

TOWARDS UNDERSTANDING FAR-IR INDUCED ISOMERISATION PROCESSES

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Conformational interconversion is a key aspect of such processes as protein folding, enzyme action via the induced fit mechanism, or the action of molecular motors. Although studies of the dynamics of interconversion exist, they are mostly limited to pump-probe spectroscopy involving electronic excitations, whereas the simplest of these interconversions take place on the ground state potential energy surface. *Ortho*- and *meta*-substituted phenols are simple model systems exhibiting *syn-anti* isomerism, with the two isomers differing by the orientation of the hydroxyl group either towards or away from the heteroatom substituent. The isomerisation reactions between *syn*- and *anti*- conformers are characterized by relatively low energy barriers and could potentially be driven using resonant IR vibrational excitation provided by a free electron laser, opening the potential to study interconversion dynamics on the ground state PES.

As a first step we have obtained isomer-specific IR spectra of 3-fluorophenol and 3-chlorophenol by means of IR-UV depletion spectroscopy. Each of these exhibit torsional –OH vibrational bands in the 250-350 cm^{-1} region, with isomer-specific frequencies observed for 3-fluorophenol (as shown in the figure). We subsequently probe the UV spectral response of these molecules following IR excitation of selected bands, employing an IR-UV double resonance scheme. We will present the results of these experiments aimed at understanding vibrational energy coupling in small aromatic systems, as well as discuss the potential for observing direct population transfer between *syn*- and *anti*-isomers.

