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Intramolecular electron transfer in transient ammonia anion resonances¹ DANIEL SLAUGHTER, HIDEHITO ADANIYA, ALI BELKACEM, TOM RESCIGNO, Lawrence Berkeley Natl Lab, CYNTHIA TREVISAN, California Maritime Academy, MARVIN WEYLAND, ALEXANDER DORN, Max Planck Institute for Nuclear Physics, ANN OREL, University of California, Davis, BILL MCCURDY, University of California, Davis and Lawrence Berkeley Natl Lab — We report a combined experimental and theoretical study of dissociative electron attachment (DEA) dynamics of ammonia. Fragment momentum imaging experiments performed at MPIK Heidelberg and LBNL Berkeley found that DEA involving two electronic Feshbach resonances produce both H- and NH2- from ammonia. Two-body dissociation producing H- occurs via direct dissociation on either of two resonant anion states, with the lower and higher energy resonances leading to ground state and electronically excited NH2^{*}, respectively. Using ab initio electronic structure theory we found that dissociation to H and NH2- involves a virtual anion state that asymptotically approaches the lower of these two dissociation limits, with nonadiabatic coupling due to electron transfer at considerable N-H distances. Through complex Kohn electron scattering calculations we examine the electron attachment probabilities in the molecular frame and compare these with measured fragment angular distributions to analyze and draw conclusions on the transient anion dynamics for each dissociation channel.

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