Scientists reveal dynamic coupling of strong hydrogen bond

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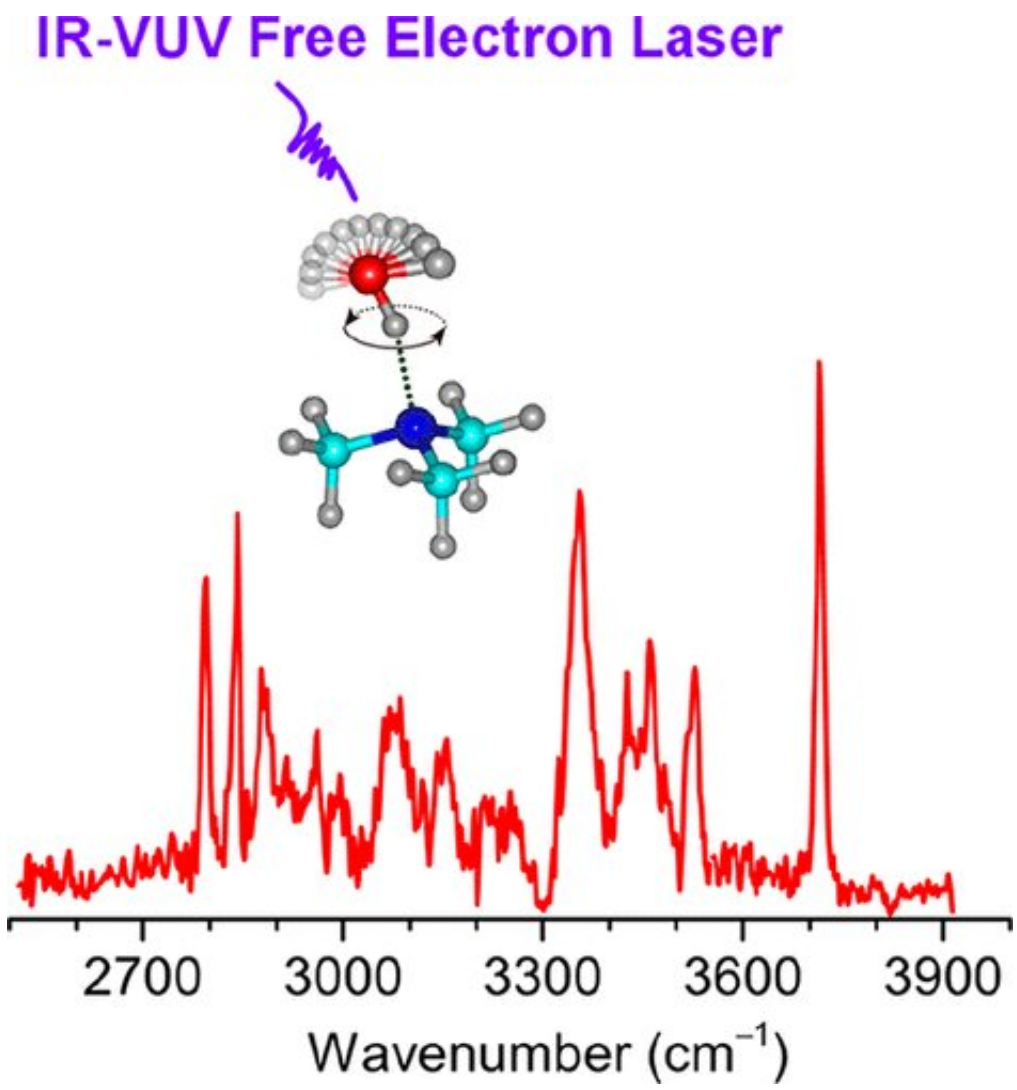

Abstract https://doi.org/10.1021/acs.jpclett.1c00168

Hydrogen bonds (HBs), the main intermolecular interactions, are inherently fluctuant in nature.

Elucidating the dynamic couplings of hydrogen bonds remains challenging for spectroscopic studies of bulk systems, because their vibrational signatures are masked by the collective effects of the fluctuation of many hydrogen bonds.

Recently, a research team led by Prof. Jiang Ling from the Dalian Institute of Chemical Physics (DICP) of the Chinese Academy of Sciences and their collaborators identified vibrational signature of dynamic coupling of a strong hydrogen bond. The study was published in the *Journal of Physical Chemistry Letters* on Feb. 26.

The study revealed that dynamic couplings were originated from strong Fermi resonance between the stretches of hydrogen-bonded OH and several motions of the solvent water/methanol, such as translation, rocking, and bending. It also highlighted a general model to elucidate the dynamic coupling of hydrogen bond in atmospheric and biological systems.

Based on the infrared spectroscopy using a tunable vacuum ultraviolet free electron laser (VUV-FEL), the research team unmasked the vibrational signatures for the dynamic couplings in neutral trimethylamine-water and trimethylamine-methanol complexes, as microscopic models with only one single hydrogen bond holding two molecules.

The broad progression of OH stretching peaks with distinct intensity modulation over ~700 cm^{-1} was observed for trimethylamine-water, while the dramatic reduction of this progression in the trimethylamine-methanol spectrum offered direct experimental evidence for the dynamic couplings.

Quantum mechanical calculations revealed that such dynamic couplings were originated from strong Fermi resonance between the stretches of hydrogen-bonded OH and several motions of the solvent water/methanol, such as translation, rocking, and bending.

More information: Shukang Jiang et al. Vibrational Signature of Dynamic Coupling of a Strong Hydrogen Bond, the *Journal of Physical Chemistry Letters* (2021). DOI: 10.1021/acs.jpclett.1c00168