

Seminar

28th of October 2021
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Zoom Virtual Meeting:

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Meeting-ID: 847 0356 4086

Password: 570173



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Every water molecule counts – structural insights on microsolvation using rotational spectroscopy

Intermolecular interactions between water and solute molecules are at the heart of many chemical processes. They are responsible for the initial steps of aerosol formation, as for example relevant for atmospheric chemistry, and for ice-grain formation, which is central for astrochemical reactions. As such, it is important to understand where, how, and why individual water molecules bind to different solute molecules, and how different solute molecules shape the water network at the molecular scale. Furthermore, it is observed that already the interaction with just a single water molecule can have a significant influence on the preferred structural arrangement of the solute. To evaluate these aspects in more detail, we employ high-resolution rotational spectroscopy in the gas phase to obtain precise structures of the solvated clusters. Our technique also provides dynamical information via the analysis of possible tunneling processes in the microsolvated clusters. The experiments are performed under the cold and collision-free conditions of a supersonic expansion, in which the isolated water-solute clusters are formed. These conditions allow for a direct comparison with and benchmarking of quantum-chemical experiments.

In the lecture, the technique of broadband rotational spectroscopy employing molecular jets will be introduced and its application to the determination of the precise structures of microsolvated complexes will be discussed, based on selected examples of astrochemical and biological relevance.

