Effects of rotation and Jahn-Teller coupling on H3+ dissociative recombination

Chris H. Greene and V. Kokoouline
Physics Department and JILA
University of Colorado
Boulder, CO 80309-0440

The enigmatic problem of describing the dissociative recombination (DR) of H3+ ions by low energy incident electrons has withstood more than a decade of serious theoretical efforts. Progress made a year ago[1] pointed out a new mechanism that apparently controls this DR process, namely Jahn-Teller coupling between the incident electron and the molecular ion. At the workshop, I will discuss a full calculation that combines multichannel quantum defect theory (MQDT) implemented at the first principles level, a hyperspherical coordinate method to include all three dimensions of vibrational motion, and the quantized rotational level structure of the target ion. A new implementation of the molecular MQDT calculation, using vibrational channel functions that obey Siegert (outgoing wave) boundary conditions, permits a simple extraction of the dissociative probability flux. The results show quantitative agreement with the average DR rate coefficient measured in the newest Stockholm storage ring experiment, although the detailed predictions of individual features show discrepancies with experiment that have not yet been resolved.

[1] V. Kokoouline, C. H. Greene, B. D. Esry, Nature 412, 891 (2001).
[2] E. L. Hamilton and C. H. Greene, Phys. Rev. Lett. (in press), and physics/0208030.