



	Experiment title: Wide-angle X-ray diffraction studies of porphyrins and their derivatives	Experiment number: MD-121
Beamline: ID15B	Date of experiment: from: 18th Juin, 2005 to: 25 Juin, 2005	Date of report: 20 Feb. 2006
Shifts:	Local contact(s): Dr Tom Fennell	<i>Received at ESRF:</i>

Names and affiliations of applicants (* indicates experimentalists):

A. Burian, A. Pasewicz, J. Koloczek

A. Chelkowski Institute of Physics, University of Silesia, ul. Uniwersytecka 4, 40-007 Katowice, Poland

T. Fennell, V. Honkomaki

ESRF, Grenoble, France

Report:

X-ray diffraction intensities of a series of 31 porphyrins and their derivatives were measured on the ID15B beamline using high-energy radiation and an image plate as a 2D detector. An aluminium foil was used to calibrate the instrument. Samples were mounted in Lindemann glass capillaries of about 1 and 2 mm in diameter on the diffractometer axis at distances 320.77 mm and 570.77 mm from the detector. The energy of the experiment was 90.45 keV and the related wavelength was 0.1374 Å. The 2D diffraction patterns were integrated over rings yielding the one dimensional intensity versus the scattering vector functions. Then two intensities, determined for both the sample to the detector distances, were merged into one data set extended to the maximum value of the scattering vector $4\pi\sin\theta/\lambda$ of about 20 Å⁻¹. The intensity of the empty capillary and the incoherent Compton contribution were subtracted from the total sample plus container signal. After normalization the intensity data were converted to a real space representation in the form of a pair correlation function via the Fourier transform. The four examples of both structure factors and pair correlation functions are shown in figures 1 and 2, respectively. The structure factor of the samples a) and b) exhibit both crystalline and amorphous features while the diffraction patterns of the samples c) and d) are typical for amorphous materials. The pair correlation functions of each sample consist of intra-molecular peaks, which extend up to about 8 Å, and slowly varying contribution resulting from inter-molecular spatial correlations

clearly visible in a range of higher values of the scattering vector. As the cores of each molecule look similar the first four peaks of the pair correlation functions have practically the same positions and amplitudes. Further work on detailed analysis of the experimental data is under development.

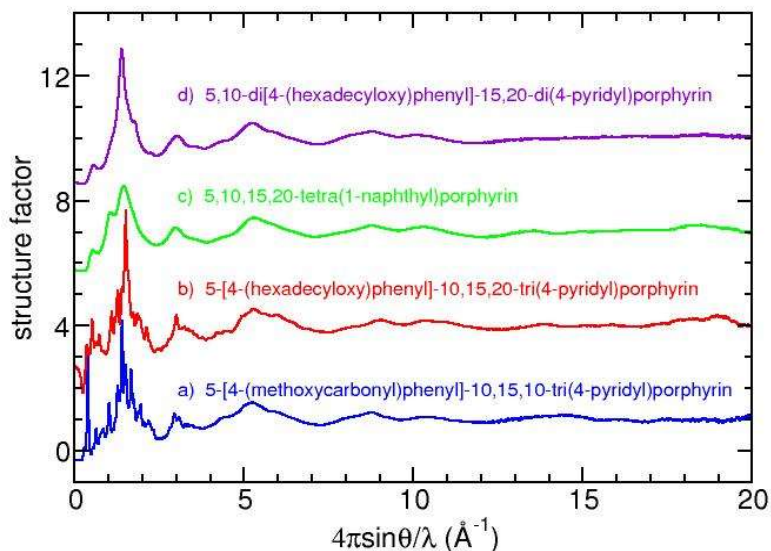


Fig. 1. Structure factors of four porphyrins samples.

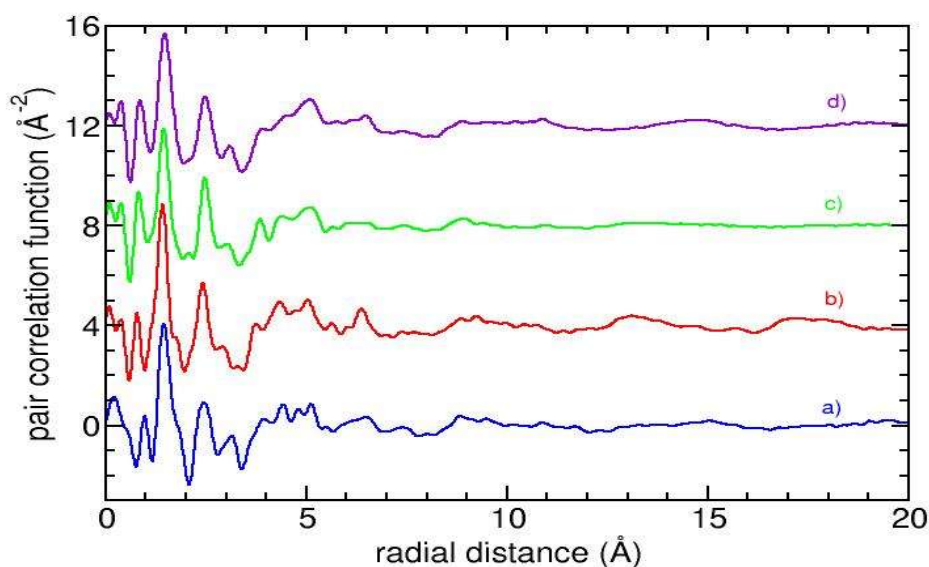


Fig. 2. Pair correlation functions computed from data shown in Fig. 1.

