	Experiment title: Localization of water sorbed in cesium exchanged ZSM-5 zeolithic materials at several loadings and temperatures. Evidence for cation migration	**Experiment number**: 01-01-653
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Report:

Cations and Cation Migration in Zeolitic Materials – I – Influence of temperature and water on the Ba migration in barium-exchanged Faujasite.

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Zeolites presenting the Faujasite structural type are widely used in petrochemical processes for selective gas separation, catalysis and detergent builders. NaY (Si/Al=2.42) zeolite has been totally Ba-exchanged and both its hydrated and dehydrated forms have been investigated by X-ray synchrotron powder diffraction (λ=0.79969Å). The samples have been filled into 0.9mm quartz capillaries, mounted on a specially designed atmosphere- controlled sample holder and investigated in the 25-450 °C temperature range.

The structural interpretation of the powder data-collections have been realized using the Rietveld method (modified DBW and GSAS). The starting T(Si,Al),O framework coordinates are those usually observed for Y faujasites (Fd3m space group) [1]. The locations of the water molecules have been estimated by molecular mechanics simulations.

In the hydrated BaY samples four Ba sites (I,I',II and III') and five water sites have been identified. In Figure 1 the Ba cation migration versus temperature at different water fillings (in parenthesis) is represented. In the anhydrous BaY only three I,I' and II Ba species are detected, and the Ba migration versus temperature is significantly less important than in the hydrated phases. These results correspond to the *dehydration* of BaY.

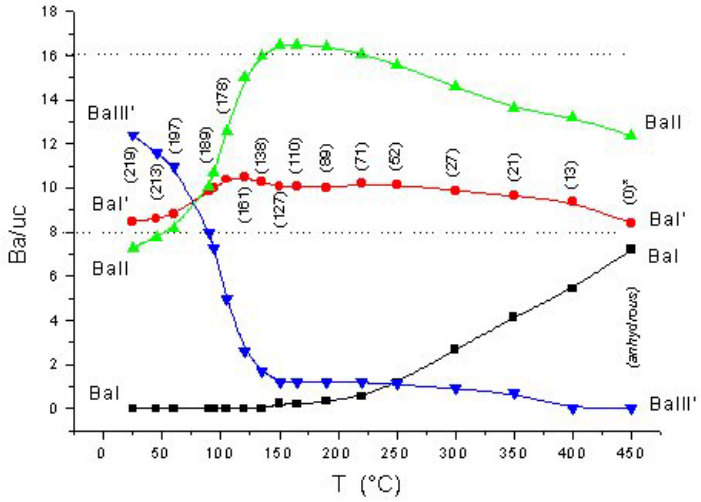

Figure 1: Ba cation migration during the dehydration of BaY.

Data collections corresponding to several rehydrated samples at ambient temperature show that the hydration process is very slow : *e.g.*, at a same overall water filling (20 water molecules/unit-cell) Ba *and* water migrate simultaneously and equilibrium is obtained after at least 12 hours. The study of the complete *hydration* process of BaY is part of future work.

References

[1] – W.L. Meier and D.H. Olson, Atlas of Zeolite Structure Types, Butterworths (1987)