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THE PYROSMALITE GROUP OF MINERALS. II. THE LAYER STRUCTURE OF McGILLITE AND FRIEDELITE

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ABSTRACT

The present study of mcGillite and friedelite by HRTEM (high-resolution transmission electron-microscopy) and electron diffraction reveals their common basic one-layer monoclinic structure ($C2/m$), whose cell dimensions can be obtained from the 12-layer hR cell (A, C) (Donnay *et al* 1980), now known to be the cell of the twin lattice, by the relations: $\mathbf{a} = \mathbf{A}_1 - \mathbf{A}_2$, $\mathbf{b} = \mathbf{A}_1 + \mathbf{A}_2$, $\mathbf{c} = (\mathbf{C} - \mathbf{A}_1 + \mathbf{A}_2)/12$, $\beta = \arctan(-C/A\sqrt{3})$; $a = A\sqrt{3}$, $b = A$, $c = C/(12 \sin\beta)$. For mcGillite: $a = 23.312$, $b = 13.459$, $c = 7.423$ Å, $\beta = 105.17°$. Stacking disorder is due to repeated incipient twinning by TLQS (twin-lattice quasisymmetry), with twin index $n = 4$ and twin obliquity $\omega = 0$. The twin lattice is a rhombohedral superlattice. Twin operations are 180° rotations about [110] and [$\bar{1}$10]; these two twin axes lie in the plane of the layers (001), which becomes composition plane. Equivalent twin operations are rotations of ± 120° about row [1.0.12], which is perpendicular to (001). Repeated twinning is universal; commonly the twin domains are only a few layers thick, a phenomenon we call "incipient twinning" when the crystals do not grow to sufficient size to give sharp X-ray reflections. Unit layers in mcGillite and pyrosmalite are similar, but the silicate sheet in mcGillite is rotated about [1.0.12] by 60° from that in pyrosmalite, for a fixed orientation of the octahedral sheet. The basic X-ray reflections that characterize the monoclinic structure, which are sharp in mcGillite, are diffuse in friedelite, which may thus be regarded as a disordered equivalent of mcGillite.

Keywords: mcGillite, layer structure, monoclinic, twinning, stacking disorder, friedelite, disordered mcGillite.

SOMMAIRE

L'étude de la mcGillite et de la friedelite par microscopie électronique de haute résolution en transmission révèle que ces deux espèces ont en commun une structure de base, monoclinique à une couche ($C2/m$), dont les dimensions de maille s'expriment comme suit, en fonction des arêtes (A, C) de la maille hR à 12 couches de Donnay *et al.* (1980): $\mathbf{a} = \mathbf{A}_1 - \mathbf{A}_2$, $\mathbf{b} = \mathbf{A}_1 + \mathbf{A}_2$, $\mathbf{c} = (\mathbf{C} - \mathbf{A}_1 + \mathbf{A}_2)/12$, $\beta = \arctan(-C/A\sqrt{3})$; $a = A\sqrt{3}$, $b = A$, $c = C/(12 \sin\beta)$. Pour la mcGillite, on obtient: $a = 23.312$, $b = 13.459$, $c = 7.423$ Å, $\beta = 105.17°$. Le désordre d'empilement provient de la répétition d'un maclage incipient (macle par pseudo-symétrie du réseau de macle, d'indice $n = 4$ et d'obliquité $\omega = 0$. Le réseau de macle est le surréseau rhomboédrique. La macle complète résulte des rotations $[110]_{180°}$ et $[\bar{1}10]_{180°}$; les deux axes de macle sont contenus dans (001), plan parallèle aux couches, qui devient plan de jonction. Les rotations $[1.0.12]_{\pm 120°}$ définissent la même macle, l'axe ternaire de macle étant normal à (001) (donnée d'observation). La macle répétée est universellement présente; les cristaux ou domaines de macle se réduisent à quelques couches d'épaisseur, phénomène que nous appelons "maclage incipient" lorsque les cristaux sont de taille trop petite pour donner des réflexions nettes aux rayons X. McGillite et pyrosmalite ont des couches élémentaires semblables, sauf que le feuillet silicate de la mcGillite est tourné de 60° par rapport à celui de la pyrosmalite, pour une orientation donnée du feuillet d'octaèdres. Les réflexions (dites réflexions B) caractéristiques de la structure monoclinique sont nettes dans la mcGillite et diffuses dans la friedelite, minéral qu'on peut donc considérer comme équivalent désordonné de la mcGillite.

Mots-clés: mcGillite, structure en feuillets, monoclinique, maclage, désordre d'empilement, friedelite, mcGillite désordonnée.

INTRODUCTION

Donnay *et al.* (1979, 1980) described the new mineral mcGillite in space group $R\bar{3}m$ and assigned it to the pyrosmalite group with A 13.459 and C 85.97 (~ 12 × 7.16) Å. No refinable structure could be determined, as X-ray diffraction gave no hint that the 12-layer cell (A, C) was a supercell. In order to elucidate the stacking sequence of mcGillite and unravel the nature of disorder in minerals of this group, which includes pyrosmalite, manganpyrosmalite, friedelite and schallerite, we decided to study these species by HRTEM. As a result, new structural features were revealed in mcGillite and friedelite; they are described in the present paper.

EXPERIMENTAL PROCEDURE

The materials used for study and their sources are as follows: manganpyrosmalite from Kyurazawa mine, Japan (University Museum, University of Tokyo PM22847), pyrosmalite from Nordmarken, Sweden (*ibid.* PM22257), friedelite from three localities: Adervielle, France (*ibid.* PM22840), Sterling Hill, N.J. (*ibid.* PM21269) and Harstig, Sweden, and mcGillite from the type locality, Sullivan mine, Kimberley, B.C.

Before preparing the samples for electron microscopy, we recorded their X-ray-diffraction patterns, by powder and precession methods, to confirm their identification. The crystals were then ground and dispersed on carbon-coated copper microgrids. Electron-diffraction patterns and micrographs were taken with a JEOL 100CX transmission electron-microscope, fitted with a double-tilt goniometer, at 100 kV and up to 650,000X magnification. In view of the perfect (albeit not micaceous) cleavage found in the minerals of the pyrosmalite group, it was not easy, in the samples thus prepared, to isolate

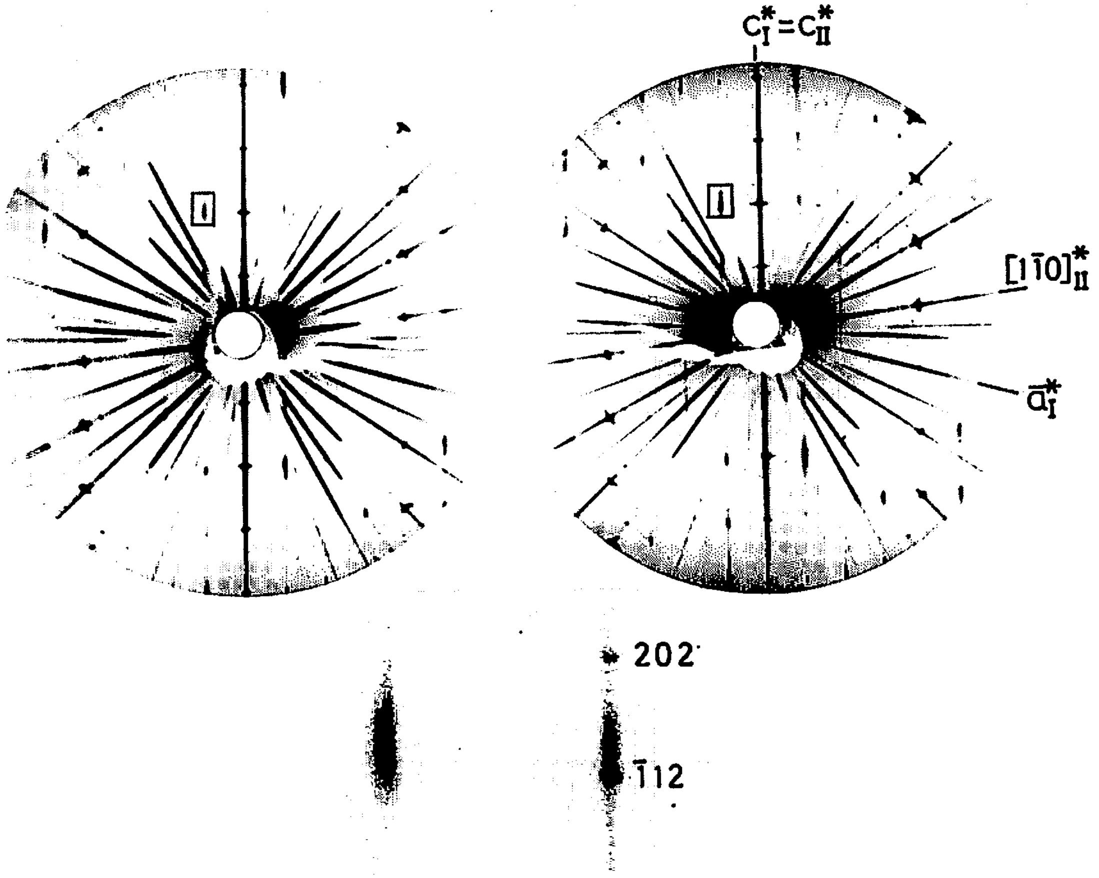


FIG. 1. Comparison of precession photographs of friedelite (*left*) and mcGillite (*right*), both are composite of $h0l$ and $\bar{h}hl$ reflections (Cu$K\alpha$). In the latter, the axes of twinned monoclinic individuals, I and II, are indicated. The *S* reflections indicated in rectangles are enlarged and shown below the pattern; the reflection 202 of mcGillite (*right*) is from individual I, whereas $\bar{1}12$ comes from II. Monoclinic indexing.

crystal fragments that could be placed in the desired orientations within the adjustment range of the goniometer stage.

EXPERIMENTAL OBSERVATIONS

Characteristics of the X-ray-diffraction patterns

The minerals of the pyrosmalite group have a pronounced substructure $Mn(OH,Cl,O)_2$, which corresponds to the structure of pyrochroite $Mn(OH)_2$, as already reported for manganpyrosmalite (Takéuchi *et al.* 1969). In general, in the minerals assigned to space group $P\bar{3}m1$ in the literature, reflections with both h and k multiples of 4 show very strong intensities, which are due to the pseudoquartering of the a_1 and a_2 edges by the Mn octahedra. Each structure type in this group may thus be regarded as a superstructure of pyrochroite, in which an attached sheet of silicon–oxygen tetrahedra defines the supercell. Hereafter, reflections with h and k both multiples of 4 will be called B reflections, and those for which either h or k is not a multiple of 4, S reflections (B and S standing for basic and superstructure reflections, respectively). As will be shown below, mcGillite and friedelite show additional complexities in their diffraction patterns.

For convenience the cell edges of mcGillite and friedelite reported in the literature will be designated A and C, instead of a and c; the diffraction symbols, when referred to these axes, will likewise be written $HK.L$ instead of the usual $hk.l$. According to the powder data in Donnay *et al.* (1980), mcGillite has cell dimensions A 13.459, C 85.97 Å and space group $R\bar{3}m$. One of the striking features of the diffraction patterns of mcGillite [Fig. 1 (right)] is the large number of "structural absences", always a strong indication of the presence of twinning. The presence criteria of $HK.L$ reflections are, in addition to the R criterion, "$-H + K + L = 0 (\text{mod } 3)$": $H - L = 0(\text{mod } 12)$ and $2H + L = 0(\text{mod } 12)$. Although the S reflections are sharp [Fig. 1 (right), monoclinic indexing], they are without exception accompanied by diffuse streaks along c^*.

Our friedelite crystals from Adervielle, France were too small for single-crystal X-ray study, so we used material labeled *friedelite* from Harstig, Sweden for the precession patterns [Fig. 1 (left)], under the same conditions as for mcGillite. A comparison of these two sets of patterns reveals that the S reflections are completely streaked out along c^* and weaker than the sharp reflections of mcGillite. If

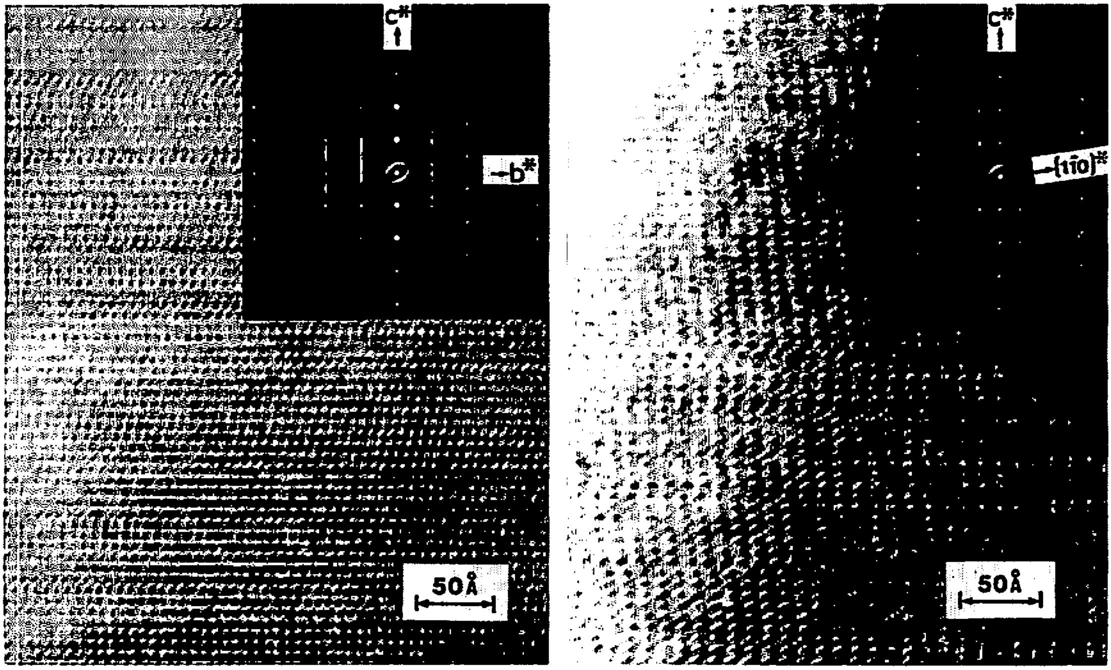


FIG. 2. Examples of $0kl$ (*left*) and $\bar{h}hl$ (*right*) electron-diffraction patterns of friedelite with corresponding structure images, showing stacking disorder.

we omit the *S* reflections, the remainders of the X-ray patterns of mcGillite and friedelite, now consisting of only *B* reflections, are both essentially the same as that of the three-layer rhombohedral lattice reported by Frondel & Bauer (1953) for friedelite.

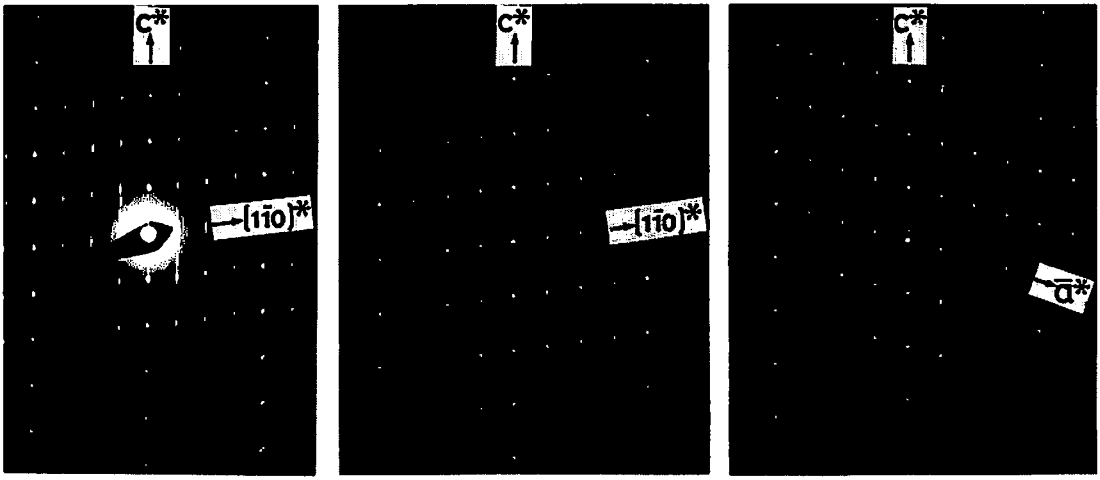
Electron-diffraction patterns and structure imaging

The electron-diffraction patterns of mcGillite and friedelite show the same difference as their X-ray patterns: the *S* reflections are sharp in mcGillite, markedly streaked in friedelite. Owing to the much smaller size of the specimens used for electron microscopy, however, features of the diffraction patterns of each mineral vary from one fragment to another, and from one area to another in the same fragment. Electron-diffraction patterns of friedelite and their corresponding structure-images (Fig. 2) indicate different degrees of stacking disorder [to be discussed in Part III, which deals with the prediction of polytypes: Takéuchi *et al.* (1983)]. The same differences are also observed in one and the same lattice plane when different portions of a fragment are examined. Applying the selected-area diffraction technique, we then looked for friedelite fragments giving *S* reflections with as short a diffuse streak as possible. We thus came across unexpected patterns that indicate monoclinic symmetry [Fig. 3(i)]. Similar patterns, though with significantly sharper *S* reflections, were obtained for mcGillite [Fig. 3(ii) and (iii)]. In addition, we observed a mcGillite pattern (Fig. 4) that is a composite of patterns [Figures 3(ii) and (iii)] and thus yields evidence of twinning.

The fact that mcGillite and friedelite exhibit such similar diffraction patterns suggests that their crystal structures are essentially the same. These patterns are clearly not rhombohedral; they show monoclinic symmetry *P*2, which should also be that of the basic structure for both mcGillite and friedelite. The "complicated" patterns of mcGillite now can be interpreted. The *hk*0 pattern of mcGillite (Fig. 5) shows that the "hexagonal symmetry" is in fact pseudosymmetry; the symmetry of this diffraction pattern is the plane group *Cmm*2, and the "mirror lines" are easily determined: the rows $[310]^*$ and $[3\bar{1}0]^*$ both make the same angle of 29° with a^*, whereas $[110]^*$ and $[\bar{1}10]^*$ are equally inclined on b^* at 31°. Note the lack of exact hexagonal symmetry in the intensity distribution, a fact that proves twinning.

Geometrical interpretation of disorder and unit cell

The diffraction patterns of Fig. 3(ii) and Fig. 3(iii) show two distinct types of oblique reciprocal-lattice nets; in one (iii) the interaxial angle is 75°; it is 82° in the other (ii). If we take the former to be the *h*0*l* net of the monoclinic lattice (Fig. 6, with $\beta^* = 75°$), we find that the



(i) (ii) (iii)

FIG. 3. Electron-diffraction patterns of friedelite (i) and mcGillite (ii) and (iii), showing monoclinic symmetry. For interpretation, refer to Figure 6.

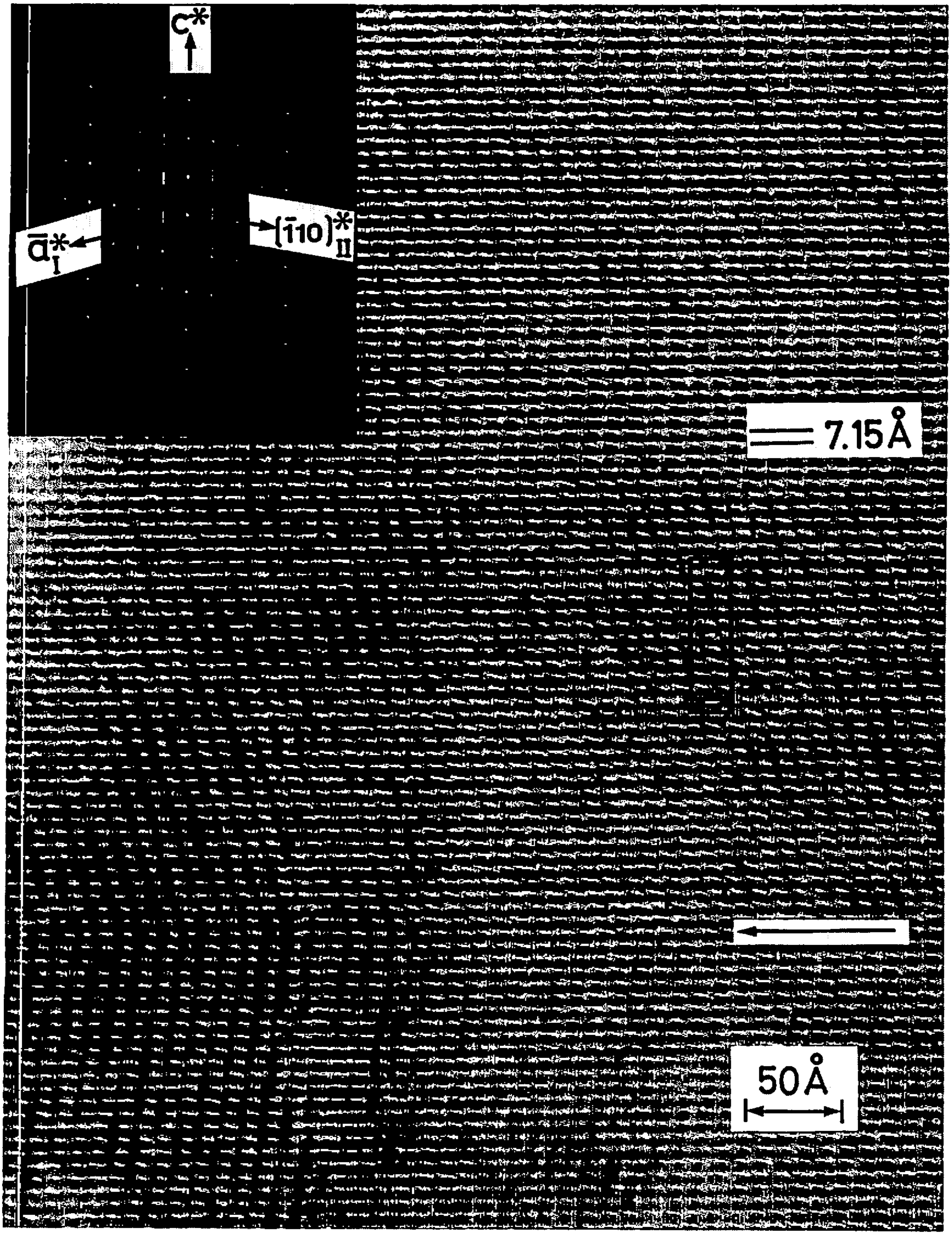


FIG. 4. An electron-diffraction pattern of mcGillite, which is a composite of the patterns of Figure 3(ii) and Figure 3(iii), and corresponding electron micrograph. One of the major twin boundaries is indicated by an arrow. One monoclinic cell and the twelvefold orthogonal cell are outlined.

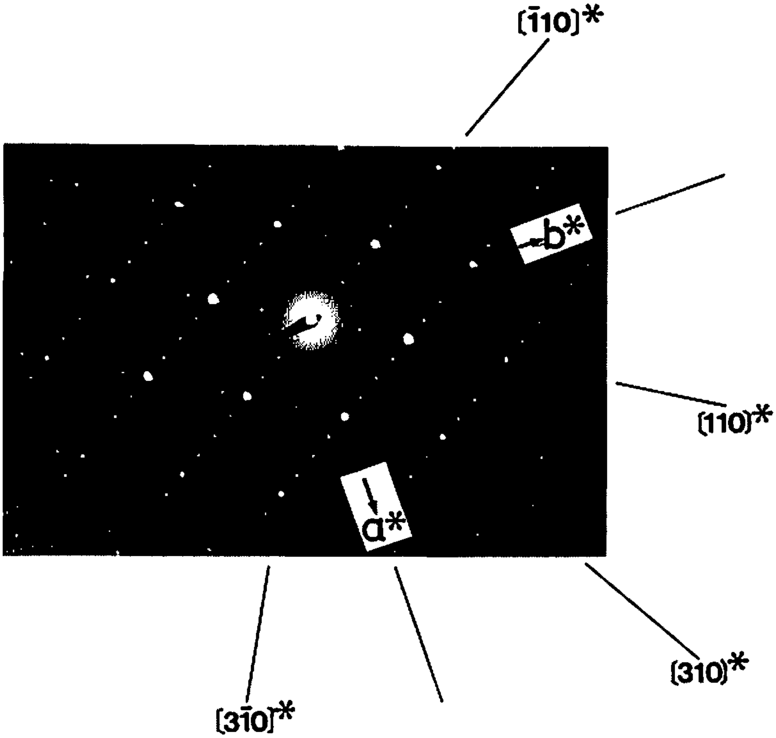


FIG. 5. An electron-diffraction pattern of mcGillite, showing *hk*0 reflections. Monoclinic indexing.

latter (Fig. 6, with $\beta^* = 82°$) corresponds to either one of the $\bar{h}hl$ or $\bar{h}\bar{h}l$ nets. Since net (001) is pseudohexagonal, $\bar{h}hl$ and $\bar{h}\bar{h}l$ are related to *h*0*l* by rotations of ± 120°. The mcGillite pattern of Figure 4 (or more generally of Fig. 1) can thus be interpreted as due to twins in which two (or three) crystal orientations are present.

The monoclinic cell

The monoclinic cell shows diffraction aspect $C^*/^*$; $C2/m$ is assumed for structural reasons. The unit vectors **a**, **b**, **c** of this cell are related as follows to the vectors $\mathbf{A}_1$, $\mathbf{A}_2$, **C** of the rhombohedral (*hR*) cell (Fig. 7), which was previously mistaken for the true cell.

$$\begin{array}{llll} \mathbf{a} = & \mathbf{A}_1 - \mathbf{A}_2 & a = & A\sqrt{3} \\ \mathbf{b} = & \mathbf{A}_1 + \mathbf{A}_2 & b = & A \\ \mathbf{c} = & (\mathbf{C} - \mathbf{A}_1 + \mathbf{A}_2)/12 & c = & C/12\sin\beta \\ \beta = & \arctan(-C/A\sqrt{3}) & & \end{array}$$

Using the cell dimensions of mcGillite determined from powder data by Donnay *et al.* (1980, Table 1), we obtained *a* 23.312(16), *b* 13.459(9), *c* 7.423(7) Å, and *β* 105.17(2)°. The powder pattern of mcGillite (Donnay *et al.* 1980) was then re-indexed on this monoclinic cell (Table 1).

A monoclinic cell was likewise derived from the *hR* cell of friedelite (Frondel & Bauer 1953); its dimensions, as determined by least-squares refinement using the program UNICS (Sakurai 1967), are *a* 23.33(5), *b* 13.396(8), *c* 7.447(4) Å, *β* 105.08(8)°. Tre powder pattern of friedelite (Frondel & Bauer 1953) has been re-indexed on the new monoclinic cell (Table 1). Note that the *S* reflections occurring in the mcGillite pattern tend to be missing in the friedelite pattern. Dunn *et al.* (1981) observed some diffuse reflections that were missed by Frondel and Bauer. Iijima (1981), at the Ottawa I.U.Cr. International Congress, announced the monoclinic symmetry of mcGillite, confirming unpublished results of R.M. Thompson, preserved in a letter that was written some thirty years ago, and gave the space group *C*2/*m*. Note that, in his abstract, Iijima erroneously referred to the mineral as "manganpyrosmalite"; the sample he studied, however, was sent to him by G. Donnay, who had identified it as mcGillite.

Twinning in mcGillite

The mcGillite twin consists of three crystals related by rotations of ± 120° about row [1.0.12], a direction that coincides with the $\bar{3}$ axis of the rhombohedral twin-lattice (Fig. 7b). The twinning is by twin-lattice quasisymmetry (TLQS) with obliquity $\omega = 0$, as observed on all examined patterns, and index $n = 4$, a rather high value, considering the observed universality of twinning (Donnay & Donnay 1974). The fact that only one-quarter of the nodes of the crystal lattice, namely the one at 000, ½½0, which are repeated after four and eight cells along the c axis, remain nodes in the twin lattice (Fig. 7a), explains the structural absences among the above-mentioned $HK.L$ reflections. Alternate and equivalent twin operations are 180° rotations about [110] and [$\bar{1}$10], which coincide with A_1 and A_2 respectively, the 2-fold axes of the twin lattice. Reflections in the planes perpendicular to these directions, namely $(\overline{12}.4.\bar{1})$ and (12.4.1), also are twin operations. These planes are mirrors in the rhombohedral twin-lattice.

Let us label the three crystals in the twin I, II and III in clockwise sense about the 3-fold twin axis [1.0.12], and let the above description of the monoclinic cell in terms of the twin cell refer to crystal I (Fig. 7b). The Roman numeral will be used as a subscript to designate the crystal in which rows are considered. The twin axis $[110]_{\mathrm{I}}$ brings $\mathbf{a}_{\mathrm{I}}$ onto $\bar{\mathbf{a}}_{\mathrm{II}}$, $\mathbf{b}_{\mathrm{I}}$ onto $\mathbf{b}_{\mathrm{II}}$ and $\mathbf{c}_{\mathrm{I}}$ onto $\bar{\mathbf{c}}_{\mathrm{II}}$; $[110]_{\mathrm{I}}$ coincides with $\bar{\mathbf{b}}_{\mathrm{III}}$, the 2-fold axis in crystal III. For twin axis $[\bar{1}10]_{\mathrm{I}}$, which coincides with $\bar{\mathbf{b}}_{\mathrm{II}}$, we find that $\mathbf{a}_{\mathrm{I}}$ is brought onto $\bar{\mathbf{a}}_{\mathrm{III}}$, $\mathbf{b}_{\mathrm{I}}$ onto $\mathbf{b}_{\mathrm{III}}$ and $\mathbf{c}_{\mathrm{I}}$ onto $\bar{\mathbf{c}}_{\mathrm{III}}$.

The perfect superposition of the reciprocal lattices of crystals I, II and III is observed for friedelite as well as for mcGillite and over a range of cell dimensions. It appears unlikely that such a superposition would be fortuitous. There appears to be restraint at work that keeps the four monoclinic cell parameters locked into the above relations with the two-parameter rhombohedral twin-lattice.

Repeated twinning is universal, and commonly the twin domains are only a few layers thick. We call this phenomenon "incipient twinning" when the crystals fail to grow to sufficient size to give sharp X-ray reflections. The stacking disorder observed in structural images (Figs. 2 and 4) can now be fully explained in terms of repeated incipient twinning.

In the high-resolution structure image of mcGillite (Fig. 4), each horizontal line of white spots (contrasts) is separated from the adjacent one by a spacing of 1/12 the period along the normal to the line of spots. The rectangle outlined in black shows a diagonal line of white spots, which divides the period (parallel to c^*) into twelve equal parts.

The crystal structure

The vector $\mathbf{c}$ of the monoclinic lattice becomes the stacking vector $\mathbf{f}$ needed to derive a possible structure for mcGillite (and friedelite). The lengths of the cell edges a, b, c and the chemical similarity suggest that the structures will be

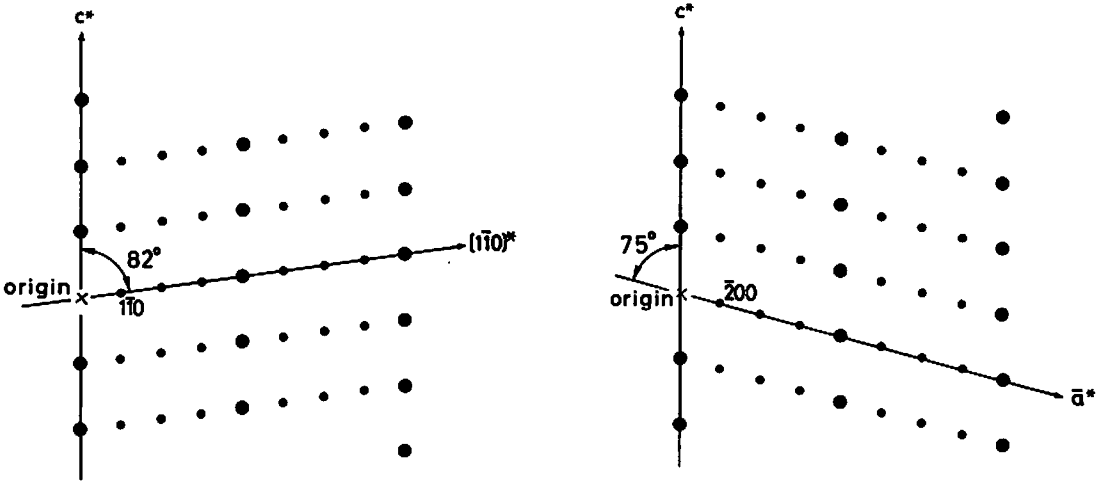


FIG. 6. Two nets of the monoclinic reciprocal lattice, one showing $\bar{h}hl$ reflections (*left*) and the other $h0l$ reflections (*right*). They correspond to the diffraction patterns shown in Figure 3(ii) and Figure 3(iii), respectively.

TABLE 1. DIFFRACTION PATTERNS OF FRIEDELITE AND McGILLITE RE-INDEXED ON THE MONOCLINIC CELL OBTAINED FROM THE RHOMBOHEDRAL CELL OF McGILLITE

Friedelite			McGillite			hkl
d_{obs}	I	d_{calc}	d_{obs}	I	d_{calc}	
11.4	10	11.51	11.67	2	11.55	110*
		11.26			11.25	200*
7.17	90	7.19	7.16	7	7.16	001
		6.70	6.75	1	6.73	020*
		6.50	6.50	1	6.49	$\bar{1}10$*
		5.45	5.44	1	5.43	201*
3.60	70	3.59	3.570	4	3.582	002
2.88	60	2.88	2.888	6	2.888	440;$\bar{8}01$
2.56	100	2.56	2.560	10	2.562	441;$\bar{8}02$
2.408	30	2.408	2.409	2	2.412	$\bar{4}42$;801
2.115	40	2.113	2.112	4	2.114	442;$\bar{8}03$
1.974	20	1.976	1.971	2	1.975	$\bar{4}43$;802
1.731	30	1.730	1.727	2	1.731	443;$\bar{8}04$
1.676	60	1.676	1.683	4	1.682	080
1.632	20	1.632	1.638	2	1.638	081
1.625	10	1.625	1.619	2	1.623	$\bar{4}44$;803
1.520	10	1.519	1.524	1	1.523	082
1.449	10	1.448	1.454	1	1.454	$\bar{8}81$;$\overline{16}$,0,1
1.439	10	1.441	1.420	2	1.438	444;$\bar{8}05$
		1.438			1.433	005
1.402	20	1.402			1.406	$\bar{8}82$;16,0,0
1.374	10	1.376			1.380	881;$\overline{16}$,0,3
		1.374			1.375	083
1.359	30	1.361	1.356	2	1.358	$\bar{4}45$;804
1.313	10	1.313	1.317	1	1.316	$\bar{8}83$;16,0,1
		1.289	1.292	1	1.294	$\bar{9}91$*
1.204	20	1.204	1.205	1	1.206	$\bar{8}84$;16,0,2
1.200	10	1.198			1.194	006
1.167	10	1.167	1.167	1	1.168	883;$\overline{16}$,0,5
1.093	10	1.092			1.093	$\bar{8}85$;16,0,3
1.090	10	1.091	1.0897	1	1.0908	085
			1.0795		1.0780	436*
1.065	10	1.063				4,12,$\bar{2}$

Diffraction pattern of friedelite after Frondel & Bauer (1953), that of mcGillite after Donnay *et al.* (1980). The calculated *d* values, d_{calc}, for friedelite were obtained from the monoclinic cell dimensions refined by least squares. Stars indicate *S* reflections.

analogous to the layer structure of manganpyrosmalite (Takéuchi *et al.* 1969), whose unit layer (Fig. 8) consists of two sheets: one octahedral, the other tetrahedral. The tetrahedral sheet is composed of six-membered rings of tetrahedra all pointing up in one ring and all down in adjacent rings, respectively away from and toward the octahedral sheet, to bond to the octahedral cations. A tetrahedral ring in the first orientation will be called a *U* ring and one in the second orientation, a *D* ring (*U* and *D* for "up" and "down", respectively). In order to stack a second layer on top of the first, to form a structure, the following condition must be satisfied: the apical oxygen atoms of the *U* rings of the first layer should become the constituent members of the bottom oxygen sheet of the second layer (Fig. 8).

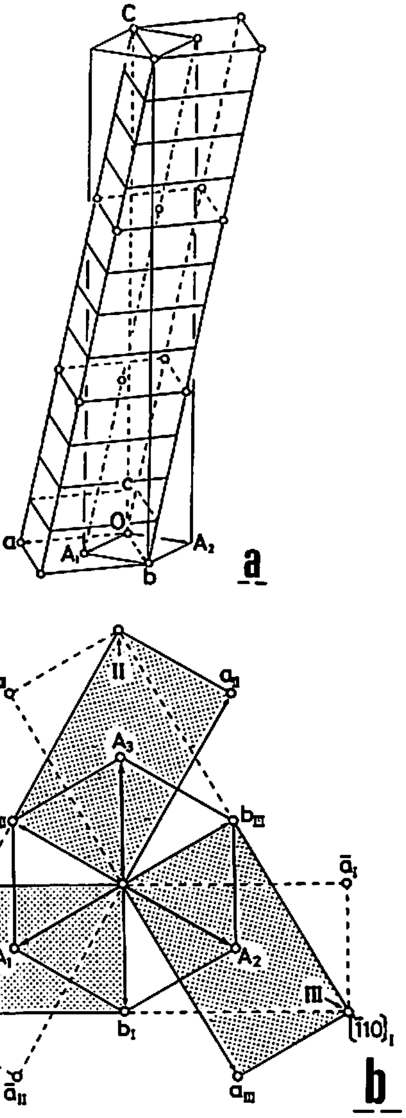


FIG. 7a. Relationships between the new monoclinic (*mC*) cell abc of mcGillite, a stack of twelve such cells, and the hexagonal (*hR*) triple cell A_1A_2C, originally, described by Donnay *et al.* (1980), showing its rhombohedral centring. b. Plan of mcGillite twin (3 crystals, numbered I, II, III). Direct lattice, monoclinic indexing.

An inspection of the pyrosmalite structure (Takéuchi *et al.* 1969) reveals that there are two distinct ways of placing the tetrahedral sheet in contact with the octahedral one to form a unit layer (Fig. 8), thus yielding two types of unit layers. These layer types differ in the relative arrangement of Si and Mn atoms; in the first one, half the Si atoms (those of the *U* rings in Fig. 8) are located nearly on top of the Mn atoms; in the second type all the Si atoms, when projected orthogonally on the plane of the layers, are nearly equally distant from Mn atoms. The first layer type will be called an **M** layer, and the second, a **P** layer. The **P** and **M** layers are notably different when viewed

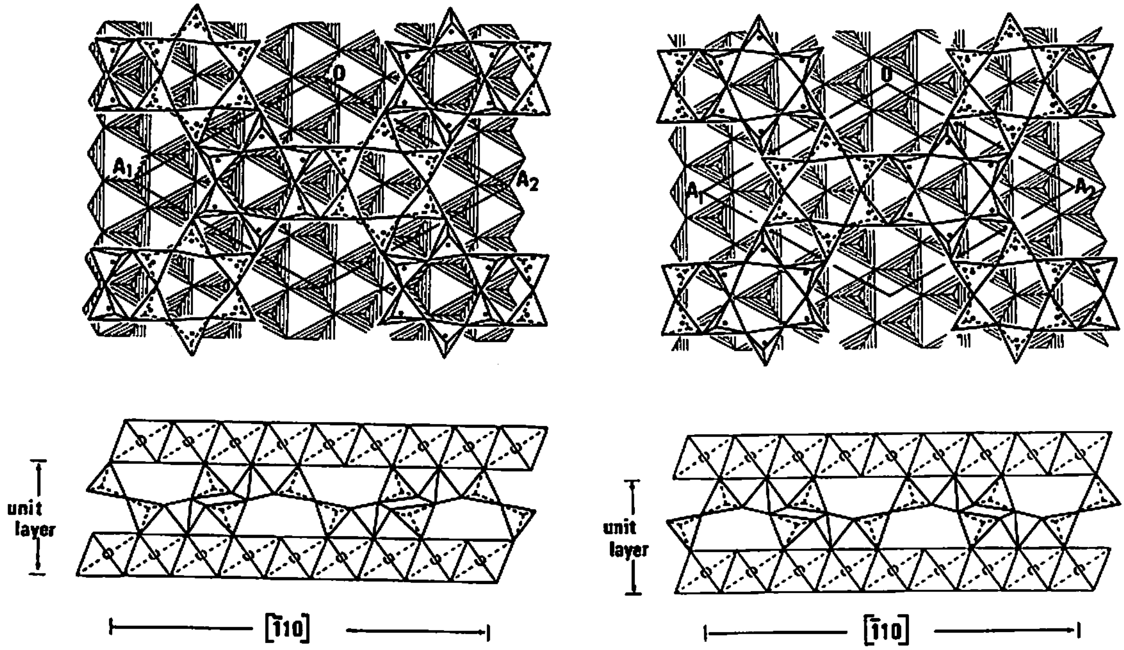


FIG. 8. Two types of unit layers, M (*left*) and P (*right*), each one shown in plan and elevation; projections along the layer normal, and along [11.0] and [11.0], respectively; in plan the downsloping faces of the octahedra are ruled. The two types of unit layers are drawn with their silicate sheets in the same oorientation; the octahedra in one type are seen to be rotated by 60° with respect to those in the other. Hexagonal indexing. Note the reversal of A_1A_2 in layer M (left).

down their monoclinic **b** axes (Fig. 8): their octahedral sheets are mirror images of each other in such a projection, whereas the silicate sheets are the same. Only in the M layer do we find that the above-mentioned vector **f** is the simplest possible stacking vector satisfying the above stacking condition. Thus the structure of mcGillite can be derived from M as a one-layer monoclinic structure, in which the stacking vector **f** occurs in one direction (Fig. 9). This structure belongs to space group *C*2/*m*. One marked feature of the structure is that the arrangement of the octahedral cations constitutes a rhombohedral superlattice. This arises from the fact that the horizontal displacement of each octahedral sheet with respect to its neighbor corresponds to the translation $\mathbf{a}_1/3 + 2\mathbf{a}_2/3$ of the hexagonal submesh of the octahedral sheet. Note that this rhombohedral superlattice is the lattice of the rhombohedral structure suggested for friedelite by Frondel & Bauer (1953).

The existence of sharp *S* reflections in the X-ray-diffraction patterns of mcGillite means that the regular stacking sequence of the monoclinic structure has an appreciable extension in the mineral species and that the regular structure can be recognized by X-ray diffraction. Accordingly, the monoclinic structure may be called the mcGillite structure-type, one of the basic structures of a series of possible polytypic structures in the pyrosmalite group. On the other hand, the fact that friedelite exhibits only diffuse *S* reflections in its X-ray-diffraction pattern means that no regular monoclinic structure in the mineral species can be identified by X-ray diffraction. Friedelite may thus be regarded as a disordered equivalent of mcGillite.

The chemical composition of mcGillite was established as $Mn_8Si_6O_{15}(OH)_8Cl_2$ when the mineral was first described (Donnay *et al.* 1979). Dunn *et al.* (1981), after examining "all available friedelite analyses", state its formula as varying from $Mn_8Si_6O_{15}(OH)_9Cl$ to $Mn_8Si_6O_{15}(OH)_{10}$, showing its Cl content to be less than half that of mcGillite. Chlorine, being a much larger anion than OH, expands the (001) layer in its plane and makes it fit. In friedelite, with less chlorine, this shared anionic plane fits less well, and more disorder results.

ADDENDUM

Iijima's two papers[1] on mcGillite (1982a, b)

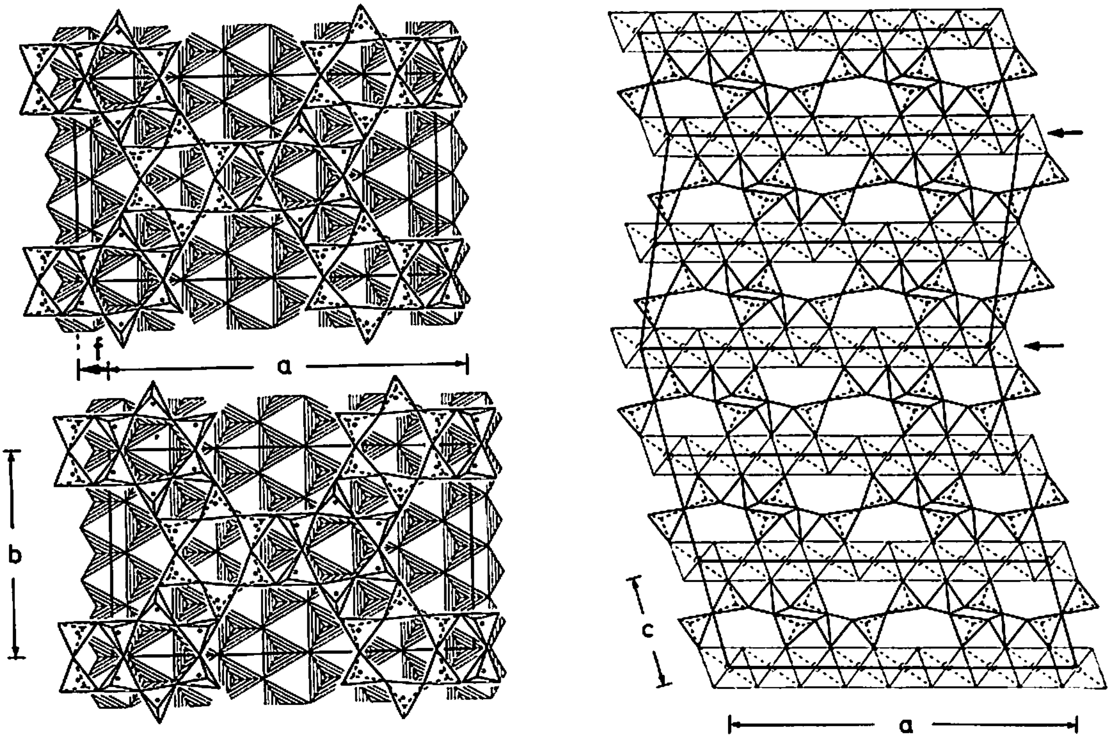


FIG. 9. The structure of mcGillite. *Left*: a pair of successive unit-layers viewed down c^*. The stacking vector **f** is indicated. *Right*: view, down *b*, of the structure in a twinned orientation. The slab between the arrows is related to the adjacent portions by a rotation of 120° around [1.0.12].

appeared in September 1982. The reader may thus be able to compare his results with ours. The layer structure of mcGillite that he proposes and the one described in this paper were both obtained by means of high-resolution electron microscopy, and show a large measure of agreement. Our study, particularly on polytypism, is more general and covers not only mcGillite but the whole pyrosmalite group of minerals.

The following errata have been noted on page 685: col. 1, line 6, *instead of* $a = 23.279$, *read* $a = 23.379$; col. 2, line 1, *instead of* $\beta = \ldots$, *read* $\beta - 90° = \ldots$: col. 2, line 7, *instead of* about [100], *read* about the normal to (001). *Cf.* abstract of Paper II (Iijima 1982b, p. 695).

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[1] In the abstract of Paper I (Iijima 1982a), p. 685, and on p. 692, Iijima (SI) describes *a, b, c* of the monoclinic cell in terms of a_o and c_o, which he defines as the dimensions of the "trigonal" cell proposed by Donnay, Bétournay and Hamill" (DBH) (1980). In fact, the DBH cell was *rhombohedral*, described in hexagonal axes (hR), and its height of 85.657 Å is equal to twelve times the c_o = 7.138 Å mentioned by SI. This value of 7.138 Å corresponds to the DBH "pseudo-repeat $c' \sim 7.16$ Å". DBH do not consider any cell of height c' except when quoting literature data in $P\bar{3}m1$ for manganpyrosmalite and pyrosmalite (in their Table 2); they point out that a layer thickness of $4c'$ is required by the *R* lattice, so that the total height of their cell is $12\ c'$.

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