observed intensities ensures that there is at least a good approximation to the atomic positions. Further work is in progress.

We wish to express our thanks to Dr L. E. Cross for providing the crystals together with information about their electrical properties, and to Dr P. Vousden for the opportunity of discussing this note before publication. One of us (M. W.) thanks D.S.I.R. for financial support while this work was carried out.

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On the Structure of Staurolite, $HFe_2Al_9Si_4O_{24}$

By I. Náray-Szabó and K. Sasvári

Central Chemical Research Institute of the Hungarian Academy, Budapest, Hungary

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A reinvestigation of the structure of staurolite has been made taking account of new chemical analyses leading to the chemical formula $HFe_2Al_9Si_4O_{24}$ or $4\,Al_2SiO_5.AlOOH.2\,FeO$ proposed by Hörner; the staurolite cell contains two of these molecules, whereas the old formula was $2\,Al_2SiO_5.Fe(OH)_2$, with four molecules in the unit cell. The two surplus Al^{3+} ions can be located reasonably and the Fe^{2+}–O^{-2} distance has been also improved. The agreement between measured and estimated intensities and measured and calculated F-values is satisfactory. The true space group is $C2/m$.

The structure of staurolite was determined long ago by one of us (Náray-Szabó, 1929), but since then some doubts have arisen about the chemical formula which had been idealized as

$$2\,Al_2SiO_5.Fe(OH)_2=H_2FeAl_4Si_2O_{12}\,.$$

Analytical evidence available in 1929 was not enough to invalidate this formula, until Skerl, Bannister & Groves (1934) showed that the cell of lusakite, a cobalt-bearing staurolite, contains 18 aluminium ions. A similar result was obtained by Juurinen (1956) for common rock-forming staurolite crystals. Meanwhile Hurst, Donnay & Donnay (1956) made a thorough study of the morphology, twinning and the optical properties of staurolite. They conclude that 'the evidence provided by X-ray diffraction is completely in favour of orthorhombic symmetry'. Optical measurements, however, showed that the real symmetry is monoclinic. These authors also took precession X-ray photographs by the method of de Jong-Bouman (1938) with a camera of the Buerger type (1939) and found some very weak reflexions indicating that the space group *Ccmm* adopted by Náray-Szabó is only a pseudo-space-group and the real one is a sub-group of it, $C2/m$. Juurinen choose $C222_1$ which is in contradiction to the monoclinic symmetry.

The structure type of staurolite SO_4 is based on *Ccmm* which was also found by Cardoso (1928). No twofold positions exist in this space group and therefore the few chemical analyses were rounded off to the first formula given above a procedure which also takes account of the close relationship of staurolite with kyanite Al_2SiO_5, which exhibits frequently a parallel growth with staurolite.

In view of the contradictions of the papers mentioned we re-examined the structure of staurolite. A series of oscillation photographs has been taken from a small staurolite crystal but we failed to find any reflexions on them to which indices prohibiting *Ccmm* could unambigously be assigned. We are much indebted to Dr V. J. Hurst by whose courtesy we obtained a precession X-ray photograph of a minute staurolite crystal, showing $(0kl)$ reflexions only. No ambiguity can arise in the indexing of this diagram and in fact some very faint reflexions forbidden in *Ccmm*, e.g. (001), (021), (041) etc. occur on it. On our own oscillation photographs, taken with Mo K radiation, a few faint reflexions coinciding with the β-spots of other reflexions appeared and have therefore been regarded as doubtful. Our own unambiguously indexed reflexions and the spots appearing on the photograph obtained from Dr Hurst indicate that the real space group is a sub-group of *Ccmm* but not $C222_1$ in which (001) could not occur. Neither Hurst, Donnay & Donnay (1956) nor the present authors were able to find a piezoelectric effect; therefore the symmetry centre required by $C2/m$ is probable and so this must be adopted as the true space group.

The content of the unit cell which has been idealized in the original work to $H_8Fe_4Al_{16}Si_8O_{48}$, should be $H_2Fe_4Al_{18}Si_8O_{48}$ according to analyses of Hörner (1915) and Skerl, Bannister & Groves (1934) and

$H_4Fe_4Al_{18}Si_8O_{48}$ according to Juurinen, but the latter formula contradicts the principle of electrostatic neutrality. The chemical analyses of the afore-mentioned authors establish the presence of 18 Al^{3+} ions in the cell, i.e. 2 more than adopted by Náray-Szabó; at the same time only 2 H^+ ions can be present. Considering the good agreement of the calculated F values and those measured or estimated according to the original structure determination, the real structure cannot be very different from the type $S0_4$. Moreover, the universally adopted structure of kyanite must be a part of the staurolite structure; therefore only the arrangement of the parallel layers (010), with the newly determined composition $Al_2Fe_4O_8H_2$ or 2 AlOOH.4 FeO should be changed and the kyanite part 4 Al_2SiO_5 remains unchanged.

The volume per oxygen ion in staurolite is 15·15 Å³, very near to the value 13·02 Å³ calculated for closest packing with an oxygen radius $r = 1{\cdot}32$ Å.—One can denote an orthogonal cell in the closest-packed cubic lattice of oxygen ions which is very nearly equal to the staurolite unit cell. Taking $r' = 1{\cdot}388$ Å³ (calculated from the volume per O^{2-} ion 15·15 Å³) then the calculated edges are $a' = 4r'.\sqrt{2}$, $b = 12r'$, $c = 4r'$; this cell contains 48 O^{2-} ions,

Edge	calc. Å	meas. Å
a	7·85	7·82
b	16·66	16·52
c	5·55	5·63

This means of course that the arrangement of O^{2-} ions is somewhat extended by the cations.

The plane (130) of the staurolite lattice is a closest-packed plane of oxygen ions. Perpendicular to this plane the identity period is six times the distance of the closest-packed O^{2-} planes. This indicates that two kinds of cation distribution parallel to (130) i.e. α and β, are following alternately (Figs. 1 and 2).

Since the cations are not equally distributed between α and β in a proportion 1:1 (although this would be possible from a chemical point of view), we may suppose that the divalent and tetravalent cations lie in one (α) layer and the monovalent ones in the other (β) layer, whereas the trivalent cations are so distributed that an equal number of cations is to be found in (α) and (β). Therefore 4 Fe^{2+} + 8 Si^{4+} + 2 Al^{3+} (16 cations with 52 valencies) should lie in (α) and 14 Al^{3+} + 2 H^+ (16 cations with 44 valencies) in (β). This is in fact the cation distribution of the type $S0_4$ plus 2 Al^{3+} ions minus 2 H^+ ions.

With the restriction of the given α and β cationic

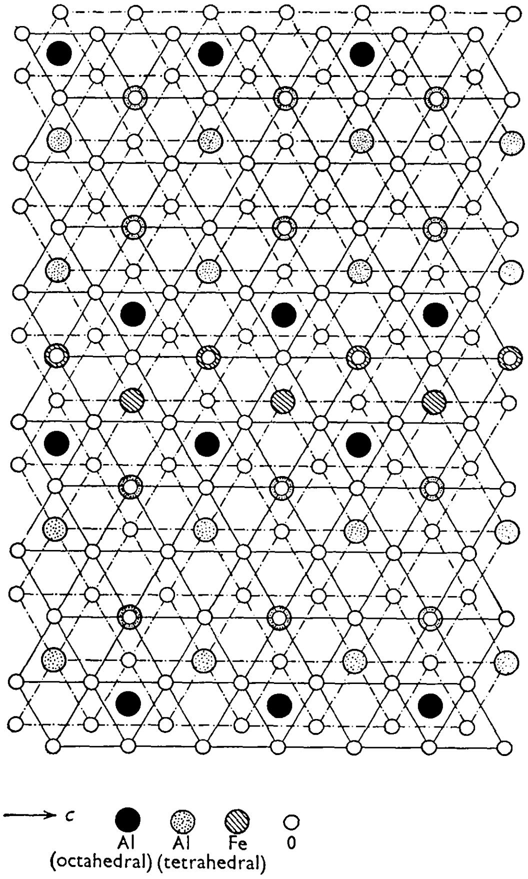

Fig. 1. A layer of the staurolite structure parallel to (130).

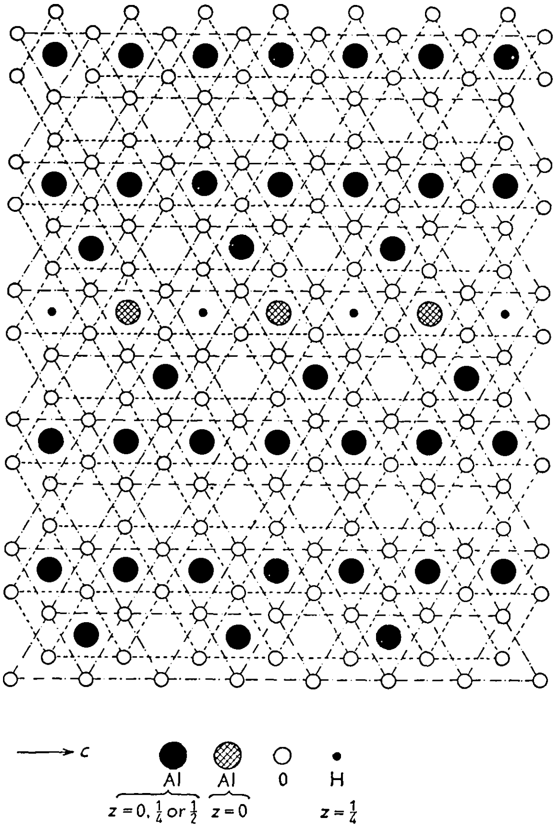

Fig. 2. Another layer of the staurolite structure parallel to (130)—to be placed above and beneath the layer shown in Fig. 1.

Table 1. *Atomic coordinates*

Group of atoms	Position	(0, 0, 0; ½, ½, 0)+	*x*	*y*	*z*
4 Fe	(*i*)	(*x*, 0, *z*)	0·389	0	0·250
8 Si	(*j*)	(*x*, *y*, *z*)	0·125	0·167	0·270
4 Al_I	(*g*)	(0, *y*, 0)	0	0·322	0
4 $Al_{I'}$	(*h*)	(0, *y*, ½)	0	0·322	0·500
8 Al_{II}	(*j*)	(*x*, *y*, *z*)	0·250	0·408	0·250
2 Al_{III}	(*a*)	(0, 0, 0)	0	0	0
4 O_I	(*i*)	(*x*, 0, *z*)	0·222	0	0·980
4 $O_{I'}$	(*i*)	(*x*, 0, *z*)	0·222	0	0·520
8 O_{II}	(*j*)	(*x*, *y*, *z*)	0·237	0·158	0·020
8 $O_{II'}$	(*j*)	(*x*, *y*, *z*)	0·763	0·158	0·520
8 O_{III}	(*j*)	(*x*, *y*, *z*)	0	0·094	0·270
8 O_{IV}	(*j*)	(*x*, *y*, *z*)	0	0·250	0·230
8 O_V	(*j*)	(*x*, *y*, *z*)	0	0·394	0·230
2 H	(*c*)	(0, 0, ½)	0	0	0·500

distribution we can place the two surplus Al^{3+} ions in 0, 0, 0 or ½, 0, 0; both are unoccupied centres of oxygen octahedra. Calculation shows that the intensities are better satisfied with the first position. Several other cation distributions have been calculated with Fe^{2+} ions in octahedral coordination, but all of them were discarded because of the discrepancies between measured and calculated intensities. The *y*-coordinate of an 8-fold group of O^{-2} ions and at the same time the *y*-coordinate of eight Al ions in the original type has been somewhat modified for producing a more reasonable Fe–O distance than in the original type. With $y_{O_V} = 0·394$ and $y_{Al_I} = 0·322$ we get Fe–O = 1·95 Å as against 1·78 Å in the original type, and Al–O = 1·85 Å as against 1·89 Å, which is still acceptable. A similar small modification of the coordinates of the silicon ions and of 4 oxygen ions also improved the agreement between measured and calculated *F* values. The new coordinates of atoms are given in Table 1. The agreement between calculated and measured intensities is better than in the original work (see Tables 2 and 3). The two H^+ ions of the cell have been placed in the centers of oxygen octahedra (Fig. 2) much in the same way as they are located in diaspore. The electrostatic valency principle of Pauling is satisfied for every ion in the cell. The new arrangement is shown in Fig. 3.

Table 2. *Measured F values* (*Náray-Szabó*, 1929) *and calculated F values* (*this work*) *of staurolite reflexions* (Rh *Kα*)

F-values smaller than about 20 could not be measured

hkl	$F_{meas.}$	$F_{calc.}$	*hkl*	$F_{meas.}$	$F_{calc.}$
020	28	+43	001	0*	+18
040	68	−58	002	146	−131
060	154	+187	003	0	+4
080	76	+70	004	355	+378
0,10,0	74	+92	005	0	+15
0,12,0	305	+314	006	54	−67
0,14,0	71	−47	007	0	+9
0,16,0	28	−6	008	117	+156
0,18,0	90	+111	009	0	+12
0,20,0	31	+74	0,0,10	48	−30
0,22,0	39	+68	0,0,11	0	−5
0,24,0	105	+94	0,0,12	49	+71
200	small	+39	110	31	−36
400	217	+222	220	79	−74
600	small	+4	330	154	+182
800	186	+256	440	89	−105
10,0,0	25	+61	550	22	+26
12,0,0	small	+56	660	25	−28
14,0,0	0	+10			

* Estimated intensity on Hurst's X-ray photograph: very weak.

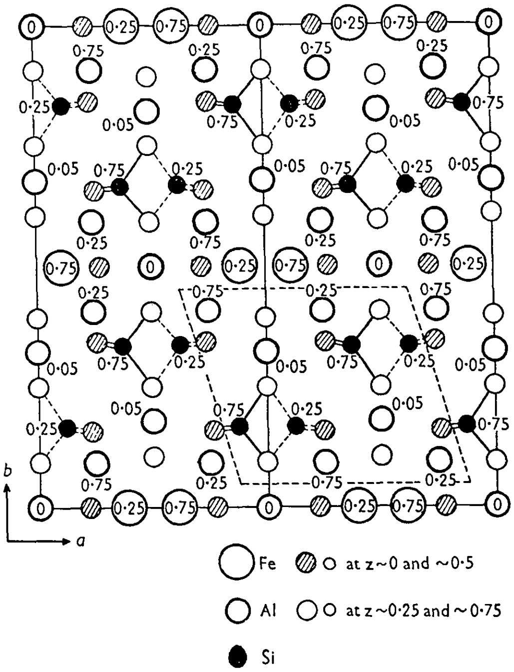

Fig. 3. Two cells of staurolite, parallel to (001). The kyanite cell inside of the staurolite structure is shown by dotted lines.

We would like to thank Dr V. J. Hurst for sending us a precession X-ray photograph of staurolite.

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Table 3. *Estimated intensities and calculated F values of staurolite reflexions*

hkl	Int.$_{\text{est.}}$ (Hurst's film)	$F_{\text{calc.}}$	*hkl*	Int.$_{\text{est.}}$ (this work)	$F_{\text{calc.}}$	*hkl*	Int.$_{\text{est.}}$ (this (work	$F_{\text{calc.}}$
021	½	+15	201	2–3	+29	132	12	+184
041	½	+29	202	8	−72	152	0	+16
061	½	+ 5	203	2	+10	172	3	+68
081	½	+28	204	2	−15	192	8	+148
0,10,1	½	+16				1,11,2	1	−28
			401	2	+39			
022	4	−67	402	9	+126	133	2	+29
042	1–2	+22	403	½	−37	153	10	+126
062	15	+201	404	7	+94	173	6	+101
082	3	−85						
0,10,2	4	−94	601	1	+25	221	10	+145
0,12,2	3	−81	602	3	+23	241	7	+134
0,14,2	1	+25	603	½	+ 1	261	0	+13
0,16,2	2	+45	604	3	+30	281	5	+115
0,18,2	1	− 6						
0,20,2	3	−65	130	½	−13	242	2	−30
0,22,2	1	−21	150	3	−60	262	0	+13
			170	2	−22	282	7	−124
023	½	+17	190	½	−41			
043	½	+ 6	1,11,0	2	−46	243	6	−72
			1,13,0	2	+41	244	3	+56
024	½	+23						
044	2	−34	240	3	+27	311	9	−134
064	6	+132	260	5	−64	331	1	− 1
084	0	+32	280	½	+ 3	351	1	+ 6
0,10,4	3	+89	2,10,0	1	+29	371	1	−11
0,12,4	15	+235				391	4	−33
0,14,4	1	−32	310	2–3	−34	3,11,1	6	−111
0,16,4	½	− 2	350	3–4	−49			
0,18,4	4	+93	370	1–2	−20	313	8	+139
0,20,4	2–3	+68	390	10	+118	332	½	−19
						333	2	+32
026	1	−29	420	1–2	−39	334	10	+147
046	½	+10	460	6	−100	352	3–4	−50
066	3	+65	480	1	− 6			
086	2	−54	4,10,0	3–4	+70	422	1	−15
0,10,6	2	−56				442	3–4	+63
0,12,6	3	−54	510	2	+55	462	15	+356
0,14,6	0	− 7	530	10	+171			
0,16,6	2	+20	590	10	+136	441	1	+31
						443	½	− 6
			620	4	−73			
						511	8	+108
			111	1	−50	513	5	−64
			131	2	+38	531	1–2	−28
			151	9	−115	551	½	+11
			171	7	−96	5,11,1	7	+94
			191	3	+63	533	5	+68
			1,11,1	½	+17	553	½	+ 4

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