Contribution ID: **72** Type: **Invited talk**

Short hydrogen bonds in the solid state: new insights from computational, infrared, inelastic neutron scattering and nuclear quadruple resonance perspective

Friday 19 September 2025 09:15 (45 minutes)

The extremely short hydrogen bonding featuring donor···acceptor separation of ~2.4 Å is still relatively poorly understood and poses a challenge for advanced experimental and theoretical treatments. Among major issues is the highly delocalized H-bonded proton, with complex dynamics driven by strong nuclear quantum effects. These systems, when paired with experimental data, provide a valuable benchmark for computational methods. Herein, we present different examples of systems containing very short H-bonds, including the picolinic acid N-oxide family, quinolinic acid, lithium hydrogenphthalate dihydrate and nitranilic acid hexahydrate. All of these systems are present in the crystalline solid state with extensive structural data available (X-ray and neutron diffraction), allowing for the construction of reliable structural models subject to periodic DFT calculations. For each of the presented systems we characterized the H-bonding by slightly different combination of experimental and computational methodologies. The latter not only proved to be of a great value for the interpretation of experimental observables (e. g., assignment of vibrational spectra), but can also provide substantial improvements in structural characterization of H-bonding, in particular determining the precise location of the proton. Among the employed experimental techniques, nuclear quadrupole resonance proved to represent a very sensitive and reliable probe for H-bond geometry. On the other side, inelastic neutron scattering vibrational spectroscopy can circumvent many drawbacks of optical spectroscopy due to simplicity of interactions between neutrons and atomic nuclei. In conjunction with advanced computational routines, both techniques provide accurate and reliable tools for detailed characterization of short H-bonds, striking a good balance between precision and computational efficiency.

Keywords

This abstract is submitted for....

HBond 2025 conference

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