ESRF	**Experiment title:** Crystal structure determination using high-resolution powder data.	**Experiment number**: CH-435
Beamline: BM16	**Date of experiment**: From: 10-5-1998 to: 13-5-1998	**Date of report**: 10-08-2004
Shifts: 6	**Local contact(s)**: Andrew Fitch	*Received at ESRF:*

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Report:

In this session the metal-organic complex A2BLAAUW ($C_{23}N_2O_3CoH_{23}$) was re-measured (see CH-342) to improve the signal/noise ratio, especially at higher diffraction angles. high-resolution powder diffraction [1] Two triacylglycerols were measured for determination of accurate cell parameters and eventually structure determination. For tristearin (SSS), a glycerol esterfied with three stearic acids, the structure has been been solved and published [2]. The structure of the triacylglycerol MPM has been solved from powder data, using the single-crystal structure of CLC as starting point [3].

For our structure determination project some organic and organo-metallic compounds have been measured. The structure of $C_{31}N_4SO_3H_{52}$ is not yet solved, but cell parameters could be determined. The structure of $C_{25}O_2H_{28}$ has been solved and refined. The results were presented at the 18th IUCR-congress in Glasgow (4-13 August, 1999) and a publication is in preparation. For $C_{10}N_2O_{13}Mo_4H_{10}$ the cell parameters have been determined, but the structure is not yet solved.

Publications

[1] Dova E., Goubitz, K., Van Langevelde A., Driessen R.A.J., Mahabiersing T., Blaauw R., Peschar R. and

Schenk H. (2001). Structure determination of two metal-organic complexes from high-resolution synchrotron powder diffraction data. , J. Synchrot. Radiat. 8 (2001), 1186-1190.

[2] Van Langevelde A., Peschar R. and Schenk H. (2001) Structure of beta-trimyristin and beta-tristearin from high-resolution x-ray powderdiffraction data. Acta Cryst B57, 372-377.

[3] Van Langevelde A, van Malssen K, Driessen R, Goubitz K, Hollander F, Peschar R, Zwart P and Schenk H. (2000) Structure of CnCn+2Cn-type (n = even) beta '-triacylglycerols. Acta Cryst. B 56(6), 1103-1111.

[4] Helmholdt R.B., Sonneveld E.J., Chernyshev V.V. and Schenk H. (2001). The crystal structure of sodiumoxamate NaC2O3NH2. Z. Kristallogr. 216, 295-297.