

Okenite and nekoite (a new mineral).

(With Plate I.)

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Summary.—The unit cell of okenite ($\text{CaO} \cdot 2\text{SiO}_2 \cdot 2\text{H}_2\text{O}$) has been determined for a specimen from Bombay, India, using a combination of X-ray, electron-microscope, and electron-diffraction methods. It is anorthic with¹ a 9.84, b 7.20, c 21.33 Å., α 90.0°, β 103.9°, γ 111.5°, elongation b , $Z = 9$. These data are compatible with the goniometric results of Bøggild (1922) and allow the latter to be interpreted.

A specimen from Crestmore, California, which Eakle (1917) had described as okenite, was also examined. It was found to be a new species, having the same composition as okenite but distinguishable from it by its optical properties, X-ray powder data, and unit cell. The latter is anorthic with¹ a 7.60, b 7.32, c 9.86 Å., α 111° 48', β 86° 12', γ 103° 54', elongation b , $Z = 3$. Because of the relation to okenite, the name *nekoite* is suggested.

PART I. OKENITE.

OKENITE ($\text{CaO} \cdot 2\text{SiO}_2 \cdot 2\text{H}_2\text{O}$) was discovered on Disko Island, Greenland. It was first analysed by von Kobell² and described by Breithaupt.³ It has since been found in other localities, usually associated with basalt. Satisfactory optical and goniometric data were first obtained by Bøggild;⁴ the former are given in table I and the latter in table IV. These data showed that okenite was anorthic, but the axial ratios could not be obtained. The optical data were confirmed by Tilley and Alderman.⁵ X-ray powder data have been reported (table II), and X-ray photographs of fibrous aggregates have shown that okenite belongs to the group of fibrous hydrated calcium silicates having a repeat distance of about 7.3 Å. in the fibre direction.⁶ No single-crystal data have been reported and the unit cell has not previously been determined.

¹ This cell is not in conventional orientation: see pp. 13 and 16, footnotes.

² F. von Kobell, Arch. gesammte Naturlehre (Kastner), 1828, vol. 14, p. 333.

³ A. Breithaupt, Ann. Phys. Chem. (Poggendorff), 1845, vol. 64, p. 170.

⁴ O. B. Bøggild, Kgl. Danske Vidensk. Selsk., Math.-fys. Medd., 1922, vol. 4, no. 8 [M.A. 2-59].

⁵ C. E. Tilley and A. R. Alderman, Min. Mag., 1934, vol. 23, p. 513.

⁶ H. F. W. Taylor, Proc. Int. Symp. Reactivity of Solids, Gothenburg, 1952 p. 677.

Optical and X-ray investigation.

A specimen from the Syhadree Mountains, Bombay, India (B.M. 27989), was employed. It consisted of fibrous aggregates showing parallel extinction, positive elongation, low birefringence, and mean

TABLE I. Optical and unit-cell data for okenite and nekoite.

<i>Optical data.</i>	Okenite.	Nekoite.
Locality:	Disko Island and Faeroe Islands	Crestmore, California
Investigator:	Bøggild	This investigation
Habit:	Usually fibrous. Single crystals are prisms with one good cleavage	Needles with one good cleavage
Twinning:	On the cleavage face, very common. On the prism axis, rare	Needles show repeated twinning with lamellae parallel to the cleavage
Indices:	α' 1.530, γ' 1.541	Mean 1.535 \pm 0.002 (Na)
Birefringence:	0.011	Very low
Extinction:	Crystals lying on the cleavage have parallel extinction, \dots elongation. In other orientations, extinction is oblique; for laths lying on edge it makes $32 \pm 2^\circ$, and for laths standing on end, 25° with the cleavage trace	Always inclined. Individual lamellae lying on the cleavage have \dots elongation, extinction angle 26° . Lamellae standing on edge have \dots elongation, extinction of adjacent twin lamellae symmetrical at 5° to the twin boundaries
Interference figure:		Individual lamellae lying on the cleavage give a poor biaxial + acute bisectrix figure
2V:	Probably large	70° approx.
Optic sign:	Negative*	Positive
Optic orientation:		X makes about 26° with the needle axis, and Z is roughly perpendicular to the cleavage
<i>Unit-cell data.</i>		
System:	Anorthic	Anorthic
Parameters:	a 9.84 Å, b 7.20 c 21.33 (3×7.11) α 90° β 103.9° γ 111.5°	c 9.86 Å, b 7.32 a 7.60 γ $103^\circ 54'$ β $86^\circ 12'$ α $111^\circ 48'$
Cell contents:	9[CaO.2SiO ₂ .2H ₂ O]	3 [CaO.2SiO ₂ .2H ₂ O]
Fibre direction:	b	b
Cleavage:	(001)	(100)

* C. E. Tilley and A. R. Alderman, loc. cit., for a specimen from Scawt Hill (Northern Ireland).

refractive index, 1.540 ± 0.003 . Similar data were obtained by Christie¹ for a specimen of a comparable degree of crystallinity, also from Bombay. The data are compatible with those obtained by Bøggild for single crystals from the type locality and elsewhere although, because they relate to fibrous aggregates, they are necessarily less detailed.

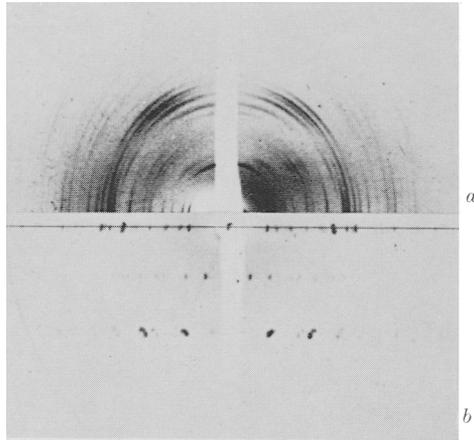


FIG. 1. X-ray rotation photographs about the needle or fibre axis. Cu- $K\alpha$ radiation. *a*, okenite, Bombay; *b*, nekoite, Crestmore.

X-ray powder data, obtained using 6-cm. and 19-cm. diameter cameras with Cu- $K\alpha$ radiation, are included in table II. They are in substantial agreement with the various sets of data obtained by previous workers, including those of McMurdie and Flint, which probably relate to material from the type locality. Minor differences exist between all the sets of data, but they can probably be attributed to the presence of impurities in some or all of the specimens, and the data indicate that all consist of substantially the same mineral.

The X-ray fibre rotation patterns previously reported, and reproduced in fig. 1*a*, showed that the repeat distance along the fibre axis (later shown to be *b*) was 7.20 \AA . They also enabled the *k*-indices of the powder reflections to be determined, and these indices are also included in table II.

Attempts to isolate single crystals of sufficient size for X-ray work were unsuccessful, even the thinnest fibres giving rotation photographs. Complete indexing of the data by X-ray means was therefore not possible, and electron diffraction was employed.

¹ W. A. K. Christie, Rec. Geol. Survey India, 1925, vol. 56, p. 199 [M.A. 3-287].

TABLE II. X-ray powder data for okenite and nekoite. Spacings in Å.

1.		2.			3.		4.		5.	
<i>d.</i>	<i>I.</i>	<i>d.</i>	<i>I.</i>	<i>k.</i>	<i>hkl.</i>	<i>d.</i>	<i>d.</i>	<i>I.</i>	<i>hkl.</i>	<i>d.</i>
10.61	30	21	vvs	0	001	20.6				
8.87	100	10.3	vw	0	002	10.3				
7.65	70	8.8	vs	0	200	8.84	9.25	vs	001	9.15
6.72	70	7.4	mw	0	201	7.46	7.45	w	100	7.39
5.72	30	6.8	vw	1	110	6.67	6.61	w	{ 01 $\bar{1}$	6.63
		6.19	w	0	20 $\bar{3}$	6.26			{ 010	6.61
		5.79	vvw	1	11 $\bar{2}$	5.86			{ (10 $\bar{1}$	5.82)
5.35	10	5.22	w	0	004	5.25	5.64	w(b)	{ 101	5.67
									{ $\bar{1}$ 11	5.55
4.57	90	4.42	w	0	400	4.42	4.55	vw	{ 002	4.57
4.23	70	4.27	vvw(b)	1	311	4.28			{ (110	4.44)
4.08	70	4.08	vw	0	401	4.11	4.14	vw	$\bar{1}$ 1 $\bar{2}$	4.20
3.90	70	3.90	vw	1	114	3.90				
3.56	90	3.56	vs	0 &	{ 405	3.56				
					{ 021	3.55				
3.35	60	3.34	vvw	2	{ 22 $\bar{1}$	3.34	3.36	vs(b)	{ 201	3.39
					{ 220	3.33			{ 020	3.30
		3.22	vvw	1	{ 510	3.18				
					{ 51 $\bar{3}$	3.18				
					{ 116	3.18				
					{ 602	3.05				
3.09	90	{ 3.07	s	0 &	{ 207	3.04	3.04	w	003	3.05
		{ 3.05	s	0	{ 222	3.08				
					{ 601	3.03				
					{ 60 $\bar{3}$	3.00				
(2.99 m)*		2.98	ms	0 &	{ 404	2.99				
				2	{ 224	3.01				
					{ 024	2.95				
					{ 600	2.95				
2.92	90	2.93	vs	0 &	{ 206	2.95	2.92	w	{ 12 $\bar{1}$	2.94
				2	{ 007	2.94			{ 20 $\bar{2}$	2.91
		2.80	w	0	{ 223	2.89			{ 202	2.84
2.78	70	2.77	ms	2	{ 407	2.81	2.82	vs	{ 12 $\bar{2}$	2.81
2.69	30	2.68	vw	0	{ 602	2.66			{ (02 $\bar{3}$	2.81)
2.53	40	2.53	w	0	{ 408	2.53			{ 103	2.79
		2.44	vvw	2	{ 423	2.45	2.47	ms	121	2.45
2.39	60	2.38	vw	0	{ 20 $\bar{9}$	2.37	2.36	vvw	301	2.36
					{ 227	2.32				
2.30	40	2.30	vw	2	{ 62 $\bar{1}$	2.32	2.28	vw		
					{ 424	2.30				
					{ 226	2.28				
2.22	40	{ 2.24	w	0	{ 608	2.25				
		{ 2.20	w	2	{ 407	2.24				
					{ 427	2.21	2.20	w		
(2.16 w)*		2.15	mw	0	{ 605	2.15	2.15	vvw		
					{ 209	2.15				
1.98	60	1.98	vw	0	{ 803	1.96	2.09	vvw		
		1.91	vw(b)	0	0.11.0	1.87				
1.88	60	1.89	w	2	{ 62 $\bar{8}$	1.91	1.90	mw		
					{ 820	1.88				
					{ 427	1.88				
		1.84	vw	2	{ 625	1.84				
					{ 821	1.82				

TABLE II (cont.)

1.		2.			3.		4.		5.	
<i>d.</i>	<i>l.</i>	<i>d.</i>	<i>l.</i>	<i>k.</i>	<i>hkl.</i>	<i>d.</i>	<i>d.</i>	<i>l.</i>	<i>hkl.</i>	<i>d.</i>
1.80	90	1.80	s	4	040	1.80	1.83	ms		
1.77	30	1.77	vw				1.79	mw		
1.73	20	1.74	vvw							
		1.71	vvw							
1.68	30	1.68	vvw				1.69	w		
1.63	10	1.64	vvw(b)				1.65	vw		
							1.615	vw		
1.58	40	1.59	ms				1.583	vvw		
1.55	30	1.56	mw				1.546	w		
1.51	40	1.52	mw							
1.45	40	1.47	vvw				1.455	vw		
1.43	30	1.45	mw				1.413	vvw		
1.39	30	1.39	vvw				1.392	vvw		
1.36	40	1.36	mw				1.357	vw		
1.33	40	1.33	w							
1.28	20	1.289	w							
1.26	20	1.256	w							
1.21	30	1.207	w							
1.19	30	1.193	vw							
1.14	10	1.146	vw							
1.11	10	1.112	w							
		1.080	w							
		1.064	w							

- Okenite, Bordø, Faeroe Islands. American Society for Testing Materials. Card File of X-Ray Diffraction Data. Cards Nos. 2 0069 and 2 0070, from data supplied by Imperial Chemical Industries Ltd., Northwich, England. Relative intensities on numerical system.*
- Okenite. B.M. 27989, Syhadree Mtns., Bombay. This investigation. Cu-K α radiation. *k*-indices deduced from fibre photographs.
- Okenite. Indices and spacings calculated on the basis of the monoclinic pseudo-cell of the present investigation.
- Nekoite, U.S.N.M. 95637, Crestmore, California. This investigation. Cu-K α radiation.
- Nekoite. Anorthic indices and calculated spacings. Indices and calculated spacings of weak reflections making minor contributions to the powder photograph are enclosed in parentheses; those of very weak reflections making negligible contributions are omitted.

* Data of McMurdie and Flint (see below); these lines were not recorded in the I.C.I. data.

† Less complete powder data for okenite were given by L. M. Clark and C. W. Bunn (Journ. Soc. Chem. Ind., 1940, vol. 59, p. 155 [M.A. 8-116]), locality and radiation not stated; and by H. F. McMurdie and E. P. Flint (Journ. Res. Nat. Bur. Stand. U.S.A., 1943, vol. 31, p. 225 [M.A. 9 45]; A.S.T.M. Index, Card No. 2-0068), Disko Island, Greenland, Cu-K α radiation.

Electron-diffraction investigation.

A Metropolitan-Vickers EM3 electron microscope was used. The operation of this type of instrument has been described elsewhere.¹ It

¹ C. E. Challice, Proc. Physical Soc., ser. B, 1950, vol. 63, p. 59; J. F. Brown and D. Clark, Acta Cryst., 1952, vol. 5, p. 615; T. B. Rymer, Brit. Journ. Appl. Phys., 1953, vol. 4, p. 297.

can be used both as an electron microscope and as a diffraction instrument. In the latter case, the area of the specimen from which the diffraction pattern is obtained can be reduced to a circle about 2μ in diameter. A pattern can thus be obtained from a very small individual crystal, and its orientation relative to the outline of the crystal can be determined. The diffraction pattern is a practically undistorted picture of the reciprocal lattice in the plane through the origin and normal to the electron beam.

Specimens were prepared by crushing a little material in water and allowing a drop of the dilute suspension to dry on a film-coated specimen grid. An electron micrograph is shown in pl. I, A, B, and C. The crystals were laths of average dimensions $6 \times 2 \times 0.5 \mu$. On closer examination these were seen to consist of very thin parallel sheets, with excellent cleavage in planes parallel to the supporting film, i.e. normal to the electron beam. Individual sheets were found by shadow-casting¹ to vary in thickness between about 20 and 250 Å. It will be shown later that these sheets are possibly twin lamellae.

The laths had well-defined edges along a direction later identified with the fibre axis of the X-ray rotation photograph, but no faces other than the one cleavage face could be distinguished.

The crystals all gave substantially identical diffraction patterns, a typical example being shown in fig. 2*a*. If the cleavage plane normal to the beam is taken as (001), two unit-cell dimensions a and b , and the angle γ , can be obtained directly from the pattern. The reciprocal lattice direction c^* coincides with the electron beam, but the $(0a^*b^*)$ plane coincides with (001) only if α and β are both 90° . Evidence will be presented to show that this is not the case, and that the pattern is therefore a projection of the $(0a^*b^*)$ plane in the direction of the beam, the large number of reflections recorded being due to the fact that the reciprocal lattice points are elongated parallel to the thin direction of the crystal.

Measurement of the pattern showed that all the reflections could be fitted geometrically on to a c -face centred monoclinic reciprocal lattice, and the resulting dimensions for the real and reciprocal cells are given in fig. 3*a*. The relative intensities depend on too many factors to confirm or disprove monoclinic symmetry, but the goniometry and optical data strongly indicate anorthic symmetry. It therefore seemed preferable to express the results in terms of an anorthic unit cell. These are given for the real and reciprocal cells in fig. 3*b*.

¹ R. E. Williams and R. W. G. Wyckoff, Journ. Appl. Phys., 1944, vol. 15, p. 712.

The other three parameters, c , α , and β , were obtained from a comparison of electron-diffraction and X-ray data. The two longest X-ray spacings (21 and 10.3 Å.; table II) have ($h0l$) indices, but are too large to correspond to any of the ($h00$) reflections, found using electron diffraction. They therefore have ($00l$) indices, and were assumed to be respectively (001) and (002), giving $c^* = 1/(20.6) \text{ \AA}^{-1}$

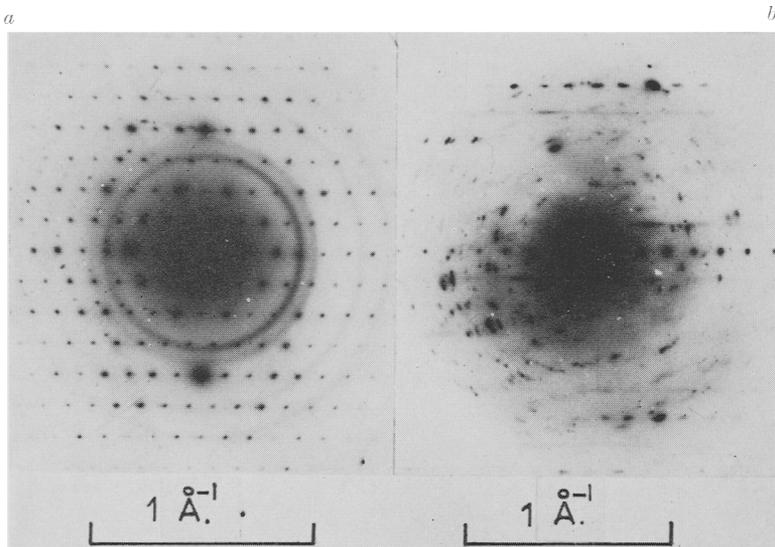


FIG. 2. Electron-diffraction patterns given by single flakes in the electron microscope. *a*, okenite lying on (001); *b*, the same after heating at 1000° C. Fibre direction vertical in each case.

The repeat distance of 7.20 Å. along the fibre direction, found using X-rays, agrees with the value of b obtained with electron diffraction. The ($0a^*b^*$) plane of the reciprocal lattice therefore coincides with (001) along the fibre direction (b), making $\alpha = 90^\circ$.

The third longest X-ray spacing, of approximately 8.8 Å., also has ($h0l$) indices. It was assumed that that of 4.42 Å. was its second order, giving a more precise value of 8.84 Å. This does not agree with any of the apparent ($h00$) spacings measured by electron diffraction, but is near enough to the apparent (100) (monoclinic (200)) spacing of 9.09 Å. (fig. 3) to suggest that the two are probably associated with the same elongated reciprocal lattice point. If this assumption is correct, the angle ($90 - \beta^*$) which a^* makes with (001) is equal to $\cos^{-1}(8.84/9.09)$,

or approximately 13° (fig. 4). β is therefore approximately $(90+13)^\circ$, or 103° .

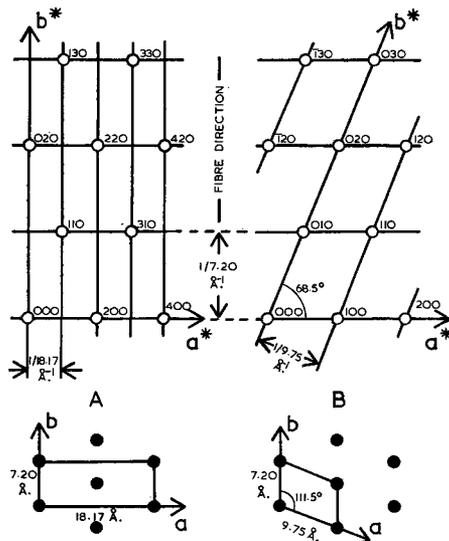


FIG. 3. Interpretation of the electron-diffraction pattern of okenite. A (left): observed reflections indexed on the (001) projection of a geometrically monoclinic c -face centred reciprocal lattice, with the corresponding real pseudo-cell below. B (right): the same reflections indexed on the (001) projection of an anorthic reciprocal lattice, with the corresponding real unit cell below.

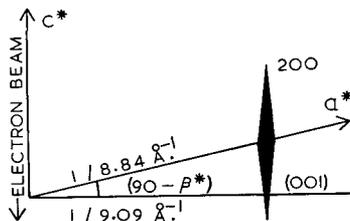


FIG. 4. Determination of the approximate value of pseudo-monoclinic $(90 - \beta^*)$ for okenite, by comparison of X-ray and electron-diffraction data. Section of the reciprocal lattice passing through the origin and normal to b , showing how the apparent a -axis of 9.09 \AA , derived from electron-diffraction data may be reconciled with the value of 8.84 \AA , given by the X-ray data.

Unit cell, twinning, and goniometric data.

From the above considerations the monoclinic pseudo-cell was assumed provisionally to have the parameters a 18·18, b 7·20, c 21·2 Å., β 103°. In order to check that these parameters were basically correct, and also to obtain a more accurate value of β , spacings were calculated and compared with the X-ray powder and fibre data. Several values of β were tried, and good agreement between observed and calculated values, as regards both spacings and k -indices, was obtained for $\beta = 105^\circ$ (table II). The revised parameters for the monoclinic pseudo-cell were thus found to be¹ a 18·30, b 7·20, c 21·33 Å., β 105°. The corresponding anorthic unit cell has² a 9·84, b 7·20, c 21·33 Å., α 90·0°, β 103·9°, γ 111·5°.

In the course of the electron-diffraction investigation, attempts were made to determine c directly by the method of Laue zones.³ These were unsuccessful, no division of the pattern into zones being observed, even though the specimen stage was tilted at angles up to 35° from the normal position, and diffraction patterns recorded for many crystals with their fibre axes approximately parallel to the axis of tilt. This remarkable absence of zoning is accounted for if the crystals have repeated lamellar twinning across the cleavage plane, so that the continuous row of lattice points along c , needed for the production of Laue zones, is not present. Twinning according to this law was found by Bøggild to be very common in larger crystals. The present results, including the appearance of the crystals in the electron microscope (pl. I), suggest that repeated twinning of this type may occur in the fibrous material from Bombay on a very small scale in which individual twin lamellae are perhaps sometimes only a few unit cells thick. This might be expected to have some influence on the X-ray pattern; in fact, Heller⁴ observed minor variations in the patterns obtained from different fibres taken from this same specimen of okenite, and mentioned complex twinning as one possible explanation.

Calculation from the unit-cell data obtained in the present investiga-

¹ This cell, having $c > a$, is not in the conventional orientation. Application of the transformation matrix $\begin{pmatrix} 001/0\bar{1}0/100 \end{pmatrix}$ gives: a 21·33, b 7·20, c 18·30 Å., β 105°; fibres parallel to b , cleavage (100).

² This cell is not in the conventional orientation. Application of the transformation matrix $\begin{pmatrix} 110/00\bar{1}/010 \end{pmatrix}$ gives: a 9·84, b 21·33, c 7·20 Å., α 90·0°, β 111·5°, γ 86·1°; fibres parallel to c , cleavage (010).

³ J. F. Brown and D. Clark, loc. cit.

⁴ L. Heller, Proc. Third Internat. Symposium Chemistry of Cement, London, 1952; Cement and Concrete Association, London, 1954, p. 237.

tion and the chemical analysis and specific gravity (2.302) determined by Christie, gave the cell contents listed in table III. They indicate the ideal formula $9[\text{CaO} \cdot 2\text{SiO}_2 \cdot 2\text{H}_2\text{O}]$ or $\text{Ca}_9\text{Si}_{18}\text{O}_{63}\text{H}_{36}$ per (anorthic) unit cell.

Bøggild obtained approximate goniometric data for very small single crystals from Disko Island and the Faeroe Isles. He described them as laths with cleavage (010) and length c . His results, obtained using a

TABLE III. Chemical analyses and unit-cell contents of okenite and nekoite.

			1.	2.				1a.	2a.
SiO_2	53.88	56.17	Si	...	16.86	6.21	
Al_2O_3	0.08	—	Al	...	0.04	—	
Fe_2O_3	0.01	—	Fe	...	—	—	
CaO	27.61	26.10	Ca	...	9.00	3.09	
SrO	0.27	—	Sr	...	0.04	—	
Na_2O	0.12	—	Na	...	0.06	—	
K_2O	0.06	—	K	...	0.02	—	
H_2O	18.02	16.83	H	...	37.8	12.4	
			100.05	99.10	O	...	61.6	21.7	
Sp. gr.	2.302	2.206					

1. Okenite, Bombay. W. A. K. Christie (analysis no. 2).

2. Nekoite, Crestmore. A. S. Eakle (analyst, W. F. Foshag).

1a. Atomic cell-contents calculated from analysis 1 (anorthic cell).

2a. Atomic cell-contents calculated from analysis 2 (anorthic cell).

two-circle goniometer, are given in table IV, which shows also that each of the faces which he measured can be satisfactorily explained on the basis of the anorthic cell found in the present investigation. Bøggild's choice of axes was not retained, because it obscures the relation between

TABLE IV. Comparison of observed and calculated goniometric data for okenite.

Indices.		Bøggild.		Calculated.	
New		ϕ .	ρ .	ϕ .	ρ .
Bøggild. (anorthic).	(001)	0°	90°	0°	90°
(010)	(102)	$56 \pm 2^\circ$	90°	58°	90°
(100)	(100)	$76(68-82)^\circ$	90°	75°	90°
(001)	(011)	$141 \pm 5^\circ$	$33 \pm 2^\circ$	139°	31°
(hkl)	(111)	118°	54°	119°	53°
(hkl)*	(102)	39°	90°	41°	90°
(010)†	(001)	0°	90°	0°	90°

For the interaxial angle β in his orientation (γ in the new anorthic orientation), Bøggild found $67-68^\circ$; we calculate 68.5° .

* Composition plane of twins about Bøggild's c [001] (new anorthic b [010]).

† Composition plane of twins across Bøggild's (010) (new anorthic (001)).

the anorthic cell and the *c*-face centred monoclinic pseudo-cell. The agreement between the present results and Bøggild's provides further evidence for the correctness of the proposed cell. It also affords further evidence for the identity of the Bombay specimen with the type material.

Dehydration.

Heller's X-ray studies showed that okenite changes to orientated wollastonite and unorientated cristobalite at 730° or above, the *b*-axis of the wollastonite coinciding in direction and approximately in length with that of the okenite from which it was formed. They did not show whether orientation was preserved in the sense of rotation around the *b*-axis, and in an attempt to settle this point a portion of the present material was heated to 1000° and then examined in the electron microscope. The micrographs (pl. I, D) confirmed that the product consisted of pseudomorphs of the original material. The flakes had a slightly mottled appearance, and on close inspection some of them appeared to be broken into parallel fibres a few hundred Ångströms wide, lying along the fibre direction. The corresponding diffraction patterns (fig. 2*b*) showed distinct layer-lines perpendicular to the fibre direction, with a repeat distance of 7.26 Å. The even layer-lines consisted of relatively sharp spots, but the odd ones consisted of streaks. There was always some disorder in the direction of the fibre axis, which varied within each flake through a few degrees from the mean position. Flakes varied considerably in the degree of order as regards rotation around this axis. In some cases, the distribution of spots along the even layer-lines was irregular, indicating that orientation around the fibre axis was probably random, but others gave a pattern approaching that characteristic of a single crystal. That shown in fig. 2*b* is of the latter type. The even layers fall on to a *c*-centred orthogonal net having $a = 15.28 \text{ \AA}$, $b = 3.63 \text{ \AA}$, which together with the presence of weak and streaky intermediate layers agrees satisfactorily with wollastonite lying on (001). There was some indication of the presence of Laue zones related to the *c*-spacing, but these were too indefinite for measurement.

PART II. NEKOITE, A NEW MINERAL.

Eakle¹ described a mineral from Crestmore, California, which was characterized by its chemical composition and optical properties as okenite. The specimen had been collected,² and some of the observations

¹ A. S. Eakle, Bull. Dept. Geol. Univ. California, 1917, vol. 10, no. 19, p. 327 [M.A. 1-20]. ² Private communication from W. F. Foshag, 20 July, 1952.

carried out by Dr. W. F. Foshag, who kindly made available a portion of the original material from the collection at the U.S. National Museum. It will be shown that the specimen was not okenite, but a new species, for which the name *nekoite* is suggested.

The specimen (U.S.N.M. 95637) consisted of a few fine, slender needles, up to 1 mm. long and $50\ \mu$ thick, and weighing in all about 0.1 mg. They were mixed with grains of calcite. This agrees with the original description.

Preliminary optical examination suggested that the needles showed parallel extinction, with very low birefringence, and mean refractive index 1.535. This agrees with the original description. On more detailed examination, however, it was seen that they showed repeated twinning, being composed of lamellae about $10\ \mu$ thick and lying parallel to the needle axis. A single lamella was detached and yielded the data given in table I. It will be seen that the apparent parallel extinction is a property of the twinned aggregates and not of the individual crystals.

X-ray examination.

Oscillation and rotation photographs (fig. 1*b*) were taken about the needle or *b*-axis of a single lamella. Weissenberg photographs were also obtained for the (*h0l*), (*h1l*), (*h2l*), and (*h3l*) layers. The unit cell was thus found to be anorthic, with¹ $a\ 7.60$, $b\ 7.32$, $c\ 9.86\ \text{\AA}$., $\alpha\ 111^\circ\ 48'$, $\beta\ 86^\circ\ 12'$, $\gamma\ 103^\circ\ 54'$; elongation *b*, cleavage (100). Pronounced pseudo-symmetry was observed. In oscillation photographs about *b*, the even layer-lines were relatively strong and showed an equatorial plane of symmetry, but the odd layer-lines were weak and showed no plane of symmetry. The pseudo-cell obtained by ignoring the odd layer-lines is thus monoclinic, and was found to be *c*-face centred with $a\ 14.78$, $b\ 3.66$, $c\ 9.15\ \text{\AA}$., $\beta\ 91^\circ\ 30'$. The relation between the true cell and the pseudo-cell is shown in fig. 5. If all three axes of the pseudo-cell are doubled, all the reflections can be indexed on monoclinic axes.

Oscillation and Weissenberg photographs were also taken of the twinned aggregates about the needle axis. They showed that two orientations were present in approximately equal amounts. The even layer-lines in the oscillation photographs were identical with those given by single crystals, but additional reflections occurred in the odd layer-lines so that these also showed an equatorial plane of symmetry. In the

¹ This cell is not in the conventional orientation. Application of the transformation matrix $\|\bar{1}00/00\bar{1}/0\bar{1}0\|$ gives: $a\ 7.60$, $b\ 9.86$, $c\ 7.32\ \text{\AA}$., $\alpha\ 111^\circ\ 48'$, $\beta\ 103^\circ\ 54'$, $\gamma\ 86^\circ\ 12'$; fibres parallel to *c*, cleavage (100).

Weissenberg photographs of the odd layers, the number of reflections along each line of constant l was doubled, causing an apparent doubling of a . Together with the optical evidence, this indicates that twinning occurs either by rotation about b , or else by reflection across the plane perpendicular to it.

X-ray powder data, obtained using a 6-cm.-diameter camera, are given in table II. Resolution was not very high because of the small

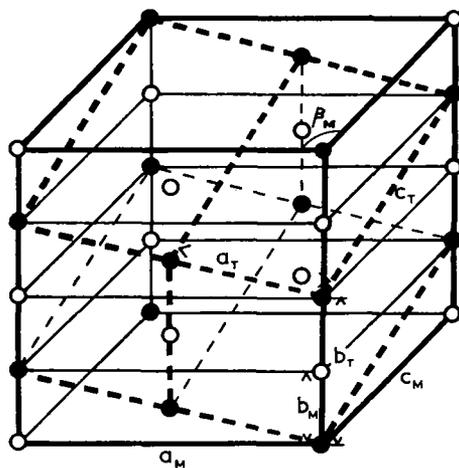


FIG. 5. Relation between the true unit cell of nekoite and the pseudo-cell. Full lines outline four c -face centred monoclinic pseudo-cells; broken lines complete the outlines of two anorthic unit cells. Full circles denote true lattice points; open circles denote additional lattice points pertaining to the pseudo-cell. Suffixes M and T denote parameters of the monoclinic and anorthic (triclinic) cells respectively.

amount of material available. The reflections were indexed by superposing single-crystal and powder photographs taken on the same camera; account was also taken of relative intensities observed on the Weissenberg photographs. Comparison of the observed and calculated spacings given in the table shows satisfactory agreement, thus affording confirmatory evidence for the correctness of the proposed unit cell.

Goniometric data and unit-cell contents.

Eakle stated that the crystals which he examined, although too slender for accurate measurement, appeared to be long prisms terminated by dull domes, and he considered them to be probably orthorhombic.

Approximate goniometric measurements by W. F. Foshag¹ gave the results quoted in table V, which shows also that each of the angles which he measured can be explained on the basis of the monoclinic, near orthorhombic, pseudo-cell of the present investigation. The number of different forms which must be assumed to occur would be reduced if,

TABLE V. Comparison of observed and calculated goniometric data for nekoite.

	Observed (Foshag).	Calculated.
Prism axis:	Not stated; assumed to be c	b
Cleavage face:	Not stated; assumed to be (010)	(100)
Crystal system:	Probably orthorhombic	Monoclinic, β $91^\circ 30'$
	(110) \wedge ($\bar{1}\bar{1}0$) $33^\circ 40'$	(102) \wedge ($\bar{1}02$) $34^\circ 24'$
	(010) \wedge (011) $52^\circ 0'$	(100) \wedge (310) $53^\circ 24'$
	(011) \wedge (0 $\bar{1}\bar{1}$) $75^\circ 0'$	(310) \wedge ($\bar{3}10$) $73^\circ 12'$

as appears probable, the crystals examined by Foshag were twinned, but the data which he obtained are inadequate to settle this point. The matrix of the transformation from Foshag's axes to the monoclinic axes of the present investigation is $\begin{pmatrix} 0 & 1 & 2 \\ 0 & 0 & 1 \\ 2 & 0 & 0 \end{pmatrix}$.

Calculation from the unit-cell dimensions found in the present investigation and Eakle's chemical analysis and specific gravity (2.206) yields the atomic cell-contents given in table III. They indicate that the ideal contents of the anorthic unit cell are $3[\text{CaO} \cdot 2\text{SiO}_2 \cdot 2\text{H}_2\text{O}]$, or $\text{Ca}_3\text{Si}_6\text{O}_{21}\text{H}_{12}$.

Not enough material was available for a further analysis to be made in the present investigation, but as a qualitative and roughly quantitative check on the composition, a crystal of which the identity had been established by X-rays was heated to 900°C ., and X-ray oscillation and rotation photographs then taken about the needle axis. These showed that the only crystalline dehydration product was a slightly disordered single crystal of wollastonite (or parawollastonite), with its b -axis parallel to the needle direction. This result indicates that the original crystal was a hydrated calcium silicate of fairly acid composition, in accordance with the analytical result.

PART III. DISCUSSION.

The data presented in the first part of this paper show that okenite may be characterized by its chemical composition, optical properties, goniometric data and habit, X-ray powder data, and unit-cell dimen-

¹ In A. S. Eakle, loc. cit.

sions. There is adequate evidence that the data given for each of these relate to material substantially the same as that occurring at the type locality (Disko).

The results given in the second part show that the crystals from Crestmore that were examined were not okenite. The chemical compositions are the same, but significant differences exist in optical properties (table I), X-ray powder data (table II), X-ray rotation photographs about the fibre axis (fig. 1), and unit-cell dimensions (table I). Further evidence, independent of the present study, is provided by the fact that Foshag's goniometric data for the Crestmore material are quite unlike those obtained by Bøggild for okenite. In contrast, Foshag's data can be satisfactorily correlated with the present X-ray results for the Crestmore specimen. This provides additional evidence that the crystals from Crestmore that were examined in the present investigation were the same as those originally described, and makes it appear unlikely that any change had taken place in the material between the original examination and the present one.

The data obtained for the Crestmore specimen were compared with those of all the other known hydrated calcium silicates, both natural and artificial. They did not agree with any of them, except in the occurrence of a strongly fibrous habit with a repeat distance of about 7.3 \AA . along the fibre axis. This is common to a number of anhydrous and hydrated calcium silicates, including the ones already mentioned.

Although the Crestmore material is not okenite, it shows certain similarities which are sufficiently close for the original characterization to be easily understood. Apart from the identical chemical compositions, the optical properties are relatively similar. The unit-cell dimensions, habits, and cell contents are also related; this is shown in table I. The cell of okenite is three times as large as that of the Crestmore mineral.

The crystal structures of the two minerals have yet to be determined. They are evidently fairly closely related to each other, and the behaviour on dehydration shows that they are also related to wollastonite. The electron-diffraction results on the dehydration of okenite show that there is a marked tendency towards an ordered transformation, in which the okenite *b*-direction becomes the wollastonite *b*-direction and the okenite (001) plane becomes, at least approximately, the wollastonite (001). The *b*-axis of okenite (7.20 \AA .) is very near to that of wollastonite (7.27 \AA .),¹ the okenite *c* (21.33 \AA .) is almost exactly three times the wollastonite *c* (7.03 \AA .), and the okenite *a* (9.84 \AA .) somewhat greater

¹ B. E. Warren and J. Bischof, *Zeits. Krist.*, 1931, vol. 80 p. 391 [M.A. 5-186].

than the wollastonite a (7.88 Å.). The unit cell of okenite contains the same number of silicon atoms (18) as three unit cells of wollastonite. These facts suggest that dehydration may occur by a process involving migration of calcium ions similar to that proposed in the case of awillite,¹ each cell of wollastonite being formed in the present case from one-third of a cell of okenite.

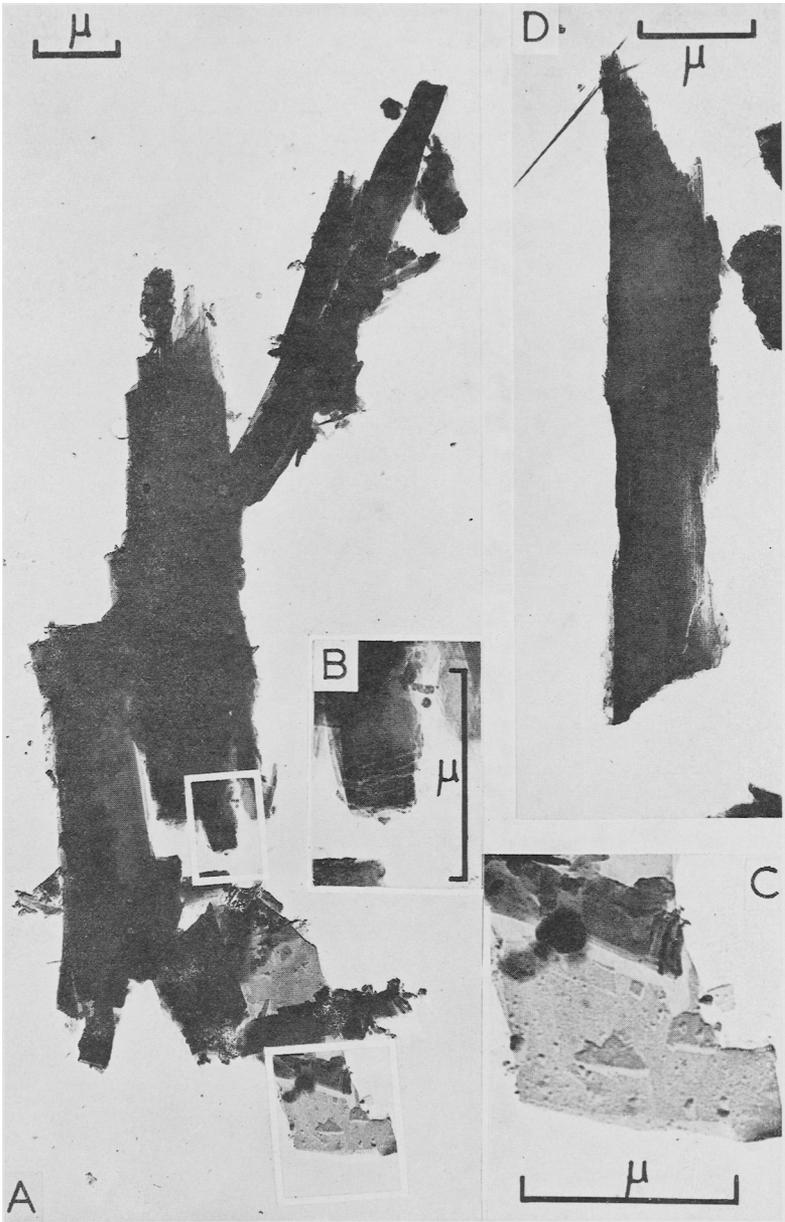
The X-ray evidence on the dehydration of the Crestmore material showed that, as with okenite, the b -direction was unchanged on conversion into wollastonite. It also showed that the product was a single crystal and not an aggregate with random orientation around b , but did not allow the orientation to be determined relative to that of the initial material. It appears likely, by analogy with the case of okenite, that the (100) plane of the original material becomes the wollastonite (001), and that one unit cell of wollastonite, containing six silicon atoms, is formed from one of the initial material.

It follows from the foregoing that the Crestmore material must be regarded as a new species. Because of the likeness to okenite, the anagram *nekoite* is suggested.

Acknowledgements.—The early part of this work was carried out by one of us (H. F. W. T.) at Birkbeck College Research Laboratory, University of London. Thanks are due to Dr. L. J. Spencer for suggesting the name *nekoite*; to the Trustees of the British Museum and to Dr. W. F. Foshag and the U.S. National Museum for the specimens from Bombay and Crestmore respectively; and to Dr. H. G. Midgley for assistance with the optical determinations.

PLATE I. A. Electron micrograph of okenite. Positive print; specimen shadow-cast with Au-Pd alloy so that the length of the shadow is four times the thickness of the projecting material. B. Enlargement from A, showing several leaves each about 20 Å. thick. C. Enlargement from A, showing a sheet about 200 Å. thick with several flakes about 20 Å. thick lying on top of it. D. Electron micrograph of okenite after heating at 1000° C., showing the minutely fibrous character of the flakes.

¹ H. F. W. Taylor, *Acta Cryst.*, 1955, vol. 8, p. 440.



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