Contribution ID: **85** Type: **Contributed talk**

Rotational and Vibrational Spectroscopic Characterisation of Hinokitiol and Its Water Complexes

Monday 15 September 2025 12:20 (20 minutes)

Hinokitiol, is a naturally occurring tropolone derivative and exhibits a range of biologically relevant activities making it a molecule of considerable interest in medicinal chemistry. Its seven-membered aromatic ring contains a hydroxy ketone moiety that contributes to its potential to form non-covalent interactions, particularly hydrogen bonds, which are key to understanding its mechanism of action in biological environments.
The bare hinokitiol was investigated using Free-Jet Absorption Millimetre-Wave (FJ-AMMW) spectroscopy. This high-resolution rotational spectroscopic technique was carried out in the 59.6–78.3 GHz frequency range under supersonic jet-cooled conditions. The recorded spectra revealed the presence of two distinct conformers of hinokitiol. These conformers arise from the rotation of the isopropyl group attached to the aromatic tropolone ring. To explore the microsolvation of hinokitiol and its ability to interact with water molecules, we employed laser-based spectroscopy in combination with time-of-flight mass spectrometry (TOF-MS). The formation of 1:1 and 1:2 hinokitiol–water complexes was investigated using Resonance Enhanced Multiphoton Ionisation (REMPI) and Ion Dip Infrared (IDIR) spectroscopic techniques. All the experimental data was contrasted with DFT calculations, which enabled conformer identification, provided insight into non-covalent interactions, and supported the assignments of the monomer and hydrated complexes.

Keywords

FJAMMW, Laser spectroscopy, Strong hydrogen bonding, Gas phase.

This abstract is submitted for....

Early-career researchers´ workshop

Primary authors: PINILLOS, Paul (University of Bologna); SONG, Wentao (University of Bologna)

Co-authors: CAMIRUAGA LEZA, Ander (Department of Physical Chemistry, University of the Basque Country); MARIS, Assimo (University of Bologna); USABIAGA, Imanol (Department of Physical Chemistry, University of the Basque Country); FERNANDEZ, Jose A. (University of the Basque Country); EVANGELISTI, Luca (University of Bologna); PARRA SANTAMARIA, Maider (University of the Basque Country (UPV/EHU)); MELANDRI, Sonia (University of Bologna)

Presenter: PINILLOS, Paul (University of Bologna)