



	Experiment title: Structure determination of new lanthanide-containing metal-organic frameworks	Experiment number: 16-01-682
Beamline: BM16	Date of experiment: from: 12 November 2006 to: 14 November 2006	Date of report:
Shifts: 6	Local contact(s): Dr. Ana LABRADOR	<i>Received at ESRF:</i>
Names and affiliations of applicants (* indicates experimentalists): Dr. Jose Luis JORDA MORET Dr. Avelino CORMA * Dr. Bogdan Vasile HARBUZARU * Dr. Fernando REY		

Report:

The objective of this project was the structural determination of two new metal-organic frameworks containing lanthanide atoms in the structure. Then, single-crystal data for both materials were collected using a wavelength of 0.97754Å.

The structure of the first material, called ITQMOF-2 (sample HB041) [monoclinic; space group $P2_1/n$; $a=7.2968(10)$, $b=25.0695(10)$, $c=29.4572(10)$ Å, $\beta=91.920(5)^\circ$], has been solved and refined using the programs SHELXS-97 and SHELXL-97 respectively, and can be described as parallel columns of metal atoms connected through the organic molecules forming a microporous 3D structure. A paper describing the details of the synthesis, crystal structure and properties of the material is going to be submitted in a few weeks to Science.

Unfortunately, although the unit cell parameters and space group of the second material (ITQMOF-1) have been obtained [hexagonal; space group $P6_3/m$ (probably); $a=b=42.1796$, $c=7.4779$ Å], its structure remains unsolved yet. This has been mainly attributed to the fact that the samples available at that moment presented a severe twinning, precluding the structure resolution. For this reason, a new proposal was submitted to BM-16 (project 16 01 688) and further calculations using the new datasets are now in progress.