CFEL SCIENCE

SEMINAR

11.06.20 - 10:00 h

At Zoom virtual meeting: https://desy.zoom.us/j/91664852751

Meeting ID: 916 6485 2751 Password: 814781

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How does the topology of a PAH influence its microsolvation? A microwave study of the phenanthrene-water and phenanthridine-water clusters

Intermolecular interactions occurring between aromatic molecules, i.e. polycyclic aromatic hydrocarbons (PAHs), and water play an important role in many areas, ranging from biomolecular recognition to astrochemistry. Although the nature of these interactions is expected to be influenced by the topology of the aromatic substrate, most of the experimental investigations have focused on their characterization in the benzene-water complex, considered as a prototype for aromatic-polar interactions. Herein, we report on the study of size-selected microhydrated clusters of the PAHs phenanthrene and phenanthidine by means of rotational spectroscopy and quantum chemical calculations. The two molecules provide a simple model to understand the impact that an extended aromatic surface and the presence of a heteroatom have on the nature of the non-covalent interactions established with the surronding water molecules. To highlight the effect that the topology of the PAH has on the aromatic-polar interaction network at play, a comparison with related PAH-water clusters will also be presented.

Host: Melanie Schnell / CFEL Molecular and Ultrafast Science Seminar