OBSERVATION OF RESONANCES IN THE F+NH_3 REACTION VIA TRANSITION-STATE SPECTROSCOPY

MARK C BABIN, *Department of Chemistry and Chemical Biology, Harvard University, Cambridge, MA, USA*; MARTIN DeWITT, *Chemistry, University of California, Berkeley, Berkeley, CA, USA*; JASCHA LAU, *Department of Chemistry, University of California, Berkeley, Berkeley, CA, USA*; HONGWEI SONG, *Wuhan Institute of Physics and Mathematics, Chinese Academy of Sciences, Wuhan, China*; HUA GUO, *Department of Chemistry and Chemical Biology, University of New Mexico, Albuquerque, NM, USA*; DANIEL NEUMARK, *Department of Chemistry, The University of California, Berkeley, CA, USA*.

Transition state spectroscopy experiments, based on negative-ion photodechament, allow for the direct probing of the vibrational structure and metastable resonances that are characteristic of the neutral reactive surface. Here, we study the four-atom F + NH_3 $\rightarrow$ HF + NH_2 reaction using slow photoelectron velocity-map imaging spectroscopy of cryogenically cooled NH_3F^- anions. The resulting spectra reveal features associated with a manifold of vibrational Feshbach resonances in the post-transition state product well of this reactive surface. Beyond this, the spectra contain structure reporting on reactive resonances in the pre-transition state reaction complex well. Quantum dynamical calculations performed on a full-dimensional potential surface show excellent agreement with the experimental results, allowing for the assignment of spectral structure and demonstrating that key dynamics of this bimolecular reaction are well described by this theoretical framework.