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A NOTE ON THE LATTICE PARAMETERS OF NEPHELINE HYDRATE I

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During an experimental investigation of the system NaAlSiO₄ – H₂O at 1,000 kg/cm² water vapour pressure, a low temperature modification of NaAlSiO₄, similar to that described by Barrer and White (1952) and termed nepheline hydrate I by these authors, was synthesized at temperatures below 415° C. in runs of 4 days duration. The starting material in these experiments was a coprecipitated gel prepared by a modification of the method described by Roy (1956) and the synthesis was carried out in the conventional cold seal pressure vessel (Tuttle, 1949).

Saha (1961) has determined that nepheline hydrate I is stable at temperatures up to approximately 425° C. at this water vapour pressure. This phase can only be preserved at room temperature by rapid quenching in water. Under conditions of air cooling, both nepheline hydrates I and II are formed. Paragonite, reported by Saha (1961), could not be detected either optically or by x-ray powder diffraction methods in runs at temperatures as low as 300° C. A trace of nepheline

hydrate II (nomenclature of Barrer and White (1952)) was observed on the x-ray diffraction patterns at this temperature. Optically, nepheline hydrate I was observed as very small crystals (5–10 microns) with irregular outlines but occasionally as blocky crystals. The mean refractive index was 1.504, this being in agreement with the values given by Saha (1961) and Barrer and White (1952).

The composition of this mineral is believed to be NaAlSiO₄ $\cdot \frac{1}{2}$ H₂O, and it has been suggested that some of the naturally occurring alteration products of nepheline, termed hydronephelites, gieseckites and ranites, may be the natural counterparts of nepheline hydrate I. Evidence for this has been summarized by Saha (1961). The writer is at present engaged in an x-ray investigation of these alteration products of natural nephelines and preliminary results indicate that no nepheline hydrate I reflections are present in the x-ray patterns.

Although Barrer and White (1952) published d values of nepheline hydrate I and suggested that the phase probably had orthorhombic symmetry, no lattice parameters or indexed pattern of this mineral have been given. These parameters are interesting because their determination may show whether there is a simple relationship between nepheline hydrate I and other tridymite type structures of the nephelinekalsilite system, and also because of a suggestion by Smith and Tuttle (1957) that pure sodium nepheline (NaAlSiO₄) may contain OH⁻⁻ ions in the structure, replacing oxygen atoms.

In the present study, no exhaustive attempt was made to completely index the x-ray pattern of this mineral, but the investigation showed that nepheline hydrate I was orthorhombic with approximate lattice parameters of a=8.20 Å, b=7.50 Å, c=5.22 Å (all values ± 1 per cent). This mineral was indexed using the Hesse-Lipson method (Azaroff and Buerger, 1958) and the lattice parameters were refined using the Q values of Donnay and Donnay (1951). The accuracy of the lattice parameters and indexing was checked on a mercury computer using a least squares analysis program kindly supplied by Mr. M. T. Frost of the British Museum of Natural History. This was done by feeding into the computer the approximate lattice parameters and indices of each reflection as determined by the Hesse-Lipson method and comparing the observed 2θ values with the 2θ values calculated by the computer. Small differences in these values indicated that the indexing and lattice parameters had been correctly determined.

The d (observed) and d (calculated) values for each reflection, together with their estimated intensities, are given in Table 1. One reflection, of low intensity could not be indexed and may represent a

MINERALOGICAL NOTES

Table 1. Indexed d Values for Nepheline Hydrate I Crystallized from a Gel at 405° C. and $P_{H_{2}0}$ =1,000 kg/cm²

hkl	Intensity (estimated)	d (obs)	d (calc)
100	60	8.19	8.19
010	50	7.49	7.49
110(?)	20	5.53	5.47
101	100	4.397	4.398
?	15	3.432	
120	100	3.408	3.407
211	35	2.960	2.959
121	10	2.850	2.853
002	10	2.607	2.608
221	10	2.445	2.442
301	5	2.420	2.419
311	5	2.303	2.302

The determinations were made from an x-ray diffractometer trace using $CuK\alpha$ radiation, with an internal Si standard

minor impurity in the crystallized product. The calculated a and c parameters of nepheline hydrate I are similar to those of the c and a parameters of β -tridymite (a=5.03 Å, c=8.22 Å), but there is no apparent relationship between the b parameter of nepheline hydrate I and the third orthogonal translation of tridymite. Smith and Tuttle (1957) have shown that nepheline has the same sized c parameter as β -tridymite, and an a parameter twice as large as that of β -tridymite. The present data may suggest that the structure of nepheline hydrate I is related to a tridymite-type structure, but this relationship is not a simple one.

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