ESRF	**Experiment title:** High resolution powder diffraction of monomeric units of side-chain thermotropic liquid crystalline polymers	**Experiment number**: CH-1511
Beamline: BM01B	**Date of experiment**: From: 17-03-2003 to: 19-03-2003	**Date of report**: 19-08-2004
Shifts: 6	**Local contact(s)**: Wouter van Beek	*Received at ESRF:*

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Report:

In total eight complete data sets have been collected at room temperature (set temp = 293 K, hutch temp ≈ 301 K) in theta mode, using continuous scans. The wavelength was 0.79942 Å, beam width 5.0 mm., beam heigth 1.0-1.5 mm. Most of the data sets were collected in the interval 1.0 – 35(or 40º) 2θ and finally binned at 0.005º2θ. Zeroshift was 0.0017 º2θ

A data collection protocol was used that consisted of a set of overlapping 2θ sections with the lower 2θ boundary being increased after each iteration. In this way each reciprocal lattice point is being exposed to approximately the same amount of radiation, like in a single-crystal diffraction experiment. According to the local contact, this scheme has two other additional advantages: (a) the slow intensity drop of the beam during the experiment, that can not (yet) be taken into consideration, has little effect on the data collection and (b) little influence of the shift of the detectors. This shift can vary in an unpredictable and non-constant way while, as yet, in the software only a constant shift is corrected for. A disadvantage of this scheme is that the amount of dead time increases with the amount of iterations but this was not considered to be decisive.

Five of the title compounds were measured, having acronyms 6A6P, HBP66, L21, MBP66 and NbOAS. Furthermore, three data collections were carried out for the compounds Ivory, Wal2025 and Atenolol.
The crystal structure of Atenolol has been solved and refined. This structure will be published together with the crystal structure of a cyclodextrin-atenolol inclusion complex that has also been solved from BM01B data (session CH-1209).
A crystal structure model for the cocoa butter Ivory in the β(V) phase has been refined and will be published soon.

Publications

Peschar, R., Pop, M.M., De Ridder, D.J.A., Van Mechelen, J.B., Driessen, R.A.J. and Schenk, H. (2004) Crystal structures of 1,3-distearoyl-2-oleoylglycerol and cocoa butter in the β(V) phase reveal the

driving force behind the occurrence of fat bloom on chocolate. *J. Phys. Chem. B.* Accepted.