



	Experiment title: Self-assembled supramolecular architectures	Experiment number: CH 918
Beamline: ID 11	Date of experiment: from:24 th february to:29 th February	Date of report: 20.02.2001
Shifts: 15	Local contact(s): G. Vaughan	<i>Received at ESRF</i>
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Report:

32 categories of samples were taken to Grenoble and 20 crystals were mounted for study. Normal x-ray diffraction measurements were carried out. Finally 14 data set could be collected. Only the structural investigations at different temperatures in order to follow one specific switching process (spin crossover of Fe^{II}-compounds) failed by reasons of phase transition in the crystals. Some of the most important data sets are discussed below:

1. [4x4] Pb(II)

Because of the uniqueness of that molecule we continued the efforts to obtain a better data set than in the previous experiment CH-832. Most of the measuring time was consumed trying to obtain an appropriate data set of this compound. Problems were the lack of long range diffraction and/or diffraction at high angle. The 16 leads are easily observed in the expected grid arrangement and finally the organic ligands were allocated too. Over 600 non hydrogen atoms will have to be refined (not including solvent molecules!)

2. Coordination Polymers of switchable Fe^{II}-grid units

Concerning this part of the experiment three data set were collected: One Fe₄^{II}-grid compound and the respective Ag^I-bridges coordination polymer. The structure exhibits a 2D sheet of meandric interwoven Fe₄^{II} switchable grid units. Unfortunately the second data collection at room temperature (to establish the switching process) failed by probably phase transitions of the crystal. In a forthcoming experiment the data collection should be persisted because of the importance of the problem. Secondly, a data set showing Fe₄^{II} switchable grid units aligned in a 1D wire by La^{III}-coordination could be established. There were some problems in refining the data and we have wait for the concluding results.

3. Further Structures

Data sets of ten different [2x2]M^{II}-Grid compounds could be collected. In addition three mononuclear compounds and one organic molecule were measured and collected. The refinement of most of the data sets is in course (in Jena and Grenoble).