EXPLORING CONFORMATION SELECTIVE FAR INFRARED ACTION SPECTROSCOPY OF ISOLATED MOLECULES AND SOLVATED CLUSTERS

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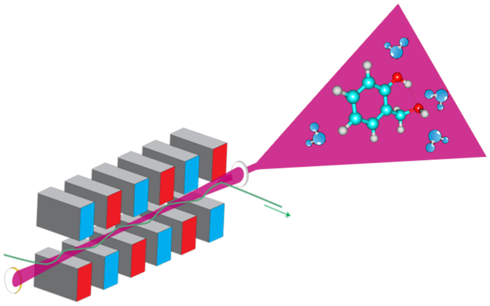
Far-Infrared (IR) spectroscopy has been labeled as a promising method for identifying structural motifs in large molecules. However, several hurdles have kept this promising spectral region from breaking through to widespread use for gas phase experiments. Normal modes in the far-IR mostly have weak intensities, and high brightness sources of far-IR radiation are rare. Moreover, standard density functional theory - applied to identify the specific molecular structure responsible for the measured IR spectra - does not reproduce features in the far-IR well. This mismatch can be attributed to the high degree of anharmonicity of many of the normal modes present in the far-IR. We have overcome these hurdles by combining an advanced laser source with novel experiments and high-level dynamical calculations.



We present far-IR spectra of a family of phenolic molecules and solvated clusters, obtained using the free electron laser FELIX. By employing IR-UV ion-dip spectroscopy in the gas phase, we are able to obtain conformer specific far-IR spectra of isolated molecules or solvated clusters. The studied systems display both intra- and intermolecular hydrogen bonding, enabling us to study the merits of far-IR action spectroscopy for direct probing of these weak interactions. Moreover, the combination of far-IR experiments with quantum chemical calculations allows us to test the limits of the harmonic approximation in DFT calculations, and to test the possibilities of employing a more sophisticated technique, namely Born-Oppenheimer molecular dynamics.