67. *Parasymplesite, a New Mineral Polymorphous with Symplesite*

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Symplesite from Felsöbánya was first described by Krenner as a monoclinic crystal.[1] Wolfe investigated with X-rays the same mineral from Lobenstein and demonstrated the triclinic nature of its lattice.[2] Unaware of Wolfe's work we analysed the crystal structure of symplesite using the fine vivianite-like specimens from Kiura, Japan.[3,4] As revealed by this study the crystals from Kiura are not triclinic but monoclinic in symmetry, being closely related to vivianite in structure. On the other hand, our recent re-examination of the original symplesite from Felsöbánya and from Lobenstein, which were kindly put at our disposal by Professor Cliford Frondel of Harvard University, has confirmed in every detail the findings of Wolfe and has placed the dimorphism of symplesite beyond question. We therefore propose here the new name *parasymplesite* (in analogy with parawollastonite,[5] paracelsian[6] etc.) for the monoclinic variety of symplesite whose structure we worked out, retaining, following Frondel,[7] the name *symplesite* for the triclinic variety originally described by Krenner and revised by Wolfe.

Occurrence

Parasymplesite from Kiura, Ohita (Bungo), Japan occurs in the contact zone of limestone with granitic diorite, forming usually radiating aggregates of fine crystals grown on massive limonite, an alteration product of various ore minerals (scorodite, arsenopyrite etc.) constituting the deposits.[4] It is these crystals we describe below.

Crystallography

The crystals of parasymplesite are about $3 \times 1.5 \times 1$ mm in dimensions and dark to light greenish blue in colour. Crystals are thick tabular after (010), with large $b(010)$ and $w(\bar{2}01)$ (Fig. 1a) or stout-prismatic with $m(110)$ and other prisms nearly equally well developed and with relatively large $E(502)$ (Fig. 1b). Numerous prismatic faces are observed in both types of crystals, other kinds of faces being only occasionally noticed.

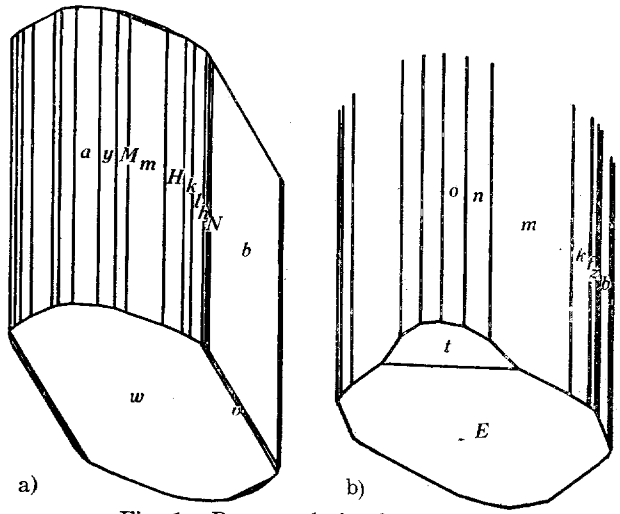


Fig. 1. Parasymplesite from Kiura

The results of measurement by means of a Goldschmidt two-circle reflexion goniometer are given in Table I. The axial ratio has been deduced from the structural data (given below) as follows:

$a:b:c=0.760:1:0.350, \beta=103°50'.$

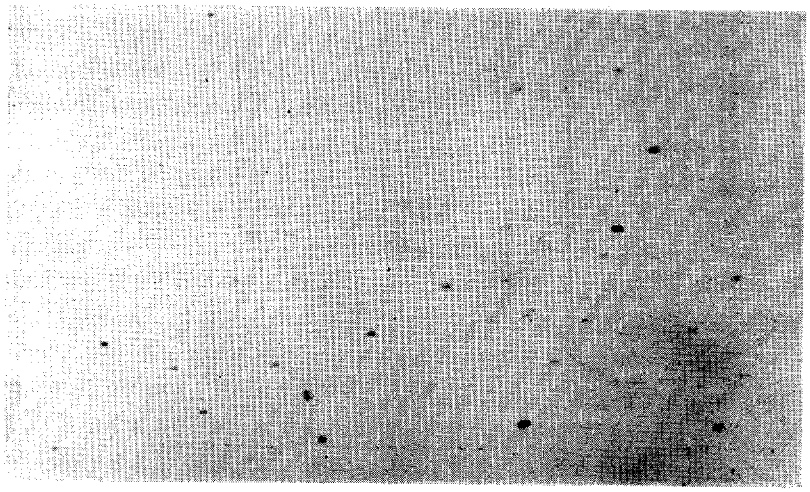
Table I. Two-circle goniometry of parasymplesite

Form	ρ_o	φ_o	ρ_c	φ_c	Nos. of faces measured
b (010)	89°43′	0°00′	90°00′	0°00′	5
z (1, 20, 0)	90 3	3 7	,,	3 58	1
N (190)	90 5	8 19	,,	8 20	1
h (170)	90 5	11 15	,,	10 56	1
f (120)	90 2	33 0	,,	34 10	1
l (580)	90 4	40 18	,,	40 15	2
k (570)	89 40	45 37	,,	44 03	4
H(560)	90 1	49 32	,,	48 28	3
m(110)	90 3	51 37	,,	53 34	6
M(430)	90 2	60 12	,,	61 02	1
Q (530)	90 8	65 51	,,	66 07	2
n (210)	90 0	69 41	,,	68 47	1
y (310)	90 1	76 13	,,	76 10	3
o (810)	89 47	83 20	,,	84 43	3
a (100)	89 53	89 20	,,	90 00	4
w($\bar{2}$01)	35 3	−90 23	34 58	−90 00	2
E ($\bar{5}$02)	42 36	−88 17	43 07	,,	1
t ($\bar{4}$01)	59 5	−93 42	58 43	,,	1
v ($\bar{2}$21)	44 44	−48 12	45 27	−47 40	3
r ($\bar{1}$11)	22 0	−32 35	22 35	−32 52	2

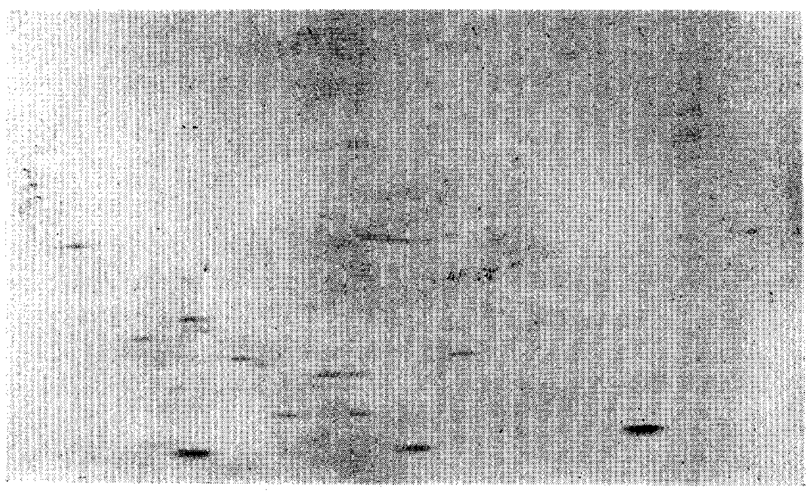
ρ_c and φ_c calculated on the basis of the axial ratio: $a:b:c=0.760:1:0.350$, $\beta=103°50'$, deduced from the structural data

The unit cell has the dimensions: $a=10.25$Å, $b=13.48$Å, $c=4.71$Å, $\beta=103°50'$,[3] containing two molecules of $Fe_3(AsO_4)_2 \cdot 8H_2O$ (Mo Kα, $\lambda=0.710$Å). The space group is $C2/m$.

We reproduce in Figs. 2 and 3, the 0-layer Weissenberg photographs of parasymplesite and symplesite (twinned on $(1\bar{1}0)$), taken with a Wiebenga integrating X-ray goniometer both about the *c* axis (Fe Kα). The X-ray powder photographs, and 'Norelco' spectrograms (Co Kα) of symplesite and parasymplesite are compared



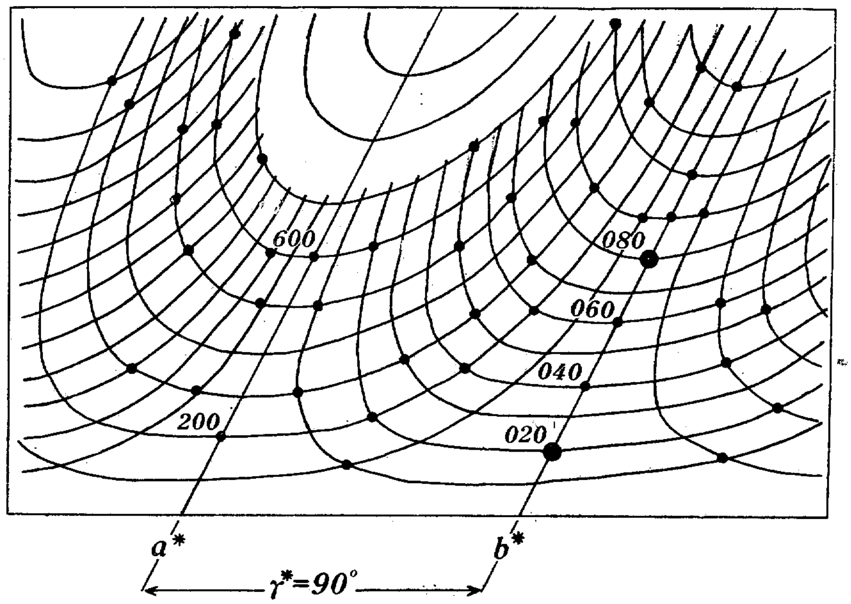
a) Parasymplesite



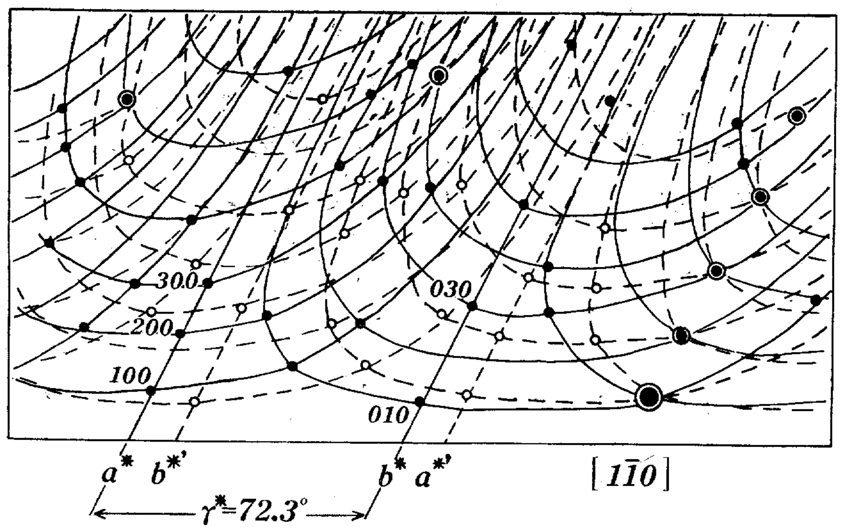
b) Symplesite

Fig. 2. Weissenberg photographs of parasymplesite and symplesite. *c*-axis, 0-layer. Fe radiations, no filter. Camera diameter 57.3 mm. Coupling 1mm to 2°

in Figs. 4 and 5. The difference as well as similarity of the two minerals in symmetry and texture is well evidenced on these diagrams. (Also see Table II.)

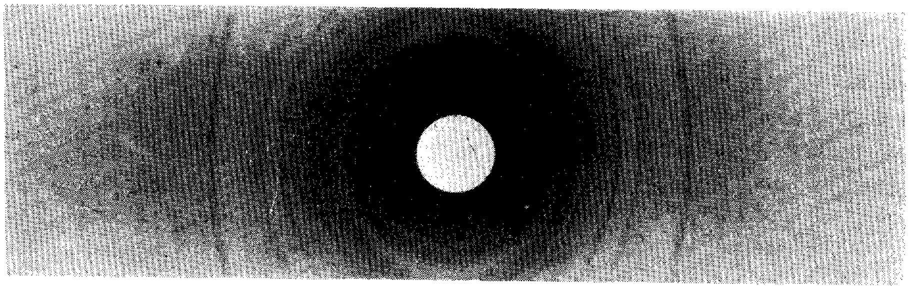


a) Parasymplesite

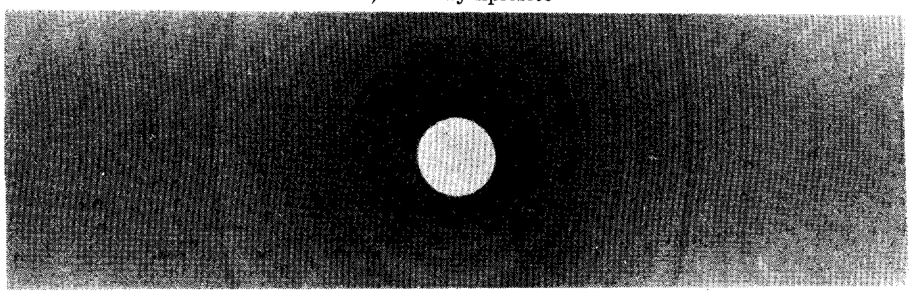


b) Symplesite

Fig. 3. Weissenbergrams corresponding to Fig. 2



a) Parasymplesite



b) Symplesite

Fig. 4. Powder photographs of parasymplesite and symplesite. Camera diameter 57.3 mm. CoKα. 3.5 KV, 9 MA, 3 hrs.

Table II. X-ray powder data of parasymplesite and symplesite

Parasymplesite from Kiura			Symplesite from Felsöbánya		
I	2θ	d (Å)	I	2θ	d (Å)
18	11.40°	9.006	15	11.45°	8.971
12	12.65	8.119			
17	13.70	7.499	16	13.70	7.499
38	14.55	7.063			
100	15.05	6.830	100	15.15	6.785
9	20.40	5.051	7	20.50	5.027
7	23.30	4.429			
8	25.55	4.051	7	25.40	4.069
9	25.90	3.991	8	25.80	4.007
10	27.80	3.723	8	27.65	3.743
{9	{30.30	{3.423	8	30.50	3.401
10}	30.55}	3.395}			
10	31.95	3.250			
10	32.70	3.177	7	32.70	3.177
9	34.25	3.038	{6	{33.20	{3.131
9	34.70	2.999	6}	33.60}	3.095}
11	36.65	2.845	7	35.05	2.970
9	38.80	2.693	7	36.75	2.838
9	40.70	2.572	5	40.60	2.578
7	42.00	2.496	{2	{42.05	{2.493
6	43.55	2.411	2}	42.50}	2.468}
{9	{45.05	{2.335	{2	{44.25	{2.375
9}	45.15}	2.330}	3}	44.65}	2.355}
6	45.65	2.306			
{6	{46.55	{2.264	2	46.15	2.282
6}	46.80}	2.252}			
8	50.45	2.099	1	55.25	1.929
6	51.50	2.059	1	57.50	1.860
{8	{63.75	{1.694	1	57.70	1.854
8	63.90	1.690	1	63.10	1.709
8}	64.00}	1.688}	2	64.20	1.683

'Norelco' X-ray spectrometer. Co Kα, λ=1.78890Å. No filter. 16-1-8 slit 1°, 0.006″, 1°. Speed 1′/min. Scale factor 16′. Multiplier 1. Time constant 8 sec.

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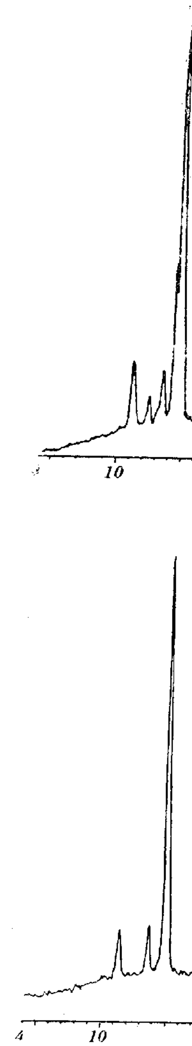

Fig. 5. '
CoKα, no filte

Chemical Composition

The chemical analysis of parasymplesite has been carried out by one of the present writers (H. M.) on the specimens which were separated from scorodite and other associated minerals with the result: As_2O_5 38.43%, Fe_2O_3 0.81%, FeO 37.70%, MgO non, CaO non, P_2O_5 non, $H_2O(+)$ 12.70%, $H_2O(-)$ 10.67%, Total 100.33%. This may be represented by the formula, $Fe_{3.03}As_{1.99}O_8 \cdot (H_2O)_{4.08+3.43}$, or very closely $Fe_3(AsO_4)_2 \cdot 8H_2O$.

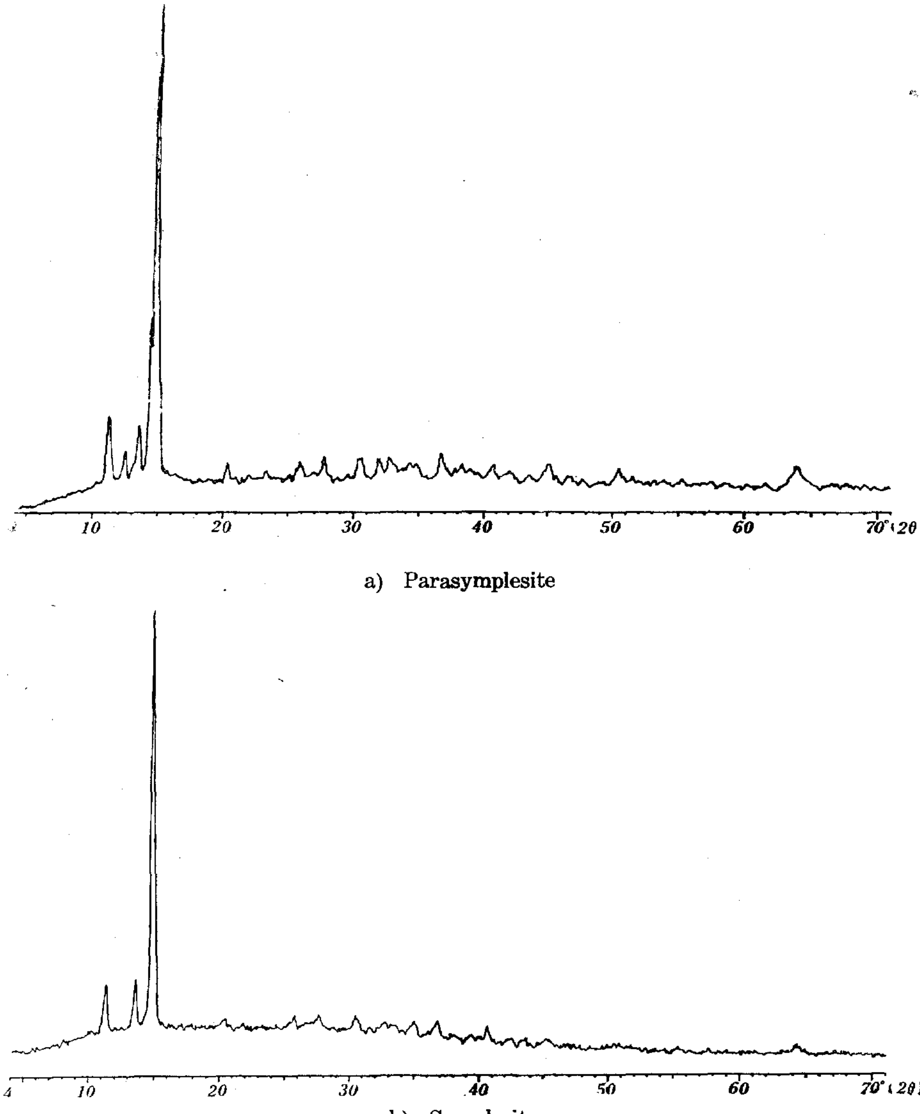

Fig. 5. 'Norelco' X-ray spectrograms of parasymplesite and symplesite. CoKα, no filter (See Table II.)

Table III. Optical properties of parasymplesite

c∧Z	...	31°20′
2V	...	large, negative (?)
Indices of refraction *		
α	...	1.628
β	...	1.660
γ	...	1.705
Pleochroism		
X	...	bluish green
Y	...	yellowish
Z	...	brownish yellow

* Determined by the immersion method using dispersion liquids and a prism monochromator

Optical and Other Physical Properties

The optical data are given in Table III. Cleavage is very perfect after (010). Hardness 2. The density has been determined with a pychnometer to be 3.07 gr/cm^3 at 20°C against 3.097 gr/cm^3 calculated on the basis of the X-ray data above given.

References

1) Krenner, J. H.: Z. Kristallogr., **13**, 70 (1887).
2) Wolfe, C. W.: Amer. Min., **25**, 801 (1940). He gave the constants: a=7.85 KX, b=9.39 KX, c=4.71 KX, α=99°55′, β=97°22′.5, γ=105°57′.5. Space group P$\bar{1}$.
3) Mori, H. and Ito, T.: Acta Cryst., **3**, 1 (1950).
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5) Peacock, M. A.: Amer. J. Sci., **30**, 495 (1935).
6) Spencer, L. J.: Mineralog. Mag., **26**, 231 (1942).
7) Frondel, C.: Dana's System of Mineralogy, 7th ed., p. 752. New York (1951).