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Simplified Theoretical Model to treat the Dissociative Recombination of polyatomic ions by strong Jahn-Teller effects: Study of H_3O^+ and H_3^+ ions[1] NICOLAS DOUGUET, University of Central Florida, Orlando, FL, CHRIS H. GREENE, Department of Physics and JILA. University of Colorado, Boulder, CO, IVAN MIKHAILOV, University of Central Florida, Orlando, FL, VIATCHESLAV KOKOOULINE, Laboratoire Aime Cotton, Orsay, France — Recent progress in theoretical treatment of dissociative recombination (DR) in closed-shell triatomic ions (H_3^+, HCO^+ or LiH_2^+) have demonstrated reasonable agreement with available experimental data. These studies take into account vibrational, rotational, electronic, and nuclear spin degrees of freedom, and for this reason, the numerical methods are rather demanding. In more recent studies, Mikhailov *et al.* and Pratt & Jungen proposed simplified theoretical methods for DR, considering that once the electron is captured by the ion into a vibrationally excited state, the system will dissociate. The probability to capture the electron is mainly determined by non-Born-Oppenheimer effects in HCO^+ (Renner-Teller effect) and H_3^+ (Jahn-Teller effect). The thermally averaged rate constants obtained with the simplified methods are in good agreement with the fully-quantum treatment. In this study we made a step further in the simplified theory of DR in small polyatomic ions and applied it to H_3O^+.

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