Contribution ID: **18** Type: **Contributed talk**

Kicking off the second HyDRA blind challenge on microhydration: Challenge details and first test set announcement

Tuesday 16 September 2025 12:10 (20 minutes)

The field of gas phase spectroscopy benefits from a robust interplay between quantum chemistry and experimental techniques. To facilitate the advancement of systematically enhanced quantum chemical predictions in vibrational spectroscopy and solvation science, we have helped to organize the first HyDRA (Hydrate Donor Red Shift Anticipation) blind challenge during the 2021/22 academic year.[1]

Within this challenge, ten cold 1:1 complexes of organic molecules with water were prepared in a vacuum and examined by infrared and Raman spectroscopy for the first time. The fundamental OH stretching vibration of the hydrogen-bonded water molecule in these complexes was measured and kept secret until ten interested theoretical research groups worldwide had made their predictions in spring 2022. The detection of a robust anharmonic resonance in some of these water complexes rendered this competition not only interesting for scaled harmonic predictions, but also for more elaborate anharmonic treatments. Now, in the sequel challenge, theoreticians are provided with a seven-fold larger training set compared to the last challenge. However, the theoretical models are now further challenged by the request to predict stronger hydrogen bonds and dihydrates.

This contribution summarizes the results of the first HyDRA challenge [2] and launches the second round of the HyDRA blind challenge by announcing for the first time the molecular test set systems which define HyDRA II.

References:

[1] Taija L. Fischer, Margarethe Bödecker, Anne Zehnacker-Rentien, Ricardo A. Mata, Martin A. Suhm, Phys. Chem. Chem. Phys., **2022**, *24*, 11442.
[2] Taija L. Fischer *et al*, Phys. Chem. Chem. Phys., **2023**, *25*, 22089-22102.

Keywords

Hydrogen bond: weak, medium and strong; cold gas phase (supersonic jet)

This abstract is submitted for....

HBond 2025 conference

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