

Probing Non-Covalent Interactions in Anisaldehyde Homodimers

Monday 15 September 2025 10:30 (20 minutes)

Non-covalent interactions (NCIs), including hydrogen bonds, π -stacking and tetrel bonds, often act in concert to stabilize molecular aggregates, playing a key role in both supramolecular chemistry and molecular recognition processes. In this work, we investigate the homodimers of *ortho*- and *para*-anisaldehyde, generated in a supersonic expansion and detected using high-resolution rotational spectroscopy. The observed configurations are stabilized by a complex network of NCIs, such as hydrogen bonds, π -stacking and tetrel bonds. Theoretical calculations support the experimental observations and provide deeper insight into the nature and relative contributions of these interactions. A comparative analysis of the homodimers and monohydrated anisaldehyde complexes highlights the distinct roles and nature of the NCIs in each system. These findings contribute to a deeper understanding of how hydrogen bonds cooperate with other non-covalent forces in shaping the structure of weakly bound molecular clusters.

Keywords

Hydrogen Bond, Gas Phase, Molecular Complexes, Rotational Spectroscopy

This abstract is submitted for....

Early-career researchers' workshop

Primary authors: VERDE, Andres (University of Valladolid); Prof. LÓPEZ, Juan Carlos (Universidad de Valladolid); Prof. BLANCO, Susana (University of Valladolid)

Presenter: VERDE, Andres (University of Valladolid)