CFEL SCIENCE

SEMINAR

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CFEL (Bldg. 99) seminar room II+III

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Hydrogen bonding in molecular complexes and atmospheric reactions

Hydrogen bonds are prevalent everywhere, yet much is still not known about their physical properties. In atmospheric research, radiative transfer, reaction mechanisms and nucleation are all affected by hydrogen bonds. We have detected and characterized hydrogen bonds, X-H···Y, for a range of different donor XH-bonds and acceptor moieties, with a focus of addressing key atmospheric questions.

The formation of a bimolecular complex, the first step in nucleation, relies on the Gibbs energy of formation, ΔG, which is difficult to obtain accurately, from pure experimental or theoretical methods. We have developed a combined experimental and theoretical hybrid approach with which ΔG of bimolecular complex formation at ambient temperature can be determined with an accuracy better than 1 kJ/mol. To facilitate this, we need to be able to calculate oscillator strengths of the vibrational transitions that are characteristic to the bimolecular complex and which can be measured. Typically, this involves absorption bands of the XH-stretching vibrations, which are mostly affected by the hydrogen bond formation, and which we can describe theoretically within a reduced dimensionality local mode framework. The calculated vibrational spectra, in turn, are key to assignment of vibrational spectra and, for atmospherically relevant molecular complexes like e.g. water dimer, important for radiative transfer in atmospheres.

The stability of intermediates and products formed in atmospheric reactions are also affected by their ability to form hydrogen bonds. Autoxidation, the repeated uptake of molecular oxygen by a molecule, is key to atmospheric oxidation and lead to highly oxygenated organic molecules with a large number of functional groups. These groups (e.g. OOH, OH, C=O) increase the ability of the molecules to form hydrogen bonds. This affects atmospheric reactions and lead to surprising stability of highly reactive compounds.

Host: Jochen Küpper/ CFEL Molecular and Ultrafast Science Seminar