INFRARED PREDISSOCIATION SPECTROSCOPY OF CATIONIC ACETYLENE CLUSTERS, $(C_2H_2)_n^+$, $n = 1 - 4$

RACHAEL A. RELPH, JOSEPH C. BOPP, JOSEPH R. ROSCIOLI, MARK A. JOHNSON, *Sterling Chemistry Laboratory, Yale University, PO Box 208107, New Haven, CT 06520.*

Infrared predissociation spectroscopic studies of systematically solvated acetylene clusters, $(C_2H_2)_n^+$, $n = 1 - 4$, reveal the structural evolution of these cations with increasing cluster size. The argon predissociation spectrum of the acetylene dimer coupled with harmonic frequency calculations suggests the dominate species adopts a cyclobutadiene-like geometry. The argon solvated trimer, $(C_6H_6)^+ \cdot$ Ar, predominantly loses $(C_2H_2)^+ \cdot$ Ar, suggesting that the trimer is composed of a covalently bonded "dimer core" which exhibits a spectrum different than cyclobutadiene, and is solvated by a weakly bound acetylene. The same spectral features are retained in the tetramer suggesting that the dimer core survives the solvation of additional acetylene molecules. The minor loss channel of $(C_6H_6)^+ \cdot$ Ar, loss of a single Ar, shows multiple features believed to be from a number of covalently bonded $(C_6H_6)^+$ species.