DETERMINATION OF THE CRYSTAL STRUCTURE OF NEPHELINE

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Abstract

The structure of nepheline has been determined by the implication method followed by Fourier synthesis. The dense atoms were all located with the aid of Harker syntheses and implication maps. With these atoms located, the oxygen atoms were found by successive electron density projections. Nepheline is based upon the tridymite framework in which all silicon atoms in tetrahedra pointing toward one end of the *c* axis are replaced by aluminum atoms, and the valence is compensated by adding alkali atoms to the voids. The true formula of nepheline is not $NaAlSiO_4$, but $KNa_3Al_4Si_4O_{16}$. The alkali atoms occur in two sets, one set occupying a larger void than the other. The smaller void is produced by a twisting of the tridymite framework about the sets of three-fold axes. The oxygen atoms on the three-fold axes are probably in motion, at least at elevated temperatures, and make contact with the surrounding sodium atoms only part of the time.

Introduction

There have been several *x*-ray diffraction investigations of the mineral nepheline.[1–7] All except Gossner and Jaeger agree on assigning nepheline to the space group $P6_3$ (C_6^6) with 8 $NaAlSiO_4$ per hexagonal cell. The structure has not been determined, although Schiebold[4,5] suggested that it is based upon a tridymite structure in which Al atoms were substituted for half the total Si atoms, Na being added to the voids of the structure to balance valances. This suggestion was accepted by Bannister and Hey[6] as well as by Nowacki.[7]

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[1] Gottfried, C., Über die Struktur des Nephelins: *Zeits. Krist.*, **65**, 100–109 (1926).

[2] Gossner, B., Über die Symmetrie von Nephelin: *Central. Mineral., etc.*, **A-1927**, 150–158 (1927).

[3] Jaeger, F. M., Westbrink, H. G. K., and van Melle, F. A., The structure of artificial ultramarines; a relation between these and the minerals haüynite, noselite, sodalite, lazurite, and nepheline: *Verslag. Akad. Wetenschappen Amsterdam*, **36**, 29–47 (1927).

[4] Schiebold, E., Zur Struktur von Nephelin und Analcim: *Naturwiss.*, **18**, 705–706 (1930).

[5] Schiebold, E., Über die Isomorphie der Feldspatmineralien: *Neues Jahrb. Min., etc. Bl. Bd.* **64A**, esp. pp. 312–313 (1931).

[6] Bannister, F. A., and Hey, M. H., A chemical, optical, and *x*-ray study of nepheline and kaliophilite: *Mineral. Mag.*, **22**, 569–608 (1931).

[7] Nowacki, W., Beziehungen zwischen $K[AlSiO_4]$ (Tief-Kaliophilit), $Ba[Al_2O_4]$, $K[LiSO_4]$, $Na[AlSiO_4]$ (Nephelin) und $[Si_2O_4]$ (β-Tridymit): *Naturwiss.*, **30**, 471–472 (1942).

We have carried out an investigation of the crystal structure of nepheline. This has proved to be a tedious task, largely because the structure lacks inversion centers and has little symmetry, and because the cell is moderately large.

We are indebted to Dr. Frederick H. Pough, formerly of the American Museum of Natural History, for a gift of several small nepheline crystals from Monte Somma, Vesuvius. Our first problem was the choice of a suitable small untwinned crystal. Since the point-group symmetry of nepheline is merely 6, it tends to twin into composites whose c axis Weissenberg photographs have diffraction symmetry $6mm$. A number of crystals which were suitable from point of size proved to be twinned in this way, so that we finally used a somewhat irregular, small fragment broken from a larger crystal which gave diffraction symmetry 6. We believe the fragment we used to be untwinned, since we tested the diffraction symmetry in several stages as the fragment was being reduced in dimensions and we failed to find any increase in contrast in the relative intensities of reflections which would be identical in intensity in a twin.

Cell and Space-Group Study

Preliminary Weissenberg photographs showed that the diffraction symbol of nepheline is $6/mP6_3/-$. This embraces the two space groups $P6_3$ and $P6_3/m$. Since nepheline is known not to have a symmetry plane normal to the hexagonal axis, the space group is uniquely fixed as $P6_3$. This confirms the space group determination of earlier investigators.

The preliminary Weissenberg study provided the following cell dimensions:

$$a = 10.01 \text{ Å}$$
$$c = 8.405$$

This cell contains 8 $NaAlSiO_4$. The atoms must be accommodated by the following sets of equipoints in space group $P6_3$:

2(*a*) along the 6_3 screw,
2(*b*) along the trigonal rotation axes,
6(*c*) in the general position.

Intensity Determination

For the subsequent quantitative work on the structure of nepheline it was necessary to have reasonably reliable estimates of the intensities of the spectra. For this purpose we used the Dawton[8] process modified so as to take advantage of the characteristics of photographic materials available in America.

[8] Dawton, Ralph H. V. M., The integration of large numbers of x-ray crystal reflections: *Proc. Phys. Soc.*, **50**, 919–925 (1938).

For the determination of the nepheline intensities, we used Weissenberg photographs made with crystal-monochromatized copper radiation. The Lorentz and polarization factors were allowed for in a manner described elsewhere.[9] Absorption was assumed to be negligible because of the small size of the crystal, and no further allowances were made in transforming intensities to $|F_{hkl}|$.

General Outline of the Structure Determination

Before proceeding to a detailed discussion of the determination of the crystal structure, the general plan of the structure determination is given here in bare outline.

The two possible Harker syntheses were first prepared and these were studied with the aid of their implication diagrams. By combining two implication diagrams, all the dense (metal) atoms could be located in xy projection.

Assuming that the diffraction phases were dominated by these metals alone, a preliminary electron density projection $\rho(xy)$ was prepared which showed not only the metals already located, but other dense areas, attributed to oxygen locations. The total number of oxygen atoms was distributed over these dense areas, and from their x,y coordinates, a new set of phases was computed and a new electron density projection $\rho(xy)$ was prepared. By repeating this procedure a number of times, an electron density projection was finally attained which required no further change in phases. The rough x,y projection of the structure was now known.

In order to determine the z parameters, several one-dimensional Patterson syntheses of the Harker type, namely $P(x_1y_1z)$, were prepared with strategic horizontal components x_1, y_1. A study of these made it evident that the nepheline structure is indeed based upon a stuffed tridymite framework, as suggested by Schiebold. The deviations of the z parameters from the ideal tridymite parameters could then be determined.

We were then in a position to prepare the electron density projection $\rho(xz)$ from the $h0l$ reflections and their phases computed with the aid of the parameters determined as above. This projection was refined by repetition until the last projection required no further phase changes.

The rough structure of nepheline was now determined. The structure type and approximate parameters were known, but the exact parameters were not known because of the lack of resolution in the electron density projection. To refine the structure requires the preparation of electron density sections. These are exceedingly tedious to prepare, because the phases of all reflections must be computed, and because each section in-

[9] Buerger, M. J., and Klein, Gilbert E., Correction of x-ray diffraction intensities for Lorentz and polarization factors: *J. Appl. Phys.*, **16**, 408–418 (1945).

FIG. 1. Nepheline, $P(xy0)$.

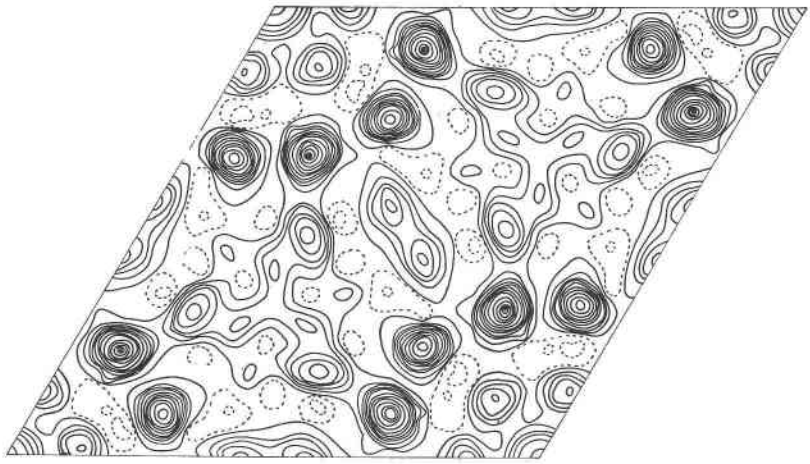

FIG. 2. Nepheline, $P(xy\frac{1}{2})$, also implication map $I6(xy\frac{1}{2})$.

volves four separate two-dimensional Fourier syntheses for the preparation of the coefficients of the two-dimensional syntheses.

HARKER SYNTHESES AND IMPLICATION MAPS

The symmetry of nepheline permits making Harker sections[10] of the Patterson[11,12] function on two levels, namely $P(xy0)$ and $P(xy\frac{1}{2})$. These were accordingly prepared from the available $|F_{hkl}|^2$ values. The Harker sections are shown in Figs. 1 and 2, respectively. The first of these can be transformed into only one *implication* map,[13] namely $I3(xy0)$,

while the second can be transformed into two implication maps, namely $I6(xy\frac{1}{2})$ and $I2(xy\frac{1}{2})$. These implication maps locate the dense atoms with the following ambiguities:

	Implication	*Ambiguity factor*
Fig. 2	$I6(xy\frac{1}{2})$	1
Fig. 3	$I3(xy0)$	3
	$I2(xy\frac{1}{2})$	4

The first and second of these were prepared and are shown in Figs. 2 and 3, respectively. The first implication, having an ambiguity factor of unity (i.e., no ambiguity) is identical with the Harker synthesis $P(xy\frac{1}{2})$.

Implication $I6(xy\frac{1}{2})$ contains satellitic peaks which are valuable in authenticating genuine Harker peaks (i.e., peaks due to "interaction" between symmetrically equivalent atoms). Each authentic Harker peak is accompanied by a satellitic peak of half the height of the Harker peak and located at twice its vector distance from the origin.[14] The authentic

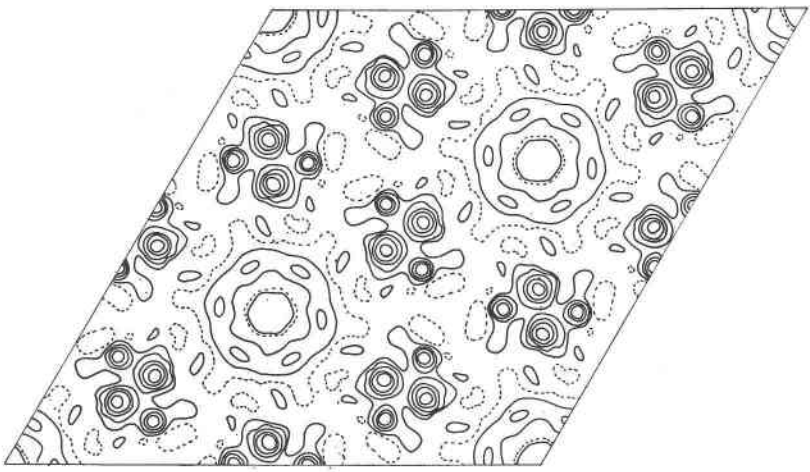

FIG. 3. Nepheline, $I3(xy0)$.

[10] Harker, David, The application of the three-dimensional Patterson method and the crystal structure of proustite, Ag_3AsS_3, and pyrargyrite, Ag_3SbS_3: *J. Chem. Phys.*, **4**, 381–390 (1936).

[11] Patterson, A. L., A Fourier series method for the determination of the components of interatomic distances in crystals: *Phys. Rev.*, **46**, 372–376 (1934).

[12] Patterson, A. L., A direct method for the determination of the components of interatomic distances in crystals: *Zeits. Krist.* (A)**90**, 517–542 (1935).

[13] Buerger, M. J., The interpretation of Harker syntheses: *J. Appl. Phys.*, **17**, 579–595 (1946).

[14] Reference 13, page 586.

peaks and their satellitic peaks are the following:

Peak	*Satellitic peak*	*Attributed to*
0, 0	0, 0	Na_1
0, .43	0, .86	Na_2
.09, .33	.18, .66	Si_2+Al_2

The atoms to which the peaks are to be attributed can be interpreted upon the assumption that nepheline is based upon a tridymite framework, Fig. 4. The other major peak of $I6(xy\frac{1}{2})$ is without an implication satellite and is therefore a non-Harker peak due to pairs of non-equivalent atoms.

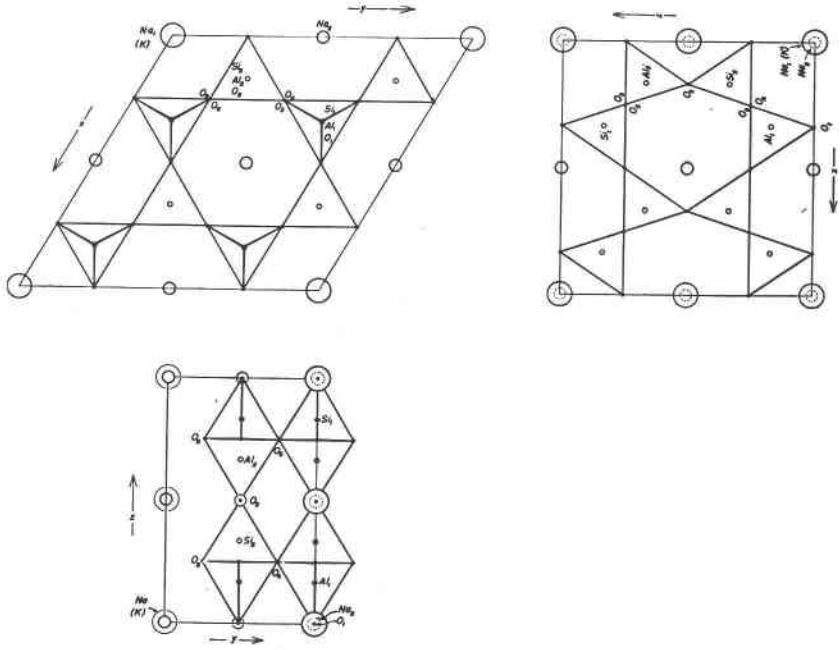

FIG. 4. Plan and elevation of ideal high tridymite referred to nepheline cell and symmetry, showing labeling of representative atoms.

On superposing the implication $I3(xy0)$ on the implication $I6(xy\frac{1}{2})$ the authenticated peaks of the latter, just listed, are found to coincide with certain of the peaks of the former. This further affirms the correctness of the positions of the atoms already located. The atoms listed in the foregoing table account for 8 Na, 6 Al, and 6 Si, out of a total of 8 Na, 8 Al, 8 Si, and 32 O. This leaves 2 Al, 2 Si, and 32 O still to be placed. Since 2 and 32 are not divisible by 6, the 2 Al, 2 Si, and at least 2 of the O's must be on either the 6-fold screw or the 3-fold axis. The former is already oc-

cupied by Na_1 atoms, which take substantially all the available space. This requires 2 Al_1, 2 Si_1, and 2 O_1, to be on the 3-fold axis. The implication peak for atoms in this location is peculiarly blurred. This is attributed to motion of the atoms so that they occupy the axis only statistically.

Determination of xy Coordinates of the Oxygen Atoms

The reasoning discussed in the last section provides the xy parameters of the atoms of nepheline as shown in column B of Table 1. The Na_1 atoms were interpreted as K atoms since the number corresponds closely to the amount of potassium in nepheline analyses.[7] The locations of thirty oxygens are unknown.

Table 1. Stages in the Determination of the Parameters of the Atoms in the Nepheline Structure

Atom	Coordinates of atoms						
	A Deduced from implication diagrams		*B* From implication diagrams plus equipoint reasoning		*C* From electron-density projection, $\rho(xy)$		*D* From lines through the Patterson function
	x	y	x	y	x	y	z
2 Na_1 (=2 K)	0	0	0	0	0	0	0
6 Na_2	0	0.43	0	0.43	0.01	0.43	0.00
2 Al_1			$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{3}$	$\frac{2}{3}$	0.18
6 Al_2	0.09	0.33	0.09	0.33	0.09	0.33	0.67
2 Si_1			$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{3}$	$\frac{2}{3}$	0.82
6 Si_2	0.09	0.33	0.09	0.33	0.09	0.33	0.33
2 O_1			$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{3}$	$\frac{2}{3}$	
6 O_2			?		0.02	0.33	
6 O_3			?		0.18	0.50	
6 O_4			?		0.17	0.53	
6 O_5			?		0.23	0.28	
6 O_6			?		0.23	0.28	

In order to locate the remaining thirty oxygen atoms it was assumed that the phases of the $hk\cdot 0$ reflections are determined, to first approximation, by the locations of the known atoms. (Fortunately, the xy projection of the space group $P6_3$ is centrosymmetrical, so the phases must be 0 or π, i.e., the signs of the F's are either positive or negative.) With this assumption, the phases of all $hk\cdot 0$ reflections were computed, and using these phases, an electron density projection, $\rho(xy)$ was prepared by the Fourier summation

$$\rho(xy) = \frac{1}{A} \sum_h \sum_k F_{hk0} \cos 2\pi(hx + ky).$$

The summation was carried out with the aid of the Patterson-Tunell method.[15] This electron density projection not only returned the atoms which were used to determine the phases, but also revealed other regions of high electron density which were interpreted to be due to the remaining oxygen atoms.

Oxygen atoms O_2, O_3, O_4, O_5, and O_6 were then distributed on these regions of high electron density and, with these new atoms located, the phases were computed again. Several sign changes occurred due to the new oxygen atoms. Utilizing these new signs, the electron density projection was again computed. The second approximation showed the new oxygen locations more clearly. Using this second electron density projection, a new set of signs for the F_{hk0}'s was computed, and the electron density projection again prepared.

This process was repeated until finally an electron density map was obtained, Fig. 5, which gave oyxgen atoms in locations such that the signs of the computed F's were the same as those which had been used for the preparation of the final electron density projection. The final set of parameters so determined is given in column C of Table 1.

This set of parameters provides a fairly good explanation of the $hk \cdot 0$ intensities. The discrepancy factor,

$$R = \frac{\sum \big| \, |F_{\text{observed}}| - |F_{\text{calculated}}| \, \big|}{\sum |F_{\text{observed}}|},$$

has a value of 0.34 for the $hk \cdot 0$; reflections, with no allowance being made for a temperature factor. That the parameters do not provide a perfect explanation of the intensities is to be expected because the parameters are approximate. This is partly because pairs of atoms which overlap in projection are unresolved, or poorly resolved, and consequently the location of each of the pair is in doubt. This kind of overlap is most annoying in derivative structure,[16] and nepheline is a derivative structure of tridymite in which the following sets of atoms overlap (see Fig. 4): Al_1,Si_1,O_1; Al_2,Si_2,O_2; O_3,O_4; O_5,O_6. The atoms in these sets are unresolved, and their parameters as determined above are probably subject to small but annoying errors.

A second reason why the discrepancy factor, R, is high, is that Al_1, Si_1, and O_1 are assumed to occupy the 2-fold equipoint, namely the 3-fold

[15] Patterson, A. L., and Tunell, George, A method for the summation of the Fourier series used in the x-ray analysis of crystal structures: *Am. Mineral*, **27**, 655–679 (1942).

[16] Buerger, M. J., Derivative crystal structures: *J. Chem. Phys.*, **15**, 1–16 (1947).

axis. There are several reasons which suggest that this is not the precise distribution of these atoms. These reasons are noted at the end of this paper.

Determination of Z Parameters

In order to determine the z parameters of the atoms, several lines through the three-dimensional Patterson function parallel to the c axis were computed. These lines were chosen to have vector components in the XY plane, equal to the vector from the K atom at the origin to each of the metal peaks. The following syntheses were made:

	to determine z parameters of
$P\ (\frac{2}{3}\ \frac{1}{3}\ z)$	Al_1, Si_1, O_1
$P\ (0.09, 0.33\ z)$	Al_2, Si_2, O_2
$P\ (0, 0.43, z)$	Na_2

The interpretation of these syntheses was again made difficult because nepheline is a derivative structure of tridymite. Nevertheless, prominent peaks were found on these lines which were consistent with the vector distances from K to the several metal atoms expected from a derivative structure of ideal high tridymite. The z coordinates so found as listed in Table 2.

Projections of the Structure Involving z

In order to refine the structure as much as possible, the phases of the 62 observed $h0 \cdot l$ reflections were computed based upon the x, y param-

Table 2

	Idealized derivative of tridymite z	Nepheline, as determined from one-dimensional Harker syntheses z
Na_1 (=K)	0	0
Na_2	0	0.00
Al_1	$\frac{1}{6}$	0.18
Al_2	$\frac{2}{3}$	0.67
Si_1	$\frac{5}{6}$	0.82
Si_2	$\frac{1}{3}$	0.33
O_1	0	—
O_2	$\frac{1}{2}$	—
O_3	$\frac{3}{4}$	—
O_4	$\frac{1}{4}$	—
O_5	$\frac{1}{4}$	—
O_6	$\frac{3}{4}$	—

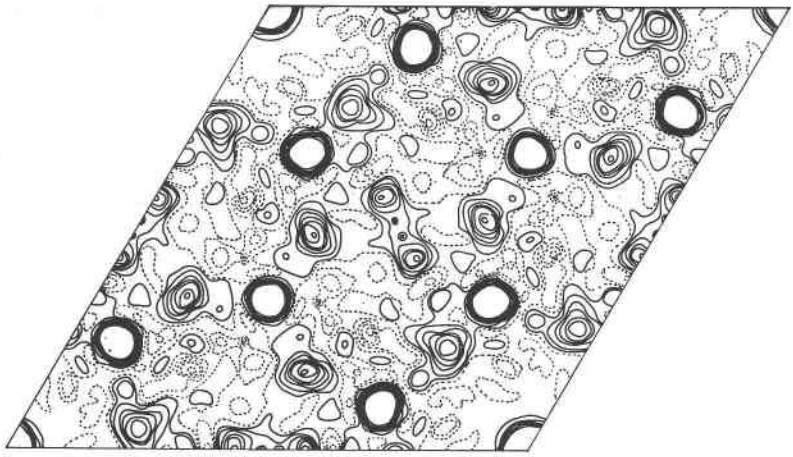

FIG. 5. Nepheline, $\rho(xy)$. The interpretation of this electron density projection is shown below in Fig. 6.

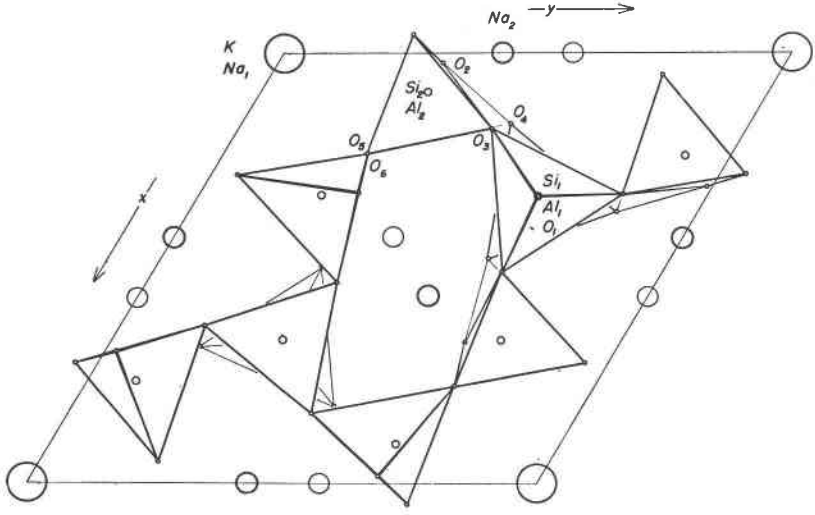

FIG. 6. Interpretation of electron density map, shown above in Fig. 5, giving designations of representative atoms.

eters determined from the $\rho(xy)$ electron density projection, and the z parameters determined from the one-dimensional Harker syntheses, plus idealized values of the z parameter for the oxygen atoms. This provided data for the determination of the electron density $\rho(xz)$ as projected parallel to a_2 onto the plane $(1\bar{2}10)$. Such a preliminary projection was prepared, and this was subsequently refined exactly as in the case of the

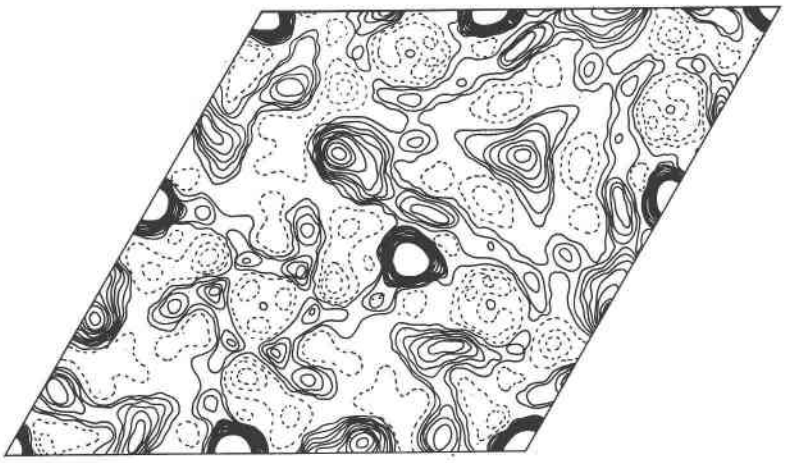

FIG. 7. Nepheline, electron density section $\rho(xy0)$.

$\rho(xy)$ projection. Unfortunately, in the $\rho(xz)$ projection no peaks corresponding to the oxygen atoms O_3, O_4, O_5, or O_6 are sufficiently resolved to permit an adequate determination of the parameters. Finally the $hh\cdot l$ reflections were used to prepare a Fourier synthesis of the electron density projected parallel to [210] onto plane (100).

FINAL ROUGH PARAMETERS

The final parameters of tridymite as determined by the study just described, are listed in Table 3. These parameters should be regarded as approximate and subject to further refinement for the following reasons:

(1) The parameters of the atoms other than K and Na are determined from electron density projections in which there is overlapping of atoms.

(2) There are reasons for believing that the Al_1, Si_1, and O_1 atoms, which were taken to occupy the equipoint 2 (*b*) because of the numbers of atoms involved, do not actually occupy this equipoint in a strict sense.

(*a*) The fundamental evidence for this is that the peak corresponding with this position on the implication map, Fig. 2, is not as high as that corresponding to the similar group of atoms, Al_2, Si_2, and O_2. This means that the density at the position accepted for Al_1, Si_1, O_1, is not as high as at the position for Al_2, Si_2, O_2. The density deficiency can be accounted for if one or more of these atoms, supposed to occupy the three-fold axis, do so only statistically, i.e., if they are actually off the axis but assume positions with time whose averages lie on the three-fold axis.

(*b*) We made an electron density section $\rho(xy0)$, Fig. 7. In this section the oxygen on the three-fold axis is more diffuse than the other oxygens in the section, and, furthermore, it is smeared so as to look like the projection of a three-bladed propeller, with the blades directed halfway between pairs of the three surrounding sodium atoms. We interpret this to mean that the oxygen is not actually on the three-fold axis,

TABLE 3. COORDINATES OF ATOMS IN NEPHELINE, COMPARED WITH THOSE OF IDEAL HIGH TRIDYMITE

Atom	Coordinates in ideal high tridymite			Coordinates in nepheline			Remarks
	x	y	z	x	y	z	
2 Na_1 (=K)	0	0	0	0	0	0	(void in tridymite)
2 Al_1	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{6}$ (.167)	$\frac{1}{3}$	$\frac{2}{3}$	.18	
2 Si_1	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{5}{6}$ (.833)	$\frac{1}{3}$	$\frac{2}{3}$	.82	
2 O_3	$\frac{1}{3}$	$\frac{2}{3}$	0	$\frac{1}{3}$	$\frac{2}{3}$	.00	
6 Na_2	0	$\frac{1}{2}$	0	$.00_8$	$.43_2$	.00	(void in tridymite)
6 Al_2	$\frac{1}{6}$ (.167)	$\frac{1}{3}$ (.333)	$\frac{2}{3}$ (.667)	$.09_2$	$.33_0$	.67	
6 Si_2	$\frac{1}{6}$ (.167)	$\frac{1}{3}$ (.333)	$\frac{1}{3}$ (.333)	$.09_2$	$.33_0$	.33	
6 O_2	$\frac{1}{6}$ (.167)	$\frac{1}{3}$ (.333)	$\frac{1}{2}$ (.500)	$.02_0$	$.33_0$	.50	
6 O_3	$\frac{1}{4}$ (.250)	$\frac{1}{2}$ (.500)	$\frac{3}{4}$ (.750)	.18	.50	~.75	
6 O_4	$\frac{1}{4}$ (.250)	$\frac{1}{2}$ (.500)	$\frac{1}{4}$ (.250)	.17	.53	~.25	
6 O_5	$\frac{1}{4}$ (.250)	$\frac{1}{4}$ (.250)	$\frac{1}{4}$ (.250)	.23	.28	~.25	
6 O_6	$\frac{1}{4}$ (.250)	$\frac{1}{4}$ (.250)	$\frac{3}{4}$ (.750)	.23	.28	~.75	

except statistically. At any one time, it is coordinating with only two of the three surrounding sodium atoms, and this connection varies with time. In other words, the oxygen atom is undergoing a kind of a rotation or gyration about the three-fold axis.

(*c*) The gyration of the oxygen atom about the three-fold axis is not unexpected. It is well-known that there is a bend in the alignment of the three atoms Si-O-Si in the silica structures, and it should be expected in the alignment Al-O-Si also. This bent alignment cannot occupy a three-fold axis, unless it does so statistically. The meaning of the three-fold axis is then that the bend takes three equivalent positions with time.

The gyration of the oxygen atom about the three-fold axis must be accompanied by a gyration of the silicon and aluminum atoms about the same axis. This would explain why the peak on this axis in the implication map $I6(xy\frac{1}{2})$ is low and propeller-shaped. Unless such deviation occurs for the silicon and aluminum atoms there is no explanation for the character of this Harker projection.

It is interesting to note that only 2 of the 32 oxygen atoms of the cell appear to gyrate. It is known that nepheline undergoes a reconstructive transformation to an isometric form, carnegieite at 1248° C. Presumably, at this temperature, all the oxygen atoms begin to gyrate with consequent increase in symmetry.

DISCUSSION

In spite of the fact that only rough parameters for the nepheline structure can be given at this time, a number of interesting mineralogical conclusions can be drawn. In the first place, as Schiebold predicted[4], the structure of nepheline is indeed based upon a generalization of the tridymite structure. If all the silica tetrahedra in the tridymite structure

which point, say, up, are replaced by alumina tetrahedra, and if the largest voids are stuffed with alkali atoms to balance the loss of positive charge due to this replacement, a nepheline-like structure results. The replacement of silicon by aluminum gives the hexagonal axis a polar character which is absent in the parent tridymite structure.

The space requirements of the alkali atoms give rise to two interesting features. In the first place, sodium is too small to occupy the voids and at the same time coordinate with the surrounding oxygen atoms. The tridymite framework therefore collapses somewhat by a twisting motion centered about the three-fold axes of the space group, and in so doing clutches the sodium atoms in the general position. This twisting collapse of the framework robs the idealized framework of its vertical symmetry planes, and therefore nepheline has no symmetry planes whatever (the horizontal plane having been lost by replacings ilicon with aluminum, as discussed above). Since the twisting motion may be either right or left, a right-or left-handed nepheline results.

The twisting motion does not significantly reduce the size of the void occupied by the alkali atom in the special position on the 6_3 axis to the same extent that it reduces the general-position void, just discussed. As a consequence, a large symmetrical hole capable of supplying a nine-fold oxygen coordination remains to be occupied by two of the eight alkali atoms of the cell. Since potassium is better suited by size to occupy such a void, it does so, provided that the nepheline crystallizes from an environment capable of supplying potassium. For this reason, natural nepheline invariably has this site substanitally filled with potassium instead of sodium. The symmetry of the nepheline structure requires that the alkali atoms be divided into two sets of 2 and 6. These two sets may, but need not, be occupied by the same chemical element, and, indeed, in general, K and Na may be expected to separate into the 2-fold and 6-fold sites respectively. Pure sodium nepheline is formed only when there is no potassium present in the environment of crystallization. Thus the ideal chemical formula for nepheline is not the currently quoted $NaAlSiO_4$, but rather $KNa_3Al_4SiO_{16}$. The analyses collected by Bannister and Hey[6] confirm this view. Since calcium is about the right size to proxy for potassium, it also may be found in the 2-fold site, thus either reducing the amount of the 2-fold alkali metal, or increasing the aluminum:silicon ratio.

Further Investigation in Progress

The members of the group which undertook the original investigation of the nepheline structure, as discussed in this paper, now reside in three different locations. The refinement of the structure is now being con-

tinued at the Crystallographic Laboratory of the Massachusetts Institute of Technology by M. J. Buerger and Theodor Han. It is expected that this refinement process will reveal more exact coordinates of the atoms, and specifically provide detailed information on the coordinates of the sodium atoms and the possible gyration of the atoms in the neighborhood of the three-fold axis.

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