

FAR-IR SPECTROSCOPY AS DIRECT PROBE OF INTERMOLECULAR DYNAMICS IN PAH-WATER COMPLEXES

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Even though the interaction between polar water and hydrophobic molecules such as PAHs is very subtle, soot or dust particles do play a key role in the water nucleation in atmospheres and in interstellar space. To understand this process and predict their structures and properties, an accurate understanding of the shallow potential energy surface between PAH-water clusters is essential. Infrared spectroscopy is a particularly well-suited technique to study the PES of such ground-state systems. Previous IR studies, as well as complementary microwave work, established that the hydrogen bonding within the water network is more important than the interactions between water substrate. However, most infrared studies focused on the XH stretch region, which only indirectly reveals information on weaker, non-covalent interactions.

This study, focusing on neutral naphthalene interacting with up to three water molecules, shows that far-IR radiation can probe the intermolecular potential directly and reveals notable effects of the substrate on the water clusters. Despite the clusters being produced in a cold environment, the weak interactions necessitate their spectra to be interpreted within a dynamic, rather than a static framework. Purely intermolecular vibrational modes are identified and changes of the far-IR water libration modes upon complexation are investigated. Both show the perturbative effect of the substrate on water and the dynamics between PAH and water.