The Capture of Electrons by Molecular Ions in Planetary Ionospheres and the Interstellar Medium

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Dissociative recombination (DR) reactions often have high rate constants allowing them to play important roles in the interstellar medium, comet atmospheres and planetary ionospheres. In these reactions, a diatomic or polyatomic ion, e.g. AB^+, captures an electron, e^-, and breaks up into neutral fragments,

$$AB^+ + e^- \rightarrow A + B \tag{1}$$

where A or B can be in the ground or an excited state. If AB^+ is a polyatomic molecule, the products can be atoms and/or molecules. The identity of the products can be sensitive to the electronic and vibrational state of the ion undergoing DR.

We describe an ab initio theoretical approach for the calculation of DR cross sections and rate coefficients. Potential curves for both molecular ions and neutral dissociative states have been determined using large scale configuration interaction wave functions. Cross sections and rate coefficients have been calculated using Multichannel Quantum Defect Theory.

In recent work [Guberman, 1997], we have identified the mechanism by which DR of O_2^+ generates the $O(^1S)$ excited state. Electron capture takes place mostly into a state which does not dissociate to $O(^1S)$ but which has a high capture probability. Vibrationally excited mixed symmetry neutral Rydberg states couple the capture state to another state which dissociates to $O(^1S)$. The calculated DR rate constant for generating $O(^1S)$ from the lowest vibrational level is $3.9x10^{-9}cm^3/sec$ at an electron temperature of 300K. Recent results for the DR of HeH^+, CO^+ and H_3^+ will also be reported.

References:

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