

Anion radical of mixed type (four $[S_4O_{12}]$ rings and P orthotetrahedra) in the structure of monoclinic fosinaite

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The authors determine the crystal structure of the monoclinic analog of fosinaite $Na_3CaPSiO_7$, discovered in Khibiny pegmatites (single-crystal diffractometer, λMo 2796 reflections, MLS in the anisotropic approximation to $R = 0.061$). The parameters of the single-crystal lattice are as follows: $a = 7.303(2)$, $b = 12.201(5)$, $c = 14.715(4)$ Å, $\beta = 91.93^\circ$, $Z = 8$, Fedorov group $P2/c$. The cationic part of the structure of monoclinic fosinaite is concentrated in geometrically similar sheets perpendicular to [100]. Chains of Ca polyhedra, constricted by pairs of Na polyhedra, are distinguished in the sheets at the $x \approx 0$ level; at the $x \approx 0.5$ level the sheets are composed of Na polyhedra. The cation framework is penetrated by the anion framework, in which there are combined tubular columns of four rings of two types: silicon–oxygen rings $[Si_4O_{12}]$ and mixed rings of P orthotetrahedra and Na polyhedra. The tetrahedral four-membered $[Si_4O_{12}]$ rings are adapted to the specific characteristics of the cation arrangements, accounting for the change in their proper symmetry.

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Following the recent discovery of the orthorhombic $Na_3Cr_2Si_2O_7$ TR silicophosphate fosinaite in alkali massifs of the Kola Peninsula,¹ it was found that Khibiny pegmatites contain a monoclinic analog of this mineral containing virtually no rare earths and corresponding in composition to the idealized formula $Na_3CaPSiO_7$.¹ According to this formula, the new silicophosphate belongs to the group of Ca minerals occupying a central position in the "Second Heading of Crystal Chemistry of Silicates."² Determination of the structure of monoclinic fosinaite, the anion part of which exhibits two types of tetrahedra, was especially interesting in the next stage of investigation of natural and synthetic minerals of the Ca, TR association.

By x-ray analysis (photographic method + recording on a single-crystal Syntex P1 diffractometer, λMo) we established the similarity of the unit-cell parameters of monoclinic Ca fosinaite and its rare earth precursor with differing symmetries (Table I). The ratio between the components in the formula of monoclinic fosinaite was determined on the basis of micro x-ray-spectral analysis.² In the unit cell with adjusted parameters contains eight $Na_3CaPSiO_7$ units.

The x-ray material (2796 nonzero $h\bar{k}0 - h\bar{k}22$ reflections) was recorded on a Syntex P1 automatic diffractom-

eter by the $(2\theta: \theta)$ method at a scanning rate of $6-24^\circ \cdot \text{min}^{-1}$ (Mo radiation, graphite monochromator). The zonal extinctions $h0l = 2n + 1$ permit two Fedorov groups – $P2/c$ and Pc . The principal structural arrangement was obtained in the $P2/c$ centrosymmetric group by the Multan program using the Syntex EXTL computing system. In the first stage of the calculations we selected 227 reflections with $|E| \geq 1.6$. Among this group, for 57 reflections we determined the signs with a probability exceeding 0.5. The 17 reflections with the most reliable signs (with a probability > 0.94), together with six other reflections selected automatically to fix the origin and the enantiomorphism, formed the reference group. Of the resulting seven alternative versions of reference group reflections with different signs, we selected one with minimal values of the "reliability indices"³: $\psi_0 = 0.201$ and $R = 25.51$.

The first electron density distribution (E synthesis) revealed the position of the heavier Ca, P, Si, and also part of the Na and O ($R_{h\bar{k}l} = 0.321$). The other Na and O atoms were located from a cycle of successive approximations using F and D syntheses. On the Fourier zero syntheses, obtained in the final stages of structural refinement, the seven distinct maxima around P_2 corresponded to the two possible mutually exclusive tetrahedra with a common vertex O_{11} . Refinement of the O atoms as-

TABLE I. Crystallographic Characteristics of Monoclinic Fosinaite and Fosinaite *

Mineral	System	Unit-cell parameters				Fedorov group	Z
		a, Å	b, Å	c, Å	β , deg		
Monoclinic fosinaite $Na_3CaPSiO_7$ Fosinaite $Na_3(Ca, Ce)SiPO_7$	Monoclinic	7.303(2)	12.201(5)	14.715(4)	91.93(3)	$P2/c$	8
	Orthorhombic	12.23	14.62	7.21		$P22_12$ or $P22_12_1$	6

* Data of Ref. 1.

TABLE II. Basis Atom Coordinates and Individual Isotropic and Anisotropic Temperature Corrections in the Structure of Monoclinic Fosnaita*

Atom	x/a	y/b	z/c	B _f
Ca ₁	0	0.5	0	0.49(4)
Ca ₂	0	0.1434(3)	0.75	1.46(5)
Ca ₃	0.0002(3)	0.1909(2)	0.5147(2)	1.22(3)
Si ₁	0.3005(4)	0.3157(3)	0.6391(2)	0.53(4)
Si ₂	0.2858(4)	0.3578(2)	0.8405(2)	0.47(4)
P ₁	0.2543(3)	0.3066(2)	0.1340(2)	0.62(4)
P ₂	0.2431(4)	0.0281(3)	0.3797(2)	0.87(4)
Na ₁	0	0.4822(6)	0.25	2.04(13)
Na ₂	0	0.1709(6)	0.25	2.56(14)
Na ₃	0.5	0.1251(8)	0.75	4.17(22)
Na ₄	0.5	0.1841(7)	0.25	3.18(17)
Na ₅	0.5	0.4545(6)	0.25	1.84(11)
Na ₆	0.5	0.5	0	0.72(8)
Na ₇	0.4841(7)	0.1760(5)	-0.0055(4)	2.70(10)
Na ₈	0.2552(5)	0.3378(3)	0.3907(3)	0.96(7)
Na ₉	0.2672(8)	0.0041(5)	0.1165(4)	3.49(13)
O ₁	0.2496(10)	0.1878(7)	0.6499(5)	1.36(12)
O ₂	0.2144(10)	0.3681(6)	0.5477(5)	1.63(13)
O ₃	0.4759(12)	0.3203(8)	0.8651(6)	2.92(18)
O ₄	0.2538(10)	0.3879(6)	0.7298(5)	1.47(13)
O ₅	0.2483(10)	0.4689(6)	0.8900(5)	1.38(12)
O ₆	0.1427(11)	0.2528(7)	0.8593(5)	2.19(16)
O ₇	0.2588(11)	0.1858(7)	0.1043(5)	2.08(14)
O ₈	0.2509(10)	0.3155(6)	0.2379(5)	1.82(13)
O ₉	0.0743(10)	0.3545(6)	0.0925(5)	1.27(12)
O ₁₀	0.4223(10)	0.3644(6)	0.0999(5)	1.21(12)
O ₁₁	0.2348(14)	0.1501(7)	0.4082(5)	1.87(14)
O ₁₂	0.0742(10)	0.0263(6)	0.9147(5)	3.87(8)
O ₁₃	0.2080(11)	0.0151(11)	0.2796(6)	3.83(11)
O ₁₄	0.4226(10)	0.0206(6)	0.9088(5)	3.69(17)
O ₁₅	0.3854(10)	0.0185(6)	0.3028(8)	0.87(5)
O ₁₆	0.2615(10)	0.0517(6)	0.9565(5)	3.19(18)
O ₁₇	0.0668(10)	0.0121(6)	0.3149(6)	3.06(17)

TABLE II (Continued)

Atom	B ₁₁	B ₂₂	B ₃₃	B ₁₂	B ₁₃	B ₂₃
Ca ₁	0.58(6)	0.67(6)	0.69(6)	--0.23(5)	0.07(5)	0.16(6)
Ca ₂	2.38(9)	0.59(7)	1.30(7)	0	1.33(7)	0
Ca ₃	1.04(5)	2.37(6)	0.71(5)	0.59(5)	--0.09(4)	0.21(5)
Si ₁	0.72(5)	0.78(6)	0.52(6)	--0.06(5)	--0.16(4)	0.03(5)
Si ₂	0.61(5)	0.89(6)	0.50(6)	0.06(5)	0.01(4)	0.03(5)
P ₁	0.72(5)	0.78(6)	0.52(6)	0.02(5)	--0.16(4)	0.13(5)
P ₂	0.68(6)	0.76(6)	0.67(7)	--0.06(5)	--0.09(5)	0.03(5)
Na ₁	1.72(19)	1.61(17)	2.71(20)	0	--0.05(15)	0
Na ₂	3.30(21)	1.22(17)	3.34(22)	0	0.56(17)	0
Na ₃	7.03(34)	0.93(18)	8.16(35)	0	-6.28(29)	0
Na ₄	5.95(30)	1.50(20)	3.52(24)	0	-2.53(22)	0
Na ₅	1.92(17)	0.90(15)	2.35(18)	0	-0.61(14)	0
Na ₆	0.88(13)	0.59(12)	0.54(12)	--0.20(11)	--0.32(10)	0.58(11)
Na ₇	2.38(14)	3.32(17)	2.30(13)	-0.79(13)	0.41(11)	-0.35(13)
Na ₈	1.37(10)	1.22(11)	0.82(9)	0.07(9)	0.04(8)	0.06(8)
Na ₉	4.08(19)	0.89(13)	6.34(21)	-0.07(13)	-0.40(16)	0.82(14)
O ₁	2.18(20)	0.61(16)	1.61(19)	-0.03(16)	0.18(16)	0.15(16)
O ₂	2.51(21)	1.70(21)	0.49(11)	1.01(17)	-0.28(15)	0.01(15)
O ₃	1.09(18)	7.20(40)	1.95(22)	1.25(24)	-0.03(16)	0.37(25)
O ₄	2.77(23)	1.07(19)	0.43(16)	0.35(17)	-0.15(15)	-0.07(14)
O ₅	3.09(23)	0.76(17)	1.26(18)	-0.08(16)	0.32(16)	-0.40(15)
O ₆	2.87(25)	1.50(21)	2.31(23)	-1.00(19)	1.02(19)	0.06(18)
O ₇	2.78(23)	0.45(18)	2.70(23)	0.06(16)	0.28(18)	-0.23(16)
O ₈	1.65(18)	2.78(23)	0.36(14)	-0.45(18)	-0.08(13)	0.21(16)
O ₉	0.79(15)	1.64(20)	1.64(19)	0.15(15)	-0.45(13)	0.45(16)
O ₁₀	0.80(16)	1.94(24)	1.48(18)	-0.26(15)	-0.09(14)	0.73(17)
O ₁₁	2.05(21)	1.42(21)	2.92(24)	-0.03(18)	0.31(18)	-1.20(19)
O ₁₂	2.50(33)	1.84(32)	11.22(62)	-0.28(27)	3.74(38)	-1.05(37)
O ₁₃	13.79(8)	2.80(46)	2.30(34)	-0.14(50)	0.87(43)	-0.49(33)
O ₁₄	2.36(34)	2.73(44)	10.65(64)	-0.46(32)	-2.74(38)	-0.56(43)
O ₁₅	2.52(75)	-0.33(51)	-0.19(47)	1.36(48)	1.60(49)	0.68(39)
O ₁₆	8.72(143)	4.04(97)	1.21(64)	-3.74(96)	3.04(80)	-3.60(20)
O ₁₇	1.29(79)	-1.62(77)	4.00(114)	0.16(86)	5.68(143)	0.78(105)

*Anisotropic thermal factors calculated from the equation $T = \exp[-1/4(B_{11}h^2a^{*2} + B_{22}k^2c^{*2} + B_{33}l^2c^{*2} + 2B_{12}hk a^* b^* + 2B_{13}hl a^* c^* + 2B_{23}kl b^* c^*)]$

signed in this position did not permit reliable section of one of the two versions of P tetrahedra, owing to the high thermal coefficients for the O₁₂₋₁₄ and O₁₅₋₁₇ atoms. (The assumption of ordered location of these two tetrahedra in the context of the acentric group P_c was not confirmed, for the same reason.) The optimal result (minimal R_{hkl}

factor with satisfactory thermal corrections) is attained by assuming statistical location of the O₁₂₋₁₄ and O₁₅₋₁₇ atoms in the structure. The number of P₂ tetrahedra formed by O₁₁, O₁₂, O₁₃, and O₁₄ is three times greater than the number of them with O₁₁, O₁₅, O₁₆, and O₁₇ in the vertices. The final value of the R_{hkl} factor with refine-

TABLE III. Structure of Monoclinic Fosinaite. Interatomic Distances, Å

Si_1-O_1	1.613(8)	Si_2-O_2	1.630(9)
O_2	1.599(8)	O_4	1.670(8)
O_3	1.637(9)	O_5	1.583(8)
O_4	1.647(8)	O_6	1.595(9)
Mean	1.624	Mean	1.620
O_4-O_2	2.673	O_3-O_4	2.600
O_1-O_3	2.591	O_3-O_5	2.647
O_1-O_4	2.714	O_3-O_6	2.568
O_3-O_3	2.628	O_4-O_5	2.575
O_2-O_4	2.698	O_4-O_6	2.670
O_3-O_4	2.653	O_5-O_6	2.730
P_1-O_7	1.535(9)	P_2-O_{11}	1.548(9)
O_8	1.533(8)	O_{12}	1.507(3)
O_9	1.546(7)	O_{13}	1.497(3)
O_{10}	1.519(7)	O_{14}	1.488(3)
Mean	1.533	Mean	1.510
O_7-O_8	2.518	$\text{O}_{11}-\text{O}_{12}$	2.455
O_7-O_9	2.463	$\text{O}_{11}-\text{O}_{13}$	2.512
O_7-O_{10}	2.491	$\text{O}_{11}-\text{O}_{14}$	2.494
O_8-O_9	2.507	$\text{O}_{12}-\text{O}_{13}$	2.302
O_8-O_{10}	2.495	$\text{O}_{12}-\text{O}_{14}$	2.550
O_9-O_{10}	2.548	$\text{O}_{13}-\text{O}_{14}$	2.461
Ca_1-O_2	2.337(7)	Ca_2-O_1	2.443(7)
O_2'	2.337(7)	O_1'	2.443(7)
O_5	2.341(7)	O_6	2.309(9)
O_5'	2.341(7)	O_6'	2.309(9)
O_9	2.291(7)	O_{12}	2.850(2)
O_9'	2.291(7)	O_{12}'	2.850(2)
Mean	2.323	O_{13}	2.488(3)
		O_{13}'	2.488(3)
		Mean	2.503
Na_1-O_4	2.624(9)	Na_2-O_7	2.903(8)
O_4'	2.624(9)	O_7'	2.903(8)
O_5	2.696(8)	O_8	2.554(9)
O_5'	2.696(8)	O_8'	2.554(9)
O_8	2.573(9)	O_{11}	2.855(8)
O_8'	2.573(9)	O_{11}'	2.855(8)
O_9	2.735(8)	O_{13}	2.464(6)
O_9'	2.735(8)	O_{13}'	2.464(6)
Mean	2.659	Mean	2.694
Na_4-O_7	2.735(8)	Na_3-O_4	2.640(9)
O_7'	2.735(8)	O_4'	2.640(9)
O_8	2.594(10)	O_8	2.488(9)
O_8'	2.594(10)	O_8'	2.488(9)
O_{13}	2.847(6)	O_{10}	2.513(7)
O_{13}'	2.847(6)	O_{10}'	2.513(7)
Mean	2.725	Mean	2.547
Na_7-O_4	2.931(9)	Na_8-O_2	2.368(8)
O_3	2.593(11)	O_5	2.373(9)
O_7	2.356(9)	O_8	2.263(8)
O_{10}	2.817(9)	O_9	2.436(8)
O_{11}	2.483(9)	O_{10}'	2.372(8)
O_{14}	2.313(5)	O_{11}	2.311(9)
O_{14}'	2.860(5)	Mean	2.354
Mean	2.622		

TABLE IV. Structure of Monoclinic Fosinaite. Local Balance of Valences on Anions

Atom	Ca_1	Ca_2	Ca_3	Si_1	Si_2	P_1	P_2	Na_1	Na_2	Na_3	Na_4	Na_5	Na_6	Na_7	Na_8	Na_9	Σ	
O_1		0.26	0.24	1.04						0.20					0.11		0.19	2.04
O_2	0.33		0.22	1.10										0.11		0.17		1.96
O_3				0.95	0.96										0.14			2.03
O_4				0.91	0.82			0.13										2.01
O_5	0.32				1.14				0.15									1.90
O_6		0.32	0.37		1.08													1.77
O_7				0.27			1.24		0.10			0.16			0.18		0.24	2.19
O_8							1.25		0.14	0.14		0.15	0.18			0.18		2.04
O_9	0.35		0.29			1.18		0.42								0.15		2.05
O_{10}						1.33								0.17	0.17	0.12	0.16	1.95
O_{11}							1.04		0.11						0.16	0.17		1.79
O_{12}		0.17	0.35					1.26									0.17	1.95
O_{13}		0.25						1.32		0.13	0.15	0.19				0.19	0.19	2.23
O_{14}								1.38		0.15					0.11	0.21	0.24	2.04

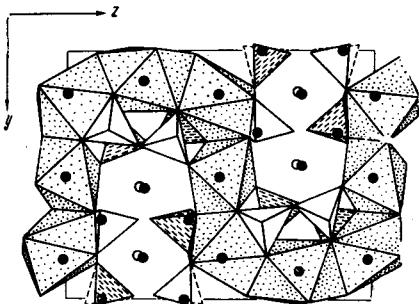


FIG. 1. Structure of monoclinic fosinaite in projection yz . In the interests of clarity, the Na atoms occupying the same points are moved somewhat apart (black and white circles).

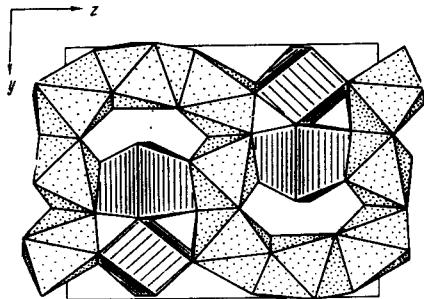


FIG. 2. Sheets of Ca and Na polyhedra at the level $x \approx 0$. The Ca polyhedra, denoted by point shading, form zigzag chains along [001]. The neighboring chains are linked to the sheet by two Na polyhedra.

ment by MLS in the isotropic approximation is 11.3%, and in the anisotropic approximation 6.1% (in neither case was a correction made for absorption, because μ was small — 15.5 cm^{-1}). Table II gives the final coordinates of the basis atoms and the individual isotropic and anisotropic temperature corrections. Taking account of the interatomic distances (Table III) we calculated the local balance of the valence states (Table IV); this confirmed the selected model. The balance quality criterion $D = 0.047$.

The principle of the internal structure of monoclinic fosinaite is clearly revealed in the yz projection (Fig. 1). The cation part of the structure is concentrated in geometrically similar sheets of two types, perpendicular to [100] (Figs. 2, 3). The sheets of the stage at the level $x \approx 0$ (Fig. 2) are formed by undulating chains of Ca polyhedra, constricted by pairs of Na polyhedra (Na_{1-2}). In the chains of Ca polyhedra are three independent Ca atoms, one of which is located in a slightly distorted octahedron, another in a low-symmetry seven-pointed polyhedron, and the third in an eight-pointed polyhedron. Both the Na polyhedra reinforcing the undulating chains have eight vertices: Na_1 has a cube, Na_2 has a prism with skewed tetragonal ends.

The sheets of the second stage at the level $x \approx 0.5$ (Fig. 3) are composed of five sorts (differing in shape) of the same Na polyhedra. The Na_{3-5} are located in somewhat distorted octahedra, the Na_{6-7} within low-symmetry seven-pointed polyhedra. The sheets of the neighboring stages are interconnected into an open three-dimensional framework which is penetrated by the anion framework. In the anion framework we distinguish tubular columns

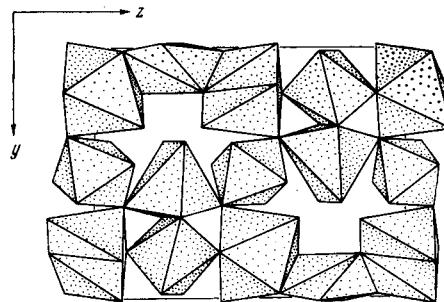


FIG. 3. Sheet of Na polyhedra distinguished in the cation framework at the level $x \approx 0.5$.

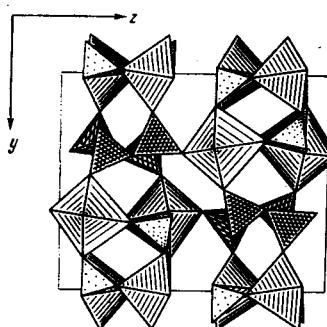


FIG. 4. Tubular columns of four rings, expressed in the anion framework of monoclinic fosinaite. The tetrahedra of silicon-oxygen rings are shaded by hatching, the P tetrahedra by dots.

elongated along the y axis and consisting of silicon and phosphorus tetrahedra, and also Na polyhedra with central cations at the levels $x \approx 0.25$ and 0.75 (Fig. 4). The columns consist of four rings of two different types. The silicon-oxygen rings Si_4O_{12} are overlain by mixed rings formed by P tetrahedra and Na polyhedra (Na_8 five-pointed polyhedra and Na_9 octahedra), similar to the four-fold centrosymmetric rings of alternate $[\text{SO}_4]$ tetrahedra and $\text{Mg}(\text{Fe})$ octahedra found in the hydrated Mg and Fe sulfates leonhardite and rosenite.⁴

Four metasilicate rings $[\text{Si}_4\text{O}_{12}]$ have been found in the structures of nine natural and synthetic minerals. Geometrically similar rings are also known in the structure of the silicate analogs — germanates and phosphates.

The adaptation of the $[\text{T}_4\text{O}_{12}]$ rings to the specific characteristics of the cation arrangements is the cause of the change in their proper symmetry. Completely asymmetric four-membered rings have been noted in joaquinite⁵ and synthetic $\text{Ca}(\text{NH}_4)_2[\text{P}_4\text{O}_{12}] \cdot 2\text{H}_2\text{O}$ (Ref. 6). Centrosymmetric rings are present in the structures of KHSiO_3 (Ref. 7), $\text{RbNd}[\text{P}_4\text{O}_{12}]$ (Ref. 8), and $\text{Na}_2\text{Pr}_6[\text{Ge}_4\text{O}_{12}][\text{Ge}_2\text{O}_7]_2$ (Ref. 9). The diorthogroups $[\text{Si}_2\text{O}_7]$ which form the rings of monoclinic fosinaite are related by the dyad rotation axis. Analogous rings, but of Ge tetrahedra, were recently found in the structure of synthetic $\text{Ca}_2\text{Ge}_2[\text{GeO}_4][\text{Ge}_4\text{O}_{12}]$ (Ref. 10). Tetranuclear rings of kainosite,¹¹ taramellite,¹² and labuntsovite¹³ are characterized by a longitudinal symmetry plane m , and verplankite¹⁴ and nenaevichite¹⁵ by an orthorhombic holohedron mmm . The most symmetrical

rings, with the axes of which the tetrad axes coincide, have been revealed in baotite,¹⁸ $\text{Ba}_5[\text{Si}_4\text{O}_{12}](\text{OH})_2$ (Ref. 17) and $\text{Al}(\text{PO}_3)_3$ (Ref. 18). Large Ca, Ba, TR, and K cations are present in all these compounds, and therefore the four-membered tetrahedral rings can be regarded as typical radicals of the "Second Heading of Crystal Chemistry." Only the smaller cyclic anions of P tetrahedra can be present in compounds with smaller cations [for example, $\text{Al}(\text{PO}_3)_3$.]³⁾

The combined anion arrangement (consisting of two types of tetrahedra — Si and P) brings monoclinic fosinaite close to lomonosovite²⁰ and innelite.²¹ However, in contrast with these minerals, this silicophosphate exhibits similar functions of the phosphate and silica tetrahedra (these tetrahedra are of four-membered rings). In lomonosovite and innelite the tetrahedra not only differ in the central cations but also play different roles. Both the latter structures are characterized by stacks consisting of cation cores with anion "chain mail" — titanium-silicon-oxygen lattices with $[\text{Si}_2\text{O}_7]$ diortho groups and Ti polyhedra. The space between the stacks contains $[\text{PO}_4]$ orthotetrahedra and Na cations (lomonosovite) or $[\text{SO}_4]$ orthotetrahedra and Ba cations (innelite).

¹⁾ The description of monoclinic fosinaite has been sent for corroboration to the Committee for New Minerals and Mineral Names, All-Union Mineralogical Society.

²⁾ The analysis was performed by Dr. H. Ronsbo (Denmark).

³⁾ At one time a profound impression was created by Pauling's determination of the latter on the basis of less than twenty reflections. In 1978, Smolin et al.¹⁹ determined with modern precision the structure of $\text{Sc}(\text{PO}_3)_3$, completely confirming the results of Pauling.

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