HYDRATION OF A LARGE ANIONIC CHARGE DISTRIBUTION - NAPHTHALENE-WATER CLUSTER ANIONS

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We report the infrared spectra of anionic clusters of naphthalene with up to three water molecules. Comparison of the experimental infrared spectra with theoretically predicted spectra from quantum chemistry calculations allow conclusions regarding the structures of the clusters under study. The first water molecule forms two hydrogen bonds with the π electron system of the naphthalene moiety. Subsequent water ligands interact with both the naphthalene and the other water ligands to form hydrogen bonded networks, similar to other hydrated anion clusters. Naphthalene-water anion clusters illustrate how water interacts with negative charge delocalized over a large π electron system. The clusters are interesting model systems that are discussed in the context of wetting of graphene surfaces and polyaromatic hydrocarbons.