



	Experiment title: Determination of the structure directing agent location and its influence on catalytic properties of zeolite ITQ-22 (IWW)	Experiment number: CH-1885
Beamline: ID-31	Date of experiment: from: 23/02/2005 to: 26/02/2005	Date of report: 20/02/2006
Shifts: 9	Local contact(s): Michella Brunelli	<i>Received at ESRF:</i>
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Report:

Five samples of the zeolite ITQ-22 in the as-prepared form, and one calcined sample, were measured. Those samples possess different chemical compositions, regarding on:

- framework composition (silicogermanates or aluminosilicogermanates)
- structure directing agent molecule

Unfortunately, two incidents occurred during the measurement, strongly reducing the useful beam time.

First, during the first night the new automatic sample exchanger was used. However, as we realized afterwards, the size and shape of the tweezers strongly limits the maximum allowed length for the capillaries fitted in the sample holder. In our case, that caused the breakage of the top of the capillaries. Then, when they were placed in the sampler spinner and rotated, the powder slowly leaks, providing observable XRD patterns, but distorting the measured intensities, forcing to repeat all the measurements collected that night.

Second, on 25th at around 6:30 AM the engine of the diffractometer broke. Then, due to the impossibility to repair it, the measurement was concluded and the last 3 shifts were not available.

However, in the remaining time it was possible to collect some diffraction patterns corresponding to several samples.

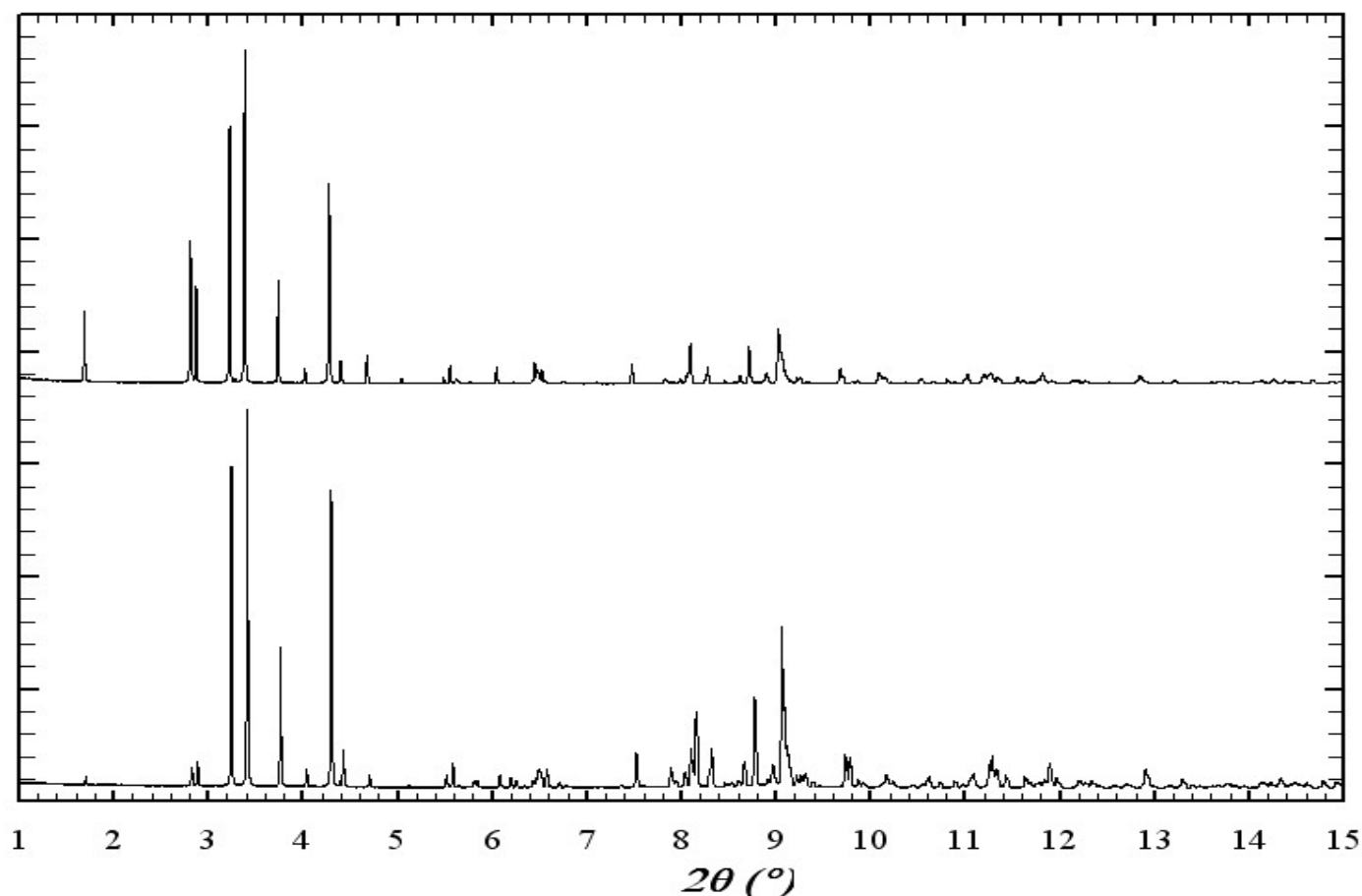


Figure 1. Diffraction patterns of calcined (top) and as-prepared (bottom) ITQ-22 (Ge/Si=0.2, Al/Si=0)

The use of difference Fourier maps, combined with ab-initio computational calculations, has allowed to tentatively locate the structure directing molecules in two different positions, one along the 12R channels, and the second one in the 10R channels.

Nowadays, we are working in properly refining the atomic positions of the organic component, in order to elucidate if those molecules are ordered or, more probably, exhibit a certain disorder, appearing slightly delocalized in the channels. This last possibility could explain the fact that the zeolite ITQ-22 have been obtained up to now using three different structure directing agents, with different sizes and lengths, that are able however to properly counter-balance the negative charges introduced by fluoride anions in fixed locations (D4R) of the framework, non being observed a significant influence of the framework chemical composition.