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Abstract for an Invited Paper for the MAR16 Meeting of the American Physical Society

Complexities in Pressure Dependent Kinetics Across a Wide-Range of Temperatures and Pressures STEPHEN KLIPPENSTEIN, Argonne Natl Lab

Sample ab initio transition state theory based master equation calculations will be used to illustrate interesting features of the kinetics for a variety of reactions of importance in astrochemistry, atmospheric, and combustion chemistry. The calculations will explore the role of long-range interactions, angular momentum conservation, tunneling, radiative emission, roaming processes, torsional motions, and prompt dissociation of incipient molecules. Comparisons with experiment will be presented to illustrate the current accuracy of such calculations.