ESRF	**Experiment title:** The Structure Elucidation of the Membrane Intrinsic Protein Complex Photosystem I by X-Ray Crystallographic Methods	**Experiment number:** LS-932
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Names and affiliations of applicants (* indicates experimentalists):

Patrick Jordan*, Norbert Krauß*, Olaf Klukas and Wolfram Saenger
Institut für Kristallographie, Freie Universitat Berlin, Takustr.6, D-14195 Berlin (Germany)

Petra Fromme*, Athina Zouni* and Horst Tobias Witt
Max-Volmer-Institut fur Biophysikalische Chemie und Biochemie, Technische Universitat Berlin, Straße des 17. Juni 135, D-10623 Berlin (Germany)

Report:

The success in finding suitable conditions for collecting X-ray diffraction data of photosystem I (PS I) crystals has opened the chance to obtain a structural model of this central complex of oxygenic photosynthesis at ≈ 3 Å resolution in a near future. This would mean that a major progress in the structure analysis of PS I could be achieved, as our present model at 4 Å resolution, which consists of α-helices including some interhelical links, the iron sulfur clusters, most of the chlorophyll *a* cofactors and one phylloquinone position (Schubert et al., 1997) could be replaced by a much more detailed model, containing the more or less complete polypeptides including side chains of the 11 protein subunits and more accurate positions and orientations of the large number of cofactors involved in electron transfer and excitation energy transfer.

After having collected native data of about 3 Å resolution during our last experiment at beam line ID02B at ESRF, our intention for this experiment was to collect data of heavy atom derivatives under cryogenic conditions. The derivatives were prepared using a platinum and a mercury compound which had already successfully been used in the preparation of heavy atom derivatives for data collection at 277 K. We succeeded in collecting complete data sets at $\lambda \approx 1$ Å of both derivatives. The mercury derivative data set is 93.4 % complete in the resolution shell from 3.0 to 2.9 Å with $R_{sym} = 0.27$ and 61 % of the reflections having $I > 3\sigma(I)$, for the platinum derivative a data set being 84 % complete between 3.27 and 3.11 Å resolution with $R_{sym} = 0.21$ and 56 % of the reflections having $I > 3\sigma(I)$ has been obtained. A native datat set was collected using the maximum wavelength ($\lambda \approx 1.4$ Å) available at this beam line in order to use the anomalous scattering signal of the iron atoms bound to PS I. So far it has not been processed completely, but the partial data are already 76 % complete in the resolution shell from 3.0 to 2.9 Å, $R_{sym} = 0.21$ and for 59 % of the reflections is $I > 3\sigma(I)$ in this shell. Anomalous Patterson syntheses calculated using these three data sets clearly showed maxima from which the major sites of the anomalous scatterers could be identified. The data sets proved to be isomorphous to each other. Consequently, isomorphous difference Patterson syntheses calculated for both derivatives confirmed the maxima found in the anomalous Patterson maps. Together, these data should provide a basis to calculate MIRAS phases up to 3.5 Å resolution or better.

As a surprising result, the crystals used for these experiments turned out to be hexagonal (space group $P6_3$, same as at 277 K) in contrast to our previous observation that PS I crystals undergo a change in symmetry upon freezing to 100 K. So far we can only suppose that the different behaviour of the crystals is caused by a modification of the treatment of the crystals prior to freezing, but an explanation can only be given if the effect of different freezing protocols is investigated systematically.

References

Schubert, W.-D., Klukas, O., Krauß, N., Saenger, W., Fromme, P. & Witt, H.T. (1997) Photosystem I of *Synechococcus elongatus* at 4 Å Resolution: Comprehensive Structure Analysis. *J. Mol. Biol. 272,741-769.*

Schubert, W.-D., Klukas, O., Saenger, W., Witt, H.T., Fromme, P. & Krauß, N. (1998) A Common Ancestor for Oxygenic and Anoxygenic Photosynthetic Systems: A Comparison Based on the Structural Model of Photosystem I. *J. Mol. Biol. 280,* 297-314.