

INFRARED SPECTROSCOPY AND STRUCTURE OF PROTONATED BENZENE CLUSTERS

B. BANDYOPADHYAY, T. CHENG, M. A. DUNCAN, *Department of Chemistry, University of Georgia, Athens, GA 30602-2556.*

Gas phase protonated benzene clusters are produced in a pulsed electrical discharge supersonic expansion cluster source. Infrared spectra of the cold argon-tagged species are obtained via infrared photodissociation spectroscopy. Theoretical investigations have been employed to probe the structures of these clusters. The infrared spectroscopy (1000 cm^{-1} to 3500 cm^{-1}) and structures of the protonated benzene dimer, trimer and tetramer will be discussed. Infrared spectrum of protonated benzene dimer shows a peak around 2840 cm^{-1} corresponding to the $\text{sp}^3\text{ CH}_2$ stretch of the benzene ring. In the case of the trimer and tetramer, this peak is shifted down to 2640 cm^{-1} , suggesting that the CH_2 moiety of the protonated benzene is interacting with another benzene. Various possible isomeric structures are explored theoretically, but the infrared spectrum of protonated benzene dimer suggests the presence of exclusively one isomer.