Resonances in Dissociative Recombination

A. E. Orel
Department of Applied Science
University of California, Davis, USA

Dissociative recombination (DR) of molecular ions:

$$AB^+ + e^- \text{-->} AB^\dagger \text{-->} A + B^*$$

transforms the kinetic energy of the incident electron into excitation of the core electrons. DR occurs when the dominant configuration of $AB^\dagger$ corresponds to a repulsive state and the chemical bond is broken. This is an important process in low temperature plasmas, such as interstellar clouds, planetary atmospheres and in plasma processing such as chemical vapor deposition[1]. With some notable exceptions[2], the process is dominated by resonances.

These resonances include both the repulsive $AB^\dagger$ states, but also bound states lying in the same energy range which lead to structure in the DR across section as a function of initial electron energy. These structures are the signature of the “indirect” recombination process. In general, they can be assigned to excited rovibrational levels of bound Rydberg states with a ground-state ion core, which couple to the initial ground-state electronic continuum by non-adiabatic interactions only.

In addition, there exists another class of resonances. These are members of a Rydberg series converging to excited states of the ion, generally referred to as “core-excited” states. These states are bound with respect to dissociation, if the ion to which the series converges is bound. They are coupled both to the electronic initial continuum and to the dissociative final channel and tend to produce broader and more prominent structures in the DR cross section[3].

We will illustrate each of these resonances for the case of dissociative recombination of the water ion. DR of the water ion is the source of OH radicals in the H I zone in dense molecular clouds[4]. Both the absolute cross section and the branching ratios in the final neutral fragment channels have been measured[5].

The ground state of water is:

$^2A_1$ $\quad (1a_1)^2(2a_1)^2(1b_2)^2(3a_1)^2(1b_1)^2$

The water ion has three low-lying excited states resulting from removing one electron from the three lowest lying orbitals.

$^2B_1$ $(1a_1)^2(2a_1)^2(1b_2)^2(3a_1)^2(1b_1)$

$^2A_1$ $(1a_1)^2(2a_1)^2(1b_2)^2(3a_1)(1b_1)^2$

$^2B_2$ $(1a_1)^2(2a_1)^2(1b_2)(3a_1)^2(1b_1)^2$

Each of these low-lying states has a Rydberg series of neutral water curves associated with it. For the case of the two higher states, some of the Rydbergs lie above the ground state of the ion, forming core-excited states. There also exist dissociative neutral autoionizing states that cross the ground state of ion that can lead to DR.

Electron-scattering calculations from the molecular ion using the complex Kohn variational method have been carried out in C_{2v} geometry. The eigenphase sums were fit to a Breit-Wigner form and the resonance energies and autoionization widths were obtained. The variation of the states as a function of the symmetric stretch and bend will be presented and the implications for dissociative recombination of the water ion and the final states resulting from this collision process discussed.

A. E. O. acknowledges useful discussions with R. van Harrevelt. This work was supported by the National Science Foundation, Grant No.PHY-99-87877.

REFERENCES

(1) For a recent review see, *Dissociative Recombination: Theory, Experiment and Applications IV*, edited by M. Larsson, B. Mitchell and I. F. Schneider (World Scientific, Singapore, 2000).

(2) See, for example, the abstract by C. Greene.

(3) L. Carata, A. E. Orel, M. Raoult, I. F. Schneider and A. Suzor-Weiner, Phys. Rev. A, **62** 052711 (2000).

(4) D. R. Bates, Astrophys. J. **306**, L45 (1986).

(5) S. Rosen, A. Derkatch, J. Semaniak, A. Neau, A. Al-Khalili, A. Le Padellec. L. Vikor, R. Thomas, H. Danared, M. af Ugglas and M. Larsson, Faraday Disc. **115**, 292 (2000).