Excitation, recombination and dissociation of molecular cations by electron-impact in cold plasmas: Application to H_2^+, HD^+, BeD^+ and BF^+

N. Pop[1,2], J. Zs. Mezei[1,3,4,5], F. Colboc[1], Y. Moulane[1,6], S. Niyonzima[7], M.D. Epée Epée[8], O. Motapon[9], F. Iacob[10], R. Boata[11],V. Laporta[1], K. Chakrabarti[12], J. Tennyson[13], I.F.Schneider[1]

[1]*LOMC, CNRS, Univ. du Havre, France,* [2]*Politehnica Univ. Timişoara, Romania,* [3]*LAC, CNRS, ENS Cachan and Univ. Paris-Sud, Orsay, France,* [4]*LSPM, CNRS, Univ. Paris 13, France,*
[5]*INRHAS, Debrecen, Hungary,* [6]*LHEPA, Cadi Ayad Univ., Marrakech, Morocco,* [7]*Univ. de Burundi, Bujumbura, Burundi,* [8]*Univ. of Douala, Cameroon,* [9]*Univ. of Maroua, Cameroon,* [10]*West University of Timişoara, Romania*
[11]*Romanian Academy, Timişoara, Romania,* [12]*Scottish Church College, Calcutta, India,*
[13]*University College London, UK.*

Reactive collisions between electrons and molecular cations have a major role in the ionized gases kinetics. Using the Multichannel Quantum Defect Theory, cross sections and rate coefficients have been obtained for different reactions induced by electrons on H_2^+, HD^+, BeH^+ and BF^+ in natural, laboratory and industrial ionized media.

1. Introduction

Dissociative recombination (DR), (ro)vibrational excitation (VE) and de-excitation (VdE), and dissociative excitation [1,2]:

$AB^+(N_i^+,v_i^+)+e^- \rightarrow A+B$, $AB^+(N_f^+,v_f^+)+e^-$, $A+B^++e^-$,

are the dominant elementary processes in numerous cold ionized media. The Multichannel Quantum Defect Theory (MQDT) has been employed for computing state-to-state cross sections and Maxwell rate coefficients relevant for the kinetic plasma models.

2. Results

In order to model and diagnose *the low-temperature fusion edge plasmas*, a complete database for electron-impact collision processes is required for molecular species containing beryllium and hydrogen. We have expanded our studies on BeH^+ [3,4] to BeD^+ and BeT^+ cations. Figure 1 shows as an example the Maxwell rate coefficients for the lowest states (v_i^+= 0-5) of BeD^+, significantly dependent on the initial vibrational level of the molecular ion: Indeed, this figure illustrates the dominance of the DR, while the VdE, clearly higher than the VE, becomes progressively important for high initial vibrational levels of the target.

The electron impact processes on BF^+ are important in the *plasma ion implantation technique* [5]. The calculated rate coefficients have revealed that the vibrational transitions in this case are more important than the dissociative recombination.

And finally, in order to describe the chemistry of the *cold environments* involved in the history of the early Universe, in the *interstellar molecular clouds* and in the *edge of the fusion plasmas*, we have extended our most recent calculations on HD^+ [6] and H_2^+ [7] to higher energy, aiming to provide a complete state-to-state collisional data-base for the hydrogen molecular cations.

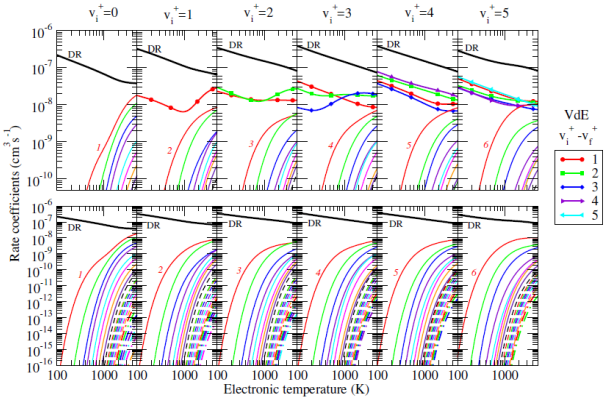

Fig.1. Dissociative recombination (DR, thick line), vibrational excitation (VE, thin lines) and vibrational de-excitation (VdE, symbols and thick lines) Maxwell rate coefficients of first excited (v_i^+ = 0-5) BeD^+ in its electronic ground state. For VE, since the rate coefficients decrease monotonically with the excitation, the lowest final vibrational quantum number of the target is indicated only, and the lower panels extend the range down to 10^{-14} cm^3/s.

In the case of the benchmark ions H_2^+ and HD^+, our reaction rates and cross sections have been thoroughly compared with those measured, mainly in the heavy-ion storage rings [2].

3. References

[1] I. F. Schneider, invited topical talk at this conference.
[2] I. F. Schneider, O. Dulieu, J. Robert, *Proceedings of DR2013: The 9th Int. Conf. on Dissociative Recombination: Theory, Experiment and Applications, Paris, 2013*, EPJ Web of Conferences **84** (2015).
[3] S. Niyonzima *et al.*, *ADNDT* (2017), in press.
[4] V. Laporta *et al*, *PPCP* **59** (2017) 045008.
[5] J. Zs. Mezei *et al.*, *PSST* **25** (2016) 055022.
[6] O. Motapon *et al*, *Phys. Rev. A* **90** (2014) 012706.
[7] M. D. Epée Epée *et al*, *MNRAS* **455** (2015) 276.