



	Experiment title: Crystal structure determination of one organic and two inorganic compounds using high-resolution powder	Experiment number: CH-342
Beamline: BM16	Date of experiment: From: 31-10-1997 to: 2-11-1997	Date of report: 10-08-2004
Shifts: 6	Local contact(s): Eric Dooryhee	<i>Received at ESRF:</i>
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Report:

In this session high-resolution powder diffraction patterns were collected of some organic, organo-metallic and inorganic powders, referred to below by their acronyms A1TAAS, A2BLAAUW, Y63, Y65, DMAN2, A9DSM and EVA1. All data sets have been collected at room temperature using the interval $3. - 38.0^\circ 2\theta$ and finally binned at $0.005^\circ 2\theta$. The wavelength used was 0.65296 \AA in all cases.

The structure of A1TAAS($C_{37}N_2OCIRhH_{40}$) has been solved and published [1]

The structure of DMAN2 has been solved and published [2]

The structure of A2BLAAUW ($C_{23}N_2O_3 CoH_{23}$) could be solved but refinement turned out to be difficult, mainly because of the poor crystallinity. In a later session (CH-435) this compound has been re-measured using a new batch.

The heavy-atom compound Y65 ($Pr_4Ge_3S_{12}$) has been solved and published [3]

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] Lasocha W., Milart P., Rafalska-Lasocha A. and Schenk H. (2001) Crystal structure of the complex of

1,8-bis(dimethylamino)naphthalene with p-nitrosophenol by powder diffraction methods. *Z. Kristall.* 216(2), 117-121.

[3] Helmholtz R.B., Goubitz K., Sonneveld E.J. and Schenk H. (2003). Pr₄Ge₃S₁₂ : structure determination from high-resolution powder diffraction data. *Acta Cryst.* E59, i119-i121.