

Investigation of the Alkaline Earth Phosphates: Synthesis and Crystal Structure of a New Strontium Hydrogen Phosphate Form

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The hydrothermal synthesis, initial characterization (EDX analysis, IR, X-ray powder pattern), and X-ray single-crystal structure are reported for a new form of strontium hydrogen phosphate (γ -SrHPO₄). The cell is orthorhombic, space group *Pbca* (No. 61) with $a = 8.131(3)$ Å, $b = 9.258(5)$ Å, $c = 18.084(7)$ Å, $V = 1361.31(2)$ Å³, and $Z = 16$. The structure was determined from 1272 observed reflections to a final *R* value of 0.039. The atomic arrangement consists of two kinds of anionic layers (P(1) and P(2)) lying parallel to (001), formed by closed dimers and infinite chains of H-bonded HPO₄²⁻ groups, respectively. These sheets are linked to each other via Sr²⁺ cations. Comparison to the crystal structure of CaBa(HPO₄)₂ is also given, the two compounds exhibiting the same arrangement. © 2000 Academic Press

Key Words: hydrothermal synthesis; initial characterization; crystal structure; strontium hydrogen phosphate; hydrogen-bond scheme.

INTRODUCTION

The chemical literature dealing with strontium hydrogen phosphate (SrHPO₄) has been well known for a long time (1–5). Mooney *et al.* (5) mentioned the existence of two allotropic varieties: the low-temperature form (β -SrHPO₄) isomorphous with the orthorhombic BaHPO₄ and the high-temperature form (α -SrHPO₄) isostructural to the triclinic CaHPO₄.

Later, Boudjada *et al.* (6) reported the preparation, the X-ray powder pattern, and the X-ray single crystal structure of α -SrHPO₄.

In this paper, we report the synthesis, the structure, and some properties of a new orthorhombic form of SrHPO₄ (γ -SrHPO₄). The relationships to the IR vibrational modes and crystal structures of other phosphates and sulfates are given.

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EXPERIMENTAL

A. Synthesis

Numerous colorless, hexagonal-shaped crystals of γ -SrHPO₄ were isolated during our systematic investigation of the system Li–Sr–P–O. They were prepared from a mixture comprising Li₂CO₃ ($\geq 99.5\%$), SrCO₃ ($\geq 98\%$), H₃PO₄ (85%), and distilled water in molar ratio Li/Sr/P/H₂O = 1/1/3/190. The reactants were introduced in a Teflon-lined Parr hydrothermal bomb, with a fill factor of approximately 50%. The bomb was heated at 180°C under autogeneous pressure for 6 days, and then slowly cooled to room temperature over 24 hours. The bomb contents were recovered by vacuum filtration and drying in air. Repeated attempts to prepare γ -SrHPO₄ hydrothermally from SrCO₃, H₃PO₄, and H₂O (Sr/P/H₂O = 1/1.9/60, $T = 140^\circ\text{C}$, 2 days) allowed us to obtain a white microcrystalline powder for this phase.

B. Initial Characterization

EDX analysis was performed with a JEOL-2010 electron microscope (TEM) operating at 200 kV and equipped with a KEVEX Energy-Dispersive X-ray analyzer. Samples were deposited on a lacey carbon film.

Infrared data were collected in the 4000–370 cm⁻¹ range with a Perkin Elmer FT-IR 1000 spectrophotometer using KBr pellet technique.

X-ray powder data were registered at room temperature using a Philips PW 3710 with CuK α radiation ($\lambda = 1.5418$ Å). A preliminary single-crystal investigation, using the Weissenberg technique, indicated an orthorhombic symmetry and space group *Pbca* (No. 61).

C. Structure Determination

A suitable single crystal, with the approximate dimensions 133 × 95 × 38 μm was selected for structure determination. Data collection was made on an AED2 Siemens-Stoe

four-circle diffractometer. The unit-cell parameters were determined by a least-squares fit of 30 reflections with 2θ ranging from 24.3 to 30.5°. The intensities were corrected for Lorentz-polarization effects. An absorption correction has been also applied (7). Atomic scattering factors were taken from the International Tables for X-ray crystallography (8). Initial heavy-atom positions (Sr, P) were located by using SHELXS-97 (9), and the O atom positions were deduced from Fourier difference maps during the refinement with the program SHELXL-97 (10). A final difference synthesis clearly revealed the hydrogen-atom coordinates, and geometrical constraints [$d_{\text{O-H}} = 0.9 \pm 0.05 \text{ \AA}$] were applied to stabilize the least-squares refinement of the H positions. The final cycle of refinement including atomic coordinates, anisotropic displacement parameters for nonhydrogen atoms, and isotropic displacement parameters for the H atoms converged to the reliability factors $R_1/wR_2 = 0.039/0.108$. Crystallographic data and some details of the structure refinement for γ -SrHPO₄ are summarized in Table 1.

TABLE 1
Summary of Crystal Data, Intensity Measurements, and Refinement Parameters for γ -SrHPO₄

Crystal data	
Formula	γ -SrHPO ₄
Formula weight (g mol ⁻¹)	183.59
Crystal dimensions	133 × 95 × 38 μm
Habit, color	Hexagonal, colorless
Crystal system	Orthorhombic
Space group	<i>Pbca</i> (No. 61)
Cell dimensions (Å)	$a = 8.131(3)$, $b = 9.258(5)$, $c = 18.084(7)$
V (Å ³), Z	1361.31(2), 16
ρ_{calc} (g cm ⁻³)	3.583
Absorption coefficient (mm ⁻¹)	$\mu(\text{MoK}\alpha) = 16.15$
Intensity measurements	
Temperature (K)	293(2)
Radiation, λ (Å)	MoK α , 0.71069
Scan mode (°)	ω - 2θ in 35 steps of $\Delta\omega = 0.035^\circ$
2θ max (°)	69.78
Standard reflections	4 0 0-8 2-4 4 0
hkl limits	$0 \leq h \leq 13$, $0 \leq k \leq 14$, $0 \leq l \leq 29$
Independent reflections	2940
Observed reflections [$I > 6\sigma(I)$]	1272
Absorption correction	SHELXA (7)
Min./Max. transmission	0.182/0.653
Structure refinement	
Parameters refined	118
Reliability factors	$R_1^a = 0.039$, $wR_2^a = 0.108$
$\Delta\rho_{\text{min/max}}$ (e Å ⁻³)	-0.97/1.01

^a R values are defined as follows: $R_1 = \sum \|F_o\| - |F_c| / \sum \|F_o\|$ and $wR_2 = [\sum w(F_o^2 - F_c^2)^2 / \sum w(F_o^2)^2]^{1/2}$ where $w^{-1} = [\sigma^2(F_o^2) + (0.0300P)^2 + 0.00P]$ and $P = (F_o^2 + 2F_c^2)/3$.

RESULTS AND DISCUSSION

A. Initial Characterization

EDX analysis of several crystals established the presence of Sr, P, and O. The obtained compositions are in good agreement with the stoichiometric formula, SrHPO₄.

The IR spectrum of γ -SrHPO₄ is reported in Fig. 1. Previous workers (11, 12) have found that the vibrational bands of inorganic phosphates are generally not very sensitive to the cations in the structure, which tend just to shift the band frequencies slightly rather than to create new bands. Thus, the IR spectrum is dominated by the HPO₄²⁻ modes. The 2800–1700 cm⁻¹ range corresponds to the OH modes of HPO₄²⁻ groups characterized by three broad bands of ABC type. Similar bands have been observed in strong hydrogen bonded crystals, such as CaBa(HPO₄)₂ (13) and PbHPO₄ (14). The presence of bands in the region 1400–1200 cm⁻¹ is characteristic of hydrogen monophosphate groups (12). They are assigned to $\delta_{\text{P-O-H}}$ in plane bending modes, two bands 1298 and 1267 cm⁻¹ are observed for these modes. In the range 1200–800 cm⁻¹ appear the PO₄³⁻ stretching modes: the high-frequency bands (1170, 1146, 1137 cm⁻¹) are assigned to the asymmetric (ν_3) mode, whereas the symmetric stretching mode of P–O(H) is observed for the low-frequency 887 cm⁻¹. The remaining bands (1070, 1016, 929, 915 cm⁻¹) are attributed to the symmetric (ν_1) mode. The bands in the range 600–370 cm⁻¹ are due to PO₄³⁻ bending modes. According to previous data (15), the two well-defined subdivisions of 600–520 and 450–370 cm⁻¹ arise from the antisymmetric (ν_4) and symmetric (ν_2) modes, respectively.

The diffraction pattern of the title compound, which differs from those of α -SrHPO₄ (JCPDS Card 33-1335) and β -SrHPO₄ (JCPDS Card 12-368) forms, was indexed using the orthorhombic cell parameters determined from the single-crystal experiment. Table 2 lists the observed and calculated interplanar distances and the intensities calculated on the basis of a LAZY-PULVERIX (16) simulation of the structure of γ -SrHPO₄.

B. Description of the Structure and Discussion

General features. Final atomic parameters for γ -SrHPO₄ are reported in Tables 3 and 4, with selected interatomic distances and angles data given in Table 5. As shown from the projection of the structure onto (010) plane (Fig. 2), the atomic arrangement consists of a succession along [001] of two kinds of alternating anionic planes denoted as P(1) and P(2). These sheets located at approximately $z = (0, 1/2)$ and $z = (1/4, 3/4)$ are formed by HP(1)O₄²⁻ (P(1)) and HP(2)O₄²⁻ (P(2)) groups, respectively. Along the c axis, two anionic planes of the same type are related by a c glide. Interleaved Sr²⁺ cations ensure the cohesion of the structure.

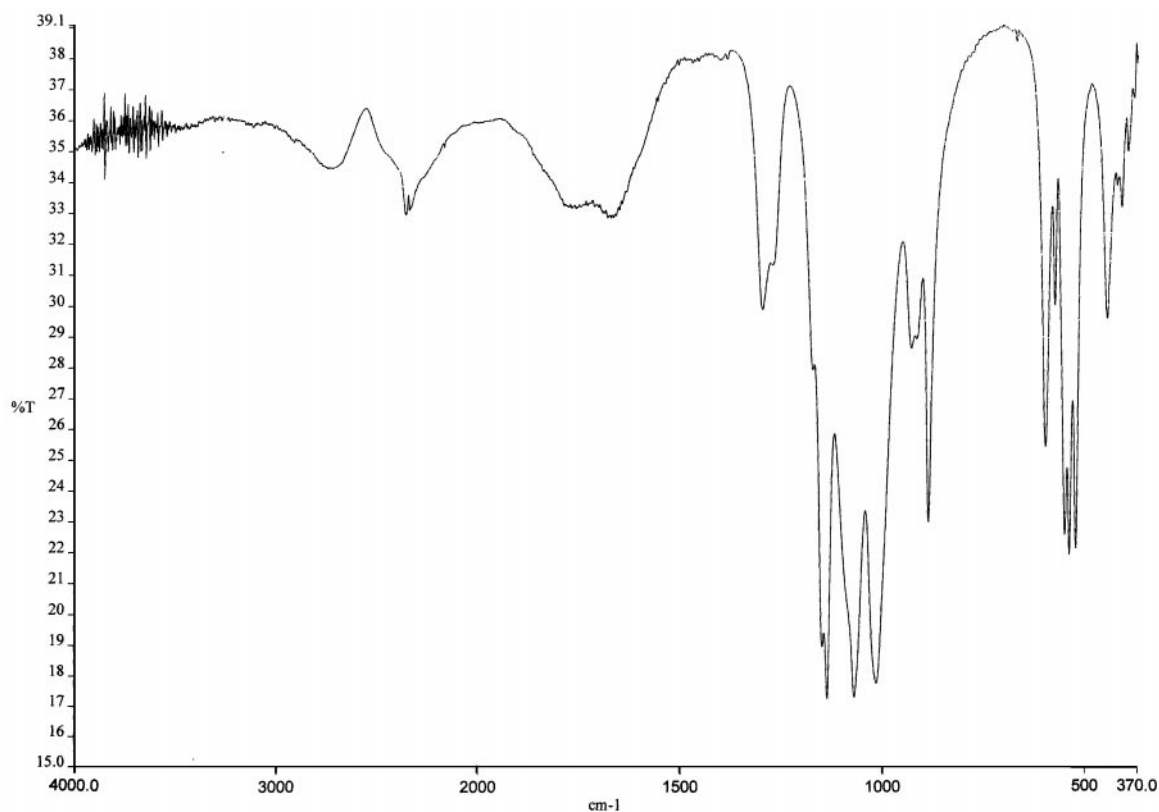


FIG. 1. Infrared spectrum of γ -SrHPO₄.

Sr²⁺ environment. The two independent Sr²⁺ ions are both 9-coordinated by oxygen atom neighbors. All oxygen atoms are involved in Sr–O bonds. The SrO₉ polyhedra are distorted as shown by the Sr–O bond lengths (Table 5). The average \langle Sr–O \rangle distances (2.703(6) and 2.660(6) Å) are quite similar to those in SrNaPO₄·H₂O (17), in which Sr²⁺ has

also a ninefold coordination, whereas these values are significantly larger than those in the SrO₈ square antiprisms of α -SrHPO₄ (7). Furthermore, the coordination choice is in agreement with results of bond valence sums (18) of 1.94 for Sr(1) and 2.14 for Sr(2). Each Sr(1)O₉ polyhedron shares one triangular face [O(2), O(3), O(7)] and two edges (O(3)–O(5),

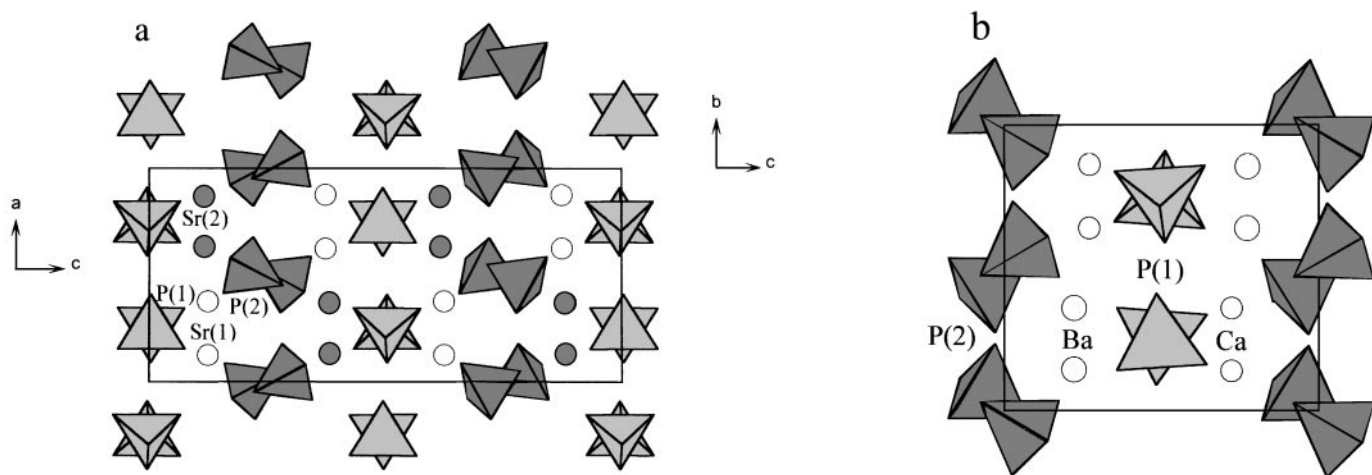


FIG. 2. (a) [010] view of the atomic arrangement of γ -SrHPO₄. (b) [100] view of the atomic arrangement of CaBa(HPO₄)₂. H atoms are not shown.

TABLE 2
X-ray Powder Data for γ -SrHPO₄

<i>h</i>	<i>k</i>	<i>l</i>	<i>d</i> _{obs.} (Å)	<i>d</i> _{cal.} (Å)	<i>I</i> / <i>I</i> ₀
1	1	1	5.76	5.78	12
0	0	4	4.50	4.52	33
0	2	2	4.11	4.12	5
1	2	1	3.92	3.92	12
2	1	0	3.71	3.72	100
2	0	2	3.71	3.70	38
1	2	3	3.33	3.34	76
0	2	4	3.22	3.23	86
1	1	5	3.10	3.11	57
1	2	4	3.00	3.05	1
2	2	2	2.88	2.89	24
2	1	4	2.88	2.87	90
2	1	4	2.86	2.87	90
1	3	1	2.841	2.849	27
1	2	5	2.683	2.689	32
3	1	1	2.570	2.574	12
2	3	0	2.450	2.458	15
3	1	3	2.382	2.388	8
3	2	1	2.315	2.319	187
0	4	0	2.315	2.314	7
2	3	3	2.279	2.276	1
0	2	7	2.256	2.255	32
3	1	4	2.250	2.254	45.5
1	4	1	2.204	2.209	31
2	3	4	2.155	2.159	9
3	1	5	2.109	2.111	7
3	3	1	2.027	2.023	17
3	3	3	1.929	1.929	7
1	4	5	1.893	1.895	14
0	0	10	1.805	1.808	4
3	3	5	1.772	1.774	23
3	2	7	1.730	1.733	7
4	2	4	1.719	1.721	6
3	4	3	1.687	1.689	12
3	3	7	1.596	1.599	6
5	1	1	1.596	1.595	1
3	4	5	1.580	1.582	13
1	2	11	1.520	1.521	2
0	6	2	1.520	1.521	1
0	0	12	1.509	1.507	3
4	4	2	1.505	1.506	1
5	2	3	1.488	1.486	1
5	2	3	1.485	1.486	1
3	5	3	1.485	1.482	5
4	2	8	1.435	1.436	9
5	3	1	1.435	1.434	2
1	5	6	1.396	1.398	3
2	1	12	1.396	1.396	16

O(2)–O(8)) with three Sr(2)O₉ polyhedra, and vice versa, resulting in a two-dimensional framework lying parallel to the *ab* plane (Fig. 3a). In the [001] direction, the Sr(1)–Sr(2) connectivity is via the O(1)–O(4) edges and the O(6) corners, forming infinite slightly corrugated ribbons (Fig. 3b), completing the three-dimensional network of the strontium polyhedra.

TABLE 3
Atomic Coordinates and Equivalent Isotropic Displacement Parameters (Å² × 10⁴) for γ -SrHPO₄

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{eq} ^a
Sr(1)	0.1244(1)	0.3213(1)	0.12536(3)	104(2)
Sr(2)	0.86913(9)	0.6821(1)	0.11737(4)	101(2)
P(1)	0.2510(2)	0.0770(1)	0.0037(1)	9(3)
P(2)	0.5227(2)	0.4790(2)	0.2057(1)	107(9)
O(1)	0.0903(5)	0.1632(5)	0.0042(3)	144(1)
O(2)	0.3450(7)	0.1013(7)	0.0754(3)	143(1)
O(3)	0.3472(7)	0.1074(7)	−0.0663(3)	115(9)
O(4)	0.2064(6)	−0.0904(5)	0.0010(4)	5(4)
O(5)	0.5793(7)	0.6203(6)	0.1718(3)	158(12)
O(6)	0.6754(7)	0.3742(6)	0.2213(3)	141(11)
O(7)	0.4484(6)	0.5019(6)	0.2828(3)	140(11)
O(8)	0.4140(7)	0.3877(6)	0.1571(3)	150(12)
H(4)	0.097(6)	−0.10(1)	0.009(7)	396(312) ^b
H(6)	0.76(8)	0.42(1)	0.215(7)	799(477) ^b

$$^a U_{\text{eq}} = 1/3 \sum_i \sum_j U_{ij} \mathbf{a}_i^* \mathbf{a}_j^* \mathbf{a}_i \mathbf{a}_j.$$

$$^b U_{\text{iso}}.$$

Anionic sheets. The mean P–O and P–O(H) bond lengths in the hydrogen phosphate groups compare well with the values 1.522 and 1.592 Å, respectively, reported by Baur in his survey of monophosphate groups (19). Both P(1) and P(2) units are involved in strong hydrogen bonds (20) (Table 5). The overall hydrogen-bond scheme in γ -SrHPO₄ is illustrated in Fig. 4. Every hydrogen phosphate tetrahedron can act both as a hydrogen acceptor and as a donor, and in such cases it has to be denoted as (D + A). Within the planes at *z* ~ (0 and 1/2) which contain the P(1) tetrahedra, closed dimers located on inversion symmetry are formed

TABLE 4
Anisotropic Displacement Parameters (Å² × 10⁴) for γ -SrHPO₄

Atom	<i>U</i> ₁₁	<i>U</i> ₂₂	<i>U</i> ₃₃	<i>U</i> ₂₃	<i>U</i> ₁₃	<i>U</i> ₁₂
Sr(1)	48(3)	108(4)	156(3)	−5(3)	−7(2)	−5(4)
Sr(2)	57(3)	92(3)	153(3)	3(3)	0(3)	4(4)
P(1)	42(6)	78(6)	147(7)	13(9)	16(11)	−1(5)
P(2)	33(7)	77(8)	147(7)	−3(7)	2(7)	2(7)
O(1)	49(18)	52(19)	221(22)	−29(25)	31(22)	11(15)
O(2)	99(28)	154(32)	179(24)	41(23)	−84(22)	−37(25)
O(3)	85(27)	162(31)	183(24)	19(23)	39(22)	−13(25)
O(4)	52(20)	114(20)	180(21)	−49(27)	−18(24)	−4(16)
O(5)	107(29)	123(28)	246(28)	102(24)	−24(23)	−5(23)
O(6)	70(24)	109(25)	247(27)	2(23)	−47(22)	40(20)
O(7)	100(22)	144(25)	178(24)	−43(23)	101(20)	−7(22)
O(8)	186(30)	167(24)	−26(24)	−39(21)	−22(24)	150(12)

Note. The form of the anisotropic thermal parameters is $\exp[-2\pi^2(h^2 \mathbf{a}^* \mathbf{a}^* U_{11} + k^2 \mathbf{b}^* \mathbf{b}^* U_{22} + l^2 \mathbf{c}^* \mathbf{c}^* U_{33} + 2hka^* \mathbf{b}^* U_{12} + 2hla^* \mathbf{c}^* U_{13} + 2k/lb^* \mathbf{c}^* U_{23})]$.

TABLE 5
Selected Interatomic Distances (Å) and Angles (°) for γ -SrHPO₄

P(1)O ₄ tetrahedron		$\langle P-O \rangle = 1.540(6)$ Å		
P(1)	O(1)	O(2)	O(3)	O(4)
O(1)	1.530(5)	2.505(7)	2.501(7)	2.532(6)
O(2)	110.2(3)	1.522(6)	2.564(7)	2.496(7)
O(3)	110.4(3)	115.1(3)	1.515(6)	2.479(8)
O(4)	108.2(2)	106.9(3)	105.8(3)	1.592(5)
D-H...A	D-H (Å)	H...A (Å)	D...A (Å)	D-H...A (°)
O(4)-H(4)...O(1) ⁽ⁱ⁾	0.90(5)	1.65(6)	2.508(6)	157(11)
P(2)O ₄ tetrahedron		$\langle P-O \rangle = 1.539(6)$ Å		
P(2)	O(5)	O(6)	O(7)	O(8)
O(5)	1.516(6)	2.569(8)	2.523(8)	2.553(7)
O(6)	111.0(3)	1.600(6)	2.458(7)	2.425(8)
O(7)	111.6(3)	103.2(3)	1.533(6)	2.523(8)
O(8)	105.9(3)	102.5(3)	112.1(3)	1.507(6)
D-H...A	D-H (Å)	H...A (Å)	D...A (Å)	D-H...A (°)
O(6)-H(6)...O(7) ⁽ⁱⁱⁱ⁾	0.89(5)	1.63(6)	2.516(8)	169(13)
Sr(1)O ₉ polyhedron		$\langle Sr(1)-O \rangle = 2.703(6)$ Å		
Sr(1)-O(1)	2.648(6)		Sr(1)-O(5) ^(v)	2.629(6)
Sr(1)-O(2)	2.859(6)		Sr(1)-O(6) ^(vii)	2.846(6)
Sr(1)-O(2) ⁽ⁱⁱⁱ⁾	2.756(6)		Sr(1)-O(7) ^(vii)	2.756(6)
Sr(1)-O(3) ^(iv)	2.579(6)		Sr(1)-O(8)	2.500(6)
Sr(1)-O(4) ⁽ⁱⁱⁱ⁾			2.758(6)	
Sr(2)O ₉ polyhedron		$\langle Sr(2)-O \rangle = 2.660(6)$ Å		
Sr(2)-O(1) ^(vii)	2.644(6)		Sr(2)-O(5)	2.617(6)
Sr(2)-O(2) ^(viii)	2.556(6)		Sr(2)-O(6) ^(viii)	2.613(6)
Sr(2)-O(3) ^(iv)	2.841(6)		Sr(2)-O(7) ⁽ⁱⁱⁱ⁾	2.541(6)
Sr(2)-O(3) ^(vii)	2.776(6)		Sr(2)-O(8) ^(viii)	2.691(6)
Sr(2)-O(4) ^(ix)			2.657(6)	

Note. Symmetry codes: (i) $-x, -y, -z$; (ii) $x + 0.5, y, -z + 0.5$; (iii) $-x + 0.5, y + 0.5, z$; (iv) $x - 0.5, -y + 0.5, -z$; (v) $-x + 0.5, y - 0.5, z$; (vi) $x - 0.5, y, -z + 0.5$; (vii) $-x + 1, -y + 1, -z$; (viii) $-x + 1.5, y + 0.5, z$; (ix) $x + 0.5, -y + 0.5, -z$.

from two H bridges O(4)-H(4)...O(1) with O...O distance of 2.508(6) Å. Whereas for the planes at $z \sim (1/4 \text{ and } 3/4)$ containing the P(2) tetrahedra, the phosphate entities are

connected through the hydrogen bonds O(6)-H(6)...O(7) with O...O distance of 2.516(8) Å, giving rise to infinite zig-zag (HPO₄²⁻)_n chains running parallel to [100]. Besides, there's no H-bond connection between the two types of anionic sheets.

Comparison to related compounds. As suggested by Figs. 2a and 2b, the atomic arrangement of the title compound shows close similarity to that observed in CaBa(HPO₄)₂ salt (13). Indeed, in the related compound, we note the same succession of two types of HPO₄²⁻ sheets which alternate with Ba²⁺/Ca²⁺ planes and an H-bonding system similar, where closed dimers are present along with infinite chains. Besides, we have observed a lowering of the lattice symmetry from orthorhombic to monoclinic with a change in the unit cell parameters ($a_o \sim b_m, b_o \sim a_m, c_o \sim 2c_m$) (Table 6).

The monoclinic deformation of the unit cell of CaBa(HPO₄)₂ can be directly related to the nature of the cation coordinations; one kind of ion, (2Sr²⁺) with average $\langle Sr-O \rangle$ distances (2.703(6) and 2.660(6) Å), is replaced by (Ba²⁺, Ca²⁺) ions with $\langle Ba-O \rangle = 2.846(5)$ Å and $\langle Ca-O \rangle = 2.462(5)$ Å in BaO₉ and CaO₇ polyhedra, respectively. The lattice distortion is coupled with small rotations of the HPO₄ tetrahedra along the a_m axis.

The slight increase of a and c lengths, from γ -SrHPO₄ to CaBa(HPO₄)₂, is caused by the radius change of the ions, where two Sr²⁺ cations ($r_{IX}(Sr^{2+}) = 1.31$ Å) are replaced by a relatively small Ca²⁺ ($r_{VII}(Ca^{2+}) = 1.07$ Å) and large Ba²⁺ ($r_{IX}(Ba^{2+}) = 1.47$ Å) cations (21). The doubling of the c parameter in γ -SrHPO₄ is due to the orientation of the tetrahedra in two successive layers either of P(1) type or of P(2) type.

Moreover, one can notice a decrease of the b parameter because the chains P(2) are rather strained in the related compound. The distance between P(2) atoms along the chains in γ -SrHPO₄ is 4.369(1) Å as compared to 4.280(5) Å for CaBa(HPO₄)₂. This decrease in the P-P distance is accompanied by a decrease in the P(2)-P(2)-P(2) angle (137.06(1)° to 135.77(1)°) and a reduction in the third lattice

TABLE 6
Comparison of Selected Structural Characteristics of γ -SrHPO₄ (I) and CaBa(HPO₄)₂ (II)

	Crystal data			HP(2)O ₄ chains		
	Lattice parameters (Å ³)	Volume (Å ³), Z	V/Z (Å ³)	O...O (Å)	P(2)-P(2) (Å)	P(2)-P(2)-P(2) (°)
I	$a_o = 8.131(3)$ $b_o = 9.258(5)$ $c_o = 18.084(7)$	1361.31(2), 16	85.08	2.516(8)	4.369(1)	137.06(1)
II	$a_m = 9.470(2)$ $b_m = 7.930(1)$ $c_m = 9.865(1)$ $\beta = 115.78(1)$	667.2(1), 4	2 × 83.4	2.466(7)	4.280(5)	135.77(1)

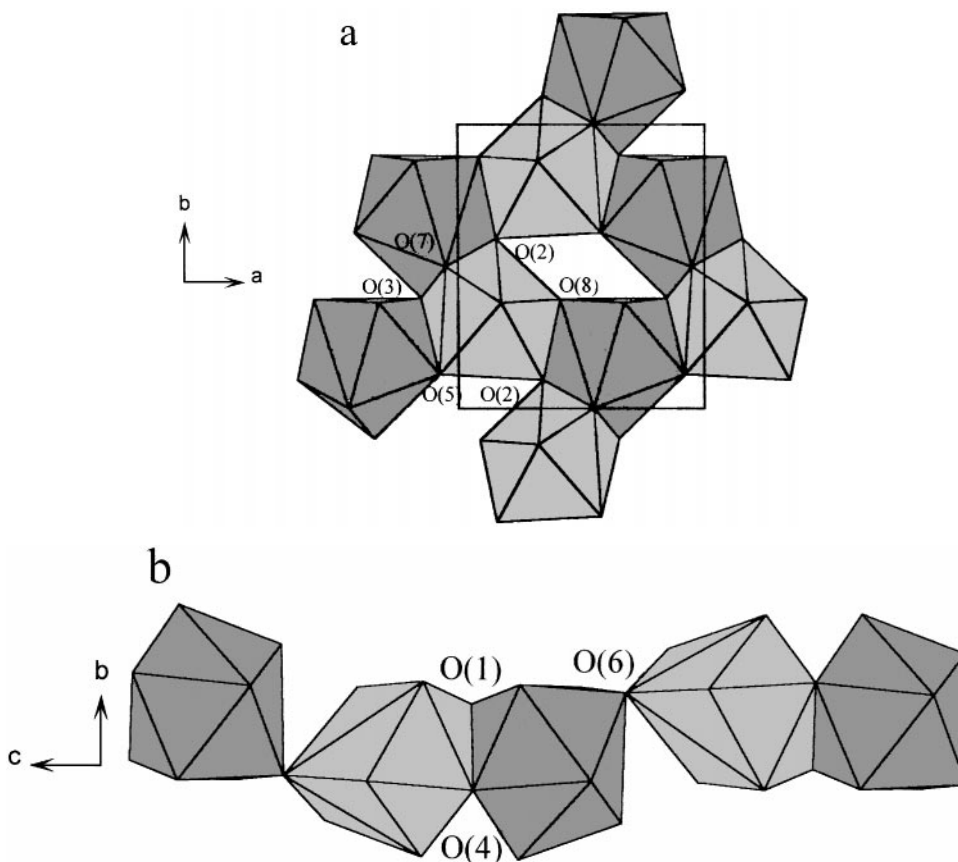


FIG. 3. The SrO₉ polyhedral connectivity into layers parallel to (001) (a) and ribbons along [001] (b). Sr(1) and Sr(2) environment are represented by light and medium gray polyhedra, respectively.

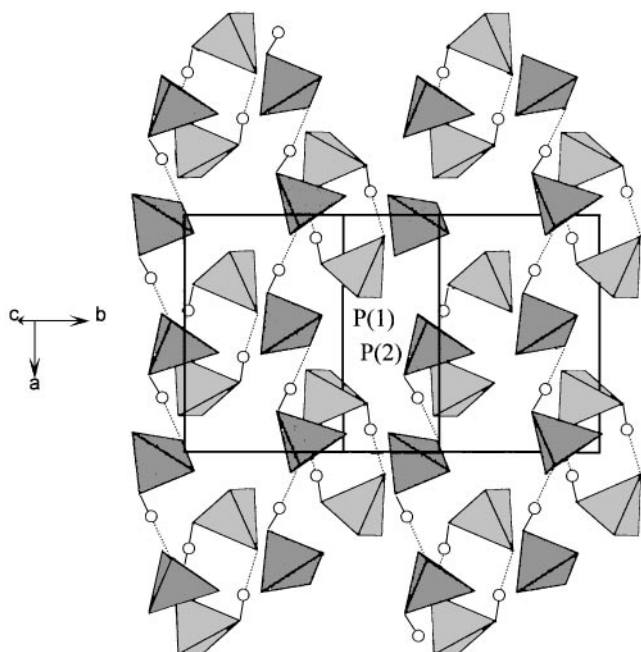


FIG. 4. Hydrogen bond scheme in γ -SrHPO₄. Small open circles represent H atoms. H bonds are indicated by dotted lines.

constant, from 8.131(3) Å (in γ -SrHPO₄) to 7.930(1) Å (in CaBa(HPO₄)₂).

As well as for both the hydrogen phosphate structures with $H/PO_4^3 = 1$, Kemnitz *et al.* (22) have found the same connectivity (dimers or/and infinite chains) in some hydrogen sulfate structures, e.g., KHSO₄, LiHSO₄, and β -NaHSO₄, where the H/SO_4^{2-} ratio is also 1. Moreover, in their investigation of Cs₅(HSO₄)₃(H₂PO₄)₂, Sossina *et al.* (23), have also observed the same behavior for the sulfate and phosphate groups.

CONCLUSION

We have described the synthesis, (EDX analysis, IR, X-ray powder pattern) characterization, and single-crystal structure of a new strontium hydrogen phosphate form. γ -SrHPO₄, like the related CaBa(HPO₄)₂ (13), has an interesting three-dimensional network consisting of phosphate sheets linked via the alkaline earth cations. Further interaction linkages are provided by strong hydrogen bonds which features are defined by the H/PO_4^3 ratio as has been found in some hydrogen sulfate structures (22). Consequently, the structural features invite us to investigate the mixed alkaline

earth of strontium–barium and strontium–calcium phosphates or/and sulfates in order to examine the effect and the influence of the cationic and anionic substitution over crystalline symmetry and physical properties.

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