ESRF	**Experiment title:** Structure determination of two new zeolitic germanosilicates	**Experiment number**: 25-01-602
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Shifts: 12	**Local contact(s)**: Dr Ignacio CARETTI	*Received at ESRF:*

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Report:

High-resolution powder diffraction data were collected for two samples: MMHX162 (zeolite ITQ33) and SR984 (zeolite ITQ35). The first material was measured in the as-prepared and in the calcined form, while the second one was measured only in the as-prepared form due to its unstability during calcination. All the measurements were performed using a wavelenght of 0.68871Å, with the samples placed in sealed glass capillaries.

Unfortunatelly, none of those data were enough in their own for structure determination of the materials, mainly due to the relatively low resolution and intensity of the data. This effects can be atributed to (a) a very short arm (50 cm) in the goniometer, which reduces the data resolution in 2-theta; (b) the presence of only a single detector, which decreases the intensity collected in the measurement, requiring a very large increase of the measurement time; and (c) the fact that the beam must travel a very long distance throught air till reaching the sample, further reducing the intensity avalilable due to absorption effects.

However, in the case of ITQ-33, the information obtained were enough to allow determining unambiguously the correct space group. That proved to be very helpful and made possible finally to determine the structure of zeolite ITQ-33 using the data collected in a reaction chamber attached to our laboratory diffractometer. The structure of this zeolite (P6/mmm, a=19.367Å, c=11.495Å), which posses a three-dimensional channel system containing 18- and 10-member rings and presents very interesting catalytic properties, has been published recently in Nature [Avelino Corma, Maria J. Díaz-Cabañas, José Luis Jordá, Cristina Martínez, Manuel Moliner, “High-throughput synthesis and catalytic properties of a molecular sieve with 18- and 10-member rings” Nature, 443, (2006), 842-845]

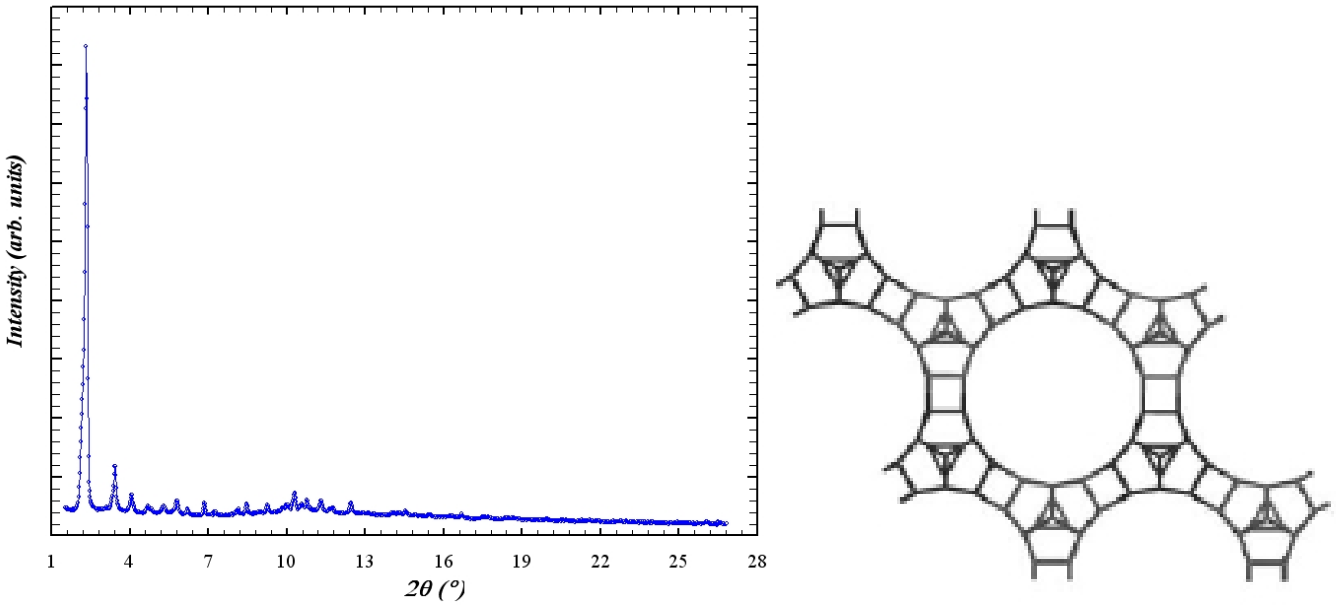

Figure 1: Powder diffraction pattern (left), and structure along [001] (right) of zeolite ITQ-33

In the case of ITQ-35, the resolution of the structure is still in progress, although the real unit cell and space group remain still ambiguous.

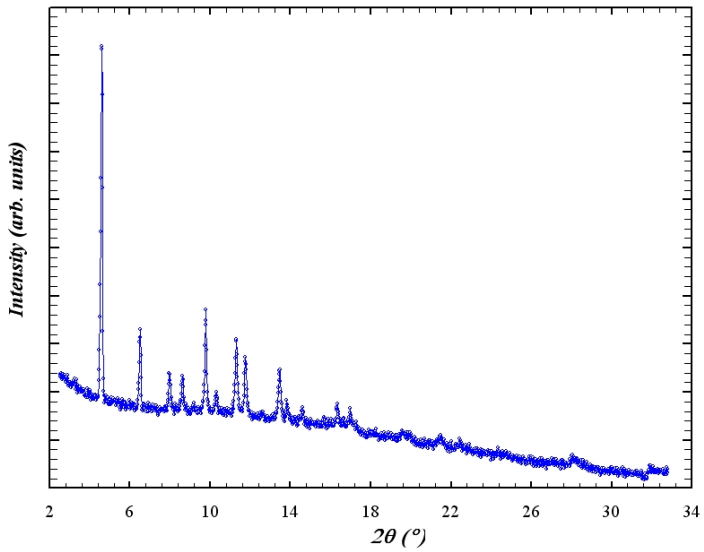

Figure 2: Powder diffraction pattern of zeolite ITQ-35 collected at BM-25A