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Theoretical description of dissociative recombination of HCO^+[1]

NICOLAS DOUGUET, VIATCHESLAV KOKOOULINE, Department of Physics, University of Central Florida, CHRIS H. GREENE, Department of Physics and JILA, University of Colorado at Boulder — Theoretical description of dissociative recombination (DR) of triatomic molecular ions is a difficult problem because several different (electronic and vibrational) degrees of freedom have to be taken into account at once. Our recent theoretical calculations of the DR cross-section of simple polyatomic ions like H_3^+, exhibited good agreement with experimental measurements. On the other hand, the previous theoretical cross-section for more sophisticated molecular ion, HCO^+, still diverges significantly from the experimental data. In this presentation, we describe our improved theoretical approach for calculation of the DR cross-section in HCO^+ and DCO^+ ions. Comparing with the previous theoretical study (Phys. Rev. A 74, 032707 (2006)) we took into account all vibrationally degrees of freedom. The Renner-Teller coupling between electronic and vibrational motion is also accounted for. The obtained theoretical cross-section is in better agreement with experiment, especially in the region of relatively high (>0.1 eV) collision energy.

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