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Unravelling Two State Reactivity: New Insights Combining Experimental, *Ab Initio*, and Statistical Modelling Techniques SHAUN ARD, AFRL, JOSHUA MELKO, University of North Florida, OSCAR MARTINEZ, AFRL, VLADIMIR USHAKOV, Max Plank Institue, ANYANG LI, RYAN JOHNSON, University of New Mexico, NICHOLAS SHUMAN, AFRL, HUA GUO, University of New Mexico, JURGEN TROE, Max Plank Institue, ALBERT VIGGIANO, AFRL — Non-Adiabatic dynamics have long played a role in understanding numerous ion molecule reactions. As calculation techniques have improved, even spin-allowed reactions have been found to be significantly impacted by low lying excited spin states, so-called Two-State reactivity. This talk will focus on recent studies of several canonical examples, FeO^+ + H_2FeO^++ CH_4, and Fe^++ N_2O. Experimentally, the kinetics of these reactions are studied from 100 to 700K. Combined with computations of the reaction surface, statistical modelling employing the Statistical Adiabatic Channel Model (SACM) of this near thermal energy range gives unique insight into kinetic details of these systems. Implications of this combined approach, specifically towards better quantifying Two-State reactivity in ion-molecule reactions, will be discussed.

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