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Sodium scandium diphosphate, $NaScP_2O_7$, isotypic with α-NaTi(III)P_2O_7

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Key indicators: single-crystal X-ray study; T = 293 K; mean σ(Sc–O) = 0.002 Å; R factor = 0.025; wR factor = 0.082; data-to-parameter ratio = 10.1.

Crystals of the title compound, $NaScP_2O_7$, were grown by a flux method. The crystal structure is isotypic with those of α-$NaTiP_2O_7$, $NaYbP_2O_7$ and $NaLuP_2O_7$, and is closely related to that of $NaYP_2O_7$. The structural set-up consists of a three-dimensional framework of P_2O_7 units that are corner-shared by ScO_6 octahedra, forming tunnels running parallel to [010]. The Na atoms are situated in the tunnels and are surrounded by nine O atoms in a distorted environment.

Related literature

Previous X-ray powder data of $NaScP_2O_7$ were reported by Vitins *et al.* (2000). $NaScP_2O_7$ is isotypic with α-$NaTiP_2O_7$ (Leclaire *et al.*, 1988), $NaYbP_2O_7$ (Férid *et al.*, 2004) and $NaLuP_2O_7$ (Yuan *et al.*, 2007) and shows similar structural features as $NaYP_2O_7$ (Hamady & Jouini, 1996). Both structure types are topologically related to β-cristobalite (Leclaire *et al.*, 1988). For a detailed review on the structures of $A^IM^{III}P_2O_7$-type diphosphates, see: Li *et al.* (2005); Schwendtner & Kolitsch (2004). For possible applications as scintillators or phosphor materials based on $A^IM^{III}P_2O_7$-type diphosphates, see: Hizhnyi *et al.* (2007, 2008). For background to structural parameters, see: Brese & O'Keeffe (1991); Robinson *et al.* (1971).

Experimental

Crystal data

$NaScP_2O_7$
M_r = 241.89
Monoclinic, $P2_1/n$
a = 8.9044 (18) Å
b = 5.3300 (11) Å
c = 12.516 (3) Å
β = 104.11 (3)°
V = 576.1 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.89 mm^{-1}
T = 293 K
0.40 × 0.15 × 0.05 mm

Data collection

Kuma KM-4-CCD diffractometer
Absorption correction: multi-scan (*CrysAlis CCD*; Oxford Diffraction, 2003) T_{min} = 0.067, T_{max} = 0.093
5082 measured reflections
1018 independent reflections
932 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.082
S = 1.18
1018 reflections
101 parameters
$\Delta\rho_{max}$ = 0.46 e Å^{-3}
$\Delta\rho_{min}$ = −0.46 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Sc—O3	2.0217 (19)	P1—O7	1.5254 (17)
Sc—O6^{i}	2.0770 (17)	P1—O4	1.5313 (18)
Sc—O7^{ii}	2.1112 (17)	P1—O5^{iii}	1.6114 (17)
Sc—O1	2.1220 (16)	P2—O3	1.5013 (19)
Sc—O2	2.1220 (16)	P2—O1^{iv}	1.5278 (16)
Sc—O4	2.1506 (18)	P2—O2^{v}	1.5332 (16)
P1—O6	1.5088 (17)	P2—O5	1.6151 (17)
P1^{vi}—O5—P2	125.47 (10)		

Symmetry codes: (i) $-x, -y+1, -z+1$; (ii) $-x, -y, -z+1$; (iii) $x-\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$; (iv) $-x+1, -y+1, -z+1$; (v) $-x+1, -y, -z+1$; (vi) $x+\frac{1}{2}, -y+\frac{1}{2}, z-\frac{1}{2}$.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2003); cell refinement: *CrysAlis CCD*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2003); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ATOMS* (Dowty, 2003); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2274).

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supplementary materials

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Sodium scandium diphosphate, $NaScP_2O_7$, isotypic with α-NaTi(III)P_2O_7

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Comment

$A^{I}M^{III}T^{V}{}_2O_7$-type compounds recently have received an increased attention, partly due to their possible applications as scintillators or phosphor materials (Hizhnyi *et al.*, 2007; Hizhnyi *et al.*, 2008). So far, the $A^{I}M^{III}P_2O_7$-type diphosphates are known to adopt eight different structure types which depends on the ratio of ionic radii of the alkali metal and the rare earth element or the three-valent metal M^{III}. Among the eight different structure types, the $KAlP_2O_7$-type structures are most common. For a detailed review including also diarsenates, see: Schwendtner & Kolitsch (2004); Li *et al.* (2005). In this article we present the structure of $NaScP_2O_7$ determined from single-crystal *x*-ray diffraction data. Previous X-ray powder data of $NaScP_2O_7$ were reported by Vitins *et al.* (2000). However, authors could not index all reflections at that time, probably because of by-products. The crystal structure of the title compound is isotypic with α-$NaTiP_2O_7$ (Leclaire *et al.*, 1988), $NaYbP_2O_7$ (Férid *et al.*, 2004) and $NaLuP_2O_7$ (Yuan *et al.*, 2007). It is also closely related to that of $NaYP_2O_7$ (Hamady and Jouini, 1996) and β-cristobalite (Leclaire *et al.*, 1988).

All atoms in the crystal structure occupy general positions. The structure is characterized by a three-dimensional framework of PO_4 tetrahedra (forming P_2O_7 groups via corner-sharing) and ScO_6 octahedra leading to narrow tunnels parallel to [010] which are occupied by Na atoms (Fig. 1). One ScO_6 octahedron is corner-linked to six tetrahedra of six different diphosphate groups, which are all oriented approximately perpendicular to (001) (Fig. 2). Tunnels are formed by stacking pseudohexagonal rings of $[Sc_2P_4O_{22}]$ units. A cage enclosing one Na atom is formed by three P_2O_7 groups, connected to four ScO_6 octahedra (Fig. 3).

The P—O bond-lengths range between 1.5088 (17) Å and 1.5332 (16) Å for terminal O of the diphosphate group that are connected to octahedra. The P1—$O5_{bridge}$—P2 angle is 125.47 (10) °, and corresponding bond lengths to the bridging O atom are 1.6114 (17) Å and 1.6151 (17) Å for <P1—O5> and <P2—O5>, respectively. The average Sc—O bond length is 2.101 Å, corresponding well with the average value for oxide compounds (2.105 Å; Brese & O'Keeffe, 1991). The ScO_6 octahedron is significantly less distorted (in terms of quadatic elongation; Robinson *et al.*, 1971) in comparison with the equivalent polyhedra in α-$NaTi^{3+}P_2O_7$, $NaLuP_2O_7$ and $NaYP_2O_7$; the polyhedral distortion is the lowest in $NaYbP_2O_7$ structure.

Experimental

$NaScP_2O_7$ crystals were grown by the flux-growth technique. The flux, sodium hexametaphosphate $(NaPO_3)_6$ (purity 3 N) was mixed together with Sc_2O_3 (purity 4 N) at a molar ratio of 6:1. The mixture was filled into a platinum crucible, covered by a loose fitting lid, and heated up to 1593 K within 3 h. The temperature was held for 24 h and afterwards slowly cooled down to 1503 K in the course of 72 h. The solidified flux was dissolved in hot water and crystals of $NaScP_2O_7$

were mechanically separated. The procedure produced transparent to translucent, colorless skeletal aggregates of tabular to acicular crystals, up to 23 mm in lengths. A fragment of a crystal was used for single-crystal structure determination.

Figures

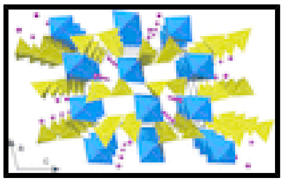

Fig. 1. Perspective view of the $NaScP_2O_7$ framework structure projected down [010]. Diphosphate groups are corner-linked to the deformed ScO_6 octahedra. Tunnels parallel to [010] are occupied by nine-coordinated atoms of Na. Displacement ellipsoids are drawn at the 50% probability level.

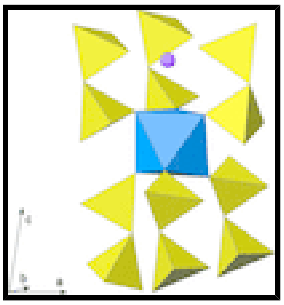

Fig. 2. View on six P_2O_7 groups corner-linked to the ScO_6 polyhedron.

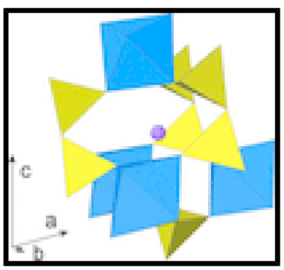

Fig. 3. Cage formed by three diphosphate groups and four ScO_6 polyhedra enclosing the Na cation.

Sodium scandium diphosphate

Crystal data

$NaScP_2O_7$	$F_{000} = 472$
$M_r = 241.89$	$D_x = 2.789$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2yn	Cell parameters from 5348 reflections
$a = 8.9044$ (18) Å	$\theta = 4.2$–27.2°
$b = 5.3300$ (11) Å	$\mu = 1.89$ mm^{-1}
$c = 12.516$ (3) Å	$T = 293$ K
$\beta = 104.11$ (3)°	Platy to fibrous fragment, colourless
$V = 576.1$ (2) Å^3	0.40 × 0.15 × 0.05 mm
$Z = 4$	

Data collection

Kuma KM-4-CCD diffractometer	1018 independent reflections
Radiation source: fine-focus sealed tube	932 reflections with $I > 2\sigma(I)$

Monochromator: graphite	R_{int} = 0.028
Detector resolution: 0.06 pixels mm^{-1}	θ_{max} = 25.0°
T = 293 K	θ_{min} = 4.2°
ω scans	$h = -10 \rightarrow 10$
Absorption correction: multi-scan (CrysAlis CCD; Oxford Diffraction, 2003)	$k = -4 \rightarrow 6$
T_{min} = 0.067, T_{max} = 0.093	$l = -14 \rightarrow 14$
5082 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0535P)^2 + 0.089P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.025	$(\Delta/\sigma)_{max}$ < 0.001
$wR(F^2)$ = 0.082	$\Delta\rho_{max}$ = 0.46 e Å^{-3}
S = 1.18	$\Delta\rho_{min}$ = −0.46 e Å^{-3}
1018 reflections	Extinction correction: SHELXL97 (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
101 parameters	Extinction coefficient: 0.080 (5)
Primary atom site location: structure-invariant direct methods	

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

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

	x	y	z	U_{iso}*/U_{eq}
Sc	0.26720 (5)	0.26098 (7)	0.52783 (4)	0.0137 (2)
P1	−0.06473 (7)	0.22372 (11)	0.61678 (5)	0.0140 (2)
P2	0.52089 (7)	0.25413 (10)	0.35283 (5)	0.0139 (2)
Na	0.35939 (11)	0.23101 (18)	0.81018 (9)	0.0278 (3)
O1	0.39845 (17)	0.4953 (3)	0.65350 (12)	0.0177 (4)
O2	0.36250 (17)	−0.0381 (3)	0.63494 (13)	0.0182 (4)
O3	0.4256 (2)	0.2456 (3)	0.43658 (14)	0.0210 (4)
O4	0.10881 (19)	0.2727 (3)	0.63286 (14)	0.0187 (4)
O5	0.39984 (18)	0.2187 (3)	0.23463 (13)	0.0175 (4)

O6	−0.16444 (17)	0.4047 (3)	0.53739 (12)	0.0220 (4)
O7	−0.10300 (18)	−0.0507 (3)	0.58783 (12)	0.0190 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sc	0.0124 (3)	0.0152 (3)	0.0135 (3)	0.00023 (15)	0.0032 (2)	0.00014 (16)
P1	0.0126 (4)	0.0155 (4)	0.0136 (4)	−0.0001 (2)	0.0025 (3)	−0.0002 (2)
P2	0.0127 (4)	0.0156 (4)	0.0134 (4)	0.0001 (2)	0.0033 (3)	0.0003 (2)
Na	0.0270 (7)	0.0245 (7)	0.0318 (7)	−0.0010 (4)	0.0069 (5)	0.0003 (4)
O1	0.0189 (8)	0.0161 (9)	0.0173 (8)	−0.0021 (6)	0.0028 (6)	0.0000 (6)
O2	0.0190 (8)	0.0172 (9)	0.0190 (8)	0.0026 (6)	0.0055 (6)	0.0014 (7)
O3	0.0208 (8)	0.0240 (11)	0.0196 (10)	0.0009 (6)	0.0077 (7)	0.0001 (6)
O4	0.0160 (8)	0.0238 (10)	0.0175 (9)	−0.0013 (6)	0.0062 (7)	−0.0020 (6)
O5	0.0149 (9)	0.0220 (10)	0.0156 (9)	−0.0018 (6)	0.0037 (7)	0.0005 (6)
O6	0.0240 (9)	0.0188 (10)	0.0215 (8)	0.0020 (7)	0.0022 (7)	0.0026 (7)
O7	0.0205 (8)	0.0168 (9)	0.0193 (8)	−0.0009 (7)	0.0041 (6)	−0.0006 (7)

Geometric parameters (Å, °)

Sc—O3	2.0217 (19)	P2—O2^{v}	1.5332 (16)
Sc—O6^{i}	2.0770 (17)	P2—O5	1.6151 (17)
Sc—O7^{ii}	2.1112 (17)	Na—O1	2.5066 (18)
Sc—O1	2.1220 (16)	Na—O7^{vi}	2.5176 (19)
Sc—O2	2.1220 (16)	Na—O4^{vii}	2.5410 (19)
Sc—O4	2.1506 (18)	Na—O2^{vi}	2.5597 (19)
P1—O6	1.5088 (17)	Na—O2	2.6264 (19)
P1—O7	1.5254 (17)	Na—O4	2.746 (2)
P1—O4	1.5313 (18)	Na—O1^{vii}	2.7505 (19)
P1—O5^{iii}	1.6114 (17)	Na—O4^{vi}	2.9710 (19)
P2—O3	1.5013 (19)	Na—O6^{viii}	2.992 (2)
P2—O1^{iv}	1.5278 (16)		
O3—Sc—O6^{i}	96.54 (6)	O4^{vii}—Na—O2^{vi}	115.31 (6)
O3—Sc—O7^{ii}	93.04 (7)	O1—Na—O2	67.77 (6)
O6^{i}—Sc—O7^{ii}	91.19 (6)	O7^{vi}—Na—O2	119.51 (6)
O3—Sc—O1	96.23 (7)	O4^{vii}—Na—O2	71.71 (6)
O6^{i}—Sc—O1	84.07 (7)	O2^{vi}—Na—O2	130.74 (5)
O7^{ii}—Sc—O1	170.01 (6)	O1—Na—O4	64.06 (6)
O3—Sc—O2	95.73 (6)	O7^{vi}—Na—O4	143.35 (6)
O6^{i}—Sc—O2	164.29 (6)	O4^{vii}—Na—O4	108.52 (6)
O7^{ii}—Sc—O2	97.93 (7)	O2^{vi}—Na—O4	69.49 (6)
O1—Sc—O2	84.87 (7)	O2—Na—O4	62.69 (6)
O3—Sc—O4	176.82 (7)	O1—Na—O1^{vii}	131.81 (5)
O6^{i}—Sc—O4	85.62 (6)	O7^{vi}—Na—O1^{vii}	141.08 (7)

O7^{ii}—Sc—O4	89.25 (6)	O4^{vii}—Na—O1^{vii}	63.57 (5)
O1—Sc—O4	81.63 (6)	O2^{vi}—Na—O1^{vii}	56.31 (6)
O2—Sc—O4	81.75 (6)	O2—Na—O1^{vii}	93.88 (6)
O6—P1—O7	113.28 (9)	O4—Na—O1^{vii}	67.92 (5)
O6—P1—O4	112.98 (9)	O1—Na—O4^{vi}	67.56 (5)
O7—P1—O4	110.77 (9)	O7^{vi}—Na—O4^{vi}	53.79 (5)
O6—P1—O5^{iii}	105.42 (9)	O4^{vii}—Na—O4^{vi}	150.38 (8)
O7—P1—O5^{iii}	108.54 (9)	O2^{vi}—Na—O4^{vi}	60.19 (5)
O4—P1—O5^{iii}	105.29 (10)	O2—Na—O4^{vi}	135.34 (6)
O3—P2—O1^{iv}	114.55 (9)	O4—Na—O4^{vi}	97.26 (6)
O3—P2—O2^{v}	113.07 (9)	O1^{vii}—Na—O4^{vi}	116.03 (6)
O1^{iv}—P2—O2^{v}	110.27 (9)	O1—Na—O6^{viii}	159.25 (6)
O3—P2—O5	105.75 (10)	O7^{vi}—Na—O6^{viii}	83.21 (6)
O1^{iv}—P2—O5	105.78 (9)	O4^{vii}—Na—O6^{viii}	61.94 (5)
O2^{v}—P2—O5	106.74 (9)	O2^{vi}—Na—O6^{viii}	67.85 (6)
O1—Na—O7^{vi}	82.54 (6)	O2—Na—O6^{viii}	132.80 (6)
O1—Na—O4^{vii}	137.09 (7)	O4—Na—O6^{viii}	123.78 (6)
O7^{vi}—Na—O4^{vii}	106.18 (6)	O1^{vii}—Na—O6^{viii}	58.46 (5)
O1—Na—O2^{vi}	101.72 (6)	O4^{vi}—Na—O6^{viii}	91.81 (5)
O7^{vi}—Na—O2^{vi}	105.53 (6)	P1^{ix}—O5—P2	125.47 (10)

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

Fig. 1

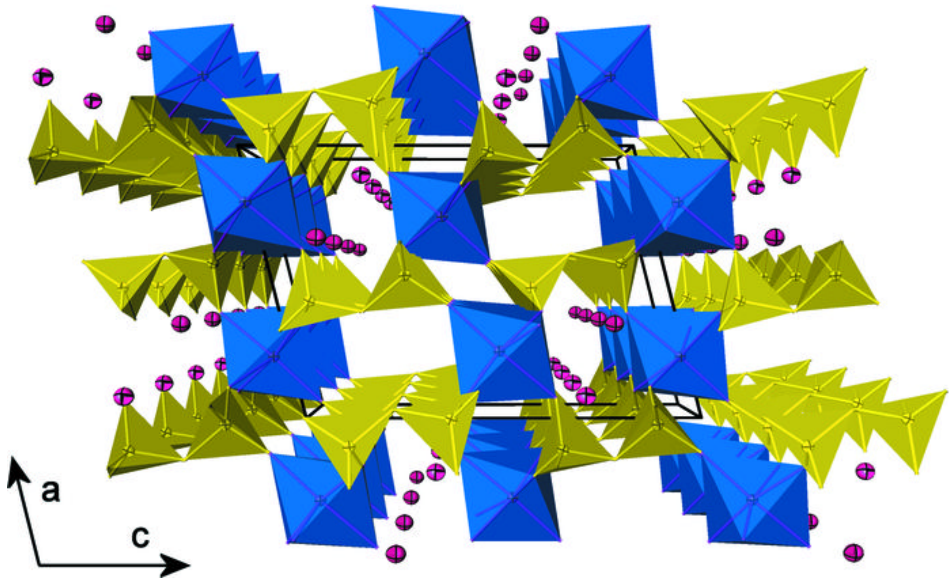

Fig. 2

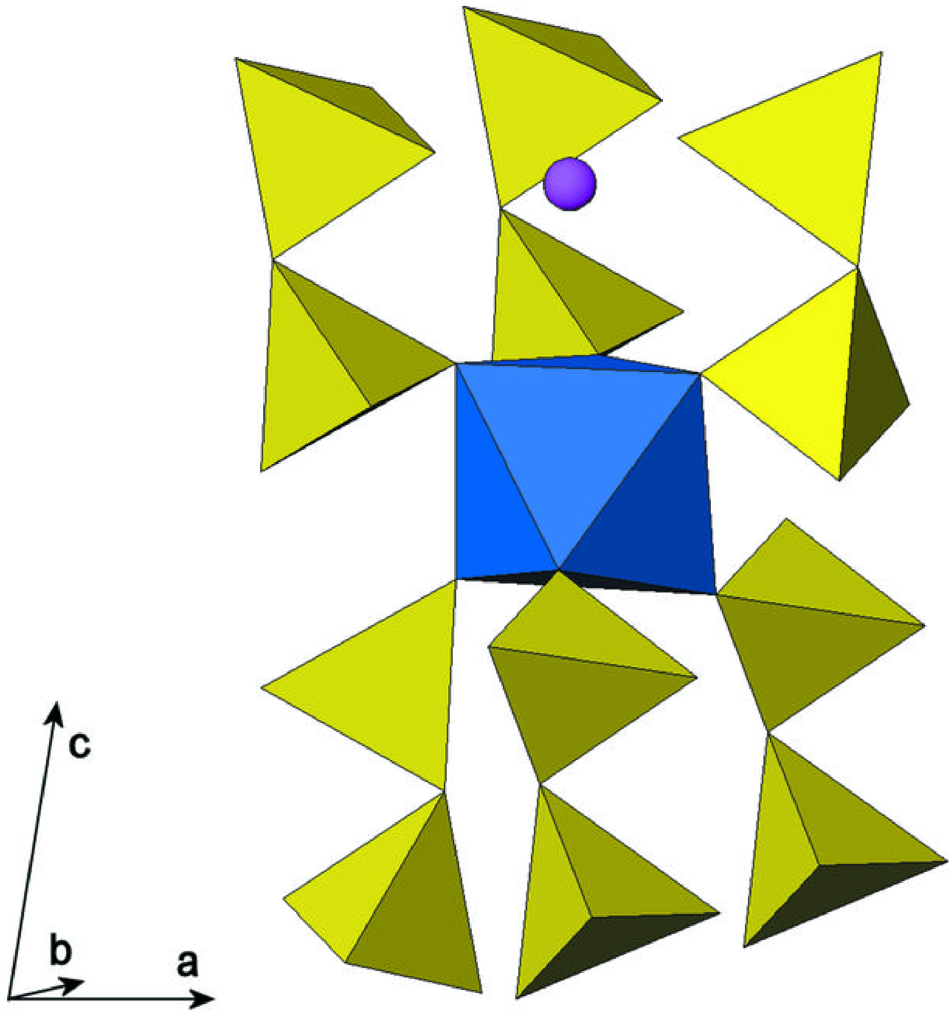

Fig. 3