THE STRUCTURE OF EPIDOTE ($HCa_2(Al, Fe)Al_2Si_3O_{13}$)

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MATERIAL

The crystals used in the present investigation came from the Prince of Wales Island, Alaska, and were given to the present writer by Dr. Edward P. Henderson of the U. S. National Museum in 1938. They are dark green crystals, ranging up to several cm. in length, out of which for the *x*-ray experiments comparatively small specimens were chosen. According to a chemical analysis made in this laboratory this epidote contains 15.53% of Fe_2O_3 and may be roughly expressed by the formula $HCa_2FeAl_2Si_3O_{13}$.

UNIT CELL AND SPACE GROUP

The unit cell and space group of epidote were already determined by H. Strunz. The results of our experiments in which Weissenberg-Buerger photographs were taken, confirm his results. The unit cell was found to be $a=8.96$Å, $b=5.63$Å, $c=10.20$Å, $\beta=115°\ 24'$, giving the axial ratio: $a:b:c=1.591:1:1.812$, in agreement with that given by N. von Koksharov. There are two molecules of $HCa_2(Al, Fe)Al_2Si_3O_{13}$ in the cell. The only possible space group for epidote is $C_{2h}^2-P2_1/m$, the reflections $(0k0)$ being absent when k is odd.

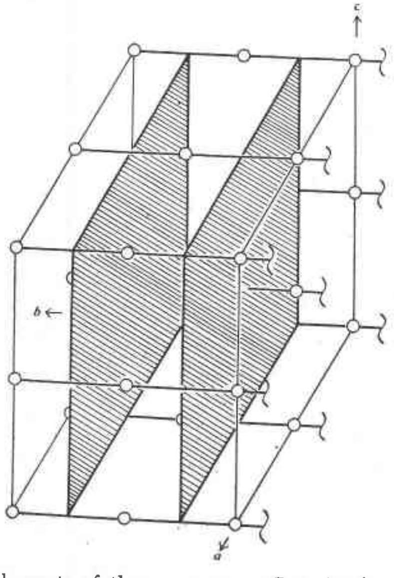


FIG. 1. Symmetry elements of the space group $C_{2h}^2-P2_1/m$. Small circles represent centers of symmetry. Shaded planes represent reflection planes. Orientation set up as in epidote.

Figure 1 shows the essential symmetry elements of the space group. There is one set of four digonal screw-axes and four sets of two symmetry centers. An atom in the general position has four equivalent positions, the intensity of reflection (hkl) being proportional to the square of $F=\Sigma 4f\cos 2\pi\,(hx+k/4+lz)\cos 2\pi\,(ky-k/4)$, where f is the atomic scattering factor appropriate to each atom.

We have to determine altogether thirty nine parameters, if no atom (except those required by the space group) lie on the reflection planes or on the centers of symmetry.

DETERMINATION OF THE POSITION OF THE ATOMS

In determining the parameters of atoms, the present writer first took into consideration the intensity of reflection measured by means of an ionization spectrometer, using Mo K_α radiation and rock salt as standard (Tables 1 and 4).

The intensity of reflection $(0k0)$ is very strong when $k/2=2n$, while it is not strong when $k/2=2n+1$. (Compare the reflections (040), (080), (0120) with the reflections (020), (060), (0100).) This suggests at once that the y-parameters of the atoms should be ones of 0, 0.25, 0.50 and 0.75 and no other values.

This can also be deduced from the geometry of the lattice and the ionic size of atoms. The b-length of the unit cell is just twice the ionic diameter of oxygen atoms. Since in the assigned space group $(010)\frac{1}{4}$ and $(010)\frac{3}{4}$ are reflection planes, oxygen atoms either lie on these reflection planes, i.e. $y=0.25$, 0.75, or just touch them, i.e., $y=0$, 0.50. As for the other atoms, they must be placed, as usual, in the centers of polyhedra formed of oxygen atoms. On the other hand, the tetrahedra of oxygen atoms around silicon atoms must also be in a position symmetrical to the reflection planes (as projected on (100) or (001), they must appear as regular or bilateral triangles), the vertices of which lie on the reflection planes or in the middle between them. It is, therefore, scarcely possible to place the silicon and other metallic atoms, which should lie in the centres of oxygen polyhedra, in positions other than $y=0$, 0.25, 0.50, 0.75.

In epidote, as in other silicates, it is reasonable to assume that the coordination of oxygen around Ca (and Fe) is eight or six, around Al six or four, while around Si is four. There are several ways to accommodate the necessary number of such ionic polyhdera in the unit cell of epidote, bearing fully in mind the restriction imposed by the space group and dimensions of the cell. The intensity of $(h0l)$ spectra may profitably be taken into consideration at this stage of analysis. The intensity of reflections $(40\bar{6})$ and $(60\bar{4})$, for example, is so strong that we can safely regard all the atoms contributing waves in the same phase. Although, according as we take the signs of $(40\bar{6})$ and $(60\bar{4})$ reflections the same or opposite, the permissible domains of atoms are different. This helped to discard some geometrically possible atomic arrangements.

A Patterson-Harker synthesis, further, was of assistance to decide between still remaining plausible atomic arrangements. Since the y-parameters of the atoms in epidote are, as above deduced, ones of 0.00, 0.25, 0.50, 0.75 the synthesis is extremely simple.

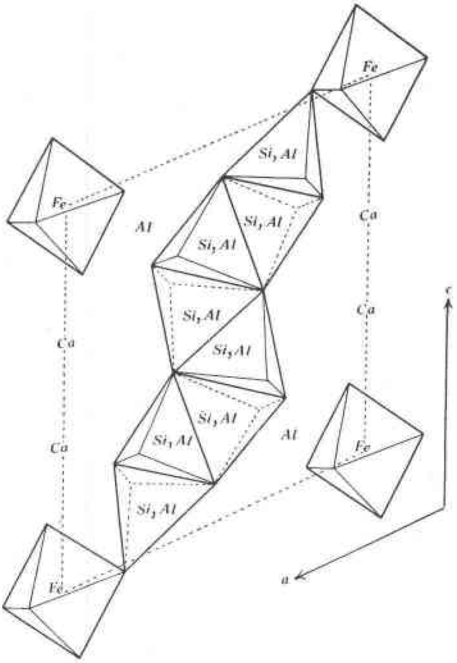


FIG. 2. The ideal structural scheme for epidote, diagrammatically shown as linked polyhedra of O and OH around metals. Projection on (010).

The structural scheme finally adopted for epidote is shown diagrammatically in Fig. 2, which is a projection on (010) of ionic polyhedra linked to each other by oxygen atoms and OH groups. Fourier synthesis was then carried out, using the F-values experimentally determined (Tables 1 and 4). The signs of the F-values are fixed provisionally by the approximate positions of atoms. We repeated this procedure several times, making necessary adjustment of the positions of atoms, assigning a renewed set of signs to the experimental F-values and improving step by step the parametral values of atoms.

TABLE 1. INTENSITY OF REFLECTIONS (*h0l*), WITH THE FINAL SET OF SIGNS AS USED IN FOURIER ANALYSIS. MEASUREMENT WITH IONIZATION SPECTROMETER (Mo K_α, $\lambda=0.707$Å)

Indices	sin θ	$\rho'\times10^6$	F′	Sign
101	.0704	25.50	45.2	+
102	.1042	55.00	82.2	+
103	.1401	3.90	28.2	+
104	.1785	14.00	57.6	+
105	.2160	8.30	40.0	+
106	.2550	3.91	37.0	+
107	.2920	6.50	56.5	−
108	.3305	4.65	53.4	+
109	.3690	2.26	38.4	−
1.0.10	.4077	1.84	37.3	+
201	.1110	7.40	33.1	+
202	.1408	44.80	95.6	+
203	.1745	20.30	74.6	+
204	.2090	9.60	52.4	−
205	.2455	1.92	27.5	−
206	.2802	3.10	40.0	+
207	.3180	5.72	55.1	−
208	.3570	1.60	30.9	+
301	.1540	0.85	16.0	+
302	.1800	4.45	33.2	+
303	.2112	6.15	42.9	+
304	.2445	11.50	64.9	+
305	.2785	14.60	83.2	+
306	.3135	2.06	33.2	+
307	.3500	0.88	22.8	−
401	.1901	3.90	32.8	+
402	.2221	3.29	31.9	−
403	.2510	7.15	51.8	+
404	.2817	10.60	71.0	+
405	.3150	2.14	33.6	−
406	.3490	2.50	38.5	+
501	.2415	0.86	14.2	+
502	.2651	13.70	78.4	+
503	.2925	1.90	31.9	+
504	.3210	0.49	16.4	+
505	.3521	6.45	62.1	−
506	.3850	2.90	43.9	−
601	.2854	0.86	24.2	+
602	.3089	2.52	35.8	−
603	.3350	4.36	48.9	+
604	.3621	2.08	36.0	+
605	.3909	0.76	22.3	−
701	.3275	3.73	45.2	+
702	.3501	1.68	35.4	−
703	.3759	5.03	56.0	+
$10\bar{1}$	.0437	17.30	28.6	+
$10\bar{2}$	.0690	67.10	73.1	+
$10\bar{3}$	.1050	5.20	25.2	+
$10\bar{4}$	.1400	14.30	55.0	+
$10\bar{5}$	.1775	10.80	44.1	+
$10\bar{6}$	.2140	44.50	116.2	+
$10\bar{7}$	.2530	6.75	44.3	−
$10\bar{8}$	.2910	1.25	24.1	+
$10\bar{9}$	.3290	2.15	33.8	−
$1.0.\overline{10}$	.3675	4.80	55.9	−
$20\bar{1}$	.0789	1.70	14.2	−
$20\bar{2}$	.0874	15.50	38.3	+
$20\bar{3}$	.1101	9.20	38.2	+
$20\bar{4}$	.1392	4.20	24.2	−
$20\bar{5}$	.1723	11.70	56.5	+
$20\bar{6}$	.2100	6.20	40.1	+
$20\bar{7}$	.2435	3.92	20.0	−
$20\bar{8}$	.2800	9.87	68.5	+
$20\bar{9}$	.3100	8.15	65.5	−
$2.0.\overline{10}$	.3550	7.90	68.5	+
$30\bar{1}$	.1195	1.30	16.0	−
$30\bar{2}$	.1204	28.25	63.3	+
$30\bar{3}$	.1311	1.86	13.9	+
$30\bar{4}$	.1521	0.80	15.2	−
$30\bar{5}$	.1780	3.70	30.8	+
$30\bar{6}$	.2088	26.80	89.5	+
$30\bar{7}$	.2420	3.65	36.5	+
$30\bar{8}$	.2760	24.00	107.0	+
$30\bar{9}$	.3150	2.60	37.3	+
$3.0.\overline{10}$	.3460	1.52	30.8	+

TABLE 1—(*continued*)

Indices	sin θ	$\rho' \times 10^6$	F′	Sign
$40\bar{1}$	.1635	41.10	99.6	−
$40\bar{2}$	.1580	1.70	23.0	+
$40\bar{3}$	.1628	12.90	55.9	+
$40\bar{4}$	.1748	1.68	18.7	+
$40\bar{5}$	.1982	1.96	24.0	+
$40\bar{6}$	.2205	46.00	119.0	−
$40\bar{7}$	.2480	0.76	14.0	+
$40\bar{8}$	.2616	3.25	40.5	+
$40\bar{9}$	.3112	3.20	41.1	−
$4.0.\overline{10}$	.3459	1.60	30.8	+
$50\bar{1}$	.2075	0.37	10.2	−
$50\bar{2}$	.1992	25.20	85.5	+
$50\bar{3}$	.1990	2.20	27.0	−
$50\bar{4}$	.2061	2.08	24.5	−
$50\bar{5}$	.2185	1.27	17.2	+
$50\bar{6}$	.2359	11.10	59.2	−
$50\bar{7}$	.2630	0.46	14.0	−
$50\bar{8}$	.2891	0.15	10.1	−
$50\bar{9}$	.3182	0.25	11.7	−
$5.0.\overline{10}$	.3486	3.47	47.0	+
$60\bar{1}$	.2509	3.51	36.4	+
$60\bar{2}$	.2391	3.63	33.2	+
$60\bar{3}$	.2368	11.00	62.5	−
$60\bar{4}$	.2409	53.60	127.0	+
$60\bar{5}$	.2490	5.92	47.0	+
$60\bar{6}$	.2622	1.22	19.1	−
$60\bar{7}$	.2810	1.04	23.3	+
$60\bar{8}$	.3042	1.01	22.6	+
$60\bar{9}$	.3298	2.70	38.4	−
$6.0.\overline{10}$	.3580	0.30	13.8	+
$70\bar{1}$	.2951	3.63	43.1	−
$70\bar{2}$	.2830	0.41	14.4	+
$70\bar{3}$	.2785	2.42	20.3	−
$70\bar{4}$	.2782	3.21	39.2	+
$70\bar{5}$	.2825	1.42	20.6	+
$70\bar{6}$	.2915	0.60	14.1	−
$70\bar{7}$	.3058	1.22	21.3	−
$70\bar{8}$	.3241	6.51	59.8	+
$70\bar{9}$	.3459	2.10	35.4	−
$7.0.\overline{10}$	.3715	11.80	89.6	−
$80\bar{1}$	.3401	5.70	57.0	−
$80\bar{2}$	.3269	9.30	71.5	+
$80\bar{3}$	.3211	11.60	79.6	−
$80\bar{4}$	.3167	2.97	40.5	+
$80\bar{5}$	.3210	2.86	39.6	+
$80\bar{6}$	.3255	1.48	28.5	−
$80\bar{7}$	.3359	1.90	32.9	+
$80\bar{8}$	.3495	1.12	22.0	−
$80\bar{9}$	.3691	0.81	22.4	−
$8.0.\overline{10}$	.3863	0.33	14.8	+

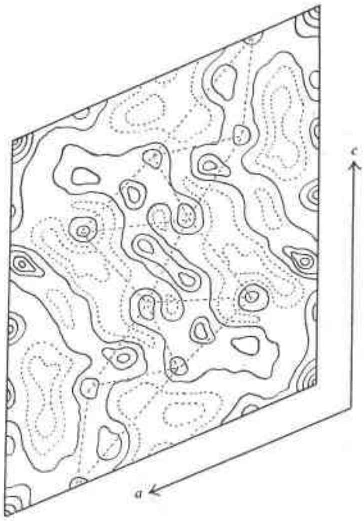


FIG. 3. The two-dimensional Fourier representation of the electron density of epidote projected on (010). An $\mathrm{AlSi_3O_9}$ group (cf. below) can be traced in the projection (dotted straight lines).

TABLE 2. COORDINATES OF ATOMS IN DECIMAL FRACTIONS OF THE AXIAL LENGTH: THE ORIGIN IS PLACED AT A CENTER OF SYMMETRY

Kind of Atom	Number in the Cell	x/a	y/b	z/c
$\mathrm{O_{I}}$	4	.042	.000	.843
$\mathrm{O_{II}}$	4	.301	.000	.742
$\mathrm{O_{III}}$	4	.783	.000	.694
$\mathrm{O_{IV}}$	2	.535	.250	.821
$\mathrm{O_{V}}$	2	.535	.750	.821
$\mathrm{O_{VI}}$	2	.420	.250	.582
$\mathrm{O_{VII}}$	2	.420	.750	.582
$\mathrm{O_{VIII}}$	2	.000	.000	.500
$\mathrm{O_{IX}}$	2	.179	.750	.033
OH	2	.179	.250	.033
$\mathrm{(Si, Al)_{I}}$	2	.394	.250	.711
$\mathrm{(Si, Al)_{II}}$	2	.604	.750	.695
$\mathrm{(Si, Al)_{III}}$	2	.582	.250	.553
$\mathrm{(Si, Al)_{IV}}$	2	.375	.750	.940
Al	2	.789	.250	.814
Al, Fe	2	.000	.000	.000
$\mathrm{Ca_{I}}$	2	.963	.250	.641
$\mathrm{Ca_{II}}$	2	.963	.750	.641

The final result of analysis is graphically represented in Fig. 3. The positions of atoms obtained are given in Table 2 and the interatomic distances calculated in Table 3. The values give a fair agreement between the theoretical and experimental *F*-values as shown in Table 4.

TABLE 3. INTERATOMIC DISTANCES IN EPIDOTE

Atom	Neighbour	Distance in A	Atom	Neighbour	Distance in A
O_{I}	O_{II}	3.5	(Si, Al)$_{III}$	O_{III}	2.3
	OH	2.8		O_{III}'	2.3
	O_{VIII}	3.2		O_{VII}	2.4
				O_{VI}'	1.4
O_{II}	O_{IV}	2.5			
	O_{VI}	2.4	(Si, Al)$_{IV}$	O_{II}	2.3
	OH	3.7		O_{II}'	2.3
				O_{V}	2.3
O_{III}	O_{IV}	3.2		O_{IX}	2.3
	O_{VI}	3.2			
	O_{VI}'	2.7	Al	O_{I}	2.7
				O_{I}'	2.7
O_{IV}	O_{VI}	2.5		O_{IV}	2.6
	O_{IX}	2.4		O_{IX}'	1.5
	OH	4.3		O_{II}'	2.0*
				O_{II}'	2.0*
(Si, Al)$_{I}$	O_{II}	1.8			
	O_{II}'	1.8	(Al, Fe)	(O_{I}, O_{I}'	1.7
	O_{IV}	1.4		O_{IX}, O_{IX}'	2.2
	O_{VI}	1.5		(OH), (OH)$'$	2.2
(Si, Al)$_{II}$	O_{III}	2.1	Ca	O_{I}, O_{I}'	2.3
	O_{III}'	2.1		O_{II}, O_{II}'	3.2
	O_{V}	1.4		O_{III}, O_{III}'	2.6
	O_{VII}	1.8		O_{VIII}, O_{VIII}'	2.5

* With no valency residue.
Prime denotes atoms in the adjoining cell.

STRUCTURAL DETAILS

The positions of atoms in the structure of epidote are shown in Fig. 4, which is a projection of the unit cell on (010). Figure 5 visualizes the structural scheme with a frame-work of linked polyhedra of oxygen atoms and the OH groups around metal atoms. We see here that some of the polyhedra are more or less deformed in contrast to those in Fig. 2, from which we started the Fourier analysis.

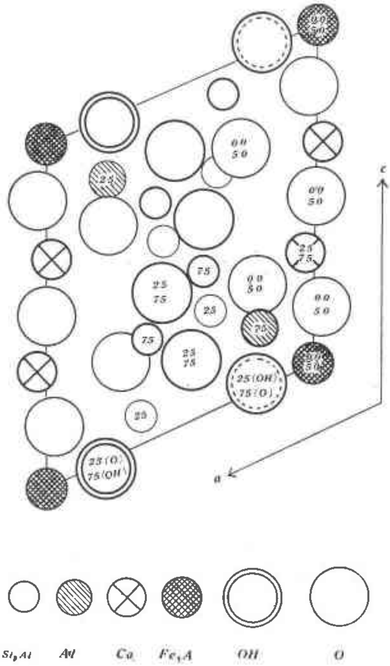


FIG. 4. The structure of epidote projected on (010). Numbers give in decimal fractions of the *b*-axis the height of atoms in the unit cell.

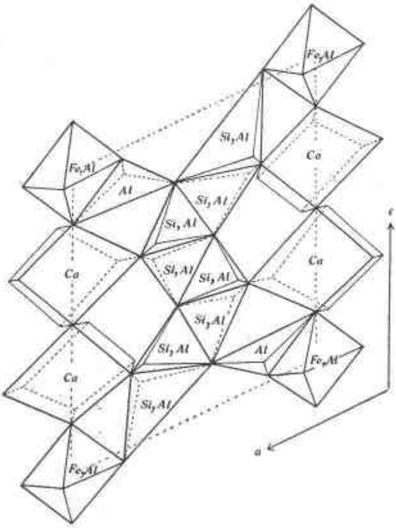


FIG. 5. The structure of epidote shown as linked polyhedra of O and OH around (Si, Al), Al, (Al, Fe) and Ca. Projection on (010). Some of the corners of polyhedra are somewhat displaced from their true positions in order to make their shape show.

TABLE 4. INTENSITY OF REFLECTIONS

(1) Measurements with ionization spectrometer
(Mo K_α radiation 0.707Å)

Indices	Sin θ	$\rho'\times10^6$	F obs.	F calc.
100	.0438	22.10	32.2	+ 48.1
200	.0876	82.80	88.6	+114.2
300	.1314	55.00	84.6	+109.2
400	.1752	27.50	75.6	+ 52.4
500	.2190	4.46	31.8	+ 19.3
600	.2628	6.50	40.5	− 39.5
700	.3066	1.35	22.4	− 3.0
800	.3504	1.24	23.2	− 33.4
900	.3942	1.24	25.4	− 15.8
10.0.0	.4380	4.50	51.0	− 43.7
11.0.0	.4818	0.93	25.4	− 15.6
020	.1257	138.70	130.0	−116.3
040	.2514	117.60	181.8	+213.6
060	.3771	18.40	93.1	− 61.8
080	.5028	16.96	112.2	+ 98.0
0.10.0	.6285	2.00	43.6	− 30.4
0.12.0	.7542	3.76	62.5	+ 64.4
001	.0385	1.16	6.4	+ 20.0
002	.0770	4.62	17.9	+ 30.1
003	.1155	8.49	30.5	+ 60.3
004	.1540	1.98	18.5	− 19.8
005	.1925	2.22	21.5	+ 30.2
006	.2310	4.92	35.0	+ 45.5
007	.2695	2.63	28.0	− 18.1
008	.3080	1.45	22.8	+ 10.9
009	.3465	1.02	20.6	− 28.3
0.0.10	.3850	0.85	20.0	− 30.5
0.0.11	.4235	5.15	54.6	+ 43.0

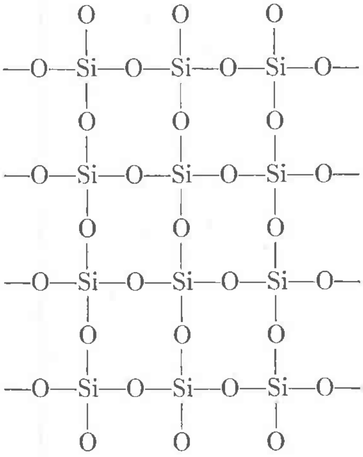
Indices	Sin θ	$\rho'\times10^6$	F obs.	F calc.
101	.0704	25.50	45.2	+ 44.1
202	.1408	44.80	95.6	+124.5
303	.2112	6.15	32.9	+ 23.2
$10\bar{1}$	.0437	17.30	28.6	+ 41.0
$20\bar{2}$	.0874	15.50	38.3	+ 37.4
$30\bar{3}$	.1311	5.86	23.9	+ 40.8
$40\bar{4}$	.1748	1.68	18.7	+ 26.0
201	.1110	7.10	33.0	− 28.0
402	.2221	3.29	31.9	+ 50.5
$20\bar{1}$	.0789	16.40	37.1	+ 54.5
$40\bar{2}$	.1580	1.80	23.0	− 42.0
$60\bar{3}$	.2368	11.00	62.5	− 57.7
203	.1745	20.30	74.6	+ 90.6
$20\bar{3}$	.1101	9.20	38.2	+ 50.0
$40\bar{6}$	.2203	46.00	119.5	+ 81.8
301	.1540	1.20	16.6	− 7.8
602	.3080	2.52	35.8	+ 48.3
$30\bar{1}$	.1185	5.00	16.0	+ 23.1
$60\bar{2}$	.2370	3.63	33.2	− 34.5
302	.1800	4.45	33.0	+ 56.6
$30\bar{2}$	.1204	14.10	43.6	− 34.9
$60\bar{4}$	.2409	53.60	127.0	+ 90.3

TABLE 4—(*continued*)

(2) Intensity estimated in the Weissenberg photographs
(Co K_α $\lambda = 1.79$Å)

Indices	Sin θ	Intensity	F calc.	Indices	Sin θ	Intensity	F calc.
110	.1936	—	+ 7.5	311	.4149	—	+11.4
210	.2760	w	+11.8	612	.7814	—	+ 2.2
310	.3680	w	+15.4				
410	.4682	w	+12.1	$31\bar{1}$	.3364	m	+33.4
				$61\bar{2}$	.6300	—	− 5.4
011	.1863	—	+ 5.1				
012	.2511	—	− 2.2	312	.4773	m	+ or −56.0
013	.3315	m	−43.5				
014	.4210	w	−32.8	$31\bar{2}$	.3424	m	+42.0
				$61\bar{4}$	.6285	w	− 8.9
111	.2362	—	+ 2.0				
212	.3859	w	−31.2	121	.3633	w	+28.0
313	.6774	w	−10.3	222	.4734	w	+33.1
				323	.6148	—	− 4.9
$11\bar{1}$	.1939	w	+36.6				
$21\bar{2}$	.2766	w	+37.4	$12\bar{1}$	.3362	—	−13.0
$31\bar{3}$	.3701	m	+43.4	222	.3880	s	+59.9
$41\bar{4}$	.4755	w	−24.0	$32\bar{3}$	.4613	w	+ 4.9
				$42\bar{4}$	.5498	s	+67.1
211	.3195	w	+ 5.6				
412	.5760	w	−26.2	221	.4212	m	+45.7
				422	.6310	w	+12.5
$21\bar{1}$	.2555	w	−31.0				
$41\bar{2}$	.4298	w	−10.0	$42\bar{2}$	.5188	m	+48.3
$61\bar{3}$	.6202	w	− 8.0	$62\bar{3}$	.6780	m	+15.4
213	.4808	—	+ 5.5	223	.5392	w	−37.4
$21\bar{3}$	.3718	w	+31.5	$22\bar{3}$	.4242	s	−121.2
$41\bar{6}$	.5850	w	+15.5	$42\bar{6}$	.6421	m	−19.8

The structure in its main feature is composed of complex chains of linked Si tetrahedra stretched in the direction of the *b*-axis. The SiO_3-chains, which can be traced in the structure, are, though in linkage similar to, in form different from those found in pyroxenes. While in pyroxenes one tetrahedron of the chain is so related to the next as if rotated ca. 109° about the chain direction (Fig. 6), in epidote this angle amounts to only ca. 71° (Fig. 7). In both minerals the chains consist of two layers of oxygen atoms. Whereas in pyroxenes two thirds of oxygen atoms of the chain lie on one layer and the remaining one third on the other, in epidote oxygen atoms are equally distributed between the two layers of the chain. In epidote four of the latter SiO_3-chains are bound with one another, holding bordering oxygen atoms in common, and build up a composite chain or band having the composition Si_4O_9, thus



In the actual structure of epidote one of four silicon atoms of the group Si_4O_9 is statistically replaced by the Al atom.

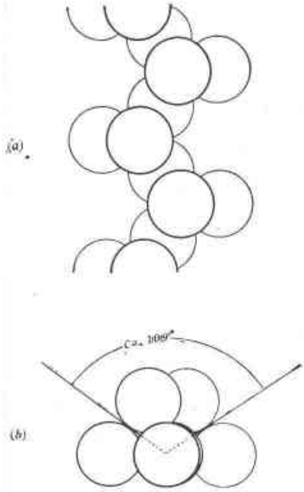


FIG. 6. The SiO_3 chain in pyroxenes. The Si atoms are omitted (a) plan; (b) viewed end on.

The composite chains or band of this type are bound together laterally by the Ca, Al(Fe) and Al atoms. The Ca atoms occupy the centers of distorted cubes formed of oxygen atoms of the chains and ones outside the chains. The Al(Fe) atoms, lying on the centers of inversion, occupy the centers of more or less regular octahedra formed of oxygen atoms and OH groups. The remaining Al atoms which cannot be replaced either by Fe or by Si atoms, occupy the centers of oxygen tetrahedra (counting only surrounding oxygen atoms with residual bonds), which share an edge with the Al(Fe) octahedra and a corner with the Si(Al) tetrahedra and another with the Ca cube.

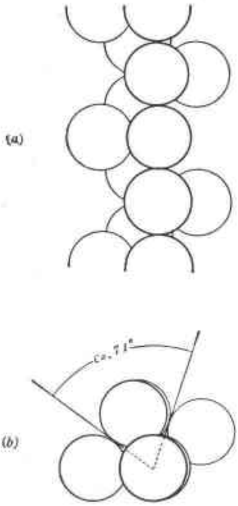


FIG. 7. The SiO_3 chain which can be traced in epidote. The Si atoms are omitted (*a*) plan; (*b*) viewed end on.

In the structure thus formed the oxygen atoms are between two Si(Al) atoms, or one Si(Al), one Al and two Al(Fe) atoms, or two Ca and two Si(Al) atoms, or two Ca, one Al and one Al(Fe) atoms, while the OH groups are always between two Al(Fe) atoms.

The structural aspect of epidote can be represented by the formula $Ca_2O \cdot (Al, Fe)O_2OH \cdot Al \cdot AlSi_3O_9$ or, in the extreme case as in epidote used in the present investigation, since Fe replaces Al to the fullest degree, by the formula $Ca_2O \cdot FeO_2OH \cdot Al \cdot AlSi_3O_9$.

Cleavages of epidote, being perfect after (001) and less so after (100), are parallel to the direction of the chains.

TWINNING OF EPIDOTE; THE STRUCTURAL RELATION OF EPIDOTE TO ZOISITE

The twinning of epidote takes place on (100). If we consider in the structure a reflection across $(100)_0$ with a glide $b/2$, the occurrence of the twin may easily be accounted for. The relative positions as well as coordination of atoms, then, in the simple and twinned structures are almost exactly the same. The only difference between them is that while in the former the shared edges of the Al(Fe) octahedron with neighbouring Al tetrahedra are *parallel* (Fig. 8*a*), in the latter they are *inclined*, meeting in a vertex (Fig. 8*b*). The Al(Fe) octahedra, further, are more symmetrical in shape in the twinned position.

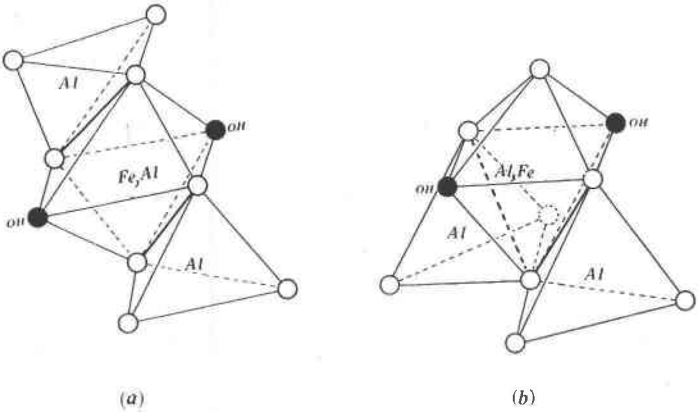


FIG. 8. Polyhedral arrangement of oxygen atoms and OH groups around Al(Fe) in epidote (*a*) and in twinned epidote (or zoisite) (*b*). Open circles represent oxygen atoms.

Zoisite may be regarded as intimately twinned epidote (or rather clinozoisite) as pointed out by several investigators. Zoisite is almost always poor in iron. The substitution of Al by Fe therefore seems to render the occurrence of twinning more haphazard and less regular. This may be due to the difference of ionic radii of the Al and Fe atoms. The (Al, Fe) octahedra are namely, though more symmetrical, less spacious in the structure in the twinned position than in the normal position to accommodate the larger Fe atoms.