ESRF	**Experiment title:** Structure determination of new lanthanide-containing metal-organic frameworks	**Experiment number**: 16-01-688
Beamline: BM16	**Date of experiment**: from: 04 March 2007 to: 05 March 2007	**Date of report**:
Shifts: 4	**Local contact(s)**: Mr. Fernando Salvador DELGADO-TRUJILLO	*Received at ESRF:*

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Report:

This project was a continuation of project 16-01-682, and the objective was the structural determination of two new metal-organic frameworks (MOFs) using single-crystal data.

The results of those two projects have been published recently in Angewandte Chemie International Edition. The full reference is:

Bogdan V. Harbuzaru, Avelino Corma, Fernando Rey, Pedro Atienzar, Jose L. Jordá, Hermenegildo García, Duarte Ananias, Luis D. Carlos, Joao Rocha, "Metal-organic nanoporous structures with simultaneous anisotropic photoluminescence and magnetic properties, and their use as sensors" *Angewandte Chemie International Edition*, 47, (6), (2008), 1080-1083 [and *Angewandte Chemie*, 120, (6), (2008), 1096-1099]

The data obtained in the first project already allowed determining the complete crystal structure of ITQMOF-2, and proposing an aproximate unit cell for ITQMOF-1.

The new measurements made in this project allowed to further refine the unit cell of the second MOF (ITQMOF-1), determining also that the isomorphic substitution of Eu with other lanthanides (or mixtures of them) do not introduce significant changes in the MOF structure. Unfortunatelly, the extremelly severe twinning in the crystals precluded the complete structure determination of that material.

Very recently, and almost simultaneously with the publication of our paper, another Spanish group independently determined the structure of a material similar to ITQMOF-1 (F. Gándara, A. de Andrés, B. Gómez-Lor, E. Gutiérrez-Puebla, M. Iglesias, M. A. Monge, D. M. Proserpio, N. Snejko, “A Rare-Earth MOF Series: Fascinating Structure, Efficient Light Emitters, and Promising Catalysts” Crystal Growth & Design, Vol. 8, No. 2, (2008), 378-380).

With that additional information, we are now carring out further studies, specially regarding the thermal behaviour of the materials, using the data obtained in this project.