

Project name: **FAMAR. New molybdenum based catalysts and coordination polymers for modern, clean technologies**

Beamtime Report

dd.mm.yyyy - dd.mm.yyyy (Date of the report to be added)

General information

Name of the rapporteur	Name of the rapporteur's organisation
Wiesław Łasocho	FAMAR
Type of research (nanotechnology/health care/chemistry etc.)	Name of the research facility
Chemistry	beamline P02.1 at PETRA 3
Date of the measurement, duration	Location of the event
28-30 January, 31 January-1 February 2013	Deutsches Elektronen-Synchrotron DESY Notkestr. 85, 22607 Hamburg
Facility personnel participating in the measurement	
Dr. Graham Appleby	

Description of the project

Research description (short summary as written in the application)
<p>New molybdenum based catalysts and coordination polymers for modern, clean technologies.</p> <p>The aim of the project was:</p> <p>1) Determination of the crystal structures of several polyoxometalate catalysts active in oxidation of hydrocarbons and other organic compounds, including renewable raw materials (for example, unsaturated fats, plant oils, hydrocarbons). The investigated compounds belonged to the group of new layered pentamolybdates of amines and several new polymeric trimolybdates.</p> <p>Significance: The aim of the research is obtaining of new catalysts for the synthesis of important industrial products (eg, dicarboxylic acids essential for the production of fibers for textile industry, plasticizers, etc.) which will be able to reduce the emission of harmful products (greenhouse gases, nitrogen oxides).</p> <p>2) Determination of the crystal structures of new group of coordination polymers (MOF type) based on different molecular linking blocks (different symmetry, size, and functionality - the ability to join and chelating) and transition metals.</p> <p>Significance: The aim of the research is obtaining new materials with high sorption capacity – materials important in the processes of gas storage (CO₂, H₂), removal of impurities, etc.</p>

Summary of activities (experiments performed, beamtime used, preliminary overview of results, next steps and other relevant information)

Obtained diffraction patterns were initially used for final test of purity (to detect even very small amounts of impurities – important in space group determination). Next all not indexed so far patterns were indexed and the most probable space groups were determined. To find crystal structure models two approaches were used – direct methods and direct space methods.

Obtained structure models were refined by Rietveld method. Crystal models were also verified by deep search in crystallographic databases, checking spectroscopy results (IR, UV VIS), SEM, chemical analysis and so on.

Up till now most of crystal structure were solved. Currently we are preparing 1st paper describing family of coordination polymers (sorption materials).

Some supplementary data are gathered to finish the second paper describing family of lithium dicarboxylates (layered materials).

Now we are correlating results of structure solution results with results of catalytic test.

How would you describe cooperation and assistance from industrial liaison officers and national contact points while preparing and carrying out the research at large scale facilities?

We are very pleased with the cooperation with prof. Krystyna Jabłńska Ławniczak from the Polish side and dr Graham Appleby from DESY side. The cooperation was very smooth. After each e-mail or phone call we obtained quick answer with suggestions, new information etc.

Even though DESY is a very big institution, with many scientific task being realized at the same time, we obtained our results very quickly, without any problems and delay.

Other personal remarks

As we mentioned above, we appreciate very much cooperation with dr Graham Appleby and prof. Krystyna Jabłńska-Ławniczak, their help and support have always been fast, efficient and friendly.

Annexes

Annexes

(list of annexes; meeting minutes, graphical illustrations, tables and other supplementary data)

We took part and reported our results during Science Link meeting in Petersburg in June 2013. We hope to send soon a manuscript (preliminary title: Design and crystal structures of a group of the new co-ordination polymers) of the first paper we are preparing based on synchrotron measurements.