Abstract Submitted
for the DAMOP17 Meeting of
The American Physical Society

Dissociative recombination of HCN+ and HNC+, a simplified approach ERIN MCBROOM, NICOLAS DOUGUET, SAMANTHA FONSECA, Drake Univ, ASA LARSON, Stockholm University, ANN OREL, UCDavis — We present the study of the Dissociative Recombination (DR) of the HCN^+ and HNC^+ molecular ions. Our calculations are based on a simplified theoretical model that captures the essence of indirectly driven DR process. We use normal modes to represent the vibrational states and the non-adiabatic couplings between them are obtained simply by computing the scattering matrix elements in this vibrational space. Electronic structure calculations, as well as scattering calculations, were carried out entirely from ab initio principles and we compare our results to available data on the literature.

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Date submitted: 27 Jan 2017 Electronic form version 1.4