

Crichtonite, a distinct species

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SUMMARY. Confusion over the status of crichtonite is due to the fact that de Bournon included two different minerals in his species: thin hexagonal plates are indeed ilmenite, as has been generally assumed, but the much rarer steep rhombohedra with basal plane are a separate species, with a distinctive X-ray powder pattern (three strongest lines: 3.39 Å,s; 2.875,s; 2.131,s) and a composition $(\text{Fe}^{2+}, \text{Fe}^{3+}, \text{Ti})_{1.71}\text{O}_3$ with $\text{Fe}^{2+}:\text{Fe}^{3+}:\text{Ti}$ near 8:7:33. There is a rhombohedral pseudo-cell containing three oxygens, with α 23° 19', a 7.117 Å but there is some evidence of twinning, and the true symmetry is probably orthorhombic or lower.

CRICHTONITE was discovered by Count J. L. de Bournon in 1788 on a small number of specimens from St. Christophe, Bourg d'Oisans, Isère, France; we have not been able to trace any record of a later find other than one by Drapiez (1818); it seems probable that Drapiez used all his material for analysis, and that the material for all subsequent studies and all now in collections came from de Bournon's find. De Bournon made a careful physical study of his scanty material, but published nothing till 1813, when he included a full description of the new mineral, which he named craitonite in honour of Sir Alexander Crichton, physician to the Tsar,¹ in the Catalogue of the de Bournon collection.²

The main part of de Bournon's description refers to very rare opaque black crystals, very steep rhombohedra with basal plane and sometimes with further small facets (fig. 1). With such scanty material he was only able to determine the hardness (H. 4½ to 5) and the crystal morphology, and his observations, included in table II, are remarkably good; his interfacial angles were probably obtained with Wollaston's then new reflecting goniometer,³ and the relatively poor value for α (18° instead of 23½°) may be due to the difficulty of measuring an interedge angle, or it may be a calculated value, the difference being the magnified reflection of a 1° error in cr or rr' .

Besides these very characteristic crystals 'On rencontre quelquefois . . . de petites

¹ The spelling craitonite was an attempt to reproduce the pronunciation for French readers; whether in fact Sir Alexander used the pronunciation KRÄITEN rather than the alternative KRİKHTEN is unknown (the latter is perhaps preferable, to avoid homophony with kreittonite). Following Sowerby (1813) and Jameson (1816) most mineralogists have preferred the spelling crichtonite; many have misspelt the name and some of these erroneous spellings are noted in the references. Crichton's collection of minerals was sold by G. B. Sowerby in 1827; it included three specimens of crichtonite (lots 733, 1995, and 2212); their later history is unknown.

² De Bournon's original collection of crichtonite was dispersed during the French Revolution, but he was able to recover many of the specimens through the good offices of Gillet de Laumont; the new collection, then including twenty crichtonites, eleven being single crystals, was offered for sale in 1813. He parted with some of his specimens to the Rt. Hon. C. F. Greville, on whose collection he worked between 1794 and 1806; on Greville's death in 1809 the Greville collections were acquired by the British Museum, but no crichtonites from this collection remain.

³ W. H. Wollaston, *Phil. Trans.* (1809), 253.

lames noires, minces et très-brillantes, appartenant aussi à la crichtonite'; he was able to distinguish these thin plates, which Beudant later (1832) was to term *crichtonite lamelliforme* in contrast to *crichtonite cristallisée*, from hematite by their lustre and their slightly bluer colour; but his conclusion that they too were crichtonite was based on nothing more than the fact that both minerals are opaque, black, and rhombohedral. In fact he may have been dealing with a second new¹ mineral, for the thin plates

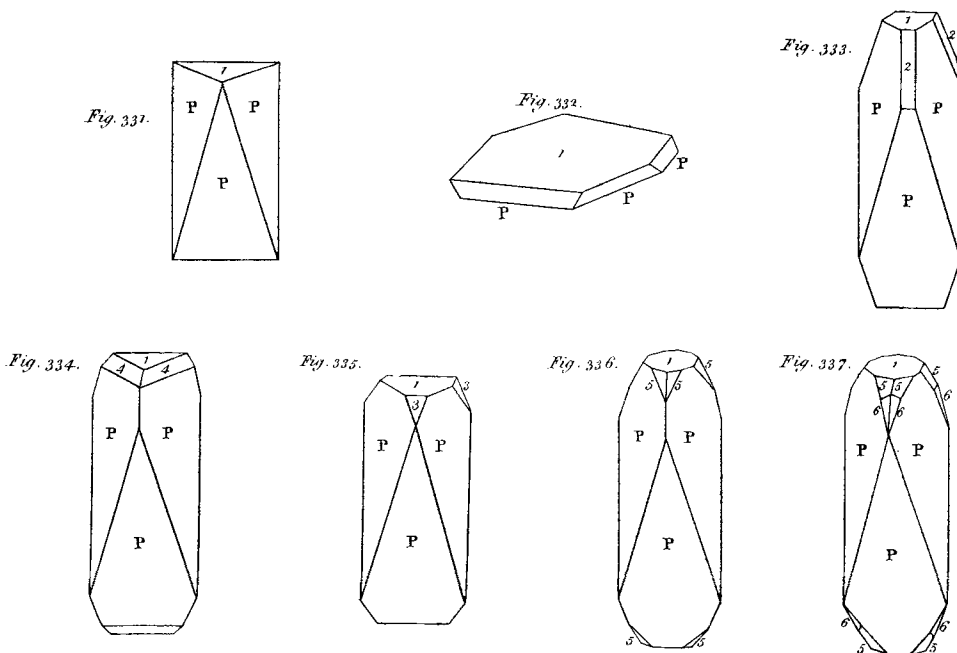


FIG. 1. Crichtonite, after de Bournon (1813).

are the mineral now known as ilmenite; they are much commoner than the true crichtonite, and all the later studies other than morphological ones were made on material that either definitely was, or that may possibly have been *crichtonite lamelliforme*.

Thus Sowerby (1813) figures two of de Bournon's specimens, 'the upper one in acute rhombs . . . the other is the laminated variety', and adds that 'Dr Wollaston found it to contain Zirconia in the greatest quantity, with Silex, Iron, and Manganese',² but there is nothing to show which mineral was examined, nor which was studied by Drapiez (1818), or by Berzelius (1819). Drapiez, like Wollaston, found, besides iron,

¹ Of the many supposedly new species now included under ilmenite, two, iserine (A. G. Werner (1797), *Reuss. Böhm.* 2, 428) and menaccanite (W. Gregor (1791), *Journ. Phys.* 72, 152), were named before 1813; but iserine is a doubtful species, possibly a titanomagnetite or an exsolution mixture (Dana, *Syst. Min.* (7th edn, 1944), 1, 541), and there is no other analysis of the Cornish menaccanite than M. H. Klaproth's of 1797 (*Beitr. Chem. Min.* 2, 226), and no modern study of it.

² We have not been able to trace any publication of this analysis, and it may have been a personal communication only.

zirconia, silica, manganese, and also alumina; he was probably led astray by the tendency of titanium salts, then but little known, to hydrolyse. Berzelius had only a few tiny fragments supplied by de Laumont, and seems to have had to rely almost entirely on a microcosmic salt bead test, but arrived at the correct composition, iron and titania in comparable amounts.

The only quantitative analysis of the St. Christophe 'crichtonite' is by Marignac (1845), and is definitely stated to be of the platy variety—that is, of ilmenite, as indeed the analysis shows. Our new analysis (table III) is the only quantitative analysis to date of the true crichtonite, and perhaps also the only qualitative one.

Unfortunately, a rather loose interpretation of Berzelius's account in the *Nouv. Syst. Min.* ('J'y ai trouvé de l'oxide de titane et de l'oxidule de fer, dans des proportions qui diffèrent peu de celles que Klaproth a trouvées dans le menacane') led to the assumption that he had shown the composition of crichtonite to be identical with that of menaccanite, and his qualifying 'mais j'ignore si la craitonite contient quelque autre chose que ces deux oxides' was disregarded. Von Leonhard (1821) writes 'Der sogenante Crichtonit (Craitonit) ist den neuesten Erfahrungen *Berzelius's* zufolge nichts, als ein Titanoxyd-haltiges späthiges Magneteisen'; and of all the authors writing from 1820 on included in the selected bibliography below, only Breithaupt, Phillips, and Dufrénoy doubt the identity of crichtonite with one or other of the minerals now included under ilmenite.¹ Phillips (1823) writes 'According to Berzelius it affords the same results as titaniferous iron before the blow-pipe; but it may be questioned whether the substance affording this result was not rather a mineral commonly sold under the name of Crichtonite, occurring in thin laminae and flat crystals . . . the chrichtonite is understood to be a compound of titanium and silex.' For Breithaupt (1823) 'der Crichtonit ist mir immer noch eine problematische Substanz'. Dufrénoy (1845) says 'Chrichtonite lamelleuse. On donne ce nom à des cristaux lenticulaires et très-minces de fer oligiste [hematite] contenant une certaine quantité de titane; la présence de titane, jointe au même gisement, sont les deux seules raisons qui ont fait réunir ces lamelles de fer oligiste à la chrichtonite . . .'; oddly enough, Dufrénoy quotes Marignac's analysis for crichtonite proper though it was the 'crichtonite lamelliforme' that he analysed.

Several authors have measured the crystals of crichtonite² (table II). Rose (1827) pointed out that the steep rhombohedron of crichtonite could be interpreted as {0551} = {11.4.4} of a crystal with the same primary rhombohedron as hematite, which he took, following Mohs, as $cr\ 57^{\circ} 38'$, and cautiously added 'auch habe ich

¹ Shepard (1832) and Dana (1837) united them all under crichtonite, but Dana (1844, 1850) used ilmenite, and this has been generally followed though in 1868 Dana (*Syst. Min.*, 5th edn) used menaccanite.

² That is, *crichtonite cristallisée*; Phillips (1823) examined a crystal from H. J. Brooke's collection, but this can no longer be traced at Cambridge; Lévy (1837) examined material from the Turner collection, one specimen from which is now in the Museum of Practical Geology (Ludlam Collection, no. L 3426). Dufrénoy's material (1845) is in the École des Mines, Paris, and is possibly the specimen studied by Lacroix and by Des Cloiseaux. For *crichtonite lamelliforme* the only goniometric data are those of A. Des Cloiseaux (*Man. de Min.* (1893), 2, 221), who found that the plates are bounded by the rhombohedra {100}, {744}, and two faces vicinal to the basal plane, approximately {11.8.8} and {13.10.10} (referred to the ilmenite axes of Dana, 6th edn).

TABLE I. *X-ray data for crichtonite, Bourg d'Oisans, Isère, France. Powder data on BM 1926, 1191, with filtered Co radiation in a camera of 11.46 cm diam.; single-crystal data on BM 32896, with filtered Cu radiation. Transformation matrix from the Bravais indices used here to the Miller indices used in the goniometry [011̄1/1̄011/1̄101]*

Powder data, with indices and calculated d-values for those lines that can be indexed on the pseudo-cell

<i>I</i>	<i>d</i>	<i>hkil</i>	<i>d_{calc}</i>	<i>I</i>	<i>d</i>	<i>hkil</i>	<i>d_{calc}</i>	<i>I</i>	<i>d</i>	<i>hkil</i>	<i>d_{calc}</i>
vww	10.92 Å	—	—	vw	1.770 Å	—	—	vwb	1.1522 Å	{ 0.0.0.18 1.0.1.16	{ 1.1533 1.1510
w	9.87	—	—	vww	1.727	0.0.0.12	1.730	vww	1.1445	—	—
vwb	8.25	—	—	m	1.704	—	—	vww	1.1321	—	—
vww	7.97	—	—	vww	1.682	—	—	w*	1.1244	} 0228	1.1241
vw	4.37	—	—	vww	1.675	—	—	w†	1.1246		
vwwb	4.16	—	—	vwb	1.650	—	—	vwwb	1.1071	1.1.2.12	1.1068
vww	3.95	—	—	vw	1.613	—	—	vww	1.0998	—	—
w	3.76	—	—	s	1.596	0.1.1.10	1.596	vww	1.0936	—	—
s	3.387	—	—	w	1.573	—	—	vww	1.0752	—	—
vww	3.335	—	—	wb	1.544	—	—	w*	1.0690	} 0.2.2.10	1.0691
vwwb	3.214	—	—	vww	1.527	—	—	w†	1.0692		
vww	3.125	—	—	m	1.503	0.1.1.11	1.505	vww*	1.0411	} 0.2.2.11	1.0405
m	3.042	—	—	vww	1.495	—	—	vww†	1.0409		
mw	2.991	—	—	vww	1.475	—	—	vww*	1.0318	—	—
s	2.875	—	—	vww	1.464	—	—	vww*	1.0176	—	—
ms	2.838	—	—	vww?	1.446	—	—	vww†	1.0169	—	—
vww	2.804	—	—	s	1.440	1120	1.440	vww*	1.0116	—	—
m	2.780	—	—	vw	1.420	—	—	vww†	1.0014	—	—
vwwb	2.688	—	—	w	1.4085	1123	1.4099	vww†	1.0005	—	—
mw-m	2.623	—	—	vww	1.3938	—	—	vww*	0.9833	—	—
mw	2.595	—	—	vww	1.3846	0.0.0.15	1.3839	vww†	0.9829	—	—
vwwb?	2.520	—	—	w	1.3747	—	—	vww*	0.9589	—	—
m	2.472	0111	2.476	vwwb	1.3572	—	—	vww†	0.9584	—	—
m	2.420	0112	2.425	vw	1.3438	0.1.1.13	1.3449	vww*	0.9421	—	—
vww	2.369	—	—	vww	1.3389	—	—	vww*	0.9391	—	—
ms	2.243	0114	2.248	vww	1.3134	—	—	vww†	0.9388	—	—
vwwb	2.175	—	—	vwb	{ 1.3018 1.2965	—	—	vww*	0.9281	—	—
s	2.131	0115	2.138	vwwb	1.2776	0.1.1.14	1.2746	vww*	0.9264	—	—
vw	2.105	—	—	vww	1.2566	—	—	mw*	0.91948	—	—
vww	2.060	—	—	vw	1.2447	0221	1.2449	mw†	0.91660	—	—
vwwb	2.020	—	—	w	1.2373	0222	1.2383	vww*	0.90977	—	—
vwb	1.960	—	—	vww	1.2266	—	—	vww†	0.90980	—	—
wb	1.912	0117	1.909	vww	1.2210	1129	1.2216	vww*	0.90515	—	—
vw	1.884	—	—	vw	1.2126	0224	1.2126	ms*	0.90061	—	—
w	1.843	—	—	vwwb	1.2025	—	—	ms†	0.90061	—	—
vww	1.825	—	—	vwb	1.1942	0225	1.1944			* K_{α_1}	† K_{α_2}
ms	1.796	0118	1.798								

Rotation photograph about an a-axis; zero layer-line and first layer-line of the pseudo-cell

Zero layer-line		ξ		hkil		'First' layer-line		ξ		hkil	
ξ	hkil	ξ	hkil	ξ	hkil	ξ	hkil	ξ	hkil	ξ	hkil
0.62	0111	1.23	0222, (0221)	0.31	1011	1.135	1129				
0.63	0112	1.285	0225	0.34	1012	1.28	1.1.2.12, (1.0.1.17)				
0.68	0009, 0114	1.33	0.1.1.16, 0.0.0.18	0.425	1014	1.44	1.1.2.15, 1.0.1.19				
0.71 ₅	0115	1.37	0228	0.48	1015	1.515	1231, 1232, (1.0.1.20)				
0.80	0117	1.44	0.2.2.10	0.60	1017	1.545	1234				
0.85	0118	1.475	0.2.2.11	0.66 ₅	1018	1.625	2138, (1.1.2.18), (2137)				
0.88 ₅	0.0.0.12	1.60	0.1.1.20	0.80	1.0.1.10	1.66	1.0.1.22				
0.96	0.1.1.10	1.74	0.1.1.22, (2.0.2.17)	0.87	1.0.1.11	1.72	1.0.1.23, 2.1.3.11				
1.02	0.1.1.11	1.85	0.2.2.19, 3033	0.925	1123, 1120	1.82	2.1.3.14				
1.14	0.1.1.13	1.925	0.2.2.20	1.01	1126						

nicht das stumpfere Rhomboëder beim Crichtonit gemessen, was nöthig wäre, um diese Frage zu entscheiden'. Lévy (1837) rightly points out that, having regard to the poor quality of the measurements, so steep a rhombohedron could be relatively simply indexed on a very wide range of primitive rhombohedra, but Rose's tentative identification has been generally accepted.

In 1952, goniometric, X-ray, and chemical studies of the three crichtonite specimens in the British Museum collections¹ were undertaken, but were not then published in full² because of difficulty in interpreting the X-ray data.

There is a prominent rhombohedral pseudo-cell with $\alpha 23^\circ 18'$, $a 7.117 \text{ \AA}$; $c_{\text{hex}} 20.759$, $a_{\text{hex}} 2.880 \text{ \AA}$), which corresponds to the steep rhombohedron of the crystals, but it does not account for many of the strongest lines of the powder photograph (table I), and while a rotation photograph around one of the hexagonal a -axes suggests a rhombohedral true cell with $a_{\text{hex}} 37.44 \text{ \AA}$, thirteen times that of the pseudo-cell (as was proposed in 1953), there are a number of unexplained peculiarities, and the true symmetry is probably lower than rhombohedral.

As there is no immediate prospect of continuing the X-ray study, it seems desirable to place the data on record, together with the new X-ray powder photograph (E. E. F.) and some further goniometric measurements (P. G. E.).

The crystals of crichtonite on the British Museum specimens and on those in the Museum of Practical Geology (L 3426 and L 8039) are essentially steep rhombohedra with basal plane, about 2–8 mm long; on some crystals the faces are dull or even matt; others are bright, but with the primary rhombohedron striated, often in a pattern suggesting twinning, and a few crystals show some re-entrant angles.³ As de Bournon noted, many of the edges and corners of the principal forms are truncated by tiny facets, the actual combinations varying from crystal to crystal, but these are not distributed with the rhombohedral symmetry shown in de Bournon's figures (see fig. 1); indeed many of the forms are represented by single facets, and suggest that the true symmetry is not higher than monoclinic.

Two crystals were measured with results in good agreement with the literature values (table II); it is clear that the principal forms are $c \{111\}$ and $r \{100\}$ referred to the pseudo-cell, but nearly all the other forms cannot be assigned simple indices on either the pseudo-cell or the large cell suggested in 1953, though a few are vicinal to simple forms.

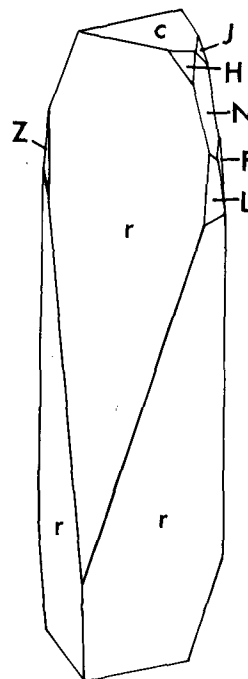


FIG. 2.

¹ BM 32896, from R. Campbell's collection, 1861; BM 67281, bought of J. R. Gregory, 1891; and BM 1926, 1191, C. O. Trechmann collection, formerly in Isaac Walker's collection, and bought by him from H. Heuland, 1837. The Museum of Practical Geology has two specimens from the Ludlam collection, nos. L 3462 and L 8039; the École des Mines, Paris, has three specimens, nos. A 9992 and A 10 1000, and one in pane no. 996, studied by A. Lacroix (*Min. de France* (1901), 3, 285).

² A short abstract of the draft paper by F. A. Bannister, G. F. Claringbull, and M. H. Hey appears in *Min. Abstr.* (1953), 12, 287.

³ On all these specimens the crichtonite crystals are implanted on crystallized quartz, mostly impregnated or coated with chlorite, but on one of the École des Mines specimens they are stated by Lacroix (loc. cit.) to be implanted directly on a fine-grained aplite.

TABLE II. *Goniometric data for crichtonite. Measured angles for two crystals, with values from the literature and angles calculated from the X-ray data. 'Small cell' indices refer to the pseudo-cell with $\alpha 23^\circ 19'$, 'large cell' to the cell with $\alpha 111^\circ 6'$; Miller (rhombohedral) indices are given; the transformation matrix to Bravais (hexagonal) indices is $[0\bar{1}1/10\bar{1}/\bar{1}10/111]$. The transformation matrix from the small rhombohedral cell to the large is $[94\bar{4}/49\bar{4}/449]$, and from the large to the small $[544/454/445]$*

Crystal from BM 1926, 1191:

Form	<i>r</i>	<i>Z</i>	<i>N</i>	<i>W</i>	<i>F</i>
Obs. $\{cX$ $\{[cX]:[cr]$	$82^\circ 47' 90^\circ$ $0^\circ 0' 44^\circ$	$66\frac{3}{4}^\circ$ $46\frac{3}{4}^\circ$	$50\frac{1}{2}^\circ$ 0°	$76^\circ 39'$ $33^\circ 12'$	
Calc. $\{cX$ $\{[cX]:[cr]$	$83^\circ 10' 90^\circ 0'$ $0^\circ 0' 43^\circ 54'$	$66^\circ 38'$ $46^\circ 6'$	$50^\circ 0'$ $0^\circ 0'$	$52^\circ 4'$ $0^\circ 0'$	$75^\circ 33'$ $33^\circ 0'$
Small cell	100	341	625	322	12.1.7
Large cell	944	341	221	511	19.1.11
					35.32.5
					19.17.3

Crystal from BM 1926, 1191 (contd.)

Form	<i>E</i>	<i>K</i>	<i>D</i>	<i>G</i>	<i>e</i> ‡
Obs. $\{cX$ $\{[cX]:[cr]$	$80^\circ 4'$ $54^\circ 35'$	$32\frac{1}{2}^\circ$ $37\frac{3}{4}^\circ$	$85\frac{1}{2}^\circ$ 55°	$78\frac{1}{4}^\circ$ 12°	— —
Calc. $\{cX$ $\{[cX]:[cr]$	$80^\circ 43'$ $54^\circ 48'$	$32^\circ 41'$ $38^\circ 13'$	$86^\circ 5'$ $55^\circ 18'$	$85^\circ 19'$ $54^\circ 48'$	$83^\circ 41'$ $56^\circ 27'$
Small cell	827	34.26.31	655	—	10.1.3
Large cell	463	623	—	23.37.19	11.18.9
					17.10.4
					76^\circ 3'
					60^\circ 0'
					101
					585

Crystal from BM 32896

Form	<i>r</i>	<i>Z</i>	<i>N</i>	<i>V</i>	<i>L</i>	<i>H</i> §	<i>J</i>
Obs. $\{cX$ $\{[cX]:[cr]$	$82^\circ 57' 90^\circ 14'$ $0^\circ 0' 44^\circ 3'$	$66^\circ 38'$ $46^\circ 31'$	77° 31°	$80^\circ 21'$ $64^\circ 43'$	$53^\circ 35'$ $75^\circ 17'$	$53^\circ 22'$ $16\frac{1}{2}^\circ$	
Calc. $\{cX$ $\{[cX]:[cr]$	$83^\circ 10' 90^\circ 0'$ $0^\circ 0' 43^\circ 54'$	$66^\circ 38'$ $46^\circ 6'$	$78^\circ 16'$ $30^\circ 0'$	$79^\circ 59'$ $64^\circ 18'$	$78^\circ 56'$ $63^\circ 12'$	$53^\circ 49'$ $73^\circ 54'$	$54^\circ 14'$ $73^\circ 54'$
Small cell	100	341	625	201	9.2.10	859	—
Large cell	944	341	221	14.12.1	—	5.10.6	17.22.20
							530

* These observed angles are weighted means. *cr* is reported as $83^\circ 20'$, $82^\circ 48'$, P.; $83^\circ 0'$, D.; $82^\circ 48'$, La. For *rr'* (calc. $118^\circ 36'$), $118^\circ 40'$, $118^\circ 45'$, R.; $118^\circ 31'$, Lé.; $118^\circ 33'$, D.; and $118^\circ 31'$, La. are reported.

† Literature values: 50° , B.; $49^\circ 17'$, D.; $49^\circ 50'$, La.

‡ Not observed on the BM specimens. Observed and fixed by zonal relation, B.; measured, *ce* $74\frac{1}{2}^\circ$, C.; $76^\circ 11'$, D.

§ This is possibly de Bournon's form 3 (obs. *cX* 54°); but if de Bournon's form is truly in the zone $[10\bar{1}]$, as it is drawn, it may be *U* 747 (small cell), with *cU* $54^\circ 40'$.

|| De Bournon observed two scalenohedra, forms 5 and 6, with *rX* 60° and 55° respectively, in roughly the same part of the crystal as *N*, *K*, and *H*. Calc. *rN* $47^\circ 13'$, *rH* $51^\circ 21'$, *rK* $58^\circ 34'$.

References: B., de Bournon, 1813; C., Cordier, 1818; D., Dufrénoy, 1845; La., A. Lacroix, *Min. de France* (1901), 3, 285; Lé., Lévy, 1837; P., Phillips, 1823; R., Rose, 1827.

We have found no trace of the basal cleavage reported by de Bournon, and in this are in agreement with Cordier (1818).

For the chemical analysis (table III), a fragment of 11.1 mg was crushed and dissolved by heating with concentrated hydrochloric acid and a small excess of iodine monochloride in a sealed tube on the waterbath; a small amount of quartz remained undissolved (its presence had been suspected during the crushing). After titration with

M/200 KIO₃ of the iodine formed by the reaction $2\text{ICl} + 2\text{Fe}^{\cdot\cdot} \rightarrow \text{I}_2 + 2\text{Cl}^{\cdot} + 2\text{Fe}^{\cdot\cdot}$, the iron was separated by extraction with ether; both iron and titanium were weighed as their dibrom-8-hydroxyquinolates.

TABLE III. Chemical analysis (recalculated to 100% assuming that the loss of 5.16% is all quartz), empirical cell contents, and atomic ratios of a 20-mg crichtonite crystal from BM 1926, 1191 (St. Christophe, Bourg d'Oisans, Isère, France). The empirical cell contents, *E*, refer to the rhombohedral pseudo-cell; the atomic ratios, *R*, refer to a rhombohedral cell containing 3×169 oxygen atoms, corresponding to the 13-fold a_{hex} suggested by Bannister, Claringbull, and Hey, *Min. Abstr.* 1953, 12-287

	Obs.	Calc. for Fe ²⁺ :Fe ³⁺ :Ti			<i>E</i>	<i>R</i>
		8:7:33	9:8:36	1:1:4		
TiO ₂	69.57	69.94	69.12	67.82	Ti 1.163	197.1
Fe ₂ O ₃	15.10	14.82	15.35	16.92	Fe 0.253	
FeO	15.33	15.24	15.53	15.24	Fe 0.285	±0.02
[100]	100.00	100.00	100.00		O 2.990	±0.03
						[507]

D_4^{20} 4.46+0.04, corrected to vacuum and for 5% quartz.

Pseudo-cell: α 23° 18', a 7.117 Å

Large cell (*Min. Abstr.* 12, 287): α 111° 6', a 22.70 Å.

The density was determined by hydrostatic weighing of a 20-mg crystal in bromoform on the microbalance, and leads to the empirical contents of the pseudo-cell shown in table III; it will be seen that while the pseudo-cell clearly contains 3 oxygen atoms, its metal content is not an integral number. Its *c*-dimension, 20.76 Å, agrees well with the dimension of nine layers of a close-pack of oxygen ions, measured along a trigonal axis, and the density is also in accord with a structure based on a close-pack of oxygen.

The atomic ratios have also been calculated on a basis of 3×169 oxygen atoms, corresponding to the large cell with α 111° 6', a 22.70 Å (a_{hex} 37.44 Å) proposed in 1953, and suggest an ideal formula Fe₁₆²⁺Fe₁₄³⁺Ti₆₆O₁₆₉; an empirical formula Fe₉²⁺Fe₈³⁺Ti₃₆O₉₃ also fits the analytical data reasonably well, but Fe₂²⁺Fe₂³⁺Ti₈O₂₁ is outside the range of probable experimental error.

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[Manuscript received 21 January 1969]