

STRUCTURAL INVESTIGATION OF HYDRATED ANIONIC PYRENE CLUSTERS WITH INFRARED SPECTROSCOPY^a

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Hydrated pyrene anions are model systems for microsolvation and hydrogen bonded (H-bonded) networks on charged graphene like materials. Tandem mass spectrometry was employed to collect mass selected messenger-tag and photodissociation infrared (IR) spectra. Photodissociation spectra of cold cluster anions of the form $C_{16}H_{10}^{-} \cdot (H_2O)_n \cdot Ar_2$ ($n=1-4$) losing Argon upon irradiation are compared to spectra of warmer $C_{16}H_{10}^{-} \cdot (H_2O)_n$ ($n=1-4$) cluster anions. Structural and dynamic information about the H-bond network is encoded in OH stretching frequencies. Experimental IR spectra are compared to density functional theory calculations, and various cluster geometries are predicted. Generally, water molecules form H-bonds with other water molecules and with the excess charge in pyrene's π -system. These binding motifs are compared to the ones found on anionic hydrated naphthalene clusters.^b

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^b1. B.J. Knurr, C.L. Adams, and J.M. Weber, Infrared Spectroscopy of Hydrated Naphthalene Cluster Anions. *J. Chem. Phys.* 137 (2012) 104303.