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Polytypes of the Two-Packet Chlorites

By V. A. Drits and Yu. V. Karavan

Geological Institute of the Academy of Sciences of the USSR, Pyzhevsky 7, Moscow, USSR

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The systematic derivation of all the possible chlorite polytypes with a two-packet unit cell is carried out. The derivation is completed for trioctahedral, dioctahedral and di-trioctahedral chlorites. The diffraction features which should identify the different chlorite polytypes are calculated.

The chlorites are layer-lattice silicates of variable composition. They consist of regularly alternating talc- and brucite-type layers (Pauling, 1930). The talc-type layer is three-storied, consisting of an octahedral net occupying the centre and two tetrahedral nets adjoining the octahedral net from above and below. The brucite-type layer is one-storied, consisting of one octahedral network. Each pair of three-storied and one-storied layers forms a chlorite packet. It would be accepted that a chlorite packet comprises one three-storied layer and two halves of two different one-storied layers, one covering it and one underlying it.

Chlorites are divided into trioctahedral, where all the octahedra are occupied by cations, and dioctahedral, in which only $\frac{2}{3}$ of all the octahedral positions are occupied. The ideal structural formula for trioctahedral chlorites is

$$(\mathrm{Mg}_{6-x-y}\mathrm{Fe}^{2+}_{y}\mathrm{Al}_{x})\,(\mathrm{Si}_{4-x}\mathrm{Al}_{x})\mathrm{O}_{10}(\mathrm{OH})_{8}\,,$$

and for dioctahedral chlorites,

$$(\mathrm{Al}_{4+x/3})\,(\mathrm{Si}_{4-x}\mathrm{Al}_{x})\mathrm{O}_{10}(\mathrm{OH})_{8}\,.$$

The structure of the chlorites is made up from chlorite packets superimposed one upon another in a varying manner. Scientific publications usually describe one-packet and semi-random chlorites (McMurchy, 1934; Zvyagin, 1964; Brown & Bailey, 1962; 1963; Shirozu & Bailey, 1965).

However, McMurchy (1934), and later Garrido (1949) and Brindley, Oughton & Robinson (1950) pointed out the occurrence of chlorites with a different periodicity of packets along the *c* axis, and discussed some polytypes possible for chlorites with more than one packet per repeat period. Chlorites with a two-packet monoclinic unit cell have been described by Drits & Lazarenko (1967) and Wlasow & Drits (1967). This paper gives a systematic determination of all the possible chlorite polytypes with a repeat period of two chlorite packets and their diffraction features are calculated in order to determine the structure of the new two-packet chlorites which we have investigated (Wlasow & Drits, 1967; Drits & Lazarenko, 1967). In deriving these polytypes the analytical method of Zvyagin (1964) was used, providing a simpler solution of this problem.

Table 1. *Components of the displacements σ and τ along the a and b axes which are possible in structures of layer silicates*

Symbols of the displacements	σ_1	σ_2	σ_3	σ_4	σ_5	σ_6	τ_0	τ_+	τ_-
	τ_4	τ_5	τ_6	τ_1	τ_2	τ_3			
Components of the displacements	$\frac{1}{3}, \frac{1}{3}$	$-\frac{1}{3}, \frac{1}{3}$	$\frac{1}{3}, 0$	$-\frac{1}{3}, -\frac{1}{3}$	$\frac{1}{3}, -\frac{1}{3}$	$-\frac{1}{3}, 0$	0, 0	$0, \frac{1}{3}$	$0, -\frac{1}{3}$

Displacement components are expressed in multiples of *a* and *b*.

This method operates on whole blocks of the structure consisting of tetrahedral and octahedral networks. Any structure of layer silicates is considered in the form of the combined patterns of parallel tetrahedral and octahedral networks, as projected along their normals onto the *ab* plane. For a complete description of a layer structure it is necessary to determine the relative displacements of adjacent networks. By measuring them from the centres of the octahedra of the octahedral network, and the centres of the hexagonal loops of the tetrahedral network, and then in a rectilinear system of coordinates with an *ab* cell, these displacements are defined by components along the axes *a* and *b*, which are given in Table 1. Here, the σ_i represent relative displacements of the octahedral and tetrahedral networks within a layer, and the τ_j represent

Table 2. *Two-packet structures consisting of the same types of trioctahedral or di-trioctahedral packets*

Group	No.	Succession of indices of structures	C_x, C_y	x_0, y_0	Space symmetry
I	1	2 | 3 4 | 3 2 |	0, 0	0, 0	C^2/c
	2	2 | 3 2 | 1 2 |	0, 0	0, 0	$C1$
	3	2 | 3 6 | 5 2 |	0, 0	0, 0	$C1$
	4	2′ 3 4′ 3 2′	0, 0	0, 0	C^2/c
	5	2′ 3 2′ 1 2′	0, 0	0, $\frac{1}{3}$	$C\bar{1}$
	6	2′ 3 6′ 5 2′	0, 0	0, 0	$C1$
	7	|3 | + |4 | + |3 |	0, 0	0, 0	$C\bar{1}$
	8	|3 | 0 |6 | 0 |3 |	0, 0	0, 0	C_{mmm}
	9	|3 | + |6 | − |3 |	0, 0	0, $\frac{1}{6}$	C_{222}
	10	|3 | + |2 | 0 |3 |	0, 0	0, 0	$C1$
	11	|3′| + |4′| + |3′|	0, 0	0, 0	$C\bar{1}$
	12	|3′| 0 |6′| 0 |3′|	0, 0	0, 0	C_{mmm}
	13	|3′| + |6′| − |3′|	0, 0	0, $\frac{1}{6}$	C_{222}
	14	|3′| + |2′| 0 |3′|	0, 0	0, 0	$C1$
II	1	3 1 3 5 3	$-\frac{1}{3}$, 0	$\frac{1}{6}$, $\frac{1}{3}$	C^2/c
	2	1 3 5 3 1	$-\frac{1}{3}$, 0	0, 0	C^2/c
	3	1 1 5 5 1	$-\frac{1}{3}$, 0	0, $\frac{1}{6}$	Cc
	4	5 3 5 5 5	$-\frac{1}{3}$, 0	$\frac{1}{6}$, $\frac{1}{3}$	$C\bar{1}$
	5	3 1 1 1 3	$-\frac{1}{3}$, 0	0, 0	$C\bar{1}$
	6	3 3 5 1 3	$-\frac{1}{3}$, 0	0, 0	$C1$
	7	3′| 1 3′| 5 3′	$-\frac{1}{3}$, 0	0, $\frac{1}{3}$	Cc
	8	1′| 3 5′| 3 1′|	$-\frac{1}{3}$, 0	0, $\frac{1}{3}$	Cc
	9	1′| 1 5′| 5 1′|	$-\frac{1}{3}$, 0	0, $\frac{1}{3}$	Cc
	10	5′| 3 5′| 5 5′|	$-\frac{1}{3}$, 0	0, 0	$C1$
	11	3′| 1 1′| 1 3′|	$-\frac{1}{3}$, 0	0, 0	$C1$
	12	3′| 3 1′| 5 3′|	$-\frac{1}{3}$, 0	0, 0	$C1$
	13	|4 | 0 |2 | 0 |4 |	$-\frac{1}{3}$, 0	0, 0	C^2/c
	14	|6 | − |6 | + |6 |	$-\frac{1}{3}$, 0	$\frac{1}{6}$, $\frac{1}{3}$	C^2/c
II	15	|4 | − |2 | + |4 |	$-\frac{1}{3}$, 0	0, $\frac{1}{6}$	Cc
	16	|2 | 0 |2 | − |2 |	$-\frac{1}{3}$, 0	$\frac{1}{6}$, $\frac{1}{3}$	$C\bar{1}$
	17	|6 | − |2 | − |6 |	$-\frac{1}{3}$, 0	0, 0	$C\bar{1}$
	18	|6 | 0 |4 | − |6 |	$-\frac{1}{3}$, 0	0, 0	$C1$
	19	|4′| 0 |2′| 0 |4′|	$-\frac{1}{3}$, 0	0, 0	C^2/c
	20	|6′| − |6′| + |6′|	$-\frac{1}{3}$, 0	$\frac{1}{6}$, $\frac{1}{3}$	C^2/c
	21	|4′| − |2′| + |4′|	$-\frac{1}{3}$, 0	0, $\frac{1}{6}$	Cc
	22	|4′| 0 |4′| + |4′|	$-\frac{1}{3}$, 0	$\frac{1}{6}$, $\frac{1}{3}$	$C\bar{1}$
	23	|6′| − |2′| − |6′|	$-\frac{1}{3}$, 0	0, 0	$C\bar{1}$
	24	|6′| 0 |4′| − |6′|	$-\frac{1}{3}$, 0	0, 0	$C1$
III	1	2 | 3 2 | 5 2 |	0, $-\frac{1}{3}$	0, 0	$C1$
	2	2 | 3 6 | 3 2 |	0, $-\frac{1}{3}$	0, 0	$C1$
	3	2 | 3 4 | 1 2 |	0, $-\frac{1}{3}$	0, 0	$C1$
	4	2′ 3 2′ 5 2′	0, $-\frac{1}{3}$	0, $\frac{1}{6}$	$C\bar{1}$
	5	2′ 3 6′ 3 2′	0, $-\frac{1}{3}$	0, 0	$C\bar{1}$
	6	2′ 3 4′ 1 2′	0, $-\frac{1}{3}$	0, 0	$C1$
	7	|3 | + |6 | + |3 |	0, $-\frac{1}{3}$	0, $\frac{1}{3}$	C^2/c
	8	|3 | 0 |2 | 0 |3 |	0, $-\frac{1}{3}$	0, $\frac{1}{3}$	$C\bar{1}$
	9	|6 | − |5 | − |6 |	0, $-\frac{1}{3}$	0, $\frac{1}{3}$	$C\bar{1}$
	10	|4 | 0 |3 | + |4 |	0, $-\frac{1}{3}$	0, 0	$C1$
	11	|4 | 0 |1 | − |4 |	0, $-\frac{1}{3}$	0, 0	$C1$
	12	|3 | + |2 | − |3 |	0, $-\frac{1}{3}$	0, 0	$C1$
	13	|3′| + |6′| + |3′|	0, $-\frac{1}{3}$	0, $\frac{1}{3}$	C^2/c
	14	|3′| 0 |2′| 0 |3′|	0, $-\frac{1}{3}$	0, $\frac{1}{3}$	$C\bar{1}$
	15	|6′| − |5′| − |6′|	0, $-\frac{1}{3}$	0, $\frac{1}{3}$	$C\bar{1}$
	16	|4′| 0 |3′| + |4′|	0, $-\frac{1}{3}$	0, 0	$C1$
	17	|4′| 0 |1′| − |4′|	0, $-\frac{1}{3}$	0, 0	$C1$
	18	|3′| + |2′| − |3′|	0, $-\frac{1}{3}$	0, 0	$C1$

C_x, C_y: Coordinates of projection of the axis *c* on the plane *ab*.
X_0, Y_0: Coordinates of the origin of the unit cell of the structure relative to the first layer.
The letters σ, τ are omitted for simplicity and shortening the designation of the structures. The succession of the indices is given and the prime and the line are preserved. For example, structure $\sigma_3'|\tau_1\sigma_1'|\tau_5\sigma_3'|$ is designated 3′|11′|53′|.

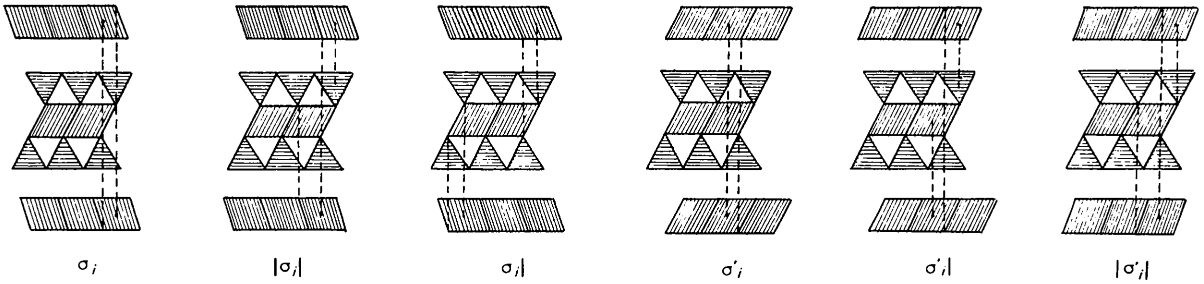

Fig. 1. Six types of chlorite packets. These are possible because, for a given three-storied layer, there are four ways of arranging an adjacent one-storied layer relative to it. These are: two opposed orientations of the one-storied layer, either parallel or antiparallel to the octahedral network of the three-storied layer, and, with these orientations fixed two possible positions, differing by *a*/3, which satisfy the condition that the OH groups of the brucite-type layer and the O atoms of the adjacent there-storied layer, are grouped in pairs to form hydrogen bonds.

displacements between the nearest networks of adjacent layers. The quantities σ, τ, can therefore be considered as the minimum number of independent parameters necessary to define any arbitrary sequence of layers. The symbol σ_i may be used to designate a type and orientation of a layer or packet.

Trioctahedral chlorites

It is accepted that six types of chlorite packet are possible for trioctahedral chlorites; they are shown in Fig. 1 and designated by the symbols σ_i; σ_i'; $\sigma_i|$; $\sigma_i'|$; $|\sigma_i|$; $|\sigma_i'|$ (Zvyagin, 1964). A prime by σ_i indicates that the octahedral networks are parallel and its absence implies that they are antiparallel. In Fig. 1 the dashed lines show atoms of the one-storied and three-storied layers which coincide in the normal projection on to the *ab* plane. When cations of a one-storied layer are superimposed on the nearest tetrahedral cations in such a projection on the *ab* plane, this is denoted by the vertical line of σ_i. Index *i* of σ_i defines one of the six identical orientations of each chlorite packet, differing only by a rotation angle which is a multiple of 60°.

A definite spatial configuration of a chlorite packet corresponds to each actual value of *i* in σ_i. Let us consider, for instance, packet $|\sigma_1'|$: first we construct a three-storied layer; we place the centre of the hexagonal loop of the tetrahedral network at the origin of the centred rectilinear cell coordinates. The coordinates of the centre of the superimposed octahedral network are $\sigma_1(\frac{1}{3},\frac{1}{3})$ (see Table 1). The centre of the hexagonal loop of the upper tetrahedral network is displaced in relation to the centre of the octahedral network, also by $\sigma_1(\frac{1}{3},\frac{1}{3})$, and in relation to the origin of the cell

Table 3. *Dioctahedral monoclinic* ($\beta = 94°$) *two-packet chlorites*

<table>
<tr><th>Succession of indices of structures containing σ_i packets</th><th>Numeration of the structures</th><th>Succession of indices of structures containing |σ_i′| packets</th><th>Numeration of the structures</th><th>Symmetry of succession packets</th><th>Space group</th></tr>
<tr><td>3 6 2 3 4 6 3</td><td>II–1<i>a</i></td><td>|6′|0 −|6′|+ 0|6′|</td><td>II–20<i>a</i></td><td>C^2/m; $C2$</td><td>$C2$</td></tr>
<tr><td>3 4 4 3 2 2 6</td><td>II–1<i>b</i></td><td>|6′|+ +|6′|− −|6′|</td><td>II–20<i>b</i></td><td>$C2$; $C2$</td><td>C^2/c</td></tr>
<tr><td>3 6 2 3 2 2 3</td><td>II–1<i>c</i></td><td>|6′|0 −|6′|− −|6′|</td><td>II–20<i>c</i></td><td>$C1$; $C\bar{1}$</td><td>$C1$</td></tr>
<tr><td>3 4 4 3 4 6 3</td><td>II–1<i>d</i></td><td>|6′|+ +|6′|+ 0|6′|</td><td>II–20<i>d</i></td><td>$C1$; $C\bar{1}$</td><td>$C1$</td></tr>
<tr><td>3 6 2 3 6 4 3</td><td>II–1<i>e</i></td><td>|6′|0 −|6′|0 +|6′|</td><td>II–20<i>e</i></td><td>$C1$; $C1$</td><td>$C1$</td></tr>
<tr><td>5 2 4 1 4 2 5</td><td>II–2<i>a</i></td><td>|4′|0 0|2′|0 0|4′|</td><td>II–19<i>a</i></td><td>C^2/m; C^2/m</td><td>C^2/c</td></tr>
<tr><td>5 4 2 1 6 6 5</td><td>II–2<i>b</i></td><td>|4′|+ −|2′|+ −|4′|</td><td>II–19<i>b</i></td><td>$C2$; $C2$</td><td>$C2$</td></tr>
<tr><td>5 4 2 1 2 4 5</td><td>II–2<i>c</i></td><td>|4′|+ −|2′|− +|4′|</td><td>II–19<i>c</i></td><td>$C\bar{1}$; $C\bar{1}$</td><td>C^2/c</td></tr>
<tr><td>5 6 6 1 6 6 5</td><td>II–2<i>d</i></td><td>|4′|− +|2′|+ −|4′|</td><td>II–19<i>d</i></td><td>$C\bar{1}$; $C\bar{1}$</td><td>C^2/c</td></tr>
<tr><td>5 2 4 1 2 4 5</td><td>II–2<i>e</i></td><td>|4′|0 0|2′|− +|4′|</td><td>II–19<i>e</i></td><td>$C1$; $C1$</td><td>$C2$</td></tr>
<tr><td>5 6 6 1 4 2 5</td><td>II–2<i>f</i></td><td>|4′|0 0|2′|+ −|4′|</td><td>II–19<i>f</i></td><td>$C1$; $C1$</td><td>$C2$</td></tr>
<tr><td>5 2 2 1 6 2 5</td><td>II–3<i>a</i></td><td>|4′|0 −|2′|+ 0|4′|</td><td>II–21<i>a</i></td><td>C^2/m; $C2$</td><td>$C1$</td></tr>
<tr><td>5 4 6 1 2 6 5</td><td>II–3<i>b</i></td><td>|4′|+ +|2′|− −|4′|</td><td>II–21<i>b</i></td><td>$C2$; $C2$</td><td>Cc</td></tr>
<tr><td>5 4 6 1 6 2 5</td><td>II–3<i>c</i></td><td>|4′|+ +|2′|0 +|4′|</td><td>II–21<i>c</i></td><td>$C1$; $C\bar{1}$</td><td>$C1$</td></tr>
<tr><td>5 4 6 1 4 4 5</td><td>II–3<i>d</i></td><td>|4′|+ +|2′|+ 0|4′|</td><td>II–21<i>d</i></td><td>$C\bar{1}$; $C1$</td><td>$C1$</td></tr>
<tr><td>5 2 2 1 4 4 5</td><td>II–3<i>e</i></td><td>|4′|0 −|2′|0 +|4′|</td><td>II–21<i>e</i></td><td>$C1$; $C1$</td><td>Cc</td></tr>
<tr><td>5 6 4 1 6 2 5</td><td>II–3<i>f</i></td><td>|4′|− 0|2′|+ 0|4′|</td><td>II–21<i>f</i></td><td>$C1$; $C1$</td><td>Cc</td></tr>
<tr><td>1 4 4 3 4 4 1</td><td>II–5<i>a</i></td><td>|2′|0 −|6′|− 0|2′|</td><td>II–23<i>a</i></td><td>C^2/m; $C\bar{1}$</td><td>$C\bar{1}$</td></tr>
<tr><td>1 2 6 3 6 2 1</td><td>II–5<i>b</i></td><td>|2′|− 0|6′|0 −|2′|</td><td>II–23<i>b</i></td><td>$C\bar{1}$; C^2/m</td><td>$C\bar{1}$</td></tr>
<tr><td>1 6 2 3 2 6 1</td><td>II–5<i>c</i></td><td>|2′|+ +|6′|+ +|2′|</td><td>II–23<i>c</i></td><td>$C\bar{1}$; $C\bar{1}$</td><td>$C\bar{1}$</td></tr>
<tr><td>1 2 6 3 2 6 1</td><td>II–5<i>d</i></td><td>|2′|+ +|6′|0 −|2′|</td><td>II–23<i>d</i></td><td>$C2$; $C1$</td><td>$C1$</td></tr>
<tr><td>1 6 2 3 4 4 1</td><td>II–5<i>e</i></td><td>|2′|+ +|6′|− 0|2′|</td><td>II–23<i>e</i></td><td>$C1$; $C2$</td><td>$C1$</td></tr>
<tr><td>1 4 4 3 6 2 1</td><td>II–5<i>f</i></td><td>|2′|0 −|6′|0 −|2′|</td><td>II–23<i>f</i></td><td>$C1$; $C1$</td><td>$C1$</td></tr>
<tr><td>5 2 2 5 2 4 5</td><td>II–4<i>a</i></td><td>|4′|0 0|4′|0 +|4′|</td><td>II–22<i>a</i></td><td>$C1$; C^2/m</td><td>$C1$</td></tr>
<tr><td>5 6 4 5 6 6 5</td><td>II–4<i>b</i></td><td>|4′|− +|4′|− −|4′|</td><td>II–22<i>b</i></td><td>$C\bar{1}$; $C2$</td><td>$C1$</td></tr>
<tr><td>5 4 6 5 2 4 5</td><td>II–4<i>c</i></td><td>|4′|+ −|4′|0 +|4′|</td><td>II–22<i>c</i></td><td>$C\bar{1}$; $C1$</td><td>$C1$</td></tr>
<tr><td>5 4 6 5 4 2 5</td><td>II–4<i>d</i></td><td>|4′|+ −|4′|+ 0|4′|</td><td>II–22<i>d</i></td><td>$C1$; $C2$</td><td>$C1$</td></tr>
<tr><td>5 2 2 5 6 6 5</td><td>II–4<i>e</i></td><td>|4′|0 (0|4′|−) −|4′|</td><td>II–22<i>e</i></td><td>$C1$; $C1$</td><td>$C1$</td></tr>
<tr><td>3 6 6 5 2 6 3</td><td>II–6<i>a</i></td><td>|6′|0 0|4′|− 0|6′|</td><td>II–24<i>a</i></td><td>C^2/m; $C1$</td><td>$C1$</td></tr>
<tr><td>3 4 2 5 2 6 3</td><td>II–6<i>b</i></td><td>|6′|0 0|4′|0 −|6′|</td><td>II–24<i>b</i></td><td>$C1$; C^2/m</td><td>$C1$</td></tr>
<tr><td>3 2 4 5 6 2 3</td><td>II–6<i>c</i></td><td>|6′|+ −|4′|+ +|6′|</td><td>II–24<i>c</i></td><td>$C\bar{1}$; $C2$</td><td>$C1$</td></tr>
<tr><td>3 2 4 5 4 4 3</td><td>II–6<i>d</i></td><td>|6′|− +|4′|+ +|6′|</td><td>II–24<i>d</i></td><td>$C2$; $C\bar{1}$</td><td>$C1$</td></tr>
<tr><td>3 4 2 5 6 2 3</td><td>II–6<i>e</i></td><td>|6′|+ −|4′|0 −|6′|</td><td>II–24<i>e</i></td><td>$C2$; $C1$</td><td>$C1$</td></tr>
<tr><td>3 6 6 5 4 4 3</td><td>II–6<i>f</i></td><td>|6′|− +|4′|− 0|6′|</td><td>II–24<i>f</i></td><td>$C1$; $C2$</td><td>$C1$</td></tr>
<tr><td>3 4 2 5 4 4 3</td><td>II–6<i>g</i></td><td>|6′|− +|4′|0 −|6′|</td><td>II–24<i>g</i></td><td>$C\bar{1}$; $C1$</td><td>$C1$</td></tr>
<tr><td>3 6 6 5 6 2 3</td><td>II–6<i>h</i></td><td>|6′|+ −|4′|− 0|6′|</td><td>II–24<i>h</i></td><td>$C1$; $C\bar{1}$</td><td>$C1$</td></tr>
<tr><td>3 2 4 5 2 6 3</td><td>II–6<i>i</i></td><td>|6′|0 0|4′|+ +|6′|</td><td>II–24<i>i</i></td><td>$C1$; $C1$</td><td>$C1$</td></tr>
</table>

The letters σ, τ are omitted for simplicity and shortening the designation of the structures. For example, structure $\sigma_1\tau_2\tau_6\sigma_3\tau_2\tau_6\sigma_1$ is designated 1 2 6 3 2 6 1.

coordinates, by $2\sigma_1(-\frac{1}{3}, -\frac{1}{3})$. In this way, the spatial orientation of the three-storied layer in relation to the chosen coordinate system is determined. The presence of a prime and vertical lines in $|\sigma_1'|$ shows how the one-storied layers should be superimposed on a given three-storied layer (see Fig. 1). (The octahedral layers of both networks are parallel, so the cations and the top apices of the octahedra of the one-storied layer coincide, in a normal projection, with the top tetrahedral cations and the lower apices of the octahedra of the bottom three-storied layer.)

It should be noted that the superposition of the one-storied layers on the three-storied layers in chlorite packets always takes place in such a way that the O atoms and hydroxyl groups, OH, of adjacent networks in different layers form pairs with hydrogen bonds.

Let us consider the sequence of layers and packets in a vertical arrangement, the three-storied layer of the initial chlorite packet being the lower, and the one-storied packet, the upper. In such a case the oxygen atoms of the tetrahedral network in the upper chlorite packet must be superimposed on the one-storied layer of the lower packet. Since the position of the one-storied layer with respect to the three-storied layer for each definite type of chlorite packet is unequivocally fixed, the displacement of adjacent packets can be defined by the values, τ_j, of the relative displacements of the centres of hexagonal loops of tetrahedral nets adjoining the one-storied layers from above and below, and belonging to different packets.

As in the case of trioctahedral chlorites, displacements of packets can be defined by displacements of three-storied layers. First we determine the various sequences of chlorite packets forming the two-packet unit-cell, independent of any definite type of chlorite packet. Furthermore, if we do not impose restrictions on the τ values, the full set of packet sequences of the type $\sigma_i\tau_k\sigma_j\tau_l\sigma_i$ can be derived from an analysis of

Table 4. $F^2(0\overset{\pm}{2}l)$, $F^2(\overset{\pm}{1}\overset{\pm}{1}l)$ *for two-packet trioctahedral chlorites with orthorhombic cell* ($l = l_{\mathrm{orth}}/3$)

Numeration of structures	l_{orth} *hkl*	0	3	6	9	12	15	18	21	24	27	30
I–1,4	$0\overset{\pm}{2}l$	11	11	30	26	7,5	1,5	4	20	2	2,5	42
	$1\overset{\pm}{1}l$	24	31	16	1	6,5	23	1	8	6	6	1
	$\overset{\pm}{1}1l$	2,5	5	10	19	0	14	8	3	2	17	2
	sum	75	94	112	90	28	75	24	63	20	51	90
I–2,5	$02l$, $\bar{1}1l$	2,5	1	5,5	30	7	1,5	67	14	6	11	1
	$0\bar{2}l$, $1\bar{1}l$	2,5	26	10	10	0	10	8	18	2	1	2
	$11l$, $\bar{1}\bar{1}l$	11	20	1	4	7	26	4	1	2	12	4
	sum	32	94	32	90	28	75	158	63	20	45	14
I–3,6	$02l$, $11l$	19	8	4	8	20	7	6	6	12	4	6
	$0\bar{2}l$, $\bar{1}\bar{1}l$	19	8	13	8	8	6	17	5	2	4	10
	$\bar{1}1l$, $1\bar{1}l$	2,5	7	23	8	6	6	11	5	11	4	2
	sum	81	46	80	45	69	38	68	32	49	26	34
I–7,11	$02l$, $1\bar{1}l$	24	31	16	1	6	23	1	8	6	6	1
	$0\bar{2}l$, $\bar{1}1l$	2,5	5	10	19	0	14	8	3	2	17	2
	$11l$	11	0	40	0	0	0	32	0	6	0	8
	$\bar{1}\bar{1}l$	11	0	22	0	27	0	27	0	26	0	2
	sum	76	72	112	39	40	72	66	22	50	37	16
I–8,12	$0\overset{\pm}{2}l$	43	0	2	0	29	0	15	0	7	0	18
	$\overset{\pm}{1}\overset{\pm}{1}l$	11	11	30	26	7	2	4	20	2	2	42
	sum	86	45	123	102	58	5	31	102	15	10	184
I–9,13	$0\overset{\pm}{2}l$	10	22	1	4	7	26	4	1	2	14	4
	$\overset{\pm}{1}\overset{\pm}{1}l$	2,5	7	23	8	6	6	11	5	11	4	2
	sum	22	50	92	35	33	48	47	21	46	32	11
I–10,14	$02l$, $\bar{1}\bar{1}l$	19	8	4	8	20	7	6	6	12	4	6
	$0\bar{2}l$, $11l$	19	8	13	8	8	6	17	5	2	4	10
	$1\bar{1}l$	2,5	26	10	11	0	10	8	18	2	1	2
	$\bar{1}1l$	2,5	1	6	30	7	2	1	14	6	11	1
	sum	80	49	50	70	63	39	54	42	35	28	34

the $\sigma_i\tau_k$ and $\sigma_j\tau_l$ combinations for all possible i,j,k,l values, except on those occasions when $i=j$ and $k=l$ simultaneously.

Such a determination of polytypes has a formal character because in this case a definite type of chlorite packet is not considered and the nature of the interlayer bonds is ignored. In principle, in this case, all possible sequences of three-storied layers only (but not chlorite packets) are revealed, which results in structures with a two-packet unit cell.

To make the data obtained more specific it should be remembered that only structures with hydrogen bonds can actually exist. This condition imposes definite restrictions on the possible values of the indices i,j,k,l in the $\sigma_i\tau_k\sigma_j$ combinations for each definite type of chlorite packet. Alternatively, definite types of chlorite packets have each to correspond to a definite set of i, k, j values. Combinations $\sigma_{2n}\tau_{2n}\sigma_{2n}$ and $\sigma_{2n+1}\tau_{2n+1}\sigma_{2n+1}$ can exist in the case of packets σ_i and $\sigma'_i|$, combinations $\sigma_{2n}\tau_{2n+1}\sigma_{2n}$ or $\sigma_{2n+1}\tau_{2n}\sigma_{2n+1}$ in the case of packets σ'_i and $\sigma_i|$, and combinations $\sigma_i|\tau_0, \pm|\sigma_j$, in the case of packets $|\sigma_i|$ and $|\sigma'_i|$. Two structures distinguished by the type of chlorite packets correspond every $\sigma_i\tau_k\sigma_j\tau_l\sigma_i$ sequence.

It can be shown that there are 148 structures with the two-packet cell but only 56 of these consist of packets of the same type (Table 2). As can be seen from Table 2, all structures are divided into three groups by the shape of their unit cells: the first group includes structures with orthogonal unit cells; the second – structures with monoclinic unit cells with $\alpha=\pi/2$ and $\beta=94°$; the third group also consists of structures with monoclinic unit cells but with $\alpha=96°$, $\beta=\pi/2$. Further discussion will be restricted to the structures of the second group. The remaining structures can be analysed in the same way.

Di-trioctahedral chlorites

This group includes structures consisting of dioctahedral three-storied layers and trioctahedral one-storied layers. In as much as a centrosymmetry of three-storied layers was assumed polytypic varieties of di-trioctahedral chlorites proved to be similar to corresponding polytypic varieties of trioctahedral chlorites, with the only difference that octahedra at a centre of symmetry of three-storied layers are empty. In order to distinguish di-trioctahedral structures we propose to single out the di-trioctahedral types of packet by a dot over the symbol σ_i, for instance, $\dot{\sigma}_3$ or $\dot{\sigma}'_3$.

Dioctahedral chlorites

As a result of one third of the octahedral positions in dioctahedral chlorites remaining unoccupied, nine dioctahedral packets are distinguished by the manner of cation distribution in the one-storied layers, and hence by space symmetry, corresponding to each di-trioctahedral chlorite packet.

The determination scheme of dioctahedral structures is as follows: in every di-trioctahedral structure of the $\dot{\sigma}_i\tau_k\dot{\sigma}_j\tau_l\dot{\sigma}_i$ type, symbols τ_k and τ_l should be replaced by $\tau_k=\tau_q+\tau_p$ and $\tau_l=\tau_n+\tau_m$, to fix the positions of empty octahedra in the one-storied layers. For each definite τ_k, in accordance with the three possible positions of empty octahedra in the one-storied layers, there are three $\tau_q\tau_p$ combinations, satisfying the $\tau_k=\tau_q+\tau_p$ equality. Thus, from each di-trioctahedral $\dot{\sigma}_i\tau_k\dot{\sigma}_j\tau_l\dot{\sigma}_i$ structure, nine structures of $\sigma_i\tau_q\tau_p\sigma_j\tau_n\tau_m\sigma_i$ type can easily be derived.

The set of independent dioctahedral monoclinic structures with an angle $\beta=94°$, constructed from packets σ_i and $|\sigma'_i|$, is given in Table 3. Similarly it is easy to obtain monoclinic structures formed by packets $|\sigma_i|$ and σ'_i.

Table 5. $F^2(0\overset{\pm}{2}l)$, $F^2(\overset{\pm}{1}\overset{\pm}{1}l)$ *for two-packet trioctahedral*

Numeration of structures	hkl_{mono} l_{orth}	$\overset{\pm}{020}$ 0	$\overset{\pm}{110}$ 1	$\overset{\pm}{\bar{1}11}$ 2	$\overset{\pm}{021}$ 3	$\overset{\pm}{111}$ 4	$\overset{\pm}{\bar{1}12}$ 5	$\overset{\pm}{022}$ 6	$\overset{\pm}{112}$ 7	$\overset{\pm}{\bar{1}13}$ 8	$\overset{\pm}{0\bar{2}3}$ 9	$\overset{\pm}{113}$ 10	$\overset{\pm}{\bar{1}14}$ 11	$\overset{\pm}{024}$ 12	$\overset{+}{114}$ 13
II–1,7		11	14	0	20	10	9	0	4	9	4	2	26	7	1
II–2,8		11	15	0	11	10	20	0	7	9	26	2	3	7	26
II–3,9		2	9	0	9	3	0	22	8	0	8	19	0	6	7
II–4,10		2	35	6	26	4	28	10	0	6	11	4	1	0	26
		2	2	9	0	2	6	6	22	0	30	10	16	6	15
II–5,11		2	2	8	5	4	0	10	30	6	20	4	28	0	2
		2	30	8	31	2	22	6	8	4	0	10	12	6	12
II–6,12		19	9	6	8	21	7	13	8	22	8	2	7	8	8
		19	8	10	8	16	8	4	8	11	8	16	7	21	6
II–13,19		11	31	8	11	2	0	0	8	6	26	10	28	7	12
II–14,20		11	3	7	20	2	28	0	22	6	4	10	1	7	15
II–15,21		2	9	10	9	22	8	22	8	11	8	2	7	7	7
II–16,22		2	14	9	26	10	6	10	24	0	11	2	16	0	1
		2	35	0	0	4	9	6	0	9	30	4	26	6	26
II–17,23		2	19	8	5	10	22	10	7	0	20	2	12	0	26
		2	2	0	31	4	20	6	31	9	0	4	3	6	2
II–18,24		12	8	24	72	16	7	13	8	5	8	16	8	8	7
		12	9	6	8	4	6	4	8	22	8	19	7	21	7

For II–4, 5, 6, 10, 11, 12, 16, 17, 18, 22, 23, 24 structures $F^2(hkl)$ and $F^2(h\bar{k}l)$ are given in same column.

Diffraction features of derived polytypes

The reflexions with indices $k \neq 3n$ are most sensitive to the strict spatial repetitiveness of the structures in layer silicates, especially $02l$, $11l$. Calculations were made of F^2 values corresponding to different polytypes for these reflexions. Tables 4, 5 and 6 give values of $F^2(0\overset{\pm}{2}l)$ and $F^2(\overset{\pm\pm}{11}l)$, calculated for the above mentioned trioctahedral structures. For each separate value of l_{orth}, both F^2 values for every combination of indices hk, and values of the F^2 sums are given, with allowances for the repetitive factor for reflexions which coincide when a method of oblique texture is used. As can be seen from Tables 4 to 6, structures with the same spatial arrangement of packets are characterized by an identical intensity distribution of reflexions $02l$, independently of their type (structures II-1,7,14,20, II-2,8,13,19 or III-3,6,11,17). Features of the intensity distribution of reflexions $\overset{\pm\pm}{11}l$ allow one to distinguish structures formed by σ_i or σ'_i packets from structures formed by $|\sigma_i|$ or $|\sigma'_i|$ packets. Thus an analysis of the $02l$ and $11l$ intensities permits us to define only two possible structures, which differ in the type of chlorite packet. In order to choose between these structures, the values of $F^2(h0l)$ given in a previous paper (Brown & Bailey, 1962; Zvyagin & Miszczenko, 1965) should be used. As a first approximation, the F^2 values obtained can be used for identification of di-trioctahedral and dioctahedral structures. This possibility was used in our investigations of the dioctahedral structures (Wlasow & Drits, 1967). F^2 values for these structures are given in Table 5 (II-1,21).

Amongst the natural chlorites investigated only a few specimens with the two-packet structure were found. Brindley *et al.* (1950) detected a two-packet Mg-chlorite, pennine. In our notation this structure can be represented as $\sigma_3\tau_1\sigma_5\tau_3\sigma_3$. In this structure, composed of σ_i packets, adjacent packets are rotated one against the other by an angle of 120° (σ_3, σ_5) and alternatively displaced by $\pm b/3$ in the b axis direction. Drits & Lazarenko (1967) have described two-packet di-trioctahedral chlorite made up of the same chlorite packets σ_i. The analytical expression of this structure is $\dot{\sigma}_3\tau_1\dot{\sigma}_3\tau_5\dot{\sigma}_3$. In the structure of this mineral, packets are alternatively displaced only by $\pm b/3$ in the b axis direction. These authors also detected a two-packet dioctahedral chlorite with $|\sigma'_i|$ type packets. In our notation this can be represented as $|\sigma'_4|\tau_+\tau_+|\sigma'_2|\tau_-\tau_-|\sigma'_4|$. In this structure, adjacent packets are rotated one against the other by an angle of 120° and alternatively displaced by $\pm b/3$ in the b axis direction. Shirozu & Bailey (1966) have described a two-packet monoclinic polytype of Mg-vermiculite, which is very similar to chlorite. This structure is made up of $|\sigma'_i|$ packets, which are displaced by $\pm b/3$ in the b-axis direction ($|\sigma'_6|\tau_-|\sigma'_6|\tau_+|\sigma'_6|$).

Thus all the above mentioned two-packet structures have a feature such that their packets can be rotated only by multiples of 120° and alternatively displaced by $\pm b/3$ in the b axis direction. In this connection, all these structures with a definite type of packet have the same projection along the b axis and are distinguishable only by projection along the a axis.

The existence of chlorites with σ_i packets is quite clear since, in their structures, the coincidence of tetrahedral and octahedral cations in the normal projection is absent. Dioctahedral chlorite packets $|\sigma'_i|$ must be the less stable. because of electrostatic repulsion between the octahedral cations of one-storied layers and the nearest tetrahedral cations of three-storied layers,

chlorites with monoclinic cell ($\beta = 94°$)

$\bar{1}\overset{\pm}{1}5$	$0\overset{\pm}{2}5$	$1\overset{\pm}{1}5$	$\bar{1}\overset{\pm}{1}6$	$0\overset{\pm}{\bar{2}}6$	$1\overset{\pm}{1}6$	$\bar{1}\overset{\pm}{1}7$	$0\overset{\pm}{2}7$	$1\overset{\pm}{1}7$	$\bar{1}\overset{\pm}{1}8$	$0\overset{\pm}{2}8$	$1\overset{\pm}{1}8$	$\bar{1}\overset{\pm}{1}9$	$0\overset{\pm}{2}9$	$1\overset{\pm}{1}9$	$\bar{1}\overset{\pm}{1}10$	$0\overset{\pm}{2}10$
14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30
3	26	5	0	4	24	4	0	4	20	2	2	10	14	0	4	4
3	2	6	24	4	0	4	20	4	1	2	17	5	2	4	12	4
0	6	8	0	11	6	0	5	7	0	12	4	0	4	6	0	2
2	10	8	19	8	6	8	18	0	9	2	9	0	0	6	5	2
9	2	0	17	0	6	1	14	6	2	6	18	4	11	0	15	0
2	14	7	4	8	18	8	3	0	12	2	10	2	17	1	11	2
9	23	0	8	0	18	1	8	6	19	6	1	8	6	2	0	0
2	6	18	6	17	6	16	5	4	6	26	5	11	4	8	4	10
17	7	4	6	3	6	2	5	16	5	12	5	20	4	0	4	6
2	2	0	4	4	18	8	20	6	12	2	1	1	2	2	11	4
2	26	0	20	4	6	8	0	6	9	2	17	0	14	0	4	4
17	6	18	12	11	6	2	5	4	6	12	4	20	4	8	4	2
9	10	5	17	8	23	1	18	4	1	2	2	4	0	1	15	2
3	2	8	0	0	6	4	14	0	20	6	10	10	11	5	4	0
9	14	5	8	8	0	1	3	4	19	2	18	8	17	4	0	2
3	23	7	24	1	18	4	8	0	1	6	10	5	6	1	12	0
15	7	4	6	17	6	6	5	16	6	26	5	4	4	0	4	10
2	7	8	6	3	6	16	6	7	6	12	5	11	4	6	4	6

which are superimposed in the normal projection. Their existence in nature is possibly the result of an ordered replacement of Al by Si in the tetrahedral network of layers and a local balance of negative charge. At present, there is not sufficient information for an evaluation of the probability of formation of two-packet chlorites and the relative abundances of the different polytypes.

Table 6. $F^2(0\overset{\pm}{2}l)$, $F^2(\overset{\pm}{1}\overset{\pm}{1}l)$ *for two-packet trioctahedral chlorites with monoclinic cell* ($\alpha=96°$)

Numeration of structures	l_{orth} hkl	1	2	4	5	7	8	10	11	13	14	16	17	19	20	22	23	25	26	28	39
III–1,4	$02l$	—	0	—	9	—	9	—	26	—	3	—	0	—	4	—	20	—	10	—	4
	$0\bar{2}l$	14	—	10	—	24	—	2	—	1	—	5	—	24	—	4	—	2	—	1	—
	$11l$	34	—	4	—	0	—	3	—	26	—	7	—	7	—	0	—	9	—	6	—
	$\bar{1}\bar{1}l$	—	9	—	6	—	1	—	16	—	9	—	16	—	1	—	2	—	4	—	15
	$\bar{1}1l$	3	—	2	—	22	—	10	—	15	—	0	—	6	—	6	—	18	—	0	—
	$1\bar{1}l$	—	7	—	28	—	6	—	1	—	2	—	20	—	8	—	9	—	0	—	5
	sum	44	16	11	39	34	11	14	30	41	12	10	36	23	10	9	21	28	9	6	22
III–2,5	$02l$	—	0	—	20	—	9	—	3	—	3	—	25	—	3	—	1	—	5	—	12
	$0\bar{2}l$	20	—	12	—	8	—	2	—	26	—	6	—	0	—	5	—	18	—	4	—
	$11l$	2	—	4	—	32	—	4	—	2	—	6	—	18	—	0	—	10	—	1	—
	$\bar{1}\bar{1}l$	—	8	—	22	—	1	—	12	—	9	—	8	—	1	—	19	—	9	—	0
	$\bar{1}1l$	32	—	1	—	8	—	10	—	12	—	0	—	18	—	6	—	1	—	2	—
	$1\bar{1}l$	—	8	—	0	—	6	—	27	—	2	—	4	—	8	—	11	—	2	—	11
	sum	42	16	12	32	44	11	14	40	28	12	10	24	36	10	9	30	20	13	5	17
III–3,6	$02l$	—	6	—	7	—	22	—	7	—	2	—	6	—	16	—	5	—	11	—	4
	$0\bar{2}l$	8	—	16	—	8	—	15	—	6	—	4	—	6	—	16	—	4	—	1	—
	$11l$	9	—	22	—	8	—	2	—	8	—	18	—	6	—	4	—	4	—	8	—
	$\bar{1}\bar{1}l$	—	8	—	8	—	11	—	7	—	17	—	6	—	6	—	6	—	20	—	4
	$\bar{1}1l$	9	—	4	—	8	—	19	—	7	—	8	—	4	—	7	—	4	—	6	—
	$1\bar{1}l$	—	23	—	7	—	6	—	8	—	15	—	6	—	10	—	6	—	4	—	4
	sum	22	35	33	18	19	28	29	18	17	33	31	16	13	25	19	13	12	30	14	10
III–7,13	$02l$	—	36	—	0	—	2	—	0	—	36	—	0	—	3	—	0	—	16	—	0
	$0\bar{2}l$	0	—	18	—	0	—	14	—	0	—	29	—	0	—	1	—	0	—	21	—
	$\overset{\pm}{1}1l$	2	—	4	—	32	—	4	—	2	—	7	—	18	—	0	—	10	—	1	—
	$\overset{\pm}{1}\bar{1}l$	—	8	—	22	—	1	—	12	—	9	—	8	—	1	—	18	—	9	—	0
	sum	3	34	16	44	63	2	14	24	5	36	28	16	35	4	1	37	19	26	13	0
III–8,14	$02l$, $\bar{1}\bar{1}l$	—	8	—	0	—	6	—	27	—	2	—	4	—	8	—	11	—	2	—	11
	$0\bar{2}l$, $11l$	32	—	1	—	8	—	10	—	12	—	0	—	18	—	6	—	1	—	2	—
	$\bar{1}1l$	0	—	6	—	0	—	38	—	0	—	1	—	0	—	24	—	0	—	0	—
	$1\bar{1}l$	—	27	—	0	—	23	—	0	—	8	—	0	—	29	—	0	—	0	—	0
	sum	63	34	8	0	13	32	53	40	18	10	1	6	28	40	33	16	2	2	3	16
III–9,15	$02l$, $\bar{1}\bar{1}l$	—	0	—	20	—	9	—	3	—	3	—	25	—	3	—	1	—	5	—	12
	$0\bar{2}l$, $11l$	20	—	12	—	8	—	2	—	26	—	6	—	0	—	5	—	18	—	4	—
	$\bar{1}1l$	0	—	42	—	0	—	6	—	0	—	20	—	0	—	18	—	0	—	3	—
	$1\bar{1}l$ a	—	0	—	0	—	36	—	0	—	12	—	0	—	14	—	0	—	41	—	0
	sum	28	0	60	30	11	50	8	4	39	16	28	38	0	18	26	1	26	48	9	23
III–10,16	$02l$, $1\bar{1}l$	—	23	—	7	—	6	—	8	—	15	—	6	—	10	—	6	—	4	—	4
	$0\bar{2}l$, $\bar{1}1l$	9	—	4	—	8	—	19	—	7	—	8	—	4	—	7	—	4	—	6	—
	$11l$	14	—	10	—	24	—	2	—	1	—	5	—	23	—	4	—	2	—	1	—
	$\bar{1}\bar{1}l$	—	0	—	9	—	9	—	26	—	3	—	0	—	4	—	20	—	10	—	4
	sum	28	35	15	19	35	18	29	37	12	25	18	9	30	20	15	28	8	16	10	9
III–11,17	$02l$, $\bar{1}\bar{1}l$	—	6	—	7	—	22	—	7	—	2	—	6	—	16	—	5	—	11	—	4
	$0\bar{2}l$, $11l$	8	—	16	—	8	—	16	—	6	—	4	—	6	—	16	—	4	—	1	—
	$\bar{1}1l$	34	—	4	—	0	—	4	—	26	—	8	—	6	—	0	—	9	—	6	—
	$1\bar{1}l$	—	9	—	6	—	1	—	16	—	9	—	16	—	1	—	2	—	4	—	15
	sum	46	18	28	17	12	33	27	27	34	13	13	26	15	25	25	10	16	20	7	21
III–12,18	$02l$, $\bar{1}\bar{1}l$	—	8	—	8	—	11	—	7	—	17	—	6	—	6	—	6	—	20	—	4
	$0\bar{2}l$, $11l$	7	—	22	—	8	—	2	—	8	—	18	—	6	—	4	—	4	—	8	—
	$\bar{1}1l$	3	—	2	—	23	—	10	—	15	—	0	—	6	—	6	—	18	—	0	—
	$1\bar{1}l$	—	7	—	28	—	6	—	1	—	2	—	20	—	8	—	9	—	0	—	5
	sum	16	19	34	39	34	22	14	12	16	27	28	23	14	18	12	17	25	31	12	1

Formula $(hkl)_{\text{orth}} \rightarrow (hkl')_{\text{mono}}/3l'_{\text{mono}} = l_{\text{orth}} - k/$ designates transmission from orthorhombic indices to monoclinic ones.

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Crystal and Molecular Structure of 6β-Bromoprogesterone

By E. M. Gopalakrishna,* A. Cooper† and Dorita A. Norton†

Center for Crystallographic Research,
Roswell Park Memorial Institute, 666 *Elm Street, Buffalo, New York* 14203, *U.S.A.*

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The steroid 6*β*-bromoprogesterone (6*β*-bromo-Δ^4-pregnene-3,20-dione, $C_{21}H_{29}O_2Br$) crystallizes in the orthorhombic space group $P2_12_12_1$ with unit-cell dimensions a = 13·431, b = 18·288 and c = 7·645 Å and with four steroid molecules per unit cell. The atomic positions of all the atoms, including the hydrogen atoms, have been refined using anisotropic temperature factors for carbon and heavier atoms and isotropic temperature factors for hydrogen atoms, giving an R value of 4·7% for 2208 independent reflections. The *A* ring is highly distorted because of the Δ^4-double bond and the ketone oxygen O(3). The rings *B* and *C* are chair-shaped. The *D* ring is a distorted half-chair. The molecules are held together in the crystalline state by van der Waals forces.

Introduction

Progesterone is unique among the steroid hormones (Applezweig, 1962) in that its role is mainly concerned with motherhood. It is produced by the corpus luteum and placenta and is involved initially in stimulating maturation of the uterine mucosa in order to prepare it for reception of a fertilized ovum; this progestational action is withdrawn by degeneration of the corpus luteum if fertilization does not occur, and the excess uterine tissue is removed through menstruation as the progesterone level drops. In the event of fertilization, however, the corpus luteum persists and continues to secrete a high level of progesterone, which now serves to maintain and protect a successful pregnancy by preventing uterine motility or further ovulation and by stimulating milk gland formation in the breasts. Any fault in the cycle of progesterone production or metabolism can give rise to numerous physiologic disorders; amenorrhea, habitual abortion, and premature delivery are all likely sequelae. While the potential usefulness of progesterone in treatment of numerous human disorders seems obvious, administration of the compound itself has proven to be a disappointment in most cases. First, progesterone differs from other steroid hormones in that a relatively large dosage is required in order to produce a physiologic effect. Secondly, since it is a time-cycle hormone, the where, when and how of its delivery becomes, as it were, a difficult problem in logistics. Since progesterone arises in some endocrine tissues which are seemingly not concerned with gestation, and since large doses are required to produce many of its so-called progestogenic effects, there is some doubt as to whether it is progesterone itself or some of its metabolites which are responsible for the different biological activities ascribed to the hormone.

Under these circumstances, a thorough and detailed investigation of the crystal and molecular structure of some of the derivatives of progesterone will certainly be useful in understanding the biological activity of this hormone and the related steroids. The present paper reports the study of the 6*β*-bromo derivative of progesterone (Fig. 1).

Experimental

The sample used in this investigation was prepared by refluxing progesterone with *N*-bromosuccinimide in

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* Present address: Material Science Laboratory, Collene of Engineering, Marquette College, Milwaukee, Wisconsin 53233, U.S.A.

† Present address: The Medical Foundation of Buffalo, 73 High Street, Buffalo, New York 14203, U.S.A.