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Crystal structure of $\text{SrCo}_4(\text{OH})(\text{PO}_4)_3$, a new hydroxyphosphate

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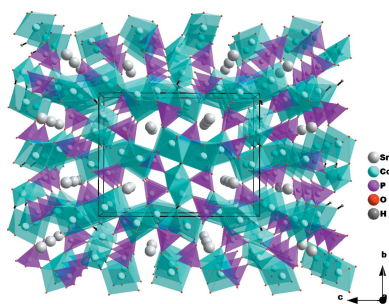
Single crystals of strontium tetracobalt tris(orthophosphate) hydroxide, $\text{SrCo}_4(\text{OH})(\text{PO}_4)_3$, were grown serendipitously under hydrothermal conditions at 473 K. The crystal structure consists of undulating chains of edge-sharing $[\text{CoO}_6]$ octahedra that are linked into (010) layers by common vertices between chains. Adjacent layers are linked along [010] into a framework structure by tetrahedral $[\text{CoO}_4]$ units and by PO_4 tetrahedra. The framework delimits channels extending along [100] in which the eleven-coordinate strontium cations are situated. Bifurcated $\text{O}—\text{H}\cdots\text{O}$ hydrogen bonds of weak strengths consolidate the crystal packing. The title compound was also characterized by infrared spectroscopy.

1. Chemical context

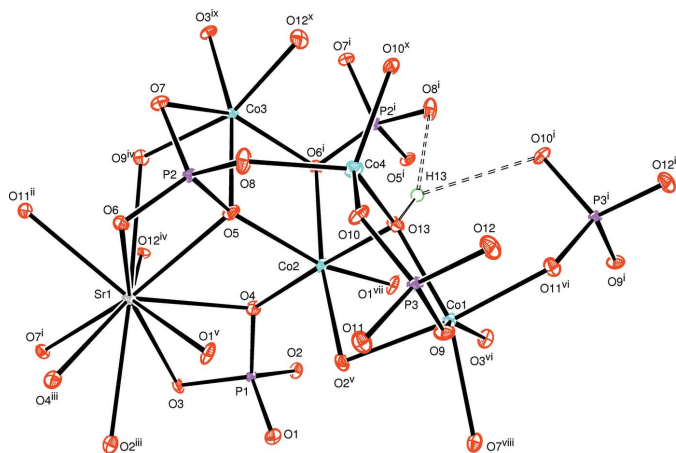
The search for new inorganic materials with open-frame structures comprising transition-metal polyhedra, $[\text{MO}_x]$, with tetrahedral phosphate or vanadate units by sharing corners or edges is still ongoing (Rghioui *et al.*, 2019; Ouaatta *et al.*, 2019; Khmiyas *et al.*, 2020). Generally, these interconnections can lead to structures with cages, interlayer spaces or channels, and the corresponding compounds are explored extensively for their excellent physical properties and various applications in electrical, electrochemical, magnetic or catalytic processes (Goodenough *et al.*, 1976; Borel *et al.*, 1991; La Parola *et al.*, 2018; Hadouchi *et al.*, 2019). The introduction of borate groups (BO_3 or BO_4) to phosphate (PO_4) units leads to a group of borophosphates with specific structural characteristics. Compounds of this family likewise exhibit remarkable physicochemical properties that allow them to be applied in different fields (Knies *et al.*, 1998; Ewald *et al.*, 2007; Lin *et al.*, 2008; Menezes *et al.*, 2008). About a decade ago, we managed to synthesize two borophosphate phases, *viz.* $(\text{Ag}_{0.57}\text{Ni}_{0.22})\text{-Ni}(\text{H}_2\text{O})_2[\text{BP}_2\text{O}_8]\cdot 0.67\text{H}_2\text{O}$ and $\text{AgMg}(\text{H}_2\text{O})_2[\text{BP}_2\text{O}_8]\cdot \text{H}_2\text{O}$ (Zouihri *et al.*, 2011*a,b*). In this context, we attempted to synthesize a strontium- and cobalt-based borophosphate, namely $\text{SrCo}_2\text{BPO}_7$, by means of the hydrothermal process. Instead, we have isolated a new hydroxyphosphate, $\text{SrCo}_4(\text{OH})(\text{PO}_4)_3$, and report here its crystal structure and its infrared spectrum.

2. Structural commentary

In the three-dimensional framework structure of $\text{SrCo}_4(\text{OH})(\text{PO}_4)_3$, an octahedral coordination of three cobalt

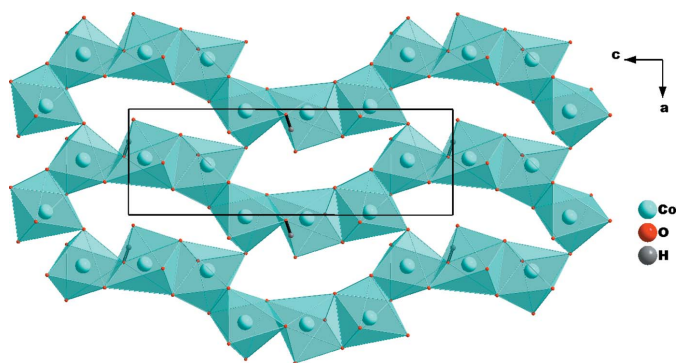


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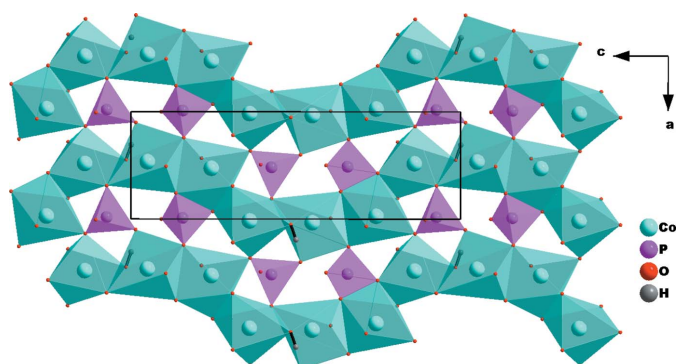

Figure 1

The interconnection of $[\text{CoO}_6]$ and $[\text{CoO}_4]$ polyhedra, and the hydroxide group linked to PO_4 tetrahedra through a bifurcated hydrogen bond (dashed lines). Displacement ellipsoids are drawn at the 50% probability level. [Symmetry codes: (i) $-x, y + \frac{1}{2}, -z + \frac{3}{2}$; (ii) $-x - \frac{1}{2}, -y + 1, z + \frac{1}{2}$; (iii) $x - 1, y, z$; (iv) $-x + \frac{1}{2}, -y + 1, z + \frac{1}{2}$; (v) $x - \frac{1}{2}, -y + \frac{3}{2}, -z + 1$; (vi) $x + 1, y, z$; (vii) $x + \frac{1}{2}, -y + \frac{3}{2}, -z + 1$; (viii) $-x + \frac{1}{2}, -y + 1, z - \frac{1}{2}$; (ix) $-x + 1, y - \frac{1}{2}, -z + \frac{3}{2}$; (x) $x + \frac{1}{2}, -y + \frac{1}{2}, -z + 1$].

atoms (Co1, Co2, Co3) and a tetrahedral coordination of the fourth cobalt (Co4) is observed. Atom O13 bears a hydrogen atom and bridges two of the six-coordinate Co atoms (Co1, Co2) and the four-coordinate Co4 atom. The hydroxide group


Figure 2

$[\text{CoO}_6]$ octahedra sharing edges to form chains that are linked together *via* a common corner every three octahedra.


Figure 3

Edge-sharing $[\text{CoO}_6]$ octahedra and PO_4 tetrahedra building a layer parallel to (010).

Table 1

Hydrogen-bond geometry ($\text{\AA}, ^\circ$).

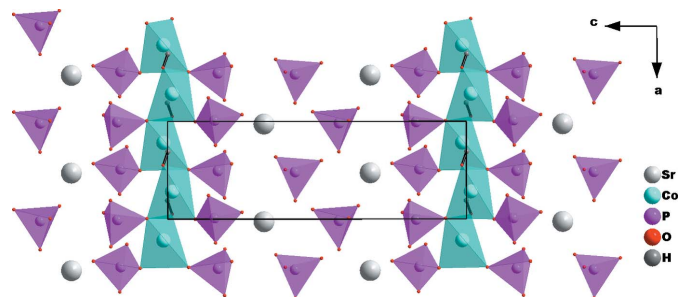
$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{O13}-\text{H13}\cdots\text{O8}^i$	0.82	2.21	2.982 (3)	157
$\text{O13}-\text{H13}\cdots\text{O10}^i$	0.82	2.40	3.010 (3)	132

Symmetry code: (i) $x + 1, y, z$.

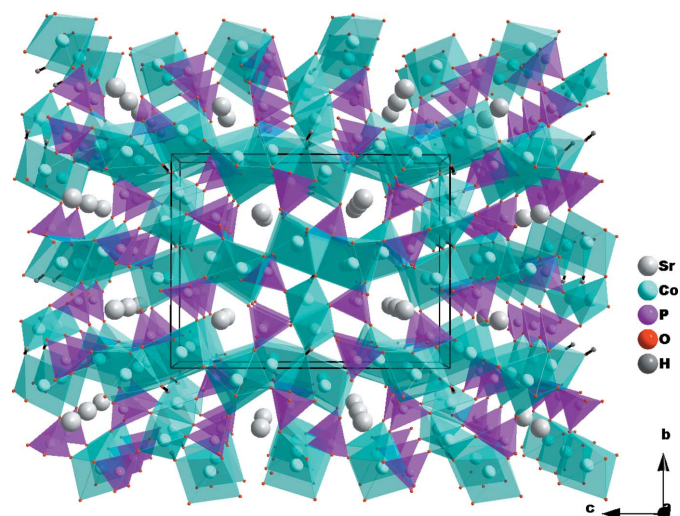
also forms a weak bifurcated hydrogen bond (Table 1) to two phosphate tetrahedra (Fig. 1).

The $[\text{CoO}_6]$ octahedra share edges to form infinite undulating chains extending parallel to [001]. Adjacent chains are cross-linked *via* common vertex atoms (O3) to build up (010) layers (Fig. 2) with the formation of oval voids surrounded by eight octahedra. Two PO_4 tetrahedra occupy the void space, whereby P1O_4 shares three of its vertices with five $[\text{CoO}_6]$ octahedra and P2O_4 shares an edge with an octahedron and a vertex with two opposite octahedra (Fig. 3).

The $[\text{Co}_4\text{O}_3\text{OH}]$ tetrahedra are linked through corners into zigzag chains running parallel to [100]; the chains are flanked by P2O_4 and P3O_4 tetrahedra into ribbons. The strontium cations and P1O_4 tetrahedra are of the same height as the ribbons, thus defining a second layer parallel to (010) (Fig. 4).


Figure 4

Ribbons formed by $[\text{CoO}_4]$ and P2O_4 and P3O_4 tetrahedra, and strontium atoms and P1O_4 tetrahedra at the same height forming the second layer parallel to (010).


Figure 5

The crystal structure of $\text{SrCo}_4(\text{OH})(\text{PO}_4)_3$ in a projection along [100], showing channels in which the strontium cations are located.

The crystal structure can be described by the stacking of the two types of layers along [010], which leads to the formation of channels extending parallel to [100] in which the strontium cations are located (Fig. 5). Each Sr^{II} atom is surrounded by eleven oxygen atoms, forming a distorted polyhedron.

Comparison of the metal–oxygen polyhedra in the title structure with the same type of polyhedra in comparable structures shows a similar behaviour. All [CoO₆] octahedra in SrCo₄(OH)(PO₄)₃ are distorted, with the Co–O distance varying between 2.022 (2) and 2.284 (2) Å. The averaged Co–O distances of 2.130 Å for Co1, 2.122 Å for Co2 and 2.124 Å for Co3 are in good agreement with those of Co₅(PO₄)₂(OH)₄ (average Co–O distances are 2.107 Å for Co1, 2.144 Å for Co2, 2.140 Å for Co3, 2.148 Å for Co4 and 2.150 Å for Co5; Ruzsala *et al.*, 1977). The distorted [Co4O₃OH] tetrahedron shows much shorter Co–O distances ranging from 1.942 (2) to 1.995 (2) Å. These distances are comparable with the averaged ⁴¹Co–O distances of 1.966, 1.955, 1.957 and 1.958 Å observed, respectively, in the phosphates NaCoPO₄, KCoPO₄, NH₄CoPO₄-Hex and NH₄CoPO₄-ABW (Feng *et al.*, 1997). The PO₄ tetrahedra in the title structure have averaged distances of 1.542 Å for P1, 1.539 Å for P2 and 1.539 Å for P3, and are compatible with the P–O distances in the orthophosphate SrCo₂Fe(PO₄)₃ (Bouraima *et al.*, 2016).

The structure model of SrCo₄(OH)(PO₄)₃ is in good agreement with calculations of the bond-valence sums (Brown & Altermatt, 1985). The obtained values (in valence units) for the cations Sr^{II}, Co^{II}, and P^V are close to the expected values: Sr1 (1.95), Co1 (1.89), Co2 (1.89), Co3 (1.88), Co4 (1.92), P1 (4.90), P2 (4.95) and P3 (4.95). The bond-valence sums calculated for the oxygen atoms range between 1.82 and 2.29 valence units.

3. Infrared spectroscopy

An infrared spectrum of SrCo₄(OH)(PO₄)₃ was recorded in order to verify the existence of the hydroxyl and PO₄ groups in the title compound (Fig. 6). The FT-IR spectrum shows characteristic vibration bands of isolated PO₄ groups. The bands observed at around 420 and 463 cm⁻¹ can be assigned to the ν₂ asymmetric stretching mode while the vibration at 573 cm⁻¹ is attributed to ν₄ asymmetric O–P–O deformation. The weak band observed at 750 cm⁻¹ most likely originates from ⁴¹Co–O vibrations, as observed in many other phosphates (Rusakov *et al.*, 2006; Antony *et al.*, 2011; Bushiri *et al.*, 2002; De Pedro *et al.*, 2010). The vibration at 1014 cm⁻¹ corresponds to the ν₃ asymmetric stretching mode of the phosphate tetrahedra. The remaining vibrations centred at 3566, 3433 and 1632 cm⁻¹ are commonly assigned to the stretching vibration of the bridging –OH group, as in Co₂PO₄OH (Wang *et al.*, 2014), in addition to the OH⁻ librational mode, which is observed at 637 cm⁻¹. We also note the presence of bands at 1384 and 875 cm⁻¹, indicating C–O bonds (Ribeiro *et al.*, 2006). This observation suggests that the powdered sample contained impurities of a carbonate. The assignments of all vibration bands are summarized in Table 2.

Table 2

Assignments of infrared vibration bands (cm⁻¹) for SrCo₄(OH)(PO₄)₃.

Position	Assignment
420	ν ₂ asymmetric stretching mode of P–O bonds
463	ν ₂ asymmetric stretching mode of P–O bond
573	ν ₄ asymmetric deformation of O–P–O
637	ν ₁ libration mode of the hydroxyl group
750	⁴¹ Co–O stretching mode
875	ν ₂ vibration of C–O bond
1014	ν ₃ asymmetric stretching mode of PO ₄ ³⁻
1384	ν ₃ vibration of C–O bond
1632	O–H stretching band
3433	O–H stretching band
3566	ν _s stretching mode of the hydroxyl group ⁻

4. Database survey

A search in the Inorganic Crystal Structure Database (ICSD; Zagorac *et al.*, 2019) revealed no match in the pseudo-quaternary system SrO/CoO/P₂O₅/OH. However, five compounds were identified in the pseudo-ternary SrO/CoO/P₂O₅ system, *viz.* triclinic SrCo₂(PO₄)₂ (*P* $\bar{1}$, *Z* = 2; El Bali *et al.*, 1993), monoclinic SrCoP₂O₇ (*P*2₁/*n*, *Z* = 4; Riou & Raveau 1991), monoclinic Sr₂Co(PO₄)₂ and SrCo₃(P₂O₇)₂ (both *P*2₁/*c*, *Z* = 6 and 2, respectively; Belik *et al.* 2001 and Yang *et al.*, 2008) and hexagonal Sr₅Co_{0.18}P₃O_{12.92} (*P*6₃/*m*, *Z* = 2; Kazin *et al.*, 2017).

5. Synthesis and crystallization

Single crystals of SrCo₄(OH)(PO₄)₃ were obtained serendipitously by attempting to synthesize the borophosphate SrCo₂BPO₇ under hydrothermal conditions. The starting materials, Sr(NO₃)₂ (0.3174 g), Co(CH₃COO)₂·4H₂O (0.7473 g), H₃BO₃ (0.0927 g) and H₃PO₄ (12 N; 0.1 ml), were mixed in the molar proportions of 1:2:1:1. The hydrothermal reaction was conducted in a 23 ml Teflon-lined autoclave, filled to 50% with distilled water and heated under autogenous pressure at 473 K for five days. After the end of the heat treatment, the autoclave was taken out of the oven and allowed to cool to room temperature. The reaction product

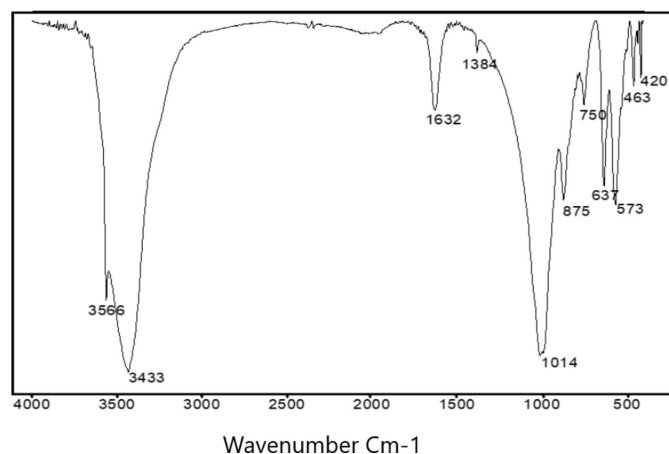


Figure 6
Infrared spectrum of SrCo₄(OH)(PO₄)₃.

Table 3
Experimental details.

Crystal data	
Chemical formula	SrCo ₄ (OH)(PO ₄) ₃
<i>M_r</i>	625.26
Crystal system, space group	Orthorhombic, <i>P</i> 2 ₁ 2 ₁ 2 ₁
Temperature (K)	296
<i>a</i> , <i>b</i> , <i>c</i> (Å)	5.1245 (1), 12.0491 (2), 15.7118 (3)
<i>V</i> (Å ³)	970.13 (3)
<i>Z</i>	4
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	12.74
Crystal size (mm)	0.35 × 0.26 × 0.17
Data collection	
Diffractometer	Bruker X8 APEX
Absorption correction	Multi-scan (<i>SADABS</i> ; Krause <i>et al.</i> , 2015)
<i>T_{min}</i> , <i>T_{max}</i>	0.391, 0.748
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	34471, 4243, 4038
<i>R_{int}</i>	0.045
(sin θ/λ) _{max} (Å ⁻¹)	0.806
Refinement	
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.022, 0.050, 1.07
No. of reflections	4243
No. of parameters	191
H-atom treatment	H-atom parameters constrained
Δρ _{max} , Δρ _{min} (e Å ⁻³)	1.60, -0.68
Absolute structure	Flack <i>x</i> determined using 1625 quotients [(<i>I</i> ⁺ - <i>I</i>)/((<i>I</i> ⁺ + <i>I</i>))] (Parsons <i>et al.</i> , 2013).
Absolute structure parameter	0.008 (3)

Computer programs: *APEX2* and *SAINT* (Bruker, 2016), *SHELXT2014/5* (Sheldrick, 2015a), *SHELXL2018/3* (Sheldrick, 2015b), *ORTEP-3 for Windows* (Farrugia, 2012), *DIAMOND* (Brandenburg, 2006) and *pubCIF* (Westrip, 2010).

was collected, filtered, rinsed with distilled water and dried in air. Optical microscopy revealed two types of crystals, *viz.* dark-purple and dark-red rectangular crystals. X-ray diffraction analysis showed the red crystals to be Co₂(OH)PO₄ (Harrison *et al.*, 1995). The purple parallelepipeds correspond to the title compound.

Infrared spectroscopic measurements were performed on a VERTEX 70 FT-IR spectrometer, using the MRI transmission technique using KBr pellets. An adequate quantity of the studied phosphate powder, obtained by grinding the SrCo₄(OH)(PO₄)₃ crystals, was diluted in KBr before being pressed into a pellet. The analysis was performed at room temperature, and the spectrum was recorded in the range 4000–400 cm⁻¹.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. The hydrogen atom of the OH group was located in a difference-Fourier map and was refined as a fixed O–H bond length of 0.82 Å and *U*_{iso}(H) = 1.5*U*_{eq}(O). The maximum and minimum remaining electron density was located at 0.69 Å from Sr1 and 0.56 Å from Co4, respectively. The reflection (011) was affected by the beam-stop (*F*_o² = 0) while reflections (052) and (053), having *F*_o² > *F*_c², were probably affected by the Renninger effect. All three reflections were omitted from the refinement.

Acknowledgements

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supporting information

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Crystal structure of SrCo₄(OH)(PO₄)₃, a new hydroxyphosphate

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Computing details

Data collection: *APEX2* (Bruker, 2016); cell refinement: *S SAINT* (Bruker, 2016); data reduction: *S SAINT* (Bruker, 2016); program(s) used to solve structure: *SHELXT2014/5* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2018/3* (Sheldrick, 2015b); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012), *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

Strontium tetracobalt tris(orthophosphate) hydroxide

Crystal data

SrCo₄(OH)(PO₄)₃

$M_r = 625.26$

Orthorhombic, $P2_12_12_1$

$a = 5.1245$ (1) Å

$b = 12.0491$ (2) Å

$c = 15.7118$ (3) Å

$V = 970.13$ (3) Å³

$Z = 4$

$F(000) = 1184$

$D_x = 4.281$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 4243 reflections

$\theta = 2.6\text{--}35.0^\circ$

$\mu = 12.74$ mm⁻¹

$T = 296$ K

Parallelepiped, violet

$0.35 \times 0.26 \times 0.17$ mm

Data collection

Bruker X8 APEX Diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

φ and ω scans

Absorption correction: multi-scan
(SADABS; Krause *et al.*, 2015)

$T_{\min} = 0.391$, $T_{\max} = 0.748$

34471 measured reflections

4243 independent reflections

4038 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.045$

$\theta_{\max} = 35.0^\circ$, $\theta_{\min} = 2.6^\circ$

$h = -8 \rightarrow 8$

$k = -19 \rightarrow 18$

$l = -25 \rightarrow 25$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.022$

$wR(F^2) = 0.050$

$S = 1.07$

4243 reflections

191 parameters

0 restraints

Hydrogen site location: difference Fourier map

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0221P)^2]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 1.60$ e Å⁻³

$\Delta\rho_{\min} = -0.68$ e Å⁻³

Extinction correction: SHELXL-2018/3
(Sheldrick, 2015b),

$F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0042 (3)

Absolute structure: Flack x determined using
1625 quotients $[(F^+)-(F^-)]/[(F^+)+(F^-)]$ (Parsons *et al.*, 2013).

Absolute structure parameter: 0.008 (3)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Sr1	0.02677 (6)	0.72309 (2)	0.67782 (2)	0.00840 (6)
Co1	0.51704 (8)	0.48429 (3)	0.35972 (3)	0.00572 (8)
Co2	0.53401 (9)	0.58186 (4)	0.54997 (3)	0.00613 (8)
Co3	0.47299 (8)	0.46200 (3)	0.74367 (3)	0.00580 (8)
Co4	0.28203 (8)	0.32358 (4)	0.51444 (3)	0.00794 (9)
P1	0.51747 (15)	0.85171 (6)	0.57349 (5)	0.00425 (12)
P2	0.01127 (15)	0.45034 (6)	0.65719 (5)	0.00471 (13)
P3	-0.00586 (15)	0.30856 (6)	0.33173 (5)	0.00413 (12)
O1	0.4003 (4)	0.8648 (2)	0.48533 (15)	0.0092 (4)
O2	0.8108 (4)	0.8848 (2)	0.57323 (15)	0.0074 (4)
O3	0.3638 (4)	0.9243 (2)	0.63798 (15)	0.0074 (4)
O4	0.4924 (5)	0.73162 (18)	0.60637 (15)	0.0095 (4)
O5	0.2427 (4)	0.5287 (2)	0.63664 (15)	0.0078 (4)
O6	-0.2433 (4)	0.5173 (2)	0.66027 (15)	0.0075 (4)
O7	0.0710 (4)	0.40910 (19)	0.74879 (15)	0.0068 (4)
O8	-0.0011 (5)	0.3572 (2)	0.59242 (14)	0.0108 (4)
O9	0.1926 (4)	0.40027 (19)	0.30856 (15)	0.0073 (4)
O10	0.0074 (4)	0.29074 (18)	0.43053 (14)	0.0080 (4)
O11	-0.2813 (4)	0.34923 (19)	0.30965 (15)	0.0075 (4)
O12	0.0671 (4)	0.20305 (19)	0.28586 (16)	0.0097 (4)
O13	0.5519 (4)	0.43152 (18)	0.48508 (15)	0.0073 (4)
H13	0.691669	0.405651	0.500919	0.011*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sr1	0.01002 (12)	0.00611 (12)	0.00908 (12)	0.00095 (10)	0.00229 (10)	0.00061 (10)
Co1	0.00609 (16)	0.00557 (17)	0.00550 (17)	-0.00054 (14)	-0.00005 (14)	-0.00035 (13)
Co2	0.00739 (17)	0.00508 (17)	0.00593 (17)	-0.00087 (15)	0.00149 (14)	-0.00104 (13)
Co3	0.00560 (16)	0.00635 (17)	0.00544 (16)	0.00038 (14)	0.00019 (14)	0.00037 (13)
Co4	0.00687 (17)	0.0095 (2)	0.00748 (18)	-0.00059 (14)	-0.00076 (14)	0.00135 (16)
P1	0.0047 (3)	0.0041 (3)	0.0039 (3)	-0.0005 (3)	0.0001 (2)	0.0001 (2)
P2	0.0044 (3)	0.0055 (3)	0.0042 (3)	0.0001 (3)	-0.0001 (2)	0.0002 (2)
P3	0.0051 (3)	0.0035 (3)	0.0038 (3)	-0.0002 (2)	-0.0002 (2)	0.0000 (2)
O1	0.0093 (9)	0.0138 (11)	0.0045 (9)	0.0012 (8)	-0.0026 (8)	-0.0010 (9)

O2	0.0044 (9)	0.0098 (10)	0.0079 (10)	-0.0026 (8)	0.0002 (7)	-0.0008 (8)
O3	0.0069 (9)	0.0083 (10)	0.0071 (10)	0.0033 (8)	-0.0001 (7)	-0.0022 (9)
O4	0.0140 (10)	0.0036 (9)	0.0109 (9)	-0.0001 (9)	0.0049 (8)	0.0008 (7)
O5	0.0058 (9)	0.0099 (10)	0.0077 (10)	-0.0020 (8)	0.0004 (7)	0.0028 (9)
O6	0.0061 (9)	0.0099 (11)	0.0065 (10)	0.0027 (8)	-0.0002 (7)	0.0016 (8)
O7	0.0069 (9)	0.0073 (10)	0.0062 (9)	-0.0016 (7)	-0.0012 (7)	0.0015 (8)
O8	0.0115 (10)	0.0114 (10)	0.0094 (10)	-0.0022 (9)	0.0030 (9)	-0.0059 (8)
O9	0.0077 (9)	0.0055 (9)	0.0088 (10)	-0.0020 (7)	0.0004 (7)	0.0022 (8)
O10	0.0095 (10)	0.0104 (10)	0.0039 (9)	-0.0020 (8)	0.0000 (8)	0.0008 (7)
O11	0.0062 (9)	0.0081 (10)	0.0082 (10)	0.0008 (8)	-0.0016 (7)	-0.0017 (8)
O12	0.0120 (10)	0.0060 (10)	0.0111 (10)	0.0014 (8)	-0.0002 (8)	-0.0035 (8)
O13	0.0068 (9)	0.0058 (9)	0.0092 (9)	0.0006 (7)	-0.0002 (8)	0.0003 (8)

Geometric parameters (Å, °)

Sr1—O7 ⁱ	2.570 (2)	Co3—O6 ^{vi}	2.067 (2)
Sr1—O11 ⁱⁱ	2.575 (2)	Co3—O3 ^{ix}	2.089 (2)
Sr1—O4	2.639 (2)	Co3—O12 ^x	2.098 (2)
Sr1—O5	2.669 (2)	Co3—O9 ^{iv}	2.125 (2)
Sr1—O2 ⁱⁱⁱ	2.779 (2)	Co3—O7	2.158 (2)
Sr1—O12 ^{iv}	2.829 (2)	Co3—O5	2.206 (2)
Sr1—O1 ^v	2.848 (2)	Co4—O8	1.942 (2)
Sr1—O6	2.853 (2)	Co4—O13	1.954 (2)
Sr1—O9 ^{iv}	2.915 (2)	Co4—O10	1.969 (2)
Sr1—O4 ⁱⁱⁱ	2.961 (2)	Co4—O10 ^x	1.995 (2)
Sr1—O3	3.041 (2)	P1—O1	1.518 (2)
Co1—O13	2.077 (2)	P1—O4	1.542 (2)
Co1—O11 ^{vi}	2.082 (2)	P1—O3	1.553 (2)
Co1—O3 ^{vii}	2.091 (2)	P1—O2	1.555 (2)
Co1—O9	2.106 (2)	P2—O8	1.517 (2)
Co1—O2 ^v	2.171 (2)	P2—O6	1.534 (2)
Co1—O7 ^{viii}	2.212 (2)	P2—O5	1.550 (2)
Co2—O4	2.022 (2)	P2—O7	1.553 (2)
Co2—O1 ^{vii}	2.060 (2)	P3—O12	1.508 (2)
Co2—O13	2.081 (2)	P3—O11	1.534 (2)
Co2—O5	2.120 (2)	P3—O9	1.545 (2)
Co2—O6 ^{vi}	2.216 (2)	P3—O10	1.569 (2)
Co2—O2 ^v	2.284 (2)	O13—H13	0.8200
O7 ⁱ —Sr1—O11 ⁱⁱ	80.73 (7)	O9—Co1—O2 ^v	98.63 (9)
O7 ⁱ —Sr1—O4	109.46 (7)	O13—Co1—O7 ^{viii}	160.47 (9)
O11 ⁱⁱ —Sr1—O4	142.85 (7)	O11 ^{vi} —Co1—O7 ^{viii}	104.92 (9)
O7 ⁱ —Sr1—O5	162.67 (7)	O3 ^{vii} —Co1—O7 ^{viii}	83.16 (8)
O11 ⁱⁱ —Sr1—O5	95.77 (7)	O9—Co1—O7 ^{viii}	79.48 (8)
O4—Sr1—O5	63.66 (7)	O2 ^v —Co1—O7 ^{viii}	82.02 (9)
O7 ⁱ —Sr1—O2 ⁱⁱⁱ	64.92 (7)	O4—Co2—O1 ^{vii}	86.30 (10)
O11 ⁱⁱ —Sr1—O2 ⁱⁱⁱ	121.22 (7)	O4—Co2—O13	175.22 (10)
O4—Sr1—O2 ⁱⁱⁱ	94.66 (7)	O1 ^{vii} —Co2—O13	95.72 (9)

O5—Sr1—O2 ⁱⁱⁱ	129.56 (7)	O4—Co2—O5	85.04 (9)
O7 ⁱ —Sr1—O12 ^{iv}	66.42 (7)	O1 ^{vii} —Co2—O5	155.36 (9)
O11 ⁱⁱ —Sr1—O12 ^{iv}	89.04 (7)	O13—Co2—O5	94.75 (9)
O4—Sr1—O12 ^{iv}	65.03 (7)	O4—Co2—O6 ^{vi}	91.44 (10)
O5—Sr1—O12 ^{iv}	96.69 (7)	O1 ^{vii} —Co2—O6 ^{vi}	81.43 (9)
O2 ⁱⁱⁱ —Sr1—O12 ^{iv}	115.29 (7)	O13—Co2—O6 ^{vi}	93.14 (9)
O7 ⁱ —Sr1—O1 ^v	133.13 (7)	O5—Co2—O6 ^{vi}	75.77 (9)
O11 ⁱⁱ —Sr1—O1 ^v	119.13 (7)	O4—Co2—O2 ^v	99.31 (9)
O4—Sr1—O1 ^v	80.64 (7)	O1 ^{vii} —Co2—O2 ^v	99.98 (9)
O5—Sr1—O1 ^v	63.27 (7)	O13—Co2—O2 ^v	76.10 (9)
O2 ⁱⁱⁱ —Sr1—O1 ^v	68.76 (7)	O5—Co2—O2 ^v	104.17 (9)
O12 ^{iv} —Sr1—O1 ^v	145.52 (7)	O6 ^{vi} —Co2—O2 ^v	169.22 (9)
O7 ⁱ —Sr1—O6	134.98 (7)	O6 ^{vi} —Co3—O3 ^{ix}	110.65 (9)
O11 ⁱⁱ —Sr1—O6	63.04 (7)	O6 ^{vi} —Co3—O12 ^x	90.20 (10)
O4—Sr1—O6	115.55 (7)	O3 ^{ix} —Co3—O12 ^x	84.17 (10)
O5—Sr1—O6	54.21 (6)	O6 ^{vi} —Co3—O9 ^{iv}	109.48 (9)
O2 ⁱⁱⁱ —Sr1—O6	111.05 (7)	O3 ^{ix} —Co3—O9 ^{iv}	84.42 (9)
O12 ^{iv} —Sr1—O6	133.49 (7)	O12 ^x —Co3—O9 ^{iv}	159.76 (10)
O1 ^v —Sr1—O6	58.64 (7)	O6 ^{vi} —Co3—O7	142.20 (9)
O7 ⁱ —Sr1—O9 ^{iv}	102.99 (7)	O3 ^{ix} —Co3—O7	106.54 (9)
O11 ⁱⁱ —Sr1—O9 ^{iv}	60.11 (7)	O12 ^x —Co3—O7	87.01 (9)
O4—Sr1—O9 ^{iv}	82.74 (7)	O9 ^{iv} —Co3—O7	80.30 (9)
O5—Sr1—O9 ^{iv}	61.25 (7)	O6 ^{vi} —Co3—O5	77.04 (9)
O2 ⁱⁱⁱ —Sr1—O9 ^{iv}	166.11 (7)	O3 ^{ix} —Co3—O5	166.41 (9)
O12 ^{iv} —Sr1—O9 ^{iv}	51.30 (6)	O12 ^x —Co3—O5	107.46 (10)
O1 ^v —Sr1—O9 ^{iv}	123.85 (7)	O9 ^{iv} —Co3—O5	82.38 (9)
O6—Sr1—O9 ^{iv}	82.19 (6)	O7—Co3—O5	68.00 (8)
O7 ⁱ —Sr1—O4 ⁱⁱⁱ	87.68 (6)	O8—Co4—O13	122.63 (10)
O11 ⁱⁱ —Sr1—O4 ⁱⁱⁱ	82.23 (7)	O8—Co4—O10	86.00 (10)
O4—Sr1—O4 ⁱⁱⁱ	132.33 (9)	O13—Co4—O10	118.80 (9)
O5—Sr1—O4 ⁱⁱⁱ	108.78 (7)	O8—Co4—O10 ^x	107.64 (10)
O2 ⁱⁱⁱ —Sr1—O4 ⁱⁱⁱ	51.92 (6)	O13—Co4—O10 ^x	98.76 (9)
O12 ^{iv} —Sr1—O4 ⁱⁱⁱ	153.73 (7)	O10—Co4—O10 ^x	124.43 (5)
O1 ^v —Sr1—O4 ⁱⁱⁱ	57.40 (6)	O1—P1—O4	111.72 (14)
O6—Sr1—O4 ⁱⁱⁱ	62.94 (6)	O1—P1—O3	109.66 (13)
O9 ^{iv} —Sr1—O4 ⁱⁱⁱ	137.82 (6)	O4—P1—O3	105.51 (13)
O7 ⁱ —Sr1—O3	60.53 (7)	O1—P1—O2	110.70 (14)
O11 ⁱⁱ —Sr1—O3	135.45 (7)	O4—P1—O2	108.80 (14)
O4—Sr1—O3	50.80 (6)	O3—P1—O2	110.33 (13)
O5—Sr1—O3	114.45 (6)	O8—P2—O6	112.00 (14)
O2 ⁱⁱⁱ —Sr1—O3	62.97 (6)	O8—P2—O5	110.08 (14)
O12 ^{iv} —Sr1—O3	56.98 (7)	O6—P2—O5	109.67 (13)
O1 ^v —Sr1—O3	103.90 (6)	O8—P2—O7	113.16 (14)
O6—Sr1—O3	161.48 (6)	O6—P2—O7	107.85 (13)
O9 ^{iv} —Sr1—O3	105.74 (6)	O5—P2—O7	103.72 (12)
O4 ⁱⁱⁱ —Sr1—O3	114.80 (6)	O12—P3—O11	112.92 (13)
O13—Co1—O11 ^{vi}	94.38 (9)	O12—P3—O9	109.08 (14)
O13—Co1—O3 ^{vii}	94.12 (9)	O11—P3—O9	108.90 (13)

O11 ^{vi} —Co1—O3 ^{vii}	89.80 (9)	O12—P3—O10	110.29 (14)
O13—Co1—O9	106.41 (9)	O11—P3—O10	107.90 (13)
O11 ^{vi} —Co1—O9	82.65 (9)	O9—P3—O10	107.61 (13)
O3 ^{vii} —Co1—O9	158.54 (9)	Co4—O13—H13	107.1
O13—Co1—O2 ^v	78.70 (9)	Co1—O13—H13	118.6
O11 ^{vi} —Co1—O2 ^v	173.06 (9)	Co2—O13—H13	102.7
O3 ^{vii} —Co1—O2 ^v	91.29 (9)		

Symmetry codes: (i) $-x, y+1/2, -z+3/2$; (ii) $-x-1/2, -y+1, z+1/2$; (iii) $x-1, y, z$; (iv) $-x+1/2, -y+1, z+1/2$; (v) $x-1/2, -y+3/2, -z+1$; (vi) $x+1, y, z$; (vii) $x+1/2, -y+3/2, -z+1$; (viii) $-x+1/2, -y+1, z-1/2$; (ix) $-x+1, y-1/2, -z+3/2$; (x) $x+1/2, -y+1/2, -z+1$.

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
O13—H13 \cdots O8 ^{vi}	0.82	2.21	2.982 (3)	157
O13—H13 \cdots O10 ^{vi}	0.82	2.40	3.010 (3)	132

Symmetry code: (vi) $x+1, y, z$.