	Experiment title: **Studies of the photo-chemistry of iodine in a variety of solvents on the sub-ns time-scale**	**Experiment number**: CH1549
Beamline: ID09B	**Date of experiment**: from: 9th May 2004 to: 15th May 2004	**Date of report**: 30/08/2005
Shifts: 12	**Local contact(s)**: Dr. Qingyu KONG (e-mail: qingyu.kong@esrf.fr)	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Panayiotis Georgiou[1*], Jonathan Vincent[1], Jens Poulsen[2], Annmarie Wöhri[2*], Magnus Andersson[2*], Pontus Gourdon[2*], Richard Neutze[2*], and Jan Davdisson[1*]

[2]Department of Physical Chemistry, Uppsala University.

[1]Department of Chemistry & Bioscience, Chalmers University of Technology.

Report:

This experiment, as proposed, aimed to study iodine in solution in a number of solvents. In addition we wished to clarify experimentally the efect of multi-photon excitation of the solvent directly. This second objective followed from an earlier experiment where we had attempted to pump CH_2I_2 disolved in CH_2Cl_2 using the third harmonic of the Ti-saphire laser system at ID09, but had recovered a signal in the control experiment (*ie.* the same time-dependent diffraction signal was seen with & without the presence of the solute).

The procedure was therefore to first study pure CH_2Cl_2 pumped with 273 nm radiation. This experiment went fairly smoothly, and we recorded data from 10 time-points, from 100 ps to 5 μs. We had also previously put quite a lot of theoretical input into the issue of modelling how liquids expand using molecular dynamics simulations. In gereral this experiment proved to be quite successful, the experimental data has been accurately modelled, and a manuscript is now at an advanced form. This work should be submitted by the end of October 2005. The major aspects remaining are that these results must be interpreted in light of a number of recent publications in the area[1-5]. We also had to give priority to the completion of a manuscript describing an earlier experiment, CH_2I_2 in methanol, which was published in Physical Review Letters this June[4]. As such we were not only the first group to present the technique through studies of a simple model system (I_2)[1], but were also the first to extend the method to the study of more complex systems[4].

Our studies on the properties of I_2 in a number of solvents, including CH_2Cl_2 and methanol, were less successful. For reasons which are not clear at this point in time, especially given the earlier successes[1,2], we did not successfully recover a signal from this photochemical in solution. There are many possible aspects such as the misalignment of the laser & x-ray beams, less than optimal choice of pump wavelength, issues of timing *etc*.... and the combination of the successful studies on pure CH_2Cl_2 plus a number of (albeit minor but accumulating) technical issues meant that we did not have the time to optimise these experiments on I_2 during the scheduled experiment. Nevertheless, in general the experimental station worked well, and there are major improvements in the on-line analysis of the experimental data which have come about as the technique matures.

References:

1. Neutze, R. et al. Visualizing photochemical dynamics in solution through picosecond x-ray scattering. *Phys Rev Lett* 87, 195508 (2001).
2. Plech, A. et al. Visualizing chemical reactions in solution by picosecond x-ray diffraction. *Phys Rev Lett* 92, 125505 (2004).
3. Lindenberg, A. M. et al. Time-resolved measurements of the structure of water at constant density. *J Chem Phys* 122, 204507 (2005).
4. Davidsson, J. et al. Structural determination of a transient isomer of CH2I2 by picosecond X-ray diffraction. *Phys Rev Lett* 94, 245503 (2005).
5. Ihee, H. et al. Ultrafast x-ray diffraction of transient molecular structures in solution. *Science* 309, 1223-7 (2005).