ESRF	**Experiment title:** The structure and rehydration kinetics of ammoniated natrolite ($Na_2Al_2Si_3O_{10}.NH_3$)	**Experiment number:** CH338
Beamline: BM16	**Date of experiment:** from: 04/09/97 to: 07/09/97	**Date of report:** 27/08/98
Shifts: 9	**Local contact(s):** A. Fitch	*Received at ESRF:* 31 AOUT 1998

Names and affiliations of applicants (* indicates experimentalists):

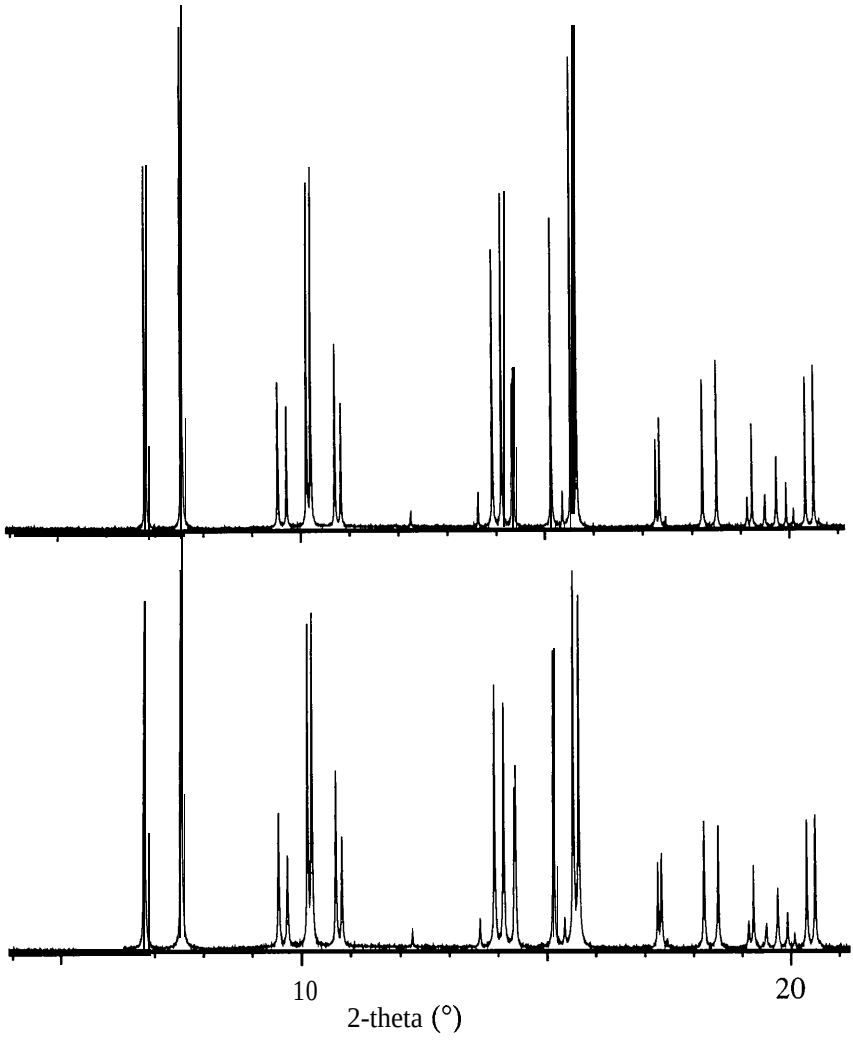
*C.M.B. Line
G. J. Kearley

Report: The interaction of ammonia with zeolites is a subject little known. Natrolite was chosen as a suitable starting point as the site for the location of guest molecules is small. The structure of hydrated natrolite is well known and the positions of the hydrogen atoms well determined (Artioli et al, 1984). Furthermore, the structure of the ammonium, NH_4^+ form is also known (Stuckenschmidt et al, 1992). However, the ammonia form, Na^+NH_3 has been previously produced (Barrer, 1938) but never before examined by high-resolution X-rays.

In a previous neutron experiment measuring the diffraction pattern of the ammoniated natrolite at 4 K, we have observed peaks not coinciding with the original hydrated natrolite peaks and therefore supposed that the ammoniated form had a different symmetry. However, the peak intensities were too dissimilar from the original form, and the data of too small a reciprocal space range, to permit a structural solution.

In this experiment we measured eight spectra, including the original form, the dehydrated form and samples with only partial loading, so as to facilitate a structural solution, as well as measuring samples of the rehydrated form. However, the same peaks were observed as for the hydrated natrolite, with only some peak intensities being dissimilar (Figure 1). The fact that no breaking of symmetry was observed may be due to the fact that the synchotron experiment was measured at a sample temperature of 70 K, as opposed to 4 K for the neutron experiment. This may therefore mean that the ammoniated form has the Fdd2 symmetry, but a phase transition to a lower symmetry at a temperature between 70 K and 4 K. Rietveld analysis of the data is in progress.

Fig 1. Synchotron diffraction pattern of hydrated natrolite (above) and ammoniated natrolite (below) at a sample temperature of 70 K. Wavelength 0.77 A.



Artioli G, Smith J. V., Kvick A. (1984) Neutron diffraction study of natrolite, $Na_2Al_2Si_3O_{10}$. 2 H_2O. Acta Cryst C40, 1658-1662.

Stuckenschmidt E, Kassner D, Joswig W, Baur W. H. (1992) Flexibility and distortion of the collapsible framework of NAT topology: the crystal structure of NT&-exchanged natrolite. Eur. J. Mineral. 4: 1229-l 240

Barrer R. (1938). The sorption of polar and non-polar gases by zeolites. Proc. Roy. Soc A 167: 392-420.