12. The Structure of Epidote.

By Teiichi ITO and Hirosada SAWADA.

Mineralogical Institute, Tokyo Imperial University.

(Rec. Dec. 28, 1944. Comm. by S. KÔZU, M.I.A., Jan. 12, 1945.)

Using the Fourier analysis as well as the usual X-ray methods, the crystal structure of epidote ($\text{HCa}_2(\text{Al}, \text{Fe})\text{Al}_2\text{Si}_3\text{O}_{13}$) was analysed. The result of analysis is graphically represented in Fig. 1. The positions of atoms are given in Table I and are shown in Fig. 2. Fig. 3 visualizes the structural scheme of epidote with a frame-work of linked polyhedra of oxygen atoms and the OH groups around metal atoms.

TABLE I. Unit cell, space group and coordinates of atoms.

1. Unit cell

$a=8.96\text{\AA}$, $b=5.63\text{\AA}$, $c=10.20\text{\AA}$

$\beta=115^\circ 24'$ (Strunz, H)

2. Space group

$C_{2h}^2-P_{21}^2/m$

3. Coordinates of atoms

Kind of atom	Number in the cell	x/a	y/b	z/c
O _I	4	.042	.000	.843
O _{II}	4	.301	.000	.742
O _{III}	4	.783	.000	.694
O _{IV}	2	.535	.250	.821
O _V	2	.535	.750	.821
O _{VI}	2	.420	.250	.582
O _{VII}	2	.420	.750	.582
O _{VIII}	2	.000	.000	.500
O _{IX}	2	.179	.750	.033
OH	2	.179	.250	.033
(Si, Al) _I	2	.394	.250	.711
(Si, Al) _{II}	2	.604	.750	.695
(Si, Al) _{III}	2	.582	.250	.553
(Si, Al) _{IV}	2	.375	.750	.940
Al	2	.789	.250	.814
Al, Fe	2	.000	.000	.000
Ca _I	2	.963	.250	.641
Ca _{II}	2	.963	.750	.641

We see that the structure is composed of complex chains of linked Si(Al) tetrahedra stretched in the direction of the b-axis corresponding to the composition AlSi_3O_9 . These composite chains or bands are bound together laterally by the Ca, Al(Fe) and Al atoms. The Ca atoms occupy the centres of cubes formed by oxygen atoms. The Al(Fe) atoms occupy the centres of octahedra formed by oxygen atoms and the OH groups. The Al atoms occupy the centres of tetrahedra formed by oxygen atoms. The structure not only gives a fair agreement between the theoretical and experimental F -values as shown in Table II, but also explains well cleavage, twinning and chemical properties of epidote. Particulars of the study will be published shortly.

TABLE II. Intensity of spectra, measurement with an ionization spectrometer. (MoK radiation 0.707Å).

Indices	$\sin \theta$	$\rho' \times 10$	F obs.	F calc.
100	.0438	22.16	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
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

Fig. 1. Two-dimensional Fourier representation of electron density of epidote, projected on (010). An AlSi_2O_6 group, a composite chain or band, may be traced in the figure. (dotted straight lines.)

Fig. 2. structure of epidote projected on (010). Numbers give in decimal fractions of the b -axis the height of atoms in the unit cell.

Fig. 3. The structure of epidote shown as linked polyhedra of oxygen atoms and the OH groups around (Si, Al), Al, (Al, Fe) and Ca atoms. Some of the corners of polyhedra are displaced from their true positions in order to make their shape show.