Abstract Submitted
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Molecular Simulations of Multi-Photon Dissociation of CaH^+ and CaD^+[1] SMITHA JANARDAN, AARON CALVIN, JOHN CONDOLUCI, RENE RUGANGO, GANG SHU, KENNETH BROWN, Georgia Inst of Tech — The vibronic and rovibronic $1^1\Sigma, \nu = 0 \rightarrow 2^1\Sigma, \nu' = 0, 1, 2, 3$ transitions are measured using molecular simulations of resonance enhanced multi-photon dissociation (REMPD) of CaH^+ and CaD^+. These measurements are vital for measuring rotational state preparation of CaH^+. The simulation method comes in two flavors: simple and full simulations, where the simple model ignores dissociation and full simulations take dissociation into account. Both methods convolute a tunable laser with an underlying rovibronic spectrum to find corresponding transition rates. By fitting the simulated spectrum to the experimental spectrum, physical constants and information, such as transition frequency, transition dipole moments, rotational constants, and dissociation pathway, is extracted. Assuming the Born-Oppenheimer Approximation (BOA), the vibronic transitions require a 687 cm^{-1} shift from their theoretically predicted values to match both CaH^+ and CaD^+. Both transition dipoles and rotational constants match relatively relatively well with theory, and we will describe possible dissociation paths through excited Σ and Π states.

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