

## Structural Dynamics in Solution probed by Time-resolved X-ray Diffraction

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The way in which a chemical reaction occurs in solution influences and is influenced by the structural rearrangements of the solvent. We are attempting to observe such local structural changes and better understand the interplay between the solute and the solvent using time-resolved x-ray scattering techniques at Beamline 5.3.1.

The ring-opening reaction of 1,3-cyclohexadiene in cyclohexane serves as model for a wide-variety of photochemical reactions. Upon excitation with ultraviolet light, it rapidly undergoes the transformations shown in Figure 1.



Figure 1. Ring-opening reaction of 1,3-cyclohexadiene.

This reaction has been studied indirectly by a wide variety of femtosecond optical techniques as well as by time-resolved electron diffraction in the gas phase. We probe this system at 5.3.1. by taking white beam from a bending magnet and quasi-monochromatizing it to a bandwidth of 3% at 9.6 keV using a W-B4C multilayer. The x-ray beam passes through a 300  $\mu\text{m}$  jet of 0.5 M cyclohexadiene in cyclohexane and the diffracted intensity is measured by scanning an avalanche photodiode across the diffraction ring. Figure 2. shows the static structure factor  $S(Q)$  and the time-resolved difference signal at  $t=200$  ps after excitation by 266 nm femtosecond light.

Structural changes are observed in both the low  $Q$  and the high  $Q$  scattering regions and work is currently underway to separate out the contributions from the solvent and from the solute.

Experiments using the same setup are also underway studying dynamics in water and in particular the structural rearrangements that occur following photoionization and injection of an electron into the liquid state.

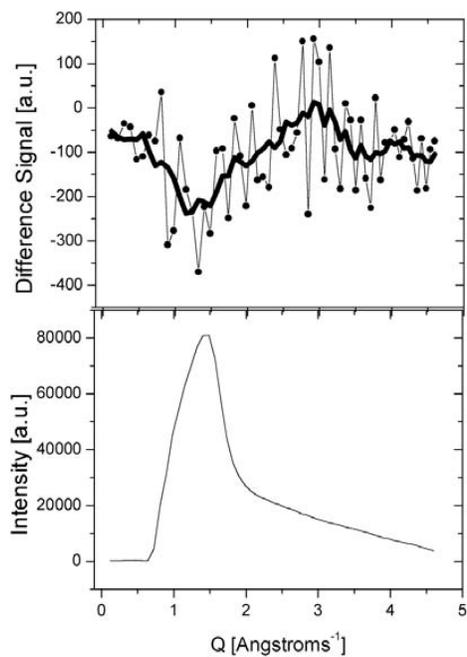


Figure 2. Bottom: 1,3-cyclohexadiene in cyclohexane diffraction curve. Top: Difference signal at 200 ps following femtosecond excitation at 266 nm.

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