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Recent Theoretical Studies of Dissociative Recombination[1]

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After decades of progress, quantitative agreement between theory and experiment for dissociative recombination (DR) cross sections has remained elusive. Using ab initio potential curves, widths and the MQDT approach (Guberman, 2012) the DR of N2+, i.e. $N2+ + e^- \rightarrow N + N$, has been analyzed for each of the lowest 5 ion vibrational levels. It is shown that agreement with future high resolution experiments requires that theory account for minor dissociative routes. The cross sections and rate constants are compared to the results of afterglow and merged beam experiments. Good agreement is obtained for the v = 0 rate constant. The only storage ring experiment (CRYRING) to measure cross sections and rate constants found that two unknown ion vibrational distributions gave similar values, (Peterson et al., 1998) leading to the conclusion that the rate constants must be similar for each of the lowest 4 ion vibrational levels. The theory finds that at low electron temperatures the rate coefficients are indeed similar but above room temperature the larger rate coefficient for v = 0 diverges from the others by factors of 2 – 3. The rate constant for "elastic" capture in which the electron is captured but emitted before dissociation has been calculated and allows for the determination of the fraction of collisional captures that lead to DR. For v = 0, DR results from 2 out of every 10 captures. Guberman, S. L., J. Chem. Phys. **137**, 074309 (2012); Peterson, J. R. et al., J. Chem. Phys. **108**, 1978 (1998).

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