bonded dimers is still possible and takes place around a centre of symmetry as usual. Double molecular sheets result which are held together by weak van der Waals forces only. This leads to the soft flaky crystals. Fatty acid crystals built up of sheets of molecules do often exhibit twinning. No twins were found, however, in this investigation.

Distortions are found in the chain packing in the vicinity of the carboxyl group where space problems exist. The long tails (C_4–C_{18}) of the molecules, however, are free to arrange in an almost regular chain packing. The main deviation seems to be a certain twist of the chain plane as the two rows of carbon atoms of one molecule are not quite parallel in the projection (Fig. 1).

I wish to thank Miss G. Ställberg for a sample of the acid and Prof. G. Hägg, Prof. E. Stenhagen and Dr E. von Sydow for their interest. I am also indebted to Messrs L. Gustavsson, E. Herberts, W. Müller and A. Westerdahl for help with the calculations. The expenses involved have been defrayed by grants from the Swedish Natural Science Research Council and the Swedish Board for Computing Machinery.

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On the Crystal Structure of 2 D-Methyloctadecanoic Acid

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2 D-methyloctadecanoic acid is monoclinic with $a = 9{\cdot}08$, $b = 5{\cdot}01$, $c = 24{\cdot}0$ Å; $\beta = 116°\ 37'$. It belongs to the space group C_2^2–$P2_1$. From a crystallographic point of view the molecule is built up of the hydrocarbon octadecane with a carboxyl group in position 2 projecting out as a side chain. The branches are as usual accommodated between the tails of the main chains. A new packing of hydrocarbon chains is found. It resembles the common orthorhombic chain packing but the symmetry elements are interchanged with respect to the subcell axes which are identical in both cases. The molecules are linked together in chains by infinite helices of hydrogen bonds.

Introduction

In connexion with synthetic work on 2-methyloctadecanoic acid (G. Ställberg, 1958) the optically active forms of the acid were found to exhibit polymorphism. As the high melting modification showed an unusual infrared spectrum for long-chain fatty acids in the solid state, a crystal structure investigation was started as a part of studies of other branched-chain acids (Abrahamsson, 1956, 1958, 1959*a*, *b*).

Preparation of crystals

One crystal form (m.p. 54·7–55·0 °C.) of the enantiomers is obtained by crystallization from solution and another (m.p. about 43 °C.) by cooling the melted acid. Crystals of the high melting form were grown from glacial acetic acid. They were well developed, long and lath-shaped and showed no twinning. Their optic sign was positive.

X-ray data

Rotation and Weissenberg photographs were taken with Cu K radiation using a calibrated camera. The following data were found:

Molecular formula: $C_{19}H_{38}O_2$.
Molecular weight: 298·49.
Unit cell: monoclinic.

$a = 9{\cdot}08 \pm 0{\cdot}03$, $b = 5{\cdot}01 \pm 0{\cdot}02$, $c = 24{\cdot}0 \pm 0{\cdot}2$ Å.
$\beta = 116°\ 37' \pm 30'$.
$U = 977 \pm 10$ Å^3.
$d(001) = 21{\cdot}46 \pm 0{\cdot}10$ Å.

Two molecules per unit cell.
Number of electrons: 336.
Density calculated: $1{\cdot}015 \pm 0{\cdot}010$ g.cm.$^{-3}$.
Density measured: $1{\cdot}015$ g.cm.$^{-3}$.
Absent reflexions: $(0k0)$ for k odd.
Space group: $P2_1$ or $P2_1/m$.

As the two identical asymmetric molecules in the cell cannot be related by a centre of symmetry the non-centrosymmetrical space group C_2^2–$P2_1$ was chosen.

The intensities of the ($h0l$) reflexions were estimated visually by two observers using an intensity scale. After correction for the Lorentz and polarization factors, a set of relative observed structure factors were evaluated. Absolute values were later obtained by comparison with calculated structure factors. No absorption correction was made.

Subcell

A very pronounced sublattice was found in the reciprocal lattice indicating a strictly periodic carbon chain in the structure. The subcell is orthorhombic with the following dimensions:

$$a_s = 7{\cdot}43,\quad b_s = 5{\cdot}01,\quad c_s = 2{\cdot}50\ \text{Å}\,.$$

The values are in good agreement with those reported for the subcell of the common orthorhombic chain packing (Bunn, 1939; Vainsthein & Pinsker, 1950; von Sydow, 1956). An inspection of the systematic absences in the sublattice revealed, however, that the subcell of the present investigation could not be identical with the common orthorhombic subcell. The extinction rules are: ($h0l$) for ($h+l$) odd and ($0k0$) for k odd. It was found during the investigation that the two subcells belong to the same space group (*Pnma*) but have the symmetry elements interchanged with respect to identical axes. The space-group symbol for the new packing is thus *Pbnm* and for the common orthorhombic packing *Pnam.*

Structure determination

The four carbon atoms of the subcell were given coordinates consistent with the subcell symmetry. The

Table 1. *Atomic coordinates*

Atom	x/a	z/c	Atom	x/a	z/c
O_1	0·1920	0·0320	C_{10}	0·2270	0·4924
O_2	0·1126	0·0500	C_{11}	0·2597	0·5534
C_1	0·2240	0·0541	C_{12}	0·1836	0·5899
C_2	0·3925	0·0970	C_{13}	0·2154	0·6519
C_3	0·4195	0·1550	C_{14}	0·1402	0·6873
C_4	0·3500	0·1985	C_{15}	0·1772	0·7494
C_5	0·3832	0·2591	C_{16}	0·0977	0·7863
C_6	0·3115	0·2968	C_{17}	0·1313	0·8468
C_7	0·3439	0·3585	C_{18}	0·0556	0·8849
C_8	0·2702	0·3950	C_{19}	0·4785	0·0595
C_9	0·3040	0·4560			

Table 2. *Observed and calculated structure factors*

hkl	F_o	F_c	hkl	F_o	F_c	hkl	F_o	F_c	hkl	F_o	F_c
000	—	336	$10\bar{1}$	15	16	2,0,13	6	5	308	6	5
001	—	6	$10\bar{2}$	24	22	2,0,14	5	6	309	7	7
002	—	12	$10\bar{3}$	29	28	2,0,15	5	5	3,0,10	9	12
003	2	7	$10\bar{4}$	34	31	2,0,16	3	4	3,0,11	20	25
004	2	3	$10\bar{5}$	35	32	2,0,17	3	2	3,0,12	8	−11
005	6	−3	$10\bar{6}$	33	30	2,0,18	< 3	1	3,0,13	< 3	1
006	8	−8	$10\bar{7}$	26	24						
007	11	−12	$10\bar{8}$	19	21	$20\bar{1}$	34	−32	$30\bar{1}$	17	−18
008	13	−14	$10\bar{9}$	19	21	$20\bar{2}$	15	−14	$30\bar{2}$	15	−18
009	16	−16	$1,0,\overline{10}$	23	−22	$20\bar{3}$	3	−2	$30\bar{3}$	11	−14
0,0,10	22	−19	$1,0,\overline{11}$	3	−3	$20\bar{4}$	7	11	$30\bar{4}$	6	−9
0,0,11	11	−14	$1,0,\overline{12}$	7	−7	$20\bar{5}$	15	18	$30\bar{5}$	2	−8
0,0,12	10	−10	$1,0,\overline{13}$	9	−10	$20\bar{6}$	17	22	$30\bar{6}$	2	−3
0,0,13	7	−7	$1,0,\overline{14}$	8	−9	$20\bar{7}$	18	23	$30\bar{7}$	4	0
0,0,14	5	−4	$1,0,\overline{15}$	7	−6	$20\bar{8}$	18	19	$30\bar{8}$	2	1
0,0,15	< 3	−2	$1,0,\overline{16}$	6	−4	$20\bar{9}$	12	14	$30\bar{9}$	36	33
0,0,16	< 3	−2	$1,0,\overline{17}$	< 3	−1	$2,0,\overline{10}$	8	8	$3,0,\overline{10}$	7	10
0,0,17	< 3	−1	$1,0,\overline{18}$	< 3	−1	$2,0,\overline{11}$	4	4	$3,0,\overline{11}$	3	5
0,0,18	6	1	$1,0,\overline{19}$	< 3	−1	$2,0,\overline{12}$	3	1	$3,0,\overline{12}$	< 3	2
0,0,19	6	5	$1,0,\overline{20}$	8	−6	$2,0,\overline{13}$	3	−1	$3,0,\overline{13}$	< 3	2
0,0,20	16	14	$1,0,\overline{21}$	4	0	$2,0,\overline{14}$	4	−3	$3,0,\overline{14}$	< 3	2
0,0,21	8	−6	$1,0,\overline{22}$	4	2	$2,0,\overline{15}$	4	−4	$3,0,\overline{15}$	< 3	2
0,0,22	< 3	−1	$1,0,\overline{23}$	3	2	$2,0,\overline{16}$	4	−3	$3,0,\overline{16}$	< 3	2
			$1,0,\overline{24}$	< 3	2	$2,0,\overline{17}$	< 3	0	$3,0,\overline{17}$	3	0
100	5	3				$2,0,\overline{18}$	5	6	$3,0,\overline{18}$	3	−2
101	5	−1	200	60	−58	$2,0,\overline{19}$	20	18	$3,0,\overline{19}$	16	−10
102	13	−13	201	125	115	$2,0,\overline{20}$	21	−16	$3,0,\overline{20}$	6	0
103	18	−21	202	20	−20	$2,0,\overline{21}$	< 3	−2	$3,0,\overline{21}$	4	1
104	20	−23	203	28	−26	$2,0,\overline{22}$	< 3	−1	$3,0,\overline{22}$	3	3
105	22	−22	204	29	−29				$3,0,\overline{23}$	3	3
106	21	−19	205	26	−26	300	19	−18	$3,0,\overline{24}$	3	2
107	18	−16	206	22	−21	301	22	−22	$3,0,\overline{25}$	3	2
108	14	−13	207	15	−15	302	19	−14			
109	6	−6	208	8	−8	303	15	−15	400	14	−16
1,0,10	10	7	209	3	−3	304	10	−10	401	24	−27
1,0,11	28	−22	2,0,10	3	1	305	4	−5	402	48	50
1,0,12	3	−4	2,0,11	< 3	−1	306	< 3	−1	403	9	7
1,0,13	< 3	−2	2,0,12	6	3	307	5	4	404	6	4

Table 2 (*cont.*)

hkl	F_o	F_c	*hkl*	F_o	F_c	*hkl*	F_o	F_c	*hkl*	F_o	F_c
405	3	2	5,0,11	<3	3	$60\bar{3}$	<3	2	$7,0,\overline{17}$	5	−4
406	<3	1	5,0,12	12	14	$60\bar{4}$	<3	2	$7,0,\overline{18}$	7	4
			5,0,13	7	−7	$60\bar{5}$	<3	2	$7,0,\overline{19}$	<3	1
$40\bar{1}$	8	−10	5,0,14	<3	−2	$60\bar{6}$	<3	2			
$40\bar{2}$	7	−9				$60\bar{7}$	3	4	$80\bar{1}$	<3	0
$40\bar{3}$	6	−8	$50\bar{1}$	4	2	$60\bar{8}$	<3	−1	$80\bar{2}$	<3	−1
$40\bar{4}$	6	−5	$50\bar{2}$	4	1	$60\bar{9}$	<3	1	$80\bar{3}$	<3	−3
$40\bar{5}$	6	−6	$50\bar{3}$	4	2	$6,0,\overline{10}$	<3	2	$80\bar{4}$	5	−4
$40\bar{6}$	6	−6	$50\bar{4}$	3	2	$6,0,\overline{11}$	3	3	$80\bar{5}$	6	−5
$40\bar{7}$	6	−6	$50\bar{5}$	<3	0	$6,0,\overline{12}$	5	3	$80\bar{6}$	5	−3
$40\bar{8}$	2	−6	$50\bar{6}$	<3	2	$6,0,\overline{13}$	5	4	$80\bar{7}$	8	−9
$40\bar{9}$	13	−10	$50\bar{7}$	<3	3	$6,0,\overline{14}$	5	4	$80\bar{8}$	5	−4
$4,0,\overline{10}$	7	−6	$50\bar{8}$	27	24	$6,0,\overline{15}$	6	5	$80\bar{9}$	<3	−3
$4,0,\overline{11}$	4	−5	$50\bar{9}$	7	−4	$6,0,\overline{16}$	6	6	$8,0,\overline{10}$	<3	−1
$4,0,\overline{12}$	<2	−3	$5,0,\overline{10}$	6	−4	$6,0,\overline{17}$	8	9	$8,0,\overline{11}$	<3	0
$4,0,\overline{13}$	<3	−1	$5,0,\overline{11}$	5	−5	$6,0,\overline{18}$	27	−24	$8,0,\overline{12}$	4	3
$4,0,\overline{14}$	3	−1	$5,0,\overline{12}$	4	−5	$6,0,\overline{19}$	<3	−2	$8,0,\overline{13}$	6	5
$4,0,\overline{15}$	5	2	$5,0,\overline{13}$	4	−4				$8,0,\overline{14}$	6	6
$4,0,\overline{16}$	7	5	$5,0,\overline{14}$	3	−4	700	<3	−3	$8,0,\overline{15}$	5	8
$4,0,\overline{17}$	10	11	$5,0,\overline{15}$	4	−3	$70\bar{1}$	5	−4	$8,0,\overline{16}$	5	8
$4,0,\overline{18}$	20	22	$5,0,\overline{16}$	<3	−4	$70\bar{2}$	5	−4	$8,0,\overline{17}$	12	−9
$4,0,\overline{19}$	29	−26	$5,0,\overline{17}$	<3	−5	$70\bar{3}$	5	−4	$8,0,\overline{18}$	<3	5
$4,0,\overline{20}$	5	−2	$5,0,\overline{18}$	14	−12	$70\bar{4}$	4	−4			
$4,0,\overline{21}$	<3	0	$5,0,\overline{19}$	8	1	$70\bar{5}$	<3	−2	900	<3	1
			$5,0,\overline{20}$	5	0	$70\bar{6}$	<3	1	$90\bar{1}$	<3	0
500	5	2	$5,0,\overline{21}$	3	2	$70\bar{7}$	17	25	$90\bar{2}$	<3	0
501	<3	5				$70\bar{8}$	6	−6	$90\bar{3}$	<3	0
502	<3	0	600	2	−1	$70\bar{9}$	<3	−1	$90\bar{4}$	<3	1
503	<3	1	601	6	−3	$7,0,\overline{10}$	<3	2	$90\bar{5}$	<3	1
504	<3	0	602	12	−8	$7,0,\overline{11}$	3	3	$90\bar{6}$	8	11
505	<3	1	603	10	9	$7,0,\overline{12}$	4	4	$90\bar{7}$	9	−10
506	<3	0	604	<3	2	$7,0,\overline{13}$	<3	4	$90\bar{8}$	6	−6
507	<3	1				$7,0,\overline{14}$	<3	4	$90\bar{9}$	4	−4
508	<3	1	$60\bar{1}$	<3	0	$7,0,\overline{15}$	<3	3	$9,0,\overline{10}$	4	−4
509	<3	1	$60\bar{2}$	<3	1	$7,0,\overline{16}$	<3	1	$9,0,\overline{11}$	<3	−3
5,0,10	<3	0									

carbon chains formed by subcell repetition were placed as required by the space group of the main cell. As the carboxyl group was assumed to project out as a side chain from a long hydrocarbon—a behaviour found in 2 DL-methyloctadecanoic acid (Abrahamsson, 1959*b*)—a trial structure mainly as shown in Fig. 2 seemed reasonable.

Cycles of structure-factor calculations and electron-density projections along the shortest axis were then carried out (the (x, z) projection has a centre of symmetry). The structure factors were computed on the BESK-computer of the Swedish Board for Computing Machinery using the atomic scattering values of Vand *et al.* (1957). The electron-density projections were performed with Beevers–Lipson strips (3°) and the Hägg–Laurent machine (1946).

Several difference syntheses were made for the final refinement. In the last stages the contribution of the hydrogen atoms to the structure factors was accounted for. The coordinates of these atoms were evaluated from the data of Vainsthein & Pinsker (1950). A temperature factor was applied $\exp(-B \sin^2 \theta/\lambda^2)$ with the final value of $B = 5{\cdot}4$ Å^2. Omitting non-observed reflexions, the reliability index R_1 is 0·16. The coordinates of the carbon and oxygen atoms are listed in Table 1 and observed and calculated structure factors in Table 2. The electron-density projection is given in Fig. 1.

Discussion of the results

The molecular arrangement is shown in Fig. 2. From a crystallographic point of view the molecule is built up like 2 DL-methyloctadecanoic acid with a carboxyl group projecting out as a side chain from position 2 of the hydrocarbon octadecane.

The molecular packing is the result of the combined effect of the steric requirements of the branches, the attractions between the polar groups and the comparatively strong van der Waals forces between the long carbon chains. As usual, the branches are accommodated between the tails of the main chains. By adopting a new chain packing and an unusual hydrogen-bond system the molecules can pack very closely as shown by the density, 1·015 g.cm.$^{-3}$, which is the highest value hitherto found for branched-chain acids. The angle of tilt of the carbon chains to the (001) planes is 57° calculated from the average difference of z-coordinates between alternate carbon atoms (C_4–C_{18}) and the subcell dimension $c_s = 2{\cdot}50$ Å. The molecular arrangement allows the main chains to assume a very regular chain packing; small deviations are found in the vicinity of the carboxyl groups.

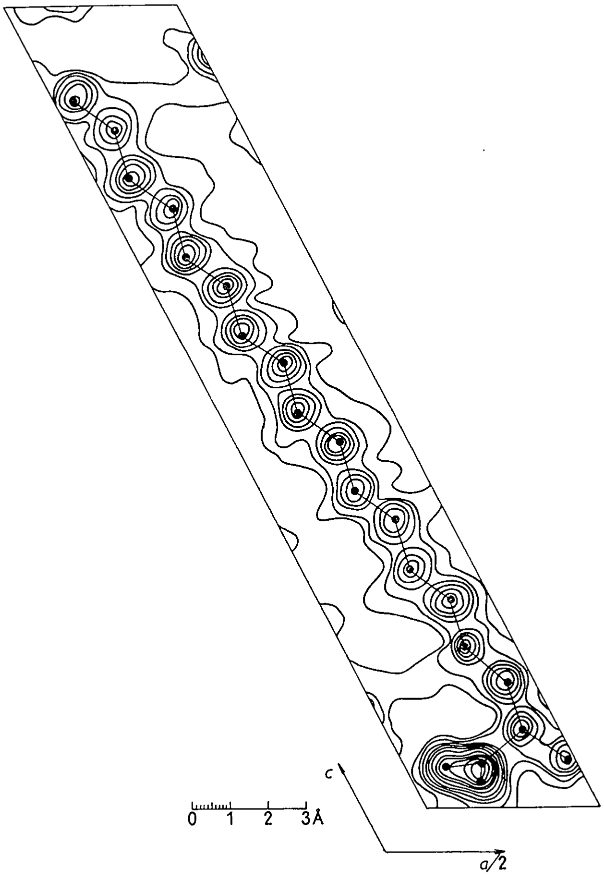

Fig. 1. Electron-density projection of 2 D-methyloctadecanoic acid along the shortest axis. Contours are given at intervals of 1 e.Å^{-2} starting with 1 e.Å^{-2}.

The subcell of the new chain packing is orthorhombic with the space group *Pbnm*. Assuming the distance 0·85 Å (Bunn, 1939) between the two rows of carbon atoms forming the planar zigzag, the subcell carbon atoms have the following coordinates:

$$\bar{x}, y, \tfrac{1}{4};\ x, \bar{y}, \tfrac{3}{4};\ \tfrac{1}{2}-x, \tfrac{1}{2}-y, \tfrac{3}{4};\ \tfrac{1}{2}+x, \tfrac{1}{2}+y, \tfrac{1}{4}$$

with $x = 0{\cdot}030a_s$ and $y = 0{\cdot}072b_s$.

The subcell is shown in Fig. 3. The angle between a chain plane and the a_sc_s face is 59°. The volume per CH_2 group is 23·3 Å^3; the same value is also found in the common orthorhombic chain packing. The van der Waals interaction between the chains is thus the same in both cases for compounds of comparable chain length. The two chain packings are related to each other by a translation of $\frac{1}{2}c_s$ of one set of structurally equivalent carbon chains with respect to the second set.

The present investigation affords a new example of a simple but evidently unusual side packing adopted in branched chain acids. Earlier von Sydow (1958) found another orthorhombic chain packing with all chain planes parallel in (−)-2-methyl-2-ethyleicosanoic acid.

The other interesting feature in the structure is the hydrogen-bond system (Fig. 4). The molecules do not form dimers as is usually the case with fatty acids but are linked together in chains by infinite helices of hydrogen bonds parallel to the *b* axis. Assuming the two carbon–oxygen distances in the carboxyl group to have the probable values 1·30 and 1·25 Å, the distance between hydrogen bonded oxygen atoms is about 2·80 Å. The value is of course rather uncertain but it is definitely larger than those listed for monocarboxylic acids by Ubbelohde & Gallagher (1955). Oxygen atoms lying on top of each other in the *b*-direction are also rather close (about 3·00 Å).

Similar hydrogen bond systems forming chains of molecules have been observed in formic acid (Holtzberg *et al.*, 1953) in acetic acid (Jones & Templeton, 1958) and in (−)-2-methyl-2-ethyleicosanoic acid (von Sydow, 1958).

The physical properties of the crystals are in agreement with the structure. As no layers of weak van der Waals forces are found, the crystals are not soft and flaky but rather hard and lath-shaped with the lath-direction parallel to the direction of the hydrogen bond helix.

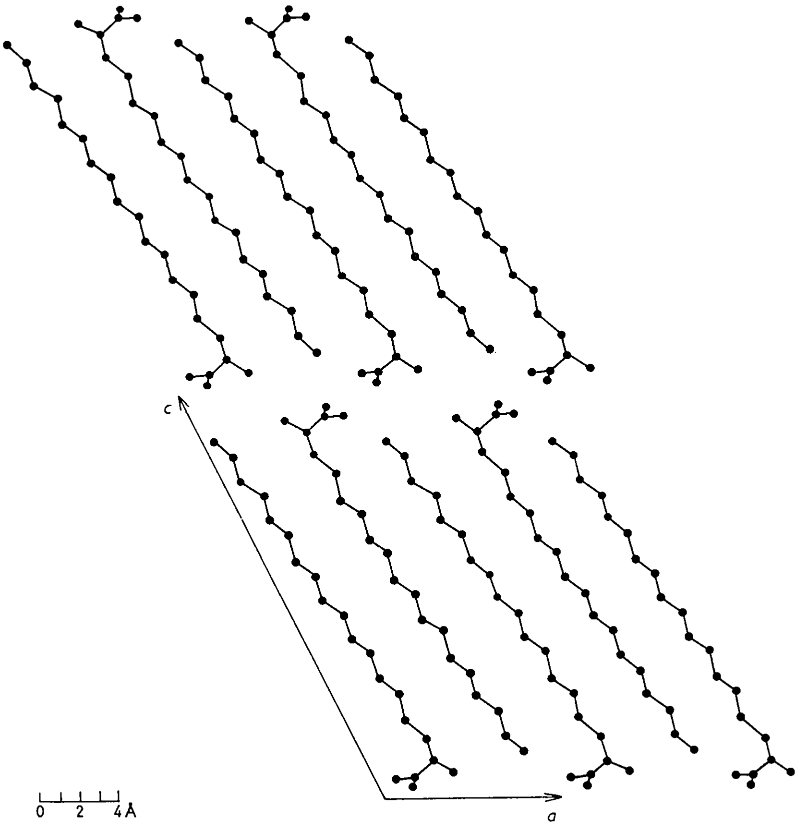

Fig. 2. Molecular arrangement of 2 D-methyloctadecanoic acid as viewed along the shortest axis.

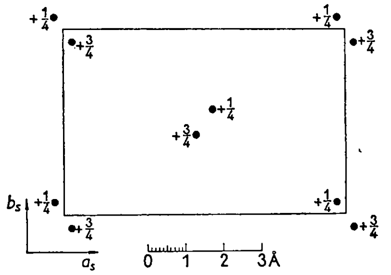

Fig. 3. The new orthorhombic subcell.

Thanks are due to Miss G. Ställberg for a sample of the acid and to Prof. G. Hägg, Prof. E. Stenhagen and Dr E. von Sydow for their interest. I am also indebted to Messrs L. Gustavsson, E. Herberts, W. Müller and A. Westerdahl for help with the computations. The expenses involved have been defrayed by grants from the Swedish Natural Science Research Council and the Swedish Board for Computing Machinery.

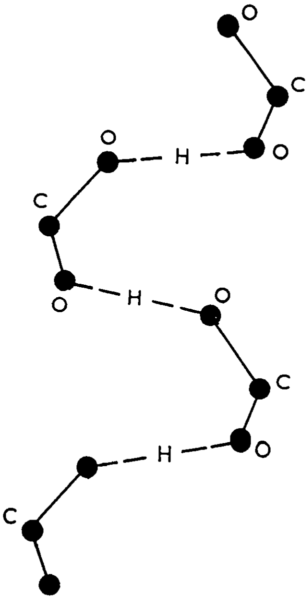

Fig. 4. The hydrogen bond system of 2 D-methyloctadecanoic acid as seen along the c axis. The b axis is vertical in the plane of the figure.

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A Re-Examination of the Structure of Tremolite

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Improved values of the x and y atomic coordinates have been obtained for the structure of tremolite $Ca_2Mg_5Si_8O_{22}(OH)_2$, and accurate lattice parameters have been derived for tremolite and actinolite from X-ray powder patterns. Tremolite has $a = 9{\cdot}840$, $b = 18{\cdot}052$, $c = 5{\cdot}275$ Å, $\beta = 104{\cdot}7°$ and actinolite $a = 9{\cdot}861$, $b = 18{\cdot}111$, $c = 5{\cdot}336$ Å, $\beta = 105{\cdot}0°$. Cell parameters of hydroxy–tremolite are larger than those of fluor–tremolite.

Introduction

The essential features of the atomic structure of amphibole minerals have been known since the work on tremolite by Warren (1930). In more recent years some attention has been given to matters of structural detail, and (x, y) electron-density projections have been derived for a magnesian crocidolite (Whittaker, 1949), an actinolite (Zussman, 1955), and for the hornblendes karinthine and barroisite (Heritsch, Paulitsch & Walitzi, 1957). Differences between each of these and the tremolite structure might be expected on various grounds, in the case of crocidolite because it is a fibrous asbestos variety, and in the case of the hornblendes because they contain additional cations in the site A $(\frac{1}{2}, 0, \frac{1}{2})$. Actinolite displays neither of these features and is different from tremolite principally in the replacement of some magnesium by iron and of silicon by aluminium. Other chemical differences are illustrated below by the approximate formulae of the minerals studied.

Tremolite		Ca_2	Mg_5	Si_8	$O_{22}(OH)_2$
Magnesian crocidolite		$(Na, Ca)_2$	$Mg_3Fe_2^{3+}$	Si_8	$O_{22}(OH)_2$
Actinolite		Ca_2	$Mg_{3\cdot5}^{2+}Fe_{1\cdot5}^{2+}$	Si_7, Al	$O_{22}(OH)_2$ (plus extra hydrogen)
Barroisite	Na	$(Ca, Na)_2$	$Mg_{2\cdot5}Fe_{1\cdot5}^{2+}Al_{1\cdot0}$	$Si_{6\cdot5}Al_{1\cdot5}$	$O_{22}(OH)_2$
Karinthine	Na	$(Ca, Na)_2$	$Mg_{3\cdot5}Fe_{0\cdot5}^{2+}Al_{1\cdot0}$	$Si_{6\cdot5}Al_{1\cdot5}$	$O_{22}(OH)_2$

Atomic coordinates and cell parameters of the four amphiboles recently studied do indeed differ from those given by Warren (1930) for tremolite, and valid comparison between the four sets of results may be

Table 1. *Tremolite: Chemical analysis**

SiO_2	57·66	CaO	13·79
TiO_2	0·01	Na_2O	0·12
Al_2O_3	1·51	K_2O	0·02
Fe_2O_3	0·23	H_2O^+	2·22
FeO	0·33	F	nil
MnO	0·01	H_2O^-	0·04
MgO	24·34	Total	100·28 %

* By R. A. Howie.

Formula on basis of 24 (O, OH):

$$\underbrace{Ca_{2\cdot00}Na_{0\cdot03}}_{2\cdot03}\ \underbrace{Mg_{4\cdot92}Fe_{0\cdot04}^{2+}Fe_{0\cdot02}^{3+}Al_{0\cdot05}}_{5\cdot03}\ \underbrace{Si_{7\cdot81}Al_{0\cdot19}}_{8\cdot00}\ O_{21\cdot99}(OH)_{2\cdot01}$$

Calculated density = 2·99 g.cm.$^{-3}$.

made (Heritsch *et al.*, 1957). Comparison with tremolite however is of little value unless results of similar accuracy are available for it. The present paper presents such results in the form of accurate x and y coordinates and accurate lattice parameters.

Experimental results

Chemical analysis of the tremolite specimen studied is presented in Table 1. A single crystal was obtained