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THE CRYSTAL STRUCTRUE OF ANAPAITE

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The structure of anapaite $Ca_2Fe(PO_4)_2 \cdot 4H_2O$ has been completely determined from ordinary and modulated projections of the Patterson function onto the xy plane. The structure is basically composed of layers of oxygenous Fe octahedra and Ca heptavertica which are parallel to (010) and joined by PO_4 tetrahedra.

Anapaite $Ca_2Fe(PO_4)_2 \cdot 4H_2O$ was first found by S. P. Popoff in 1899 in the Zhelezny Rog deposit near Anapa on the Tamansk peninsula and was described by him under the name of tamanite [1]. According to [1] the pale green anapaite crystallites belong to the triclinic holohedry and are characterized by the following parameters: $a:b:c = 0.7069:1:0.8778$, $\alpha = 97°12'$, $\beta = 95°17'$, $\gamma = 70°11'$; cleavage planes coinciding with (101) and (010) are reported in this work.

Almost simultaneously the same mineral, except for the name anapaite, was described by Sachs [2] who proposed a different setting: $a:b:c = 0.8757:1:0.5975$, $\alpha = 132°22'$, $\beta = 106°47'$, $\gamma = 83°28'$.

In 1933, Palache [3] made a more detailed study of anapaite; his setting differs from the two preceding ones: $a:b:c = 0.8575:1:0.9401$, $\alpha = 108°56'40''$, $\beta = 104°05'40''$, $\gamma = 78°25'24''$. The transformation from Popoff's setting to that of Palache is described by the matrix $101/020/\bar{1}01$, and from Sach's to Palache's by the matrix $112/1\bar{1}0/00\bar{2}$.

Wolfe [4] was the first to study anapaite by x-ray diffraction. In Palache's setting he interchanged *a* and *c*, so as to make the *c* axis shorter than *a* and *b*. This transformation can be represented by the matrix $00\bar{1}/010/\bar{1}00$. In the new setting, the best cleavage is on (001), whereas the worst coincides with (010) [3]. Wolfe obtained from oscillation patterns and unfoldings of the layer lines, as well as from goniometric measurements, the cell parameters given in many well-known handbooks: $a = 6.41$ A, $b = 6.88$ A, $c = 5.86$ A ($a:b:c = 0.9317:1:0.8512$), $\alpha = 101°34'30''$, $\beta = 104°05'30''$, $\gamma = 71°03'30''$. In 1948, an attempt was made to determine the anapaite crystal structure [5] which turned out to be unsuccessful, since there is a considerable disparity between the calculated and the experimental intensity values, and the results of this work were not included in the International Handbook "Structure Reports" [6], in which there is only a reference to [5].

The objects of our study were samples from the Zheleznyi Rog deposits made available to N. A. Kruglova through the courtesy of the Mineralogical Museum of the Academy of Sciences of the USSR. Oscillation patterns were obtained from them around the *a*, *b*, and *c* axes with Mo radiation, and also unfolding of the zero layer oscillation lines around *b* and *c* and of the first oscillation layer line around *c*. Later, the unfolding of the zero oscillation line around *a* became essential. The cell parameters of anapaite were obtained from the x-ray patterns: $a = 6.39$ A, $b = 6.86$ A, $c = 5.89$ A, $\alpha = 101°$, $\beta = 104°$, $\gamma = 71°$, and turned out to be in good agreement with the data of [4]. With a specific gravity of $\delta = 2.812$ g/cm^3, a cell with such dimensions contains one formula unit $Ca_2Fe(PO_4)_2 \cdot 4H_2O$. The reflection intensities of each unfolding were evaluated visually with the aid of a blackening scale made from several photographs with different exposures.

That there is a center of symmetry in anapaite was determined on the basis of goniometric data, as indicated above in article [1]. We checked this assertion by Wilson's method [7] which states that for a crystal without a center of symmetry the ratio of the mean-square-value of the structure factor to the mean intensity square $(\overline{F})^2/\overline{F^2}$ is $0.785 = \pi/4$, but for one with a center of symmetry it is $0.637 = 2/\pi$. For the anapaite hk0 reflections without taking the zero F_{hk0} into account, the value of $(\overline{F}_{hk0})^2/\overline{F^2_{hk0}} = 0.652$, but allowing for the zero F_{hk0}'s it is 0.474. For the zone of reflections hk1 discounting the zero F_{hk1}'s the magnitude $(\overline{F}_{hk1})^2/\overline{F^2_{hk1}} = 0.674$, but including the zero ones it is 0.530. These results proved the presence of a center of symmetry in the structure, and the anapaite space group is taken to be $C_i^1 = P\bar{1}$.

To decipher the structure, ordinary and modulated Patterson projections were studied. From 180 nonzero hk0 reflections and 134 h0l reflections, we first constructed the interatomic vector diagrams P(x, y) and P(x, z); the rules of the arrangement of the peaks on these confirmed the centrosymmetricity of anapaite [8]. From the projection P(x, y) the arrangement of the heavier Ca atoms was determined (the single Fe atom could be only at the center of symmetry), and further, with the aid of the Fe and Ca, the arrangement of the lighter P and part of the O atoms was determined. However, it was very difficult to determine the z coordinates, since the majority of the peaks on the projection P(x, y) overlapped and merged into a large region of diffuse and unresolved maxima. This difficulty was overcome with the aid of modulated Patterson projections. In particular, from the 298 nonzero F_{hk1}'s were constructed

$$P_1^c(x, y) = \int_0^c P(x, y, z)\cos\frac{2\pi z}{c}\,dz = \frac{1}{A_c}\sum_{h=-\infty}^{\infty}\sum_{k=-\infty}^{\infty}|F_{hk1}|^2\cos 2\pi(hx+ky)$$

and

$$P_1^s(x, y) = \int_0^c P(x, y, z)\sin\frac{2\pi z}{c}\,dz = \frac{1}{A_c}\sum_{h=-\infty}^{\infty}\sum_{k=-\infty}^{\infty}|F_{hk1}|^2\sin 2\pi(hx+ky),$$

from which we succeeded in determining approximately the z coordinates of the majority of the atoms, and also to mark the (x, y) coordinates of the two O atoms which overlapped in the projection on xy.

TABLE 1

The Coordinates of the Basic Atoms in the Structure of Anapaite

Atoms	Number atoms in cell	x/a	y/b	z/c	Atoms	Number atoms in cell	x/a	y/b	z/c
Fe	1	0	0	0	O_{III}	2	0.324	0.878	0.978
Ca	2	0.341	0.210	0.710	O_{IV}	2	0.409	0.847	0.575
P	2	0.433	0.721	0.776	H_2O_I	2	0.101	0.216	0.309
O_I	2	0.319	0.370	0.116	H_2O_{II}	2	0.053	0.759	0.248
O_{II}	2	0.308	0.552	0.681					

Then the structure was refined by the usual method of recomputing the signs of the structure factors, alternating with the construction of electron density syntheses. The final projections of the electron density σ(x, y) and σ(x, z) are illustrated in Fig. 1 a and b. All the calculations were carried out on the rapid calculating machine "Strela" (Arrow). Inasmuch as because of overlapping in these projections not all the coordinates could be determined exactly, an additional projection σ(y, z) had to be constructed from the 127 F_{0kl}'s (Fig. 1 c). The basic atomic coordinates definitively accepted on the strength of these projections are assembled in Table 1. The values of F_{hk0} and F_{0kl} (allowing for an isotropic temperature factor) calculated from them are compared with the corresponding experimental data (Tables 2 and 3). The coefficient of divergence R_{hk0}

$$(R = \Sigma\,||F_e| - |F_t||\,/\,\Sigma\,|F_e|),$$

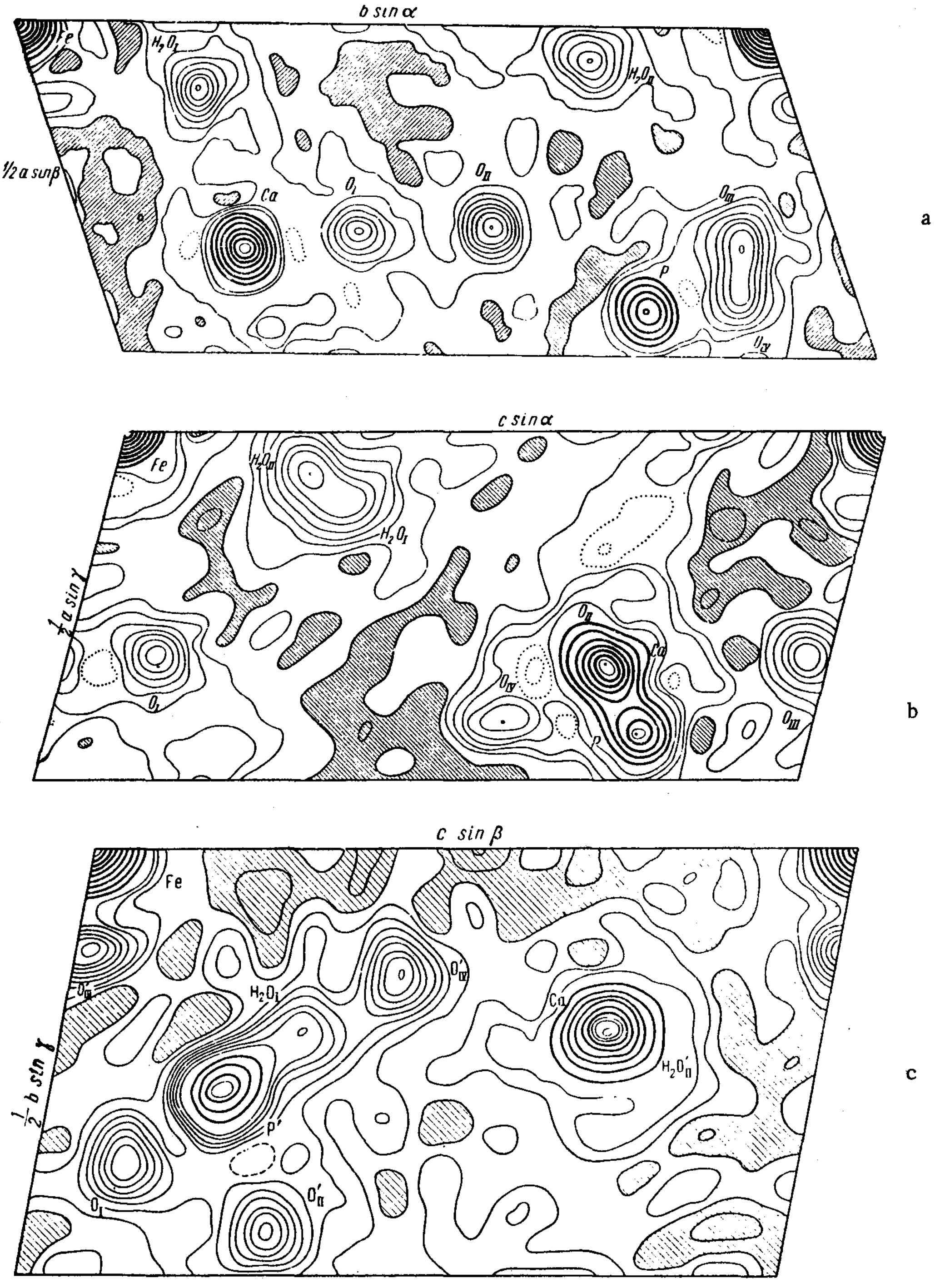

Fig. 1. Electron density projections. a) $\sigma(x, y)$; b) $\sigma(x, z)$; c) $\sigma(y, z)$. Fine contours are drawn through $3e/A^2$; heavy ones through $10e/A^2$. Primes mark the atoms connected by the basic center of symmetry. The regions of negative values are striated. The dotted contours correspond to hollows.

TABLE 2

The Experimental and Calculated Values of the Structure Factors F_{hk0}

(The Temperature Factor $\exp\left[-0.65\text{A}^2\left(\frac{\sin\vartheta}{\lambda}\right)^2\right]$ is Introduced into F_{calc}.)

k h	0	1	2	3	4	5	6	7	8	9	10	11	12	13
1			12.9 +12.4		< 5.8 + 2.7		6.6 — 5.4	7.4 + 7.4	9.7 +11.6					
9	20.2 +21.5	< 5.4 — 0.9	6.5 — 7.9		13.0 +14.1	5.8 + 6.6	7.8 + 9.9	< 5.7 — 1.3	< 5.8 + 0.9	8.5 + 8.2			6.1 — 6.8	
8	11.6 —10.6	27.9 +28.9	20.9 +21.7	7.6 — 6.7	7.8 — 8.7	16.9 +16.6	21.9 +22.6	< 5.4 + 2.5	6.1 — 5.5	< 6.0 + 3.8	7.9 + 9.2		6.8 + 5.4	
7	8.5 + 8.8	< 4.5 + 1.3	10.2 +10.7	21.4 +19.5	10.8 +10.6	< 4.6 — 0.9	5.9 — 4.5	22.6 +21.4	7.9 + 9.0	< 5.5 — 4.4	< 5.9 + 3.9	8.1 + 9.6	6.7 + 6.3	
6	14.7 +15.6	5.5 + 6.6	18.1 +16.6	< 3.9 + 1.5	< 4.0 + 2.9	19.4 +20.0	18.0 +18.3	12.9 —11.7	< 5.1 + 1.7	22.2 +23.8	9.9 +12.6	< 6.0 — 1.0	8.1 — 7.7	
5	< 3.5 + 0.4	54.6 +50.5	8.1 + 9.9	8.2 — 9.5	6.1 + 6.1	9.6 +10.9	24.2 +24.4	18.7 +18.1	< 5.4 + 5.6	11.8 —10.6	< 5.5 + 2.4	13.8 +12.2	8.1 +11.0	
4	12.2 —12.0	22.7 —21.3	38.4 +35.4	63.2 +52.6	9.4 + 9.3	< 3.6 + 0.2	< 3.9 — 2.8	17.4 +16.8	4.8 + 6.3	10.3 + 8.2	6.3 + 8.1	< 5.8 — 0.5	7.6 + 8.6	8.7 + 9.8
3	66.0 +64.7	44.2 +37.9	< 2.8 + 0.2	19.0 —18.6	28.2 +26.2	34.3 +32.0	5.7 — 4.8	7.6 —10.6	23.2 +24.8	23.0 +26.7	< 5.4 — 0.4	< 5.5 — 0.1	< 5.7 — 2.3	< 6.0 + 3.8
2	18.7 +16.1	27.9 +23.1	12.0 — 9.7	14.6 +14.8	19.8 +19.5	< 3.4 + 1.6	41.0 +39.9	19.4 +21.3	7.2 — 5.6	8.7 — 7.5	10.2 + 9.2	10.1 + 9.8	< 5.5 + 8.3	< 5.8 + 3.6
1	—23.9	+10.9	44.6 +37.1	54.6 +42.4	36.4 +33.3	21.4 +21.9	25.7 —25.6	< 4.1 — 1.8	25.4 +24.1	18.8 +19.9	< 5.2 — 0.9	7.1 — 7.4	12.4 +12.9	7.5 + 8.8
0	+200	+26.9	44.4 —45.3	13.4 —11.2	30.4 +31.9	32.3 +25.1	< 3.8 + 1.4	7.6 + 6.3	8.1 + 9.6	10.4 +11.4	11.1 +10.0	10.4 + 7.4	8.7 — 7.5	< 6.1 + 4.2
$\bar{1}$	—23.9	28.9 +33.4	31.1 +29.9	< 3.3 + 1.4	5.3 + 4.2	16.5 +15.6	40.4 +38.4	< 4.4 + 2.1	< 4.9 — 4.3	< 5.3 + 4.5	6.3 + 5.5	6.8 + 6.0	8.1 + 7.4	
$\bar{2}$	18.7 +16.1	30.3 +27.4	3.8 + 4.0	29.4 +32.3	39.1 +37.2	< 3.7 + 0.7	20.6 —20.8	16.5 +16.0	21.9 +22.1	< 5.6 + 2.0	< 5.8 — 0.6	< 6.0 + 2.0	7.6 + 8.5	

TABLE 2 (Continued)

$\bar{3}$	66.0 +64.7	<2.7 −1.7	7.3 + 6.8	< 3.5 + 0.3	< 3.7 − 1.6	23.7 +23.6	18.0 +17.4	< 5.6 + 0.6	9.7 + 6.3	12.8 +10.8	10.8 +12.0	6.1 + 4.6	< 6.2 − 3.7
$\bar{4}$	12.2 −12.0	29.1 +33.5	23.8 +27.0	< 3.9 + 2.2	5.8 + 5.8	< 4.4 + 0.6	11.0 +14.8	11.0 +12.9	9.8 + 9.2	< 6.1 − 3.6	< 6.2 − 4.5	10.6 +10.0	8.4 + 6.6
$\bar{5}$	< 3.5 + 0.4	14.0 −16.3	6.8 + 7.7	33.3 +37.9	13.3 +13.6	8.0 − 9.6	< 5.2 − 1.3	12.5 +15.1	5.9 + 7.3	< 6.1 − 2.0	< 6.2 + 3.4	< 6.3 + 0.7	
$\bar{6}$	14.7 +15.6	13.2 +14.5	12.9 +11.3	< 5.2 − 1.5	< 5.4 + 4.1	19.6 +20.2	< 5.6 + 0.9	< 5.8 − 3.4	< 5.9 + 4.0	7.6 + 7.7	< 6.3 + 4.0	< 6.4 + 3.7	
$\bar{7}$	8.5 + 8.8	< 4.6 + 0.6	8.4 +10.7	13.4 +12.7	< 5.5 + 2.2	9.8 − 9.8	11.0 +14.0	15.3 +16.3	< 6.0 + 0.5	< 6.1 − 0.6	< 6.4 − 0.3	6.8 + 7.0	
$\bar{8}$	11.6 −10.6	5.2 − 5.9	9.1 + 8.7	13.6 +13.1	9.1 + 5.1	< 6.1 + 2.8	< 6.2 + 0.9	< 6.2 − 1.1	6.3 + 4.2	6.7 + 4.4			
$\bar{9}$	20.2 +21.5	10.5 +13.0	< 6.2 − 1.2		6.1 − 6.9	7.5 + 9.0	< 6.4 − 2.2						
$\overline{10}$			8.5 +10.8				9.6 +12.1						

TABLE 3

The Experimental and Calculated Values of the Structure F_{0kl}

(The Temperature Factor $\exp\left[-0.5\ A^2\left(\frac{\sin\vartheta}{\lambda}\right)^2\right]$) is Introduced into F_{calc}.)

k \ l	0	1	2	3	4	5	6	7	8	9	10
10	11.1 +10.2	17.6 +17.9									
9	10.8 +12.2	8.7 — 7.2	< 9 + 6.2	17.4 +18.1							
8	9.6 + 9.4	< 7.9 — 1.6	16.7 +15.1	13.6 +13.5	9.0 +10.1						
7	7.0 + 5.8	13.8 +12.4	17.9 +21.2	< 9.5 — 2.1	13.4 +13.2	25.3 +25.7	11.5 +11.6				
6	< 5.8 + 1.5	35.7 +33.3	11.9 +14.8	12.3 —10.4	< 8.6 + 4.7	18.5 +20.2	< 9.0 + 2.3	11.6 +12.1			
5	24.7 +25.3	< 5.9 + 2.7	< 6.1 + 1.6	31.3 +33.3	< 7.2 + 3.2	11.0 — 9.7	< 8.3 + 3.3	15.5 +16.1			
4	30.9 +32.4	17.6 —12.4	31.0 —32.4	36.5 +36.4	25.4 +26.1	7.2 — 6.1	< 7.9 + 6.3	< 8.5 + 2.1			
3	12.0 —11.4	17.1 +16.5	27.7 +27.6	15.4 —13.6	9.6 —13.0	20.8 +20.1	14.7 +15.3	10.1 — 9.2	< 8.8 + 0.3	11.8 +10.9	
2	51.5 —45.5	61.0 +51.8	75.5 +71.0	9.5 — 7.5	< 5.6 — 3.2	11.7 +12.6	11.4 +12.0	< 7.9 — 2.8	< 8.3 + 3.4	< 9.6 + 7.2	
1	+26.9	11.4 +12.4	25.0 +18.6	4.9 + 3.8	36.0 +39.2	11.4 +15.7	7.6 — 8.8	19.3 +14.0	14.1 +17.3	< 9.6 + 0.9	
0	+200	+19.9	37.2 —34.5	40.0 +42.0	37.9 +40.7	< 5.7 — 0.8	< 6.7 + 1.2	16.9 +18.8	< 6.8 + 2.4	11.0 +11.4	11.9 +12.3
$\bar{1}$	+26.9	30.1 +27.0	47.0 +43.7	42.8 +42.1	6.2 + 4.1	17.8 +16.0	23.2 +26.0	10.5 +14.4	8.1 — 7.8	< 8.8 + 2.5	15.2 +19.2
$\bar{2}$	51.5 —45.5	< 3.6 + 0.8	58.3 + 5.5	29.1 +26.7	23.2 —20.9	17.2 +19.3	26.0 +29.5	9.3 + 8.3	< 8.0 + 4.5	< 8.8 + 8.7	
$\bar{3}$	12.0 —11.4	57.0 +50.0	12.1 +11.6	7.9 —10.2	23.0 +24.2	18.9 +22.0	9.6 —11.3	< 8.8 — 4.3	21.8 +27.8	< 8.9 + 1.8	
$\bar{4}$	30.9 +32.4	23.1 +20.7	19.9 —18.6	< 5.4 — 2.7	27.5 +31.2	13.8 +14.6	< 7.1 + 2.4	< 7.8 — 5.7	< 8.4 + 6.6	< 9.1 + 4.3	
$\bar{5}$	24.7 +25.3	< 5.6 + 1.2	< 5.8 — 2.4	14.1 +15.3	6.4 + 6.3	16.4 —18.9	13.1 +16.5	< 8.0 + 1.2	< 8.6 — 4.7	< 9.4 — 3.6	
$\bar{6}$	< 5.8 + 1.5	21.4 —17.5	29.0 +32.0	26.6 +27.4	< 7.0 — 2.5	7.5 — 5.1	< 7.9 — 4.5	< 8.3 + 1.4	< 8.9 — 4.2	10.1 + 6.2	
$\bar{7}$	7.0 + 5.8	10.0 +10.2	11.4 +11.4	< 7.3 — 2.9	7.6 + 8.8	27.2 +26.6	< 8.6 + 4.5	< 8.9 — 5.1	< 9.5 + 1.3	12.0 +12.2	
$\bar{8}$	9.6 + 9.4	31.4 +30.5	11.2 +11.0	10.0 —10.4	< 8.3 + 2.5	23.7 +24.5	< 8.9 + 5.1	< 9.4 — 3.3	14.4 +13.4		
$\bar{9}$	10.8 +12.2	8.7 +10.2	< 8.8 + 1.3	19.7 +22.7	12.7 +12.7	< 9 —8	< 9.5 + 4.6	14.4 +15.1			
$\overline{10}$	11.1 +10.2			15.0 +17.1	9.6 +11.6		< 9.7 + 2.7	9.9 +12.9			
$\overline{11}$							9.9 +10.4				

taken from all the nonzero experimental F_{hk0} is equal to 10.2%, but when allowing for the zero F_{hk0} it is 15.8% for $\sin\vartheta/\lambda \leq 0.8$; R_{0kl}, calculated from all the 127 nonzero F_{0kl}, is equal, respectively, to 10.35% and to 17.8% when allowing for the zero ones for $\sin\vartheta/\lambda \leq 0.8$.

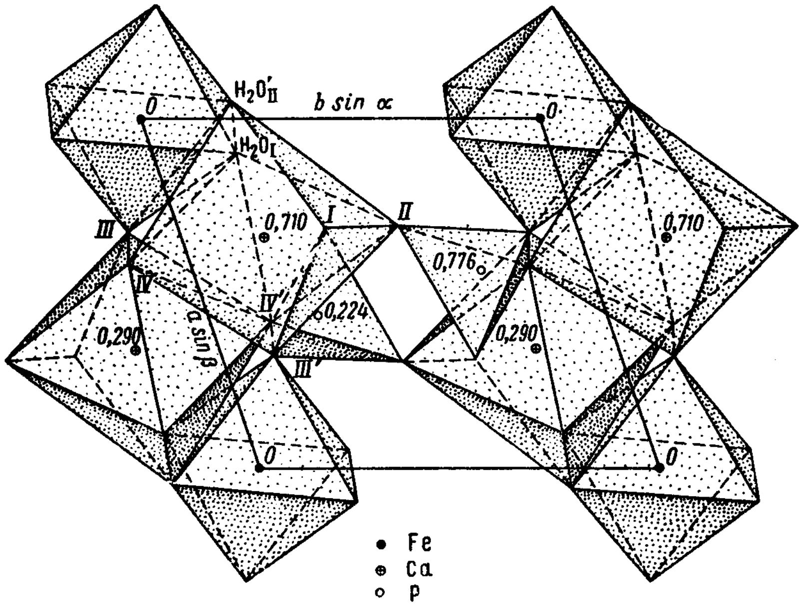

Fig. 2. The polyhedral structure of anapaite. Projection in the direction of the c axis. Roman numerals indicate the oxygen atoms. Primes stand for atoms connected by the basic symmetry center. The numbers correspond to the z/c values for cations.

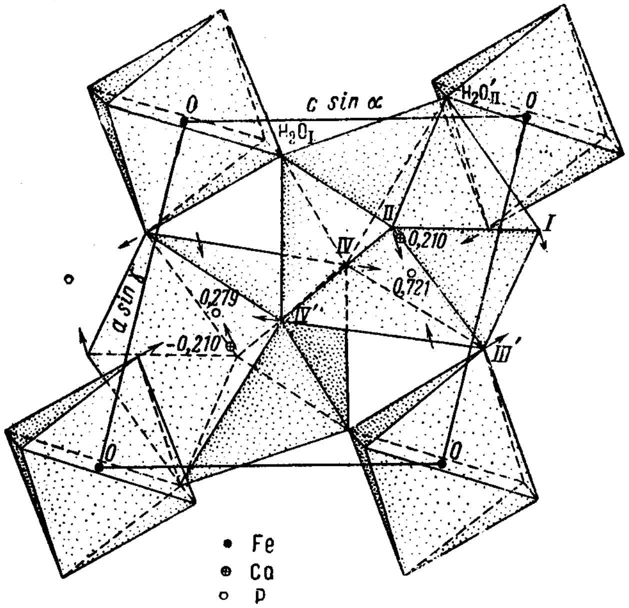

Fig. 3. Layer of Fe – Ca – polyhedra in the structure of anapaite. Projection along b. The O – P bonds connecting two adjacent polyhedral layers are indicated by arrows; arrows abutting the vertices indicate the bonds between O and P, in the illustrated layer, arrows that do not abut the vertices indicate bonds between the overlying O and P layer.

The characteristic architectural features of the anapaite structure are the layers of Fe and Ca polyhedra parallel to (010) which are quite apparent in Figs. 2 and 3. The Fe atoms occupy the centers of oxygen octahedra distributed in the (010) plane, from which the Ca atoms emerge from both sides. The latter form around themselves a complex oxygen heptaverticon similar to the one recently described for the Zr cations in baddeleyite, zirconium oxide [9]. In each layer,two adjacent Ca heptavertica have the same $O_{IV}-O'_{IV}$ edge and are surrounded by four Fe octahedra; in addition, each Ca heptaverticon is bound to three Fe octahedra by the same vertices. Separate layers are connected by PO_4 tetrahedra.

TABLE 4

Interatomic Distances in the Structure of Anapaite*

P tetrahedron		Fe octahedron		Ca polyhedron			
$\mathrm{P-O'_{I}}$	1.53 A	$\mathrm{Fe-O_{III}}$	2.00 A	$\mathrm{Ca-O_{I}}$	2.43 A	$\mathrm{O_{II}-O'_{IV}}$	3.08 A
$\mathrm{P-O_{II}}$	1.56 A	$\mathrm{Fe-H_2O_{I}}$	2.21 A	$\mathrm{Ca-O_{II}}$	2.33 A	$\mathrm{O'_{III}-O_{IV}}$	3.36 A
$\mathrm{P-O_{III}}$	1.56 A	$\mathrm{Fe-H_2O_{II}}$	2.31 A	$\mathrm{Ca-O'_{III}}$	2.45 A	$\mathrm{O'_{III}-O'_{IV}}$	3.45 A
$\mathrm{P-O_{IV}}$	1.55 A	$\mathrm{O_{III}-H_2O_{I}}$	2.93 A	$\mathrm{Ca-O_{IV}}$	2.40 A	$\mathrm{O_{IV}-O'_{IV}}$	3.07 A
$\mathrm{O'_{I}-O_{II}}$	2,57 A	$\mathrm{O_{III}-H_2O_{II}}$	2.99 A	$\mathrm{Ca-O'_{IV}}$	2.48 A	$\mathrm{O_{I}-H_2O'_{II}}$	3.02 A
$\mathrm{O'_{I}-O_{III}}$	2,48 A	$\mathrm{O_{III}-H_2O'_{I}}$	3.02 A	$\mathrm{Ca-H_2O_{I}}$	2.48 A	$\mathrm{O_{II}-H_2O_{I}}$	3.23 A
$\mathrm{O'_{I}-O_{IV}}$	2.52 A	$\mathrm{O_{III}-H_2O'_{II}}$	3.11 A	$\mathrm{Ca-H_2O'_{II}}$	2.54 A	$\mathrm{O_{II}-H_2O'_{II}}$	3.76 A
$\mathrm{O_{II}-O_{III}}$	2,56 A	$\mathrm{H_2O_{I}-H_2O_{II}}$	3.20 A	$\mathrm{O_{I}-O_{II}}$	3.04 A	$\mathrm{O_{IV}-H_2O_{I}}$	3.10 A
$\mathrm{O_{II}-O_{IV}}$	2,54 A	$\mathrm{H_2O_{I}-H_2O'_{II}}$	3.25 A	$\mathrm{O_{I}-O'_{III}}$	2.48 A	$\mathrm{O_{IV}-H_2O'_{II}}$	3.51 A
$\mathrm{O_{III}-O_{IV}}$	2.50 A			$\mathrm{O_{II}-O'_{III}}$	3.72 A	$\mathrm{O'_{IV}-H_2O_{I}}$	2.96 A
						$\mathrm{H_2O_{I}-H_2O'_{II}}$	2.95 A

* Primes indicate atoms connected by the basic symmetry center.

Table 4 gives a complete list of the most important interatomic distances in the structure of anapaite. The P – O distances are all within the narrow range 1.53-1.56 A, the Fe – O = 2.00 A is considerably smaller than the $Fe-H_2O$ (2.21 - 2.31 A), a fact which we shall discuss in more detail below. The Ca – O distances are in a very narrow range 2.33-2.54 A for the "porous" Ca cation. The next in size is the Ca – O = 3.07 A distance which exceeds substantially the first seven distances, and,therefore,the heptaverticon must be considered as the coordination polyhedra of Ca.

TABLE 5

The Balance of Valences in the Structure of Anapaite

Anions	Cations			sum of valences
	P	Fe	Ca	
O_I	$^5/_4$		$^2/_7$	1.54
O_{II}	$^5/_4$		$^2/_7$	1.54
O_{III}	$^5/_4$	$^2/_6$	$^2/_7$	1.87
O_{IV}	$^5/_4$		$2\cdot{}^2/_7$	1.82
H_2O_I		$^2/_6$	$^2/_7$	0.62
H_2O_{II}		$^2/_6$	$^2/_7$	0.62

Table 5 gives the valence balance calculated according to Pauling's second rule. At first it does not seem to be quite satisfactory, inasmuch as the excess of positive valence for the H_2O particles is 31% of the charge on the O atom, and has a magnitude exceeding the generally accepted maximum (25%); while the sum of the positive valence which converges at O is clearly insufficient. As Table 4 indicates, to compensate for this the distances $Fe-H_2O$ and $Ca-H_2O$ increase noticeably in comparison with the Fe – O and Ca – O distances, so that the true balance of the valences can be considered satisfactory.

According to articles [1-4] there are cleavages in anapaite along the (001) and (010) planes, the better one along (001) and the poorer one along (010) [3]. Consulting Figs. 2 and 3 we see that a discontinuity plane (010) passes parallel to the layers of Fe and Ca polyhedra through the Ca heptavertica,and only two $Ca-O_{II}$ bonds are disturbed in the cell. The cleavage plane (001) also passes through the Ca heptavertica and destroys only two $Ca-O'_{IV}$ and $2Ca-H_2O$ bonds in the cell; these are very weak due to the large Ca – O distances and the small number of Ca^{2+} charges. The cleavage along (001) is better than that along (010) because the length of the $Ca-O'_{IV}$ bonds (2.48 A) is greater than that of the $Ca-O_{II}$ (2.33 A).

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