

## THE HyDRA BLIND CHALLENGE: INVITING THEORY TO PREDICT UNKNOWN VIBRATIONAL SPECTROSCOPY DATA

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There is a myriad of quantum-chemical methods which can be used to predict the OH stretching spectrum of cold, vacuum-isolated hydrate clusters, with a perspective to deepen our understanding of aqueous solution dynamics. They range from uniformly scaled harmonic DFT predictions to fully anharmonic high level wave function theory treatments.

Fortuitous error compensation is a major issue in such a situation, in particular if the experimental result is known beforehand. The HyDRA (Hydrate Donor Redshift Anticipation) blind challenge is an effort to circumvent previous knowledge, by inviting theory groups to make predictions for 10 not yet vibrationally characterized organic monohydrates and performing the corresponding experiments in parallel.

This contribution will present the procedure<sup>a</sup> and discuss results of the recently finished blind challenge HyDRA by comparing the theoretical predictions to our experimental results.

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