

WEAKLY-BOUND COMPLEX FORMATION BETWEEN HCN AND CH₃Cl: A MATRIX-ISOLATION AND COMPUTATIONAL STUDY

EMILY K HOCKEY, *Department of Chemistry and Biochemistry, University of Maryland, College Park, College Park, MD, USA*; KORINA VLAHOS, *Chemistry and Biochemistry, University of Maryland, College Park, College Park, MD, USA*; THOMAS HOWARD, JESSICA PALKO, LEAH G DODSON, *Department of Chemistry and Biochemistry, University of Maryland, College Park, MD, USA*.

Matrix-isolation spectroscopy is used to characterize the weakly-bound complex(es) of hydrogen cyanide with methyl chloride, two astrophysically relevant molecules. HCN and its polymers captivate interstellar discussions of prebiotic monomers and other life-bearing polymers, while CH₃Cl leads as the first organohalogen detected in space. This highlights the importance of studying their reactivity. In this talk, we will describe our new matrix-isolation instrument, constructed at the University of Maryland, and how we identify the structure of the weakly-bound complexes [(HCN)_nCH₃Cl] that form upon co-condensation of HCN and CH₃Cl in an argon matrix. Infrared spectroscopy is used in tandem with quantum chemistry calculations to characterize the vibrational spectrum of the resulting complexes. Our work reveals preferential formation of matrix-isolated HCN trimer species in the presence of CH₃Cl, qualitatively characterized by non-covalent interactions through natural bond orbital calculations. Finally, we will discuss the astrochemical implications of the resulting complexes and HCN trimer formation.