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Invisible Forces, Precise Spectra: A Journey Through Noncovalent Interactions via Gas-Phase Rotational Spectroscopy

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Hydrogen bonding is one of the most fundamental and widespread noncovalent interactions in chemistry and biology, governing the structure, dynamics, and function of countless molecular systems. Despite its apparent simplicity, hydrogen bonding displays remarkable diversity in geometry, strength, and electronic character, especially when studied in isolation from environmental effects.

Rotational spectroscopy in the gas phase provides an exceptionally precise and unambiguous way to characterize hydrogen bonds. By isolating molecular complexes in supersonic expansions, it becomes possible to access their intrinsic structural and energetic features, free from solvation or packing forces. The analysis of rotational constants, nuclear quadrupole interactions, and dipole moment components offers detailed insight into bond directionality, donor–acceptor distances, and subtle electronic rearrangements induced by hydrogen bonding.

In this contribution, several gas-phase studies of hydrogen-bonded complexes involving small organic molecules and relevant ligands such as water are presented. The role of secondary interactions and cooperative effects will also be discussed, particularly in systems where multiple H-bonds coexist or compete with other weak forces. Special attention is given to fluorinated aromatic acceptors, where hydrogen bonding competes with lone pair···π-hole interactions, offering a rich scenario for structural analysis.

These experimental results, supported by high-level quantum-chemical calculations, provide benchmark data for understanding hydrogen bond geometries and for validating theoretical models. This journey through "invisible forces"demonstrates the powerful synergy between microwave spectroscopy and theoretical chemistry in elucidating fundamental aspects of molecular aggregation.

Keywords

Rotational spectroscopy, Noncovalent interactions, Hydrogen bonding, Quantum chemical calculations, Molecular complexes, Supersonic Expansion

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