

# Decoding Hydrogen-Bonded Clusters: Structural Insights from Rotational Spectroscopy

*Wednesday 17 September 2025 10:00 (30 minutes)*

The investigation of hydrogen-bonded clusters in the gas phase, where the effect of the environment is removed, is crucial to understand the interplay of intra- and intermolecular forces and how modest changes influence structural outcomes. Rotational spectroscopy, with its direct dependence of mass distribution and its unparalleled capability to differentiate between conformers and isomers, is an ideal technique to study such clusters. Specifically, microsolvated clusters where water is added to solutes in a stepwise fashion provide insight into how the transition from isolated to fully solvated molecule proceeds. In this talk we will discuss our findings on several clusters of water with molecules of atmospheric and biological interest, investigated by a combination of broadband rotational spectroscopy in supersonic jets and quantum chemical calculations. We will comment on the preferred structural choices and relevant non-covalent interactions, as well as on the performance of the various theoretical approaches.

## Keywords

hydrogen bond, complexes, rotational spectroscopy, supersonic jet, gas, DFT and ab initio calculations

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