ESRF	**Experiment title:** Structure determination of the novel zeolite ITQ-38	**Experiment number**: CH-2493
Beamline: BM01B	**Date of experiment**: from: 1/02/2008 to: 4/02/2008	**Date of report**: 24/02/2009
Shifts: 6	**Local contact(s)**: Hermann Emerich	*Received at ESRF:*

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Report:

High resolution powder diffraction data were collected for four samples containing different Si/Ge ratios in their framework compositions.

Also, we collected data at different temperatures for two of the samples, (a) to exploit the anisotropic expansion of the unit cell in order to resolve highly overlapped peaks, and (b) to study the thermal behaviour of the zeolite at different temperatures.

In this case, the synchrotron data allowed us to determine that the previously proposed unit cell was incorrect; then, the material has now been indexed with a monoclinic cell with a= 21.25Å, b=12.70Å, c=13.02Å, and beta=96.87º; the absence of systematic extinctions suggest that the space group is *P2*, *Pm* or *P2/m*.

Unfortunately, the low symmetry of the material, together with its relatively large unit cell and density indicates that it contains at least 14 Si and 28 O atoms in the asymmetric unit (space group *P2/m*) or 28 Si and 56 O (space groups *P2* and *Pm*). Then, due to the large complexity of the structure, all the attempts made up to now to determine its structure have failed. Nowadays, we are making further efforts for determining the structure of this material,

with the introduction of the "charge flipping method", a new technique described recently by other authors for determining the structure of other highly-complex zeolites [Ch. Baerlocher, et al. *Science*, **315**, 1113-1116 (2007)], and attempts to introducing HRTEM and electron diffraction data in the structural analysis.

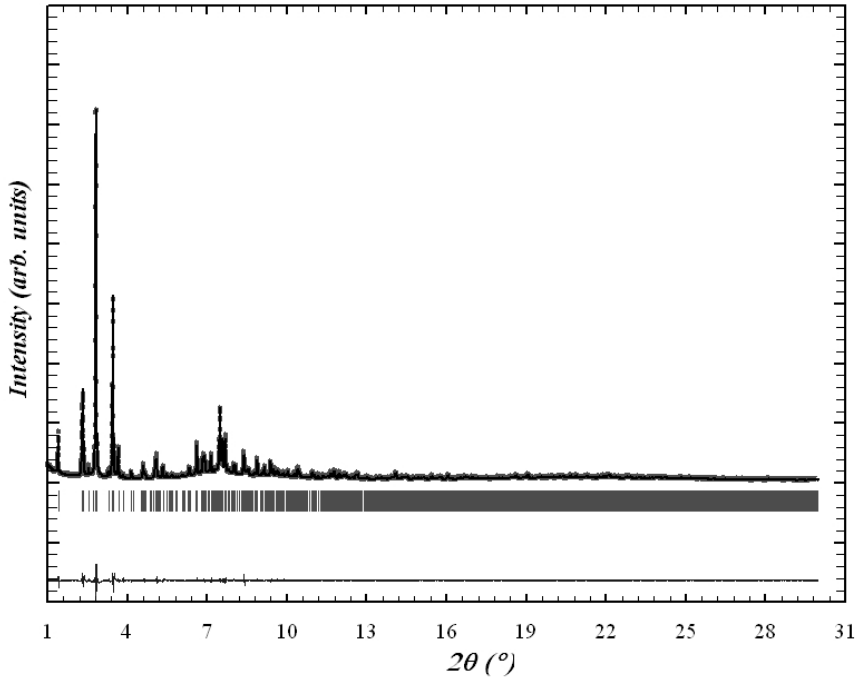

Figure 1: Profile fitting of a ITQ-38 sample (a= 21.25Å, b=12.70Å, c=13.02Å, and beta=96.87º, space group *P2*)

Regarding the thermal behaviour of the zeolite, it presents a high anisotropy; as shown in Figure 2, the *b* parameter increases with temperature; *a* increases from 10 to 300K, and then it decreases, while *c* follow the opposite trend; last, *beta* is almost constant between 300 and 700K, but increases at 100K. As a result, (a) the unit cell volume is almost constant in the range 300-700K, and is slightly smaller at 100K, and (b) the large anisotropy suggests that the shape of the pores will probably change significativelly with the temperature, modifying the diffusion properties of the material.

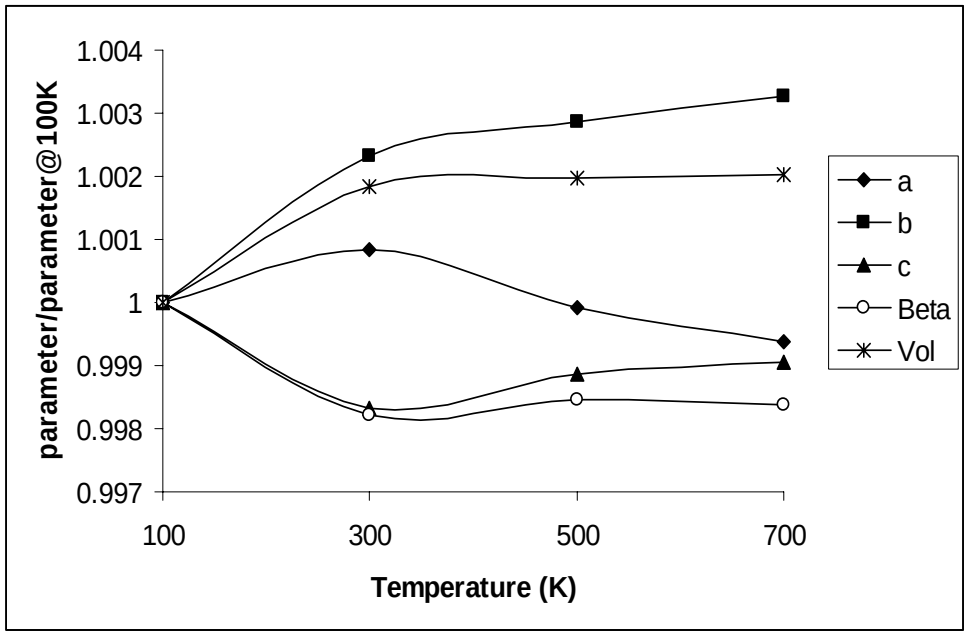

Figure 2: Variation of the cell parameters with temperature