



	Experiment title: Photo-induced isomerisation of organic chromophors	Experiment number: CH1910
Beamline: ID09B	Date of experiment: from: 07 May 2005 to: 12 May 2005	Date of report: 15/08/2006
Shifts: 12	Local contact(s): Dr. Q. Kong	<i>Received at ESRF:</i>
Names and affiliations of applicants (* indicates experimentalists): PD Dr. Simone Techert *, Max Planck Institute for Biophysical Chemistry, 37077 Göttingen Dr. M Goulakov *, Max Planck Institute for Biophysical Chemistry, 37077 Göttingen A. Debnarova *, Max Planck Institute for Biophysical Chemistry, 37077 Göttingen M. Cammarata *, ESRF		

Report:

In **CH1910** we wanted to finish the experiment started in Exp-No **CH-707** and **SC-811**, namely the investigation of a photo-induced large amplitude motion in the liquid phase, here the trans / cis isomerisation of stilbene in methanol [1-3]. As method we used picosecond time-resolved wide angle x-ray scattering with high resolution in space (scattering to high q values).

Figure 1 presents the x-ray scattering difference map for a negative and a positive time-point near the overlap of laser pump and x-ray probe pulse in time. This time the quality of the TR-WAXS data were sufficient enough to probe the photoisomerisation process in methanol. For the simulation in the difference map, the difference map of pure methanol as a function of time convoluted with the signal changes due to the isomerisation processes are presented. Data analysis of all the experimental data leads to the plot of figure 1 / right. It essentially emphasizes that the isomerisation process is ultrafast (simulation curve) and that the signal changes essentially monitor the natural halfwidth of the x-ray probe pulse (black experimental curve).

The summarised results are important parameters in order to find out which kind if WAXS experiments might be possible to be monitored with future ultrafast x-ray sources, like the XFEL [1,2]. The comparison of experimental and theoretical scattering curve based on a pure quantumchemical treatment of the system emphasizes the need of high-resolution WAXS experiments [3]. Most of the differences between classical Debye and full-quantummechanical description do come from the aromaticity of the system which is not reflected in the structure factor of carbon which is used for the description in the Debye equation. At very short time scales (about the first 100 fs) other interference effects based on wavepacket dynamics are predicted [2] and it would be of great interest to measure them on some stage in future experimentally.

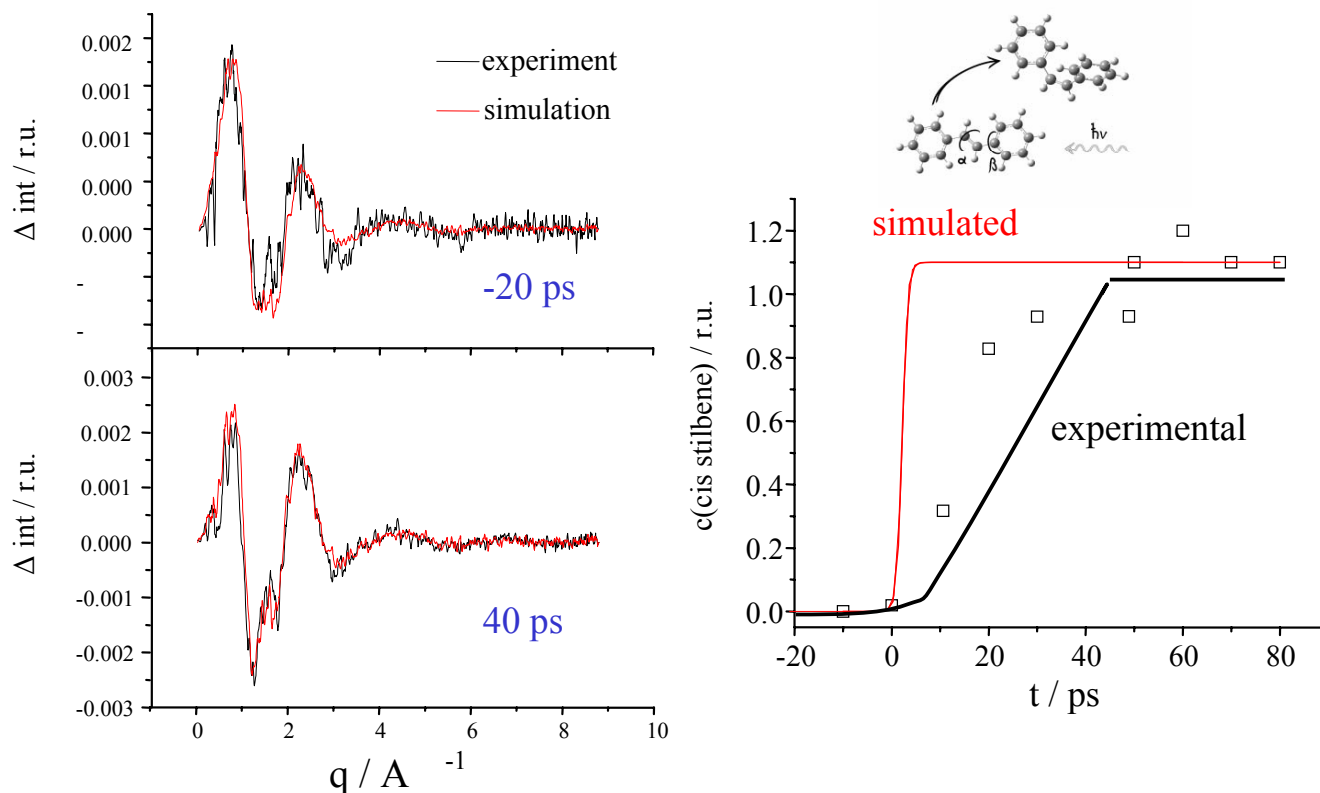


Figure 1: Left: X-ray scattering difference map for a negative (top) and a positive (bottom) time-point near the overlap of laser pump and x-ray probe pulse in time. Right: Data evaluation of the TR-WAXS experiments yield that the isomerisation process is ultrafast, monitoring the halfwidth of the x-ray probe pulse [3].

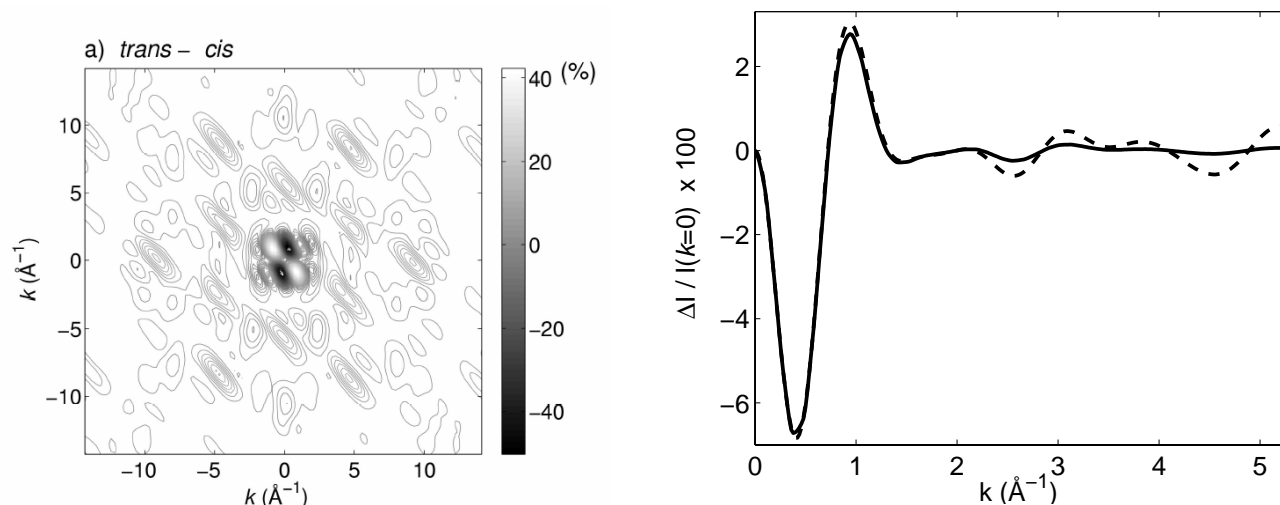


Figure 2: Left: Difference map of x-ray scattering signal as derived from a full quantummechanical description in internal coordinates 180° (trans) – 10° (cis). 1D cut through the 2D counter map (dotted line) in comparison to classical Debye description (dashed line). The predicted maximal changes are about 10 % [2], as been confirmed by the experiment [3].

References

- [1] S. Techert, S. Schmatz, *Z. Phys. Chem.* **216**, 575-583 (2002).
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- [3] A. Debnarova, M. Camaratta, M. Wulff, S. Schmatz, S. Techert, *J. Chem. Phys.*, *to be submitted* (2006).