Indirect Dissociative Recombination of Small Ions

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Dissociative recombination (DR) is a process is which a free electron with a positive kinetic energy is captured by a molecular ion while breaking one or several chemical bonds,

$$e^- + AB^+ \rightarrow A + B\,.$$

This is a very efficient chemical process, but is rarely described in chemical textbooks. It is considered to be the most complex of gas-phase reactions leading to the production of neutral atoms and molecules [1].

Historically, we distinguish two different mechanisms for the DR process. In the direct mechanism the reaction is mediated by an electronic resonant state AB^*(shape or core-excited resonance), while in the indirect mechanism no such electronic state exists in the Frank-Condon region and the AB^* state is formed by an internal rovibrational excitation (rovibrational Feshbach resonance). For most of the molecular systems both mechanisms interfere resulting in a complicated structures of the DR rates. However, for a number of molecular cations (LiH+, LiHe+, HeH+, . . .) the indirect process dominates in the dissociation.

Although the theoretical models [2, 3] describing the indirect DR with multichannel quantum defect theory (MQDT) have been successfully used [4] for several decades, the recent experimental advances [5] put the accuracy of these models to a test. In this paper we show how the theory helps to setup the experiment and we also report on our progress in development of accurate indirect DR theory and its application to several molecular targets.

References

[1] A. E. Orel and M. Larsson, *Dissociative recombination of molecular ions* (Cambridge University Press, New York, 2008).
[2] A. Giusti, *J. Phys. B: Atom. Molec. Phys.*, **13**, (1980), 3867.
[3] E. L. Hamilton and C. H. Greene, *Phys. Rev. Lett.*, **89**, (2002), 263003.
[4] R. Čurík and C. H. Greene, *Phys. Rev. Lett.*, **98**, (2007), 173201.
[5] R. von Hahn, A. Becker, F. Berg, K. Blaum, C. Breitenfeldt, H. Fadil, F. Fellenberger, M. Froese, S. George, J. Goeck, et al., *Rev. Sci. Instrum.*, **87**, (2016), 063115.