ESRF	**Experiment title:** Determination of the structure directing agent location and its influence on catalytic properties of zeolite ITQ-22 (IWW)	**Experiment number**: CH-2034
Beamline: ID-31	**Date of experiment**: from: 10/09/2005 to: 13/09/2005	**Date of report**: 20/02/2006
Shifts: 9	**Local contact(s)**: Irene Margiolaky	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

*** Jose Luis Jordá Moret, Instituto de Tecnologia Quimica (UPV-CSIC)**

*** Maria José Díaz Cabañas, Instituto de Tecnologia Quimica (UPV-CSIC)**

Fernando Rey García, Instituto de Tecnologia Quimica (UPV-CSIC)

*** Sandra Leiva Herrero, Instituto de Tecnologia Quimica (UPV-CSIC)**

Report:

In this experiment, we had two main objectives.

The first one is a continuation of experiment CH-1885, which consists on the measurement of three as-prepared and calcined ITQ-22 samples that couldn't have been measured in experiment CH-1885 due to the failure of the engine of the diffractometer.

As presented in the report corresponding to that experiment, the structure directing agent seems to be slightly delocalized in the 10R and 12R channels of the structure. Nowadays further efforts are been made in order to propely refine the atomic positions.

The second objective was focused on the thermal behaviour of zeolite ITQ-22 at non-ambient temperatures (100 to 1000K), using three silicogermanate and aluminosilicogermanate samples.

As shown in figure 1, this extremelly complex material posses an unusual thermal behaviour. It has been reported previously that several zeolites exhibit a negative thermal expansion when increasing the temperature. In zeolite ITQ-22, however, the thermal expansion is extremelly anisotropic; in fact, in this material the thermal expansion can be positive, negative or almost negligible depending on the choosen direction. A detail of the peak shifts corresponding to some selected reflections along he axis directions is shown in figure 2

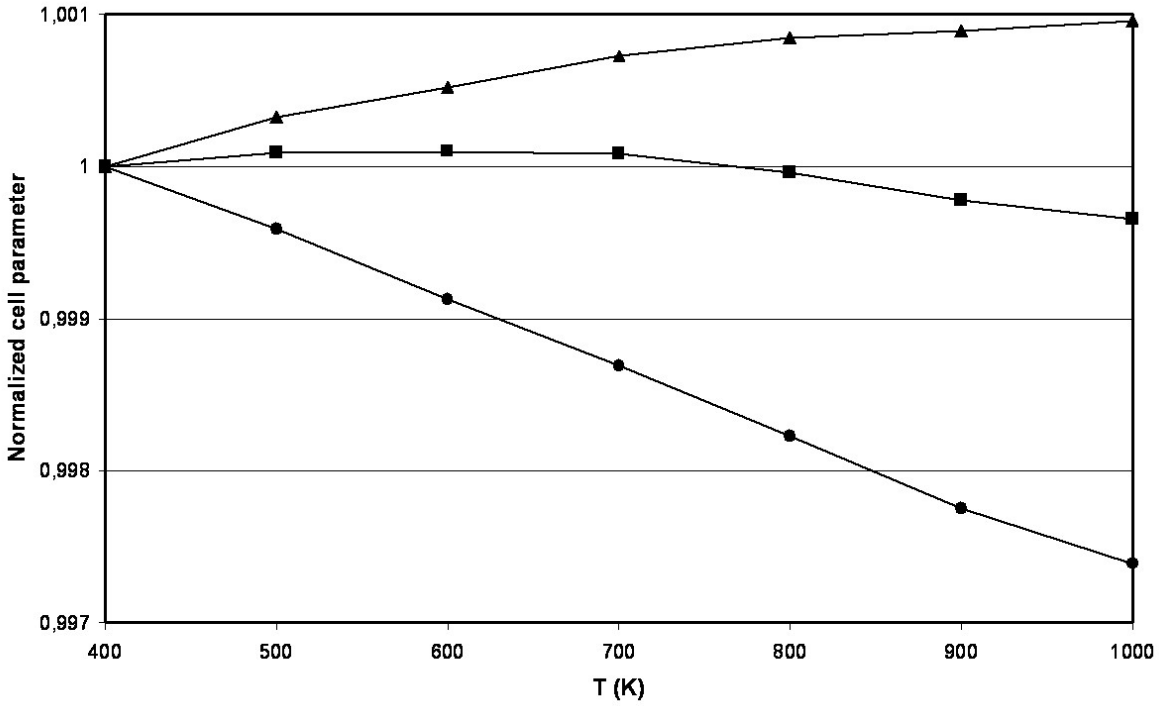

Figure 1: Variation of cell parameters at high-ambient temperature, normaliced respect to the cell parameters at 400K. Circle, square and triangle correspond to parameters a, b and c, respectively.

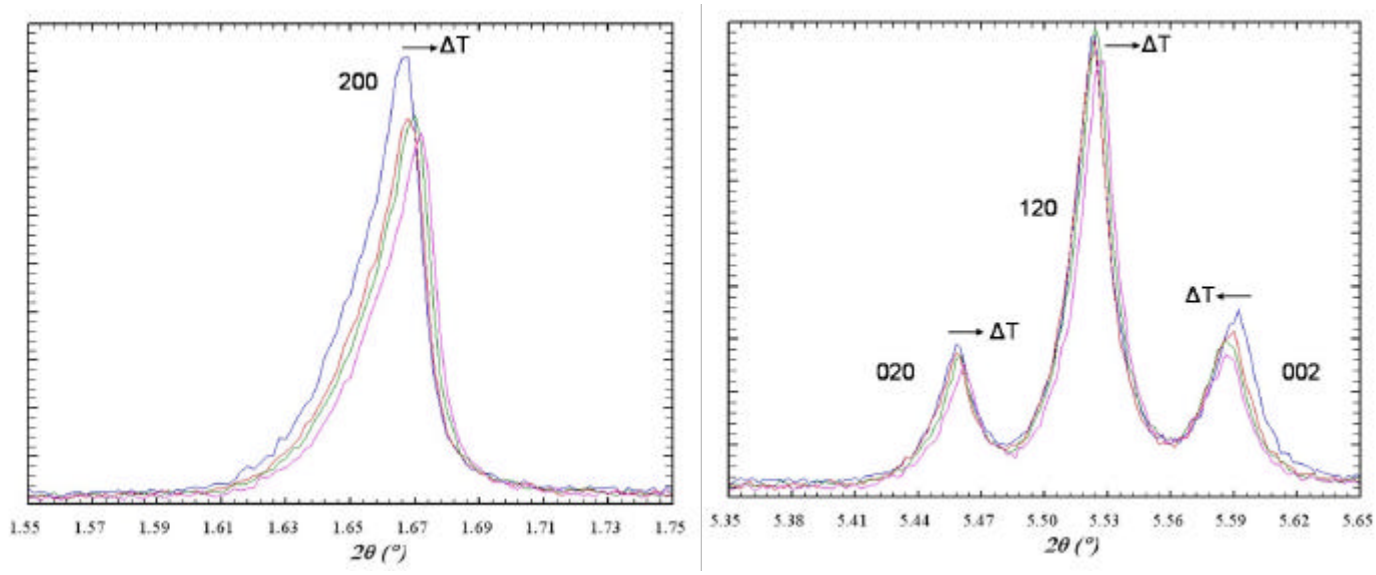

Figure 2: Peak shifts at high temperatures (400, 600, 800 and 1000K). Arrows indicate the direction of peak shifts when increasing temperature.

The thermal expansion along the c axis has been atributed to the presence of germanium-containing D4R in this direction; the increase of the temperature could produce and increase of the T-O-T angles in these units, expanding and distorting them.

Although the large number of parameters involved difficults and slows extremelly the required calculations, the Rietveld refinements at different temperatures are being carried out nowadays, in order to fully understand those results.