

*In-House Report concerning the 01-01-677 experiment at the SNBL (ESRF) on BM01B.*

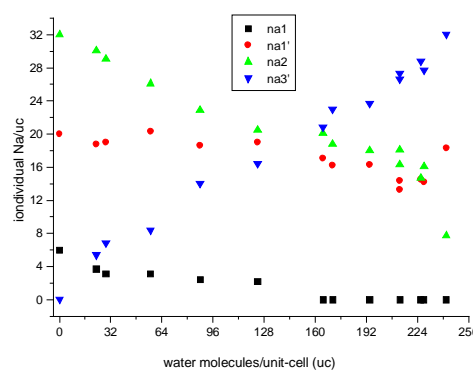
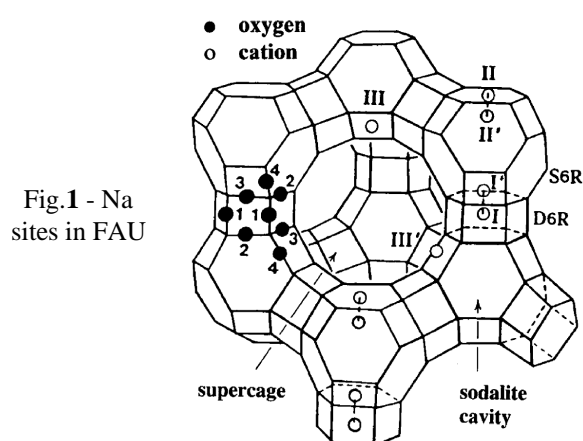
B.F. Mentzen - H. Emerich - April 20 2005 to April 25 2005.

**Title of Exp. 01-01-677** : Localization of water sorbed in sodium exchanged Y ( $\text{Na}_{58}\text{Y}$ ) zeolite ( $\text{Si}/\text{Al} = 2.31$ ) at several loadings. Cation migration versus temperature and water adsorption.

**Subject** : Structural evolution of zeolitic sorbent/sorbate systems - *Continuation* of experiments CH-1838 (CsMFI/water system) and 01-01-653 (BaY/water system).

**Aim** : Description of the structural evolution during the dehydration/hydration mechanism versus temperature and sorbate (water) fillings.

**Report** : During the present 01-01-677 In-House experiment three series of zeolitic sorbent/water systems have been investigated : (1) - the NaY/water, (2) - the BaY/water and (3) - the CsMFI/water system. In all cases the samples (12 to 14 for each series) correspond to powder filled glass-capillaries heated and sealed at increasing temperatures in order to obtain, *at room temperature* after *equilibration* (2 weeks), several hydration degrees. For systems (2) and (3) ESRF Reports have already been deposited. Accordingly, the present report is restricted to preliminary results concerning the structural evolution of a  $\text{Na}_{58}\text{Y}$ /water system *during dehydration*.



The labelling of the cationic Na sites in FAU type zeolites is given in figure 1. In figure 2 the migration of the Na cations versus water fillings is represented. These results represent the *very first example* of a complete description of the structural evolution at RT of a zeolitic sorbent/water system. The water molecules are located on *five* distinct sites and the distribution of their populations versus water fillings is presently established. The most unexpected result is the presence of the NaIII' site (blue triangles) at all water fillings except at total dehydration. Once again it must be emphasized that figure 2 represents the Na migration at *room temperature* in progressively *dehydrated*  $\text{Na}_{58}\text{Y}$ /water samples : in fact, in the case of *rehydrated* samples at room temperature calorimetric results seem to show that the structural evolution is quite different. Therefore, a *continuation experiment* concerning progressively rehydrated samples has to be performed.