Electron-impact excitation and recombination of molecular cations in cold ionized gases: application to H_2^+, BeH^+, CH^+, CO^+, N_2^+, BF^+ and AlO^+

N. Pop[1,2], J. Zs Mezei[1,3,4,5], S.Niyonzima[1,6], F. Colboc[1], S. Ilie[1,2], M. D. Epée Epée[1,7], D. A. Little[8], B. Peres[9], V. Morel[9], O. Motapon [1,7], K. Chakrabarti[1,10], A. Bultel[9], K. Hassouni[4], J. Tennyson[8], I. F. Schneider[1,3]

[1]Laboratoire Ondes et Milieux Complexes, CNRS, Université du Havre, Le Havre, France
[2]Department of Physical Foundation of Engineering, Politehnica University Timișoara, Timișoara, Romania
[3]Laboratoire Aimé Cotton, CNRS, ENS Cachan and Univ. Paris-Sud, Orsay, France
[4]Laboratoire des Sciences des Procédés et des Matériaux, CNRS, Univ. Paris 13, France
[5]Instititute of Nuclear Research of the Hungarian Academy of Sciences, Debrecen, Hungary
[6]Département de Physique, Université du Burundi, Bujumbura, Burundi
[7]Department of Physics, Faculty of Sciences, University of Douala, Douala, Cameroon
[8]Department of Physics and Astronomy, University College London, United Kingdom
[9]Complexe de Recherche Interprofessionnel en Aérothermochimie (CORIA) CNRS, Université de Rouen, France
[10]Department of Mathematics, Scottish Church College, Kolkata

The Multichannel Quantum Defect Theory (MQDT) has been employed in computing cross sections and Maxwell rate coefficients for electron-driven reactions involving molecular cations. These data are used in the modelling of the kinetics of various cold ionized media of fundamental and applied interest.

1. Introduction

The detailed collisional-radiative modelling of cold ionized gasses requires accurate cross sections and rate coefficients of the major elementary processes. Among them, data on Dissociative Recombination (DR):

$$AB^{+}+e^{-}\rightarrow AB^{*},\ AB^{**}\rightarrow A+B, \qquad (1a)$$

as well as on its competitive processes Vibrational/Rotational Excitation (VE/RE) and deExcitation (VdE/RdE):

$$AB^{+}(N^{+},v^{+})+e^{-}\rightarrow AB^{*},\ AB^{**}\rightarrow AB^{+}(N^{+\prime},v^{+\prime})+e^{-} \qquad (1b)$$

and Dissociative Excitation (DE):

$$AB^{+}+e^{-}\rightarrow AB^{*},\ AB^{**}\rightarrow A+B^{+}+e^{-} \qquad (1c)$$

are badly needed [1].

Using the Multichannel Quantum Defect Theory (MQDT) [2], we have evaluated these data for a variety of ionized media.

2. Results

For the <u>fusion plasma edge</u>, extensive cross sections and rate coefficients have been produced for HD^+, H_2^+ [3], BeH^+ [4] - Figure 1 - and CH^+. The role of the DE for the hydrogen isotopomers, and that of the core-excited Rydberg states for CH^+, have been clearly put in evidence by an appropriate account of the mixing of the various reaction channels, *open* and *closed* [3, 5].

The same core-excited effects have been included successfully in the study of the DR of N_2^+ [5] – Figure 2 - required for the modelling of the plasma formed at the <u>hypersonic entry of space-crafts</u> in the Titan's atmosphere. This study succeeded extensive computations on NO^+ DR for the Terrestrial re-entries [6, 7], and on CO^+ DR, VE and VdE [8] for the Martian entries.

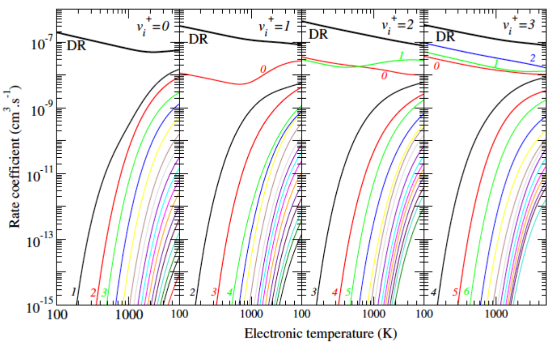

Figure 1. Maxwell rate coefficients for the DR, VE and VdE of BeH^+ ion in its electronic ground state and on its initial vibrational states v_i^+. The numbers label the final vibrational state of the transition [4].

We are currently about to produce DR rate coefficients for BF^+, involved in the <u>Plasma Ion Implantation</u> technique [9], as well as for AlO^+, formed in the LIBS-type experiments performed on Aluminium targets using picosecond laser sources [10].

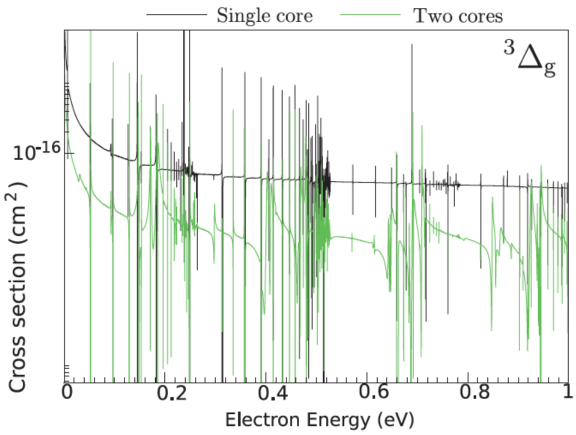

Figure 2. Core-excited Rydberg effects in the DR of N_2^+ [5]. Black curve: Rydberg series associated to the ground electronic state of N_2^+ included only. Green curve: both Rydberg series associated to the ground and to the first excited electronic states of N_2^+ included.

And finally, in order to model the excessively cold environments involved in the chemistry of the early Universe [11], interstellar molecular clouds [12], supernovae and planetary atmospheres, rate coefficients for VE, VdE, RE, RdE and DR have been produced for HD^+ - Figure 3 - H_2^+ [13] CO^+ [8] and CH^+.

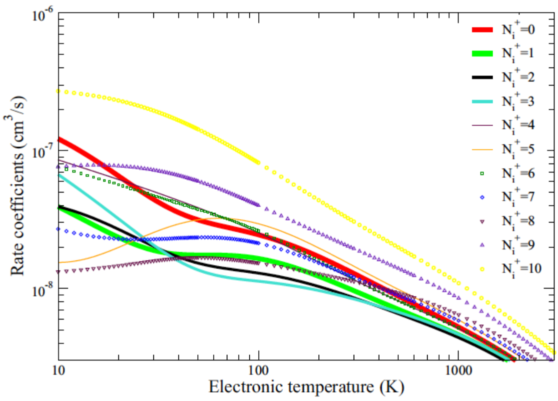

Figure 3. Maxwell rate coefficients for the DR of HD^+ on various initial rotational levels N_i^+ at low temperature [13].

Our calculations resulted in good agreement with the CRYRING (Stockholm) and TSR (Heidelberg) *magnetic* storage ring results, and our approach is permanently improved in order to face the new generation of *electrostatic* storage rings, as CSR (Heidelberg) and DESIREE (Stockholm) [1].

3. References

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