

International Master 2 Atmospheric Sciences: Research Training 2022-2023

Laboratory: PhLAM

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Eventually CaPPA Work Package: WP-1 From gas phase to aerosols

Gas phase microsolvation of atmospheric SOAs precursors

Volatile organic compounds (VOCs) are emitted into the atmosphere from natural and anthropogenic sources. Terpenoids are VOCs emitted by plant and on the global scale they represents about 11% of the total biogenic emission. They are generally highly reactive compounds that play an essential role in atmospheric chemical interactions. They undergo oxidation and degradation processes and react with other abundant atmospheric species (O_3 , OH, NO_x) to produce large amounts of new species. They are considered as precursors of secondary organic aerosols (SOAs) which have an impact on human health and affect also the overall energy balance of our planet by scattering or absorbing incoming radiation and by acting as cloud condensation nuclei. The aerosol's formation processes are far to be well understood at the molecular level. Hydrogen bond interaction has been shown to enhance the nucleation process leading to new particle formation. In-depth information about the molecular systems formed in the gas phase is important and mandatory to better understand their physico-chemical properties and behavior. The combination of microwave spectroscopy with quantum chemical calculations is a powerful tool to study molecular structure and microsolvation in the gas phase through the analysis of their pure rotational spectra.

The project aims to study isolated molecules in order to characterize their conformational landscape by recording and analyzing their rotational spectrum with the help of quantum chemical calculations. Afterwards, the same strategy will be applied to the same molecule in the presence of other atmospheric species such as water to characterize the solvation sites and to evidence the structural modifications upon hydration. These data are then extremely useful to describe the nature of the non-covalent intermolecular interactions involved in the stabilization of the complexes and understand at the molecular scale the first steps in the process of aerosols formation.

For this purpose, a selected terpenoid will be studied isolated and microsolvated by means of Fourier transform microwave spectrometer coupled to a supersonic jet. Then, recorded spectra will be analyzed using available least squares fitting software. The comparison with theoretical calculations finally allows to interpret these parameters in terms of physical properties of the observed system.

Key words: Molecular physics, Spectroscopy, Atmospheric VOC, Microsolvation