ESRF	**Experiment title:** High resolution powder diffraction of alpha-cyclodextrins complexed with hydrophobic guest molecules	**Experiment number**: CH-1536
Beamline: BM01B	**Date of experiment**: From: 19-09-2003 to: 21-09-2003	**Date of report**: 18-08-2004
Shifts: 6	**Local contact(s)**: Hermann Emerich	*Received at ESRF:*

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Report:

Low angle (< ~ 2.0 º 2 θ) intensities as recorded in a previous session at BM01B seemed too low, compared with laboratory data, and suggested a potential shielding-off effect because of the position of the beam stop. This problem was discussed in detail with the local contact and, after testing, solved satisfactorily before the data collection was started. Also an artifact peak was observed at ~1.0 º 2θ that, afterwards, could be retraced by the local contact to a satellite reflection of the monochromator.

In total seven complete data sets have been collected at room temperature (set temp = 293 K ± 0.5 K) in theta mode, using continuous scans. The wavelength was 0.800001 Å, beam width 4.4 mm., beam heigth ~ 2.2 – 2.3 mm. Most of the data sets were collected in the interval 0.5 – 35 (or 40º) 2 θ and finally binned at 0.005º2θ. Zeroshift has been corrected for.

A data collection protocol was used that consisted of a set of overlapping 2θ intervals 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.

Eight data sets were collected in this session, four alphacyclodextrin (α-CD) inclusion compounds, 3-alfa(inclusion: tolfenamic acid) 4-alfa (flufenamic acid), 5-alfa (ciprofloxacin) and 6-alfa(omeprazol), two betacyclodextrion inclusion compounds β-CD (ketoprofen) and β-CD (z-8-dedecen-1-ol) , the inclusion compound metoprolol. Indexing and structure determination has been started by Dr. Borodi who has been awarded a grant for this purpose.