

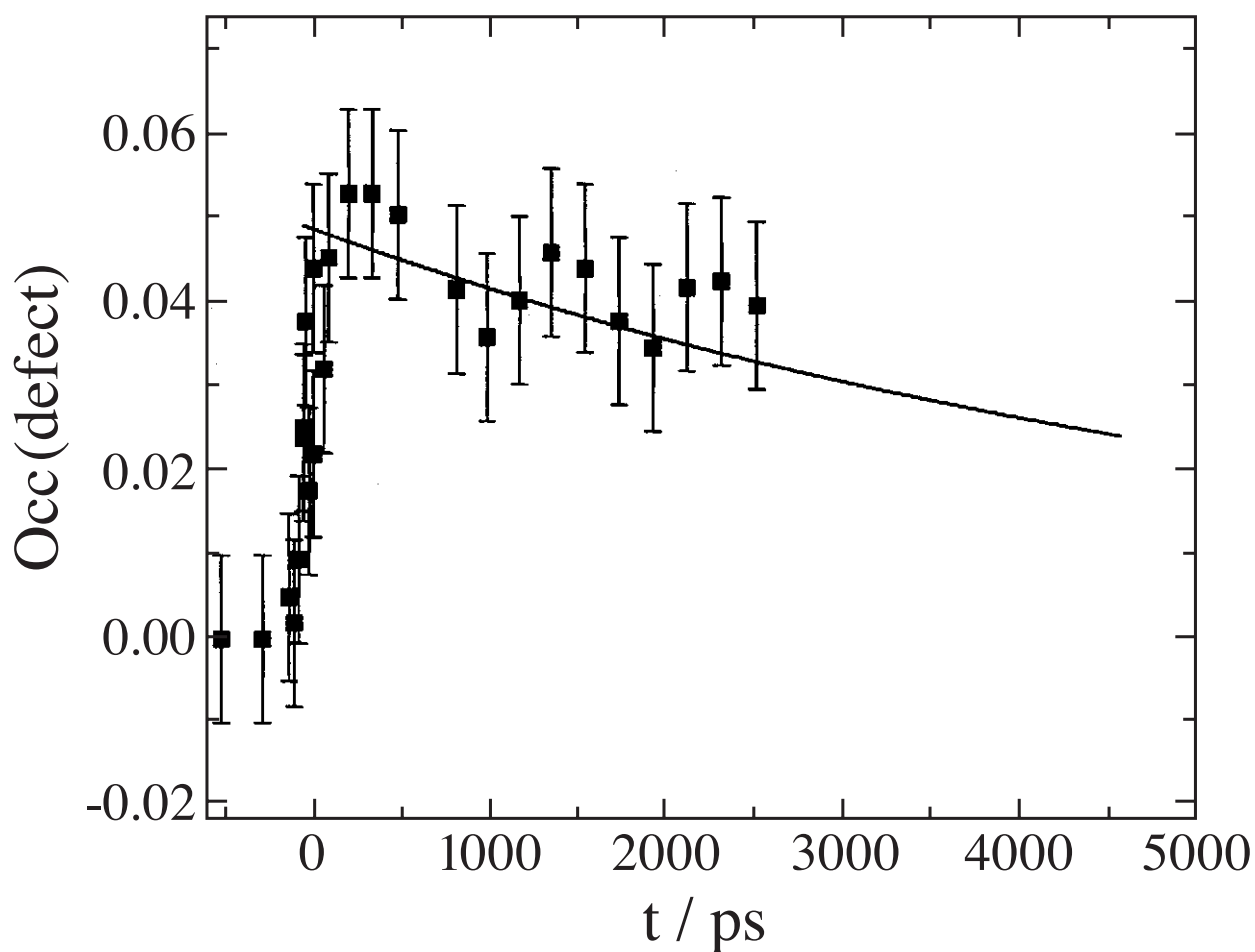


	<b>Experiment title:</b> Picosecond time-resolved x-ray scattering probed conical intersection: The TICT (twisted intramolecular charge transfer)...	<b>Experiment number:</b> CH 1114
<b>Beamline:</b>	<b>Date of experiment:</b> from: 31/10/01 to: 05/11/01	<b>Date of report:</b> 31/08/04
<b>Shifts:</b> 15	<b>Local contact(s):</b> A. Plech	<i>Received at ESRF:</i>
<b>Names and affiliations of applicants (* indicates experimentalists):</b> * Simone Techert, MPibpc – Structural dynamics of (Bio)chemical Systems, 37077 Goettingen, Germany * Linda Woo, MPibpc – Structural dynamics of (Bio)chemical Systems, 37077 Goettingen, Germany		

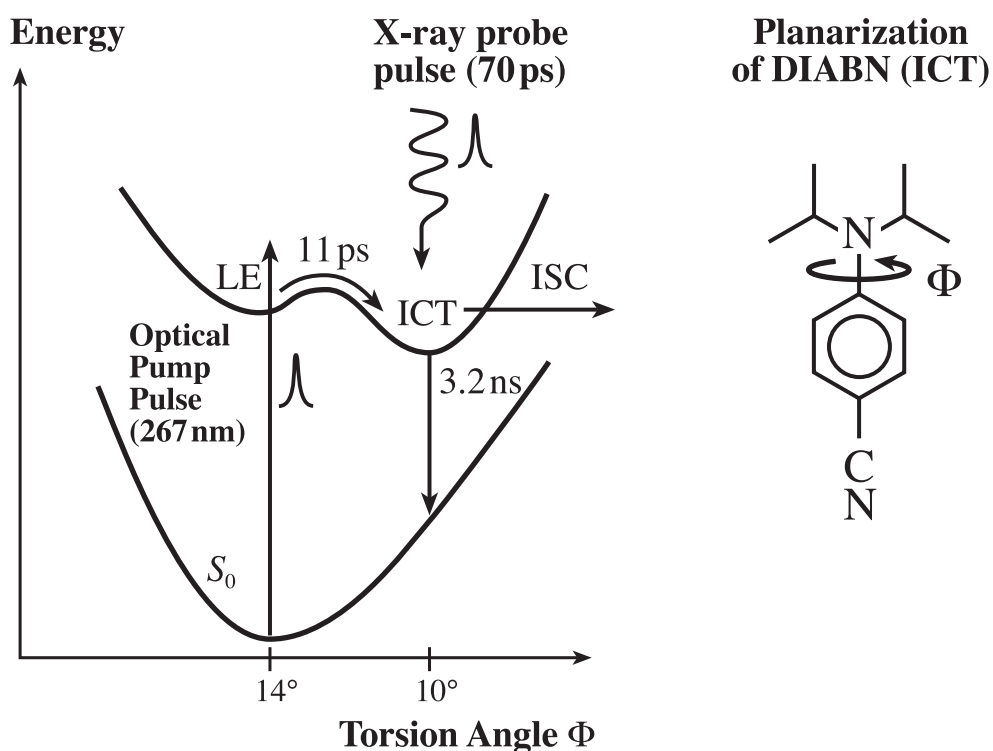
### Report:

In the experiment No **CH-1114** we investigated the photo-induced structural reorganisation of *N,N*-diisopropylaminobenzonitrile in powders by time-resolved powder diffraction. We investigated *N,N*-diisopropylaminobenzonitrile in the powder – and not in the liquid phase - since spectroscopic investigations indicated a large amplitude motion to a twisted intramolecular charge transfer in the crystalline phase. In contrast to the scattering experiments in the liquid phase, monochromatic powder diffraction provide a more accurate method to determine intramolecular distances and angles which we wanted to determine as most accurate as possible. In **CH-1114** we could follow the structural rearrangement after electron transfer on the picosecond time scale. Figure 1 illustrates a typical result of this study, where we could refine the occupancy and the structure of the transient intermediate which has a lifetime of about 3 - 4 ns. The photophysical pathway of *N,N*-diisopropylaminobenzonitrile with the refined structural changes is summarised in Figure 2. More results from experiment No **CH-1114** can be found in the following publications:

- S. Techert und K. A. Zachariasse, *Planar Structure of the Intramolecular Charge Transfer State in Crystalline 4-(Diisopropylamino)benzonitrile from Picosecond X-ray Diffraction*, *J. Am. Chem. Soc.* **126**, 5593 (2004).
- S. Techert, *First, Second und Third Order Correlation Function in Time-resolved X-ray Diffraction*, *J. Appl. Cryst.* **37**, 445 (2004).
- J. Davaasambuu, P. Durand und S. Techert, *Experimental Conditions for Light-induced Reactions in Powders Investigated by Time-resolved X-ray Diffraction*, *J. Appl. Cryst.*, in press (2004).



**Figure 1:** Time evolution of the occupancy of the intramolecular charge transfer state of *N,N*-diisopropylaminobenzonitrile.



**Figure 2:** The photophysical pathway of *N,N*-diisopropylaminobenzonitrile with the refined structural changes.