



Experiment title: Crystal structure determination using high-resolution powder data.

Experiment number:
CH-435

Beamline:
BM16

Date of experiment:
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Shifts:
6

Local contact(s):
Andrew Fitch

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Names and affiliations of applicants (* indicates experimentalists):

Henk Schenk*, Rene Peschar, Anke Etz, Wieslaw Lasocha, Wim Molleman* and Rob Helmholdt*.

Laboratory for Crystallography
Institute for Molecular Chemistry (IMC)
Universiteit van Amsterdam
Nieuwe Achtergracht 166
1018 WV Amsterdam
The Netherlands

Report:

In this session the metal-organic complex $C_{23}H_{27}N_2O_3Co$ was re-measured (see CH-342) to improve signal/noise ratio, especially at higher diffraction angles. Unfortunately, the problems with the refinement were not solved with this new measurement.

Two triacylglycerols were measured for determination of accurate cell parameters and eventually structure determination. For tristearin (SSS), a glycerol esterified with three stearic acids, the cell parameters are determined and the structure is solved and refined. A publication about this structure determination for powder data is in preparation. For MPM, a triacylglycerol with unequal chain-lengths, the cell parameters are determined but the structure is not yet solved.

For our structure determination project some organic and organo-metallic compounds are measured. The structure of $C_{31}H_{52}N_4SO_3$ is not yet solved, but the cell parameters could be determined. The structure of $C_{25}H_{28}O_2$ is solved and refined. The results were presented on

the 18th IUCr-congress in Glasgow (4-13 August 1999) and a publication is in preparation.

For $C_{10}H_{10}N_2O_{13}Mo_4$ the cell parameters are determined, but the structure is not yet solved.