Control. Fusion **59**, 045008 (2017).
[7] K. Chakrabarti, *et al* J. Phys. B: At. Mol. Opt. Phys. **50**, 175202 (2017).