

Master 2: Research Training 2023-2024

Laboratory: PhLAM

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

Characterizing Gas Phase Atmospheric Organic Compounds: a Rotational Spectroscopic Approach

Volatile organic compounds (VOCs) are emitted into the atmosphere from both natural and human-made sources. Among these VOCs, sesquiterpenes ($C_{15}H_{24}$) are predominantly released by plants and vegetation, exceeding the emission of monoterpenes in northern wetlands. These highly reactive compounds play a crucial role in atmospheric chemistry, reacting with other abundant atmospheric species such as O_3 , OH, and NO_x to form significant quantities of new compounds. Secondary organic aerosols (SOAs) formed from biogenic volatile organic compounds (BVOCs) constitute a significant fraction of atmospheric particulate matter and have been recognized to significantly affect the climate and air quality.

Despite their significance, the mechanisms involved in aerosol formation are not fully understood at the molecular level. Research suggests that hydrogen bond interactions can enhance the nucleation process, leading to the creation of new particles. Obtaining in-depth information about the molecular systems formed in the gas phase is essential for a better understanding of their physico-chemical properties and behavior.

This project employs a powerful approach that combines microwave spectroscopy with quantum chemical calculations to investigate molecular structure and microsolvation in the gas phase. By analyzing their pure rotational spectra, the primary objective is to characterize the conformational landscape of the species through the recording and analysis of their rotational spectrum with the help of quantum chemical calculations.

To achieve these objectives, a selected sesquiterpene will be studied in isolation and in presence of water conditions using a Fourier transform microwave spectrometer coupled to a supersonic jet expansion. The recorded spectra will then be analyzed with available least squares fitting software. Finally, by comparing experimental data with provided theoretical calculations, we can interpret these parameters in terms of the physical properties of the observed system.

These data will shed light on the non-covalent intermolecular interactions involved in stabilizing the complexes with water and help understand, at the molecular scale, the initial steps in the process of aerosol formation.

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