Contribution ID: **13** Type: **Contributed talk**

Hydrogen bonding enables detection of Elusive conformers: interplay between supersonic jet relaxation and complex formation in 4-(4-methoxyphenyl)aniline

Tuesday 16 September 2025 15:20 (20 minutes)

Understanding conformational relaxation pathways is essential for characterizing flexible molecular systems with multiple low-lying rotamers in supersonic jets. To investigate in depth the relaxation pathways, the conformational dynamics of 4-(4-methoxyphenyl)aniline (4-MPA), a newly synthesized molecule, were studied in a supersonic expansion using high-resolution rotational spectroscopy in the 2-8 GHz range. Only the most stable of two potentially populated conformers of 4-MPA was detected in the spectrum, with the absence of the higher-energy form attributed to collisional conformational relaxation in the supersonic jet. Using quantum-chemical calculations, four plausible pathways for the conversion of the higher-energy conformer to the global minimum were identified. Among them, only one involves a feasible motion with a low barrier consistent with relaxation, while the other pathways present rather high energy barriers. Upon complexation with water, the formation of a hydrogen-bonded complex alters the potential energy surface, hindering the relaxation. The complexation through hydrogen bonding traps the higher-energy conformer in the first stages of the supersonic expansion, before the relaxation processes occur, enabling its detection. The interplay between relaxation and complexation highlights the role of microsolvation in modulating intramolecular dynamics and opens a possible route to detect otherwise non-detectable conformers

Keywords

Hydrogen bonding, conformational relaxation, molecular complexes, gas-phase interactions

This abstract is submitted for....

HBond 2025 conference

Primary author: PINACHO MORANTE, PABLO (University of Valladolid)

Co-authors: VERDE, Andres (University of Valladolid); BLANCO, Susana (Universidad de Valladolid); ESTEBAN, Victor (University of Valladolid); Prof. COCO, Silverio (University of Valladolid); Prof. LÓPEZ, Juan Carlos (Universidad de Valladolid)

Presenter: PINACHO MORANTE, PABLO (University of Valladolid)