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Silver indium diphosphate, $AgInP_2O_7$

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Key indicators: single-crystal X-ray study; T = 296 K, P = 0.0 kPa; mean σ(P–O) = 0.002 Å; R factor = 0.021; wR factor = 0.048; data-to-parameter ratio = 36.9.

Polycrystalline material of the title compound, $AgInP_2O_7$, was synthesized by traditional high-temperature solid-state methods and single crystals were grown from the melt of a mixture of $AgInP_2O_7$ and B_2O_3 as flux in a platinium crucible. The structure consists of InO_6 octahedra, which are corner-shared to PO_4 tetrahedra into a three-dimensional network with hexagonal channels running parallel to the *c* axis. The silver cation, located in the channel, is bonded to seven O atoms of the $[InP_2O_7]$ framework with Ag–O distances ranging from 2.370 (2) to 3.015 (2) Å. The P_2O_7 diphosphate anion is characterized by a P—O—P angle of 137.27 (9) and a nearly eclipsed conformation. $AgInP_2O_7$ is isotypic with the $M^IFeP_2O_7$ (M^I = Na, K, Rb, Cs and Ag) diphosphate family.

Related literature

For properties of $M^IFeP_2O_7$ (M^I = Na, K, Rb, Cs and Ag) diphosphates, see: Terebilenko *et al.* (2010); Hizhnyi *et al.* (2008); Whangbo *et al.* (2004); Vitins *et al.* (2000). For isotypic structures, see: Belkouch *et al.* (1995); Gabelica-Robert *et al.* (1982); Moya-Pizarro *et al.* (1984); Mercader *et al.* (1990).

Experimental

Crystal data

$AgInP_2O_7$
M_r = 396.63
Monoclinic, $P2_1/c$
a = 7.4867 (3) Å
b = 8.2620 (3) Å
c = 9.8383 (5) Å
β = 112.038 (2)°
V = 564.09 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 8.11 mm^{-1}
T = 296 K
0.08 × 0.06 × 0.05 mm

Data collection

Bruker X8 APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1999)
T_{min} = 0.563, T_{max} = 0.667
21692 measured reflections
3730 independent reflections
3245 reflections with $I > 2\sigma(I)$
R_{int} = 0.035

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.021
$wR(F^2)$ = 0.048
S = 1.03
3730 reflections
101 parameters
$\Delta\rho_{max}$ = 1.62 e Å^{-3}
$\Delta\rho_{min}$ = −2.04 e Å^{-3}

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BR2154).

References

Belkouch, J., Monceaux, L. & Courtine, P. (1995). *Mater. Res. Bull.* **30**, 149–160.
Bruker (2005). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Gabelica-Robert, M., Goreaud, M., Labbe, Ph. & Raveau, B. (1982). *J. Solid State Chem.* **45**, 389–395.
Hizhnyi, Y. A., Oliynyk, A., Gomenyuk, O., Nedilko, S. G., Nagornyi, P., Bojko, R. & Bojko, V. (2008). *Opt. Mater.* **30**, 687–689.
Mercader, R. C., Terminiello, L., Long, G. J., Reichel, D. G., Dickhaus, K., Zysler, R., Sanchez, R. & Tovar, M. (1990). *Phys. Rev. B Condens. Matter*, **42**, 25–32.
Moya-Pizarro, T., Salmon, R., Fournes, S. L., Le Flem, G., Wanklyn, B. S. & Hagenmuller, P. (1984). *J. Solid State Chem.* **53**, 387–397.
Sheldrick, G. M. (1999). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Terebilenko, K. V., Kirichok, A. A., Baumer, V. N., Sereduk, M., Slobodyanik, N. S. & Gütlich, P. (2010). *J. Solid State Chem.* **183**, 1473–1476.
Vitins, G., Kanepe, Z., Vitins, A., Ronis, J., Dindune, A. & Lusis, A. (2000). *J. Solid State Electochem.* **4**, 146–152.
Whangbo, M.-H., Dai, D. & Koo, H.-J. (2004). *Dalton Trans.* pp. 3019–3025.

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supplementary materials

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Silver indium diphosphate, $AgInP_2O_7$

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Comment

The diphosphates $A^IM^{III}P_2O_7$ (A^I = Li, Na, K, Rb, Cs and Ag; M^{III} = Al, Ga, Cr, Fe, In, Y) are extensively studied for their electrical and optical properties and for its perspective application as magnetic materials (Terebilenko *et al.* (2010); Hizhnyi *et al.* (2008); Whangbo *et al.* (2004); Vitins *et al.* (2000)). The crystal structures of most of these compounds are known except a few cases in which the crystal growth is difficult. In this context, the present paper reports on the determination of $AgInP_2O_7$ crystal structure from X-ray diffraction single-crystal data.

The structure of this phosphate is characterized by a three-dimensional network built up from indum octahedra linked to diphosphate groups by a corner-sharing. Each InO_6 octahedra is surrounded by six PO_4 tetrahedra belonging to five different P_2O_7 groups (see Fig.1 and Fig.2). As a result of these blocks, assemblage three-dimensional-framework is formed with hexagonal channels, where silver cations reside. Although, the coordination sphere of Ag^+ cations is composed of seven O^{2-} anions in an irregular geometry, located at Ag–O distances between 2.370 (2) and 3.015 (2) Å (see Fig.2). Furthermore, the diphosphate group contains two distorted PO_4 tetrahedra sharing one corner and display a nearly eclipsed conformation. The P–O bond-lengths range between 1.492 (2) Å for terminal P1–O1 and 1.606 (2) Å for the bridging P2–O7 bond. Therefore, a P1–O7–P2 angle of 137.27 (9) ° is wider than 133.6 (3)° and 132.9 (3) ° reported for both $AgFeP_2O_7$ and $NaFeP_2O_7$ respectively (Belkouch *et al.* (1995); Gabelica-Robert *et al.* (1982); Moya-Pizarro *et al.* (1984); Mercader *et al.* (1990)).

Silver indium diphosphate (pyrophosphate) is isostructural to $A^IFeP_2O_7$ (A^I = Na, K, Rb, Cs and Ag) diphosphates family and is categorized as a dichromate type.

Experimental

$AgInP_2O_7$ in the form of single crystals was prepared by stoichiometric reaction of $AgNO_3$, $(NH_4)_2HPO_4$ and In_2O_3 in B_2O_3 flux. The mixture was heated at 773 K under ambiante atmosphere for 6 h and 973 K for 2 h with intermediate grindings to ensure complete reaction. Subsequent melting at 1323 K followed by slow cooling to room temperature at a rate of 12°K h^{-1} resulted in colourless crystals of the title compound.

Refinement

The highest and deepest hole residual peak in the final difference Fourier map are located at 0.49 Å and 0.58 Å, respectively from Ag1 atom. The not significants bonds and angles were removed from the CIF file.

Figures

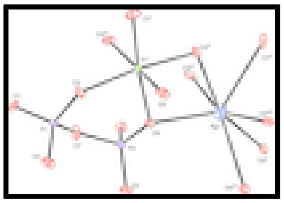

Fig. 1. Partial plot of $AgInP_2O_7$ crystal structure shawing plyhedra linkage. Displacement ellipsoids are drawn at the 50% probability level. Symmetry codes: (i) $-x + 1, y - 1/2, -z + 1/2$; (ii) $-x, y - 1/2, -z + 1/2$; (iii) $-x + 1, -y + 1, -z + 1$; (iv) $x, -y + 3/2, z - 1/2$; (v) $x - 1, y, z$; (vi) $x - 1, -y + 3/2, z - 1/2$; (vii) $-x, -y + 1, -z + 1$.

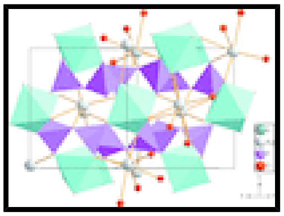

Fig. 2. Perspective view along [101] of the $AgInP_2O_7$ framework structure shawing tunnel where silver cations are located.

Silver indium diphosphate

Crystal data

$AgInP_2O_7$	$F(000) = 728$
$M_r = 396.63$	$D_x = 4.670$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 317 reflections
$a = 7.4867$ (3) Å	$\theta = 2.5–30.2°$
$b = 8.2620$ (3) Å	$\mu = 8.11$ mm^{-1}
$c = 9.8383$ (5) Å	$T = 296$ K
$\beta = 112.038$ (2)°	Block, colourless
$V = 564.09$ (4) Å^3	0.08 × 0.06 × 0.05 mm
$Z = 4$	

Data collection

Bruker X8 APEXII CCD area-detector diffractometer	3730 independent reflections
Radiation source: fine-focus sealed tube	3245 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.035$
ω and φ scans	$\theta_{max} = 41.0°$, $\theta_{min} = 2.9°$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1999)	$h = -13\rightarrow13$
$T_{min} = 0.563$, $T_{max} = 0.667$	$k = -15\rightarrow15$
21692 measured reflections	$l = -18\rightarrow18$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map

$R[F^2 > 2\sigma(F^2)] = 0.021$	$w = 1/[\sigma^2(F_o^2) + (0.017P)^2 + 0.9979P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.048$	$(\Delta/\sigma)_{max} = 0.001$
$S = 1.03$	$\Delta\rho_{max} = 1.62$ e Å^{-3}
3730 reflections	$\Delta\rho_{min} = -2.04$ e Å^{-3}
101 parameters	Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
0 restraints	Extinction coefficient: 0.0171 (4)

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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}
In1	0.242354 (15)	0.495357 (12)	0.247622 (11)	0.00618 (3)
Ag1	−0.20911 (3)	0.52697 (2)	0.30478 (2)	0.02442 (4)
P1	0.57689 (6)	0.74758 (5)	0.46083 (4)	0.00600 (6)
P2	0.17589 (6)	0.78735 (5)	0.45174 (4)	0.00656 (6)
O1	0.6810 (2)	0.86792 (17)	0.40464 (15)	0.0141 (2)
O2	0.6836 (2)	0.71622 (16)	0.62241 (14)	0.0136 (2)
O3	0.52473 (17)	0.59259 (15)	0.36935 (14)	0.01027 (19)
O4	0.04427 (18)	0.91166 (17)	0.35059 (15)	0.0123 (2)
O5	0.1917 (2)	0.79561 (16)	0.60976 (14)	0.0126 (2)
O6	0.13231 (18)	0.61348 (15)	0.39564 (14)	0.01054 (19)
O7	0.37868 (18)	0.83601 (16)	0.44239 (16)	0.0128 (2)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
In1	0.00656 (4)	0.00614 (4)	0.00593 (4)	−0.00024 (3)	0.00244 (3)	−0.00045 (3)
Ag1	0.01913 (7)	0.02720 (8)	0.03341 (9)	−0.00235 (6)	0.01725 (7)	−0.01071 (7)
P1	0.00574 (14)	0.00643 (14)	0.00582 (14)	−0.00025 (11)	0.00217 (11)	0.00044 (11)
P2	0.00588 (14)	0.00706 (14)	0.00644 (14)	0.00073 (11)	0.00195 (11)	−0.00090 (12)
O1	0.0185 (6)	0.0141 (5)	0.0133 (5)	−0.0053 (4)	0.0104 (5)	0.0012 (4)
O2	0.0195 (6)	0.0098 (5)	0.0070 (4)	−0.0006 (4)	−0.0001 (4)	0.0018 (4)
O3	0.0072 (4)	0.0099 (5)	0.0130 (5)	−0.0012 (3)	0.0030 (4)	−0.0040 (4)
O4	0.0084 (5)	0.0135 (5)	0.0135 (5)	0.0034 (4)	0.0023 (4)	0.0041 (4)

O5	0.0211 (6)	0.0099 (5)	0.0072 (4)	−0.0009 (4)	0.0058 (4)	−0.0023 (4)
O6	0.0116 (5)	0.0097 (5)	0.0123 (5)	−0.0019 (4)	0.0067 (4)	−0.0039 (4)
O7	0.0078 (5)	0.0100 (5)	0.0217 (6)	0.0010 (4)	0.0069 (4)	−0.0020 (4)

Geometric parameters (Å, °)

In1—O1^{i}	2.0799 (13)	Ag1—O5^{vii}	2.7829 (14)
In1—O4^{ii}	2.1120 (12)	Ag1—O6^{vii}	3.0153 (14)
In1—O2^{iii}	2.1133 (13)	P1—O1	1.4919 (13)
In1—O5^{iv}	2.1401 (13)	P1—O2	1.5097 (13)
In1—O3	2.1562 (12)	P1—O3	1.5292 (13)
In1—O6	2.1569 (12)	P1—O7	1.6021 (13)
Ag1—O3^{v}	2.3703 (12)	P2—O4	1.5101 (13)
Ag1—O6	2.4757 (13)	P2—O5	1.5158 (13)
Ag1—O4^{ii}	2.4865 (14)	P2—O6	1.5295 (13)
Ag1—O2^{vi}	2.6991 (14)	P2—O7	1.6062 (13)
Ag1—O7^{ii}	2.7744 (15)		
O1^{i}—In1—O4^{ii}	90.70 (6)	O3^{v}—Ag1—O5^{vii}	94.99 (4)
O1^{i}—In1—O2^{iii}	86.35 (6)	O6—Ag1—O5^{vii}	104.03 (4)
O4^{ii}—In1—O2^{iii}	89.82 (6)	O4^{ii}—Ag1—O5^{vii}	80.85 (4)
O1^{i}—In1—O5^{iv}	89.04 (5)	O2^{vi}—Ag1—O5^{vii}	157.25 (4)
O4^{ii}—In1—O5^{iv}	93.79 (5)	O7^{ii}—Ag1—O5^{vii}	71.00 (4)
O2^{iii}—In1—O5^{iv}	174.18 (6)	O3^{v}—Ag1—O6^{vii}	72.37 (4)
O1^{i}—In1—O3	96.36 (5)	O6—Ag1—O6^{vii}	88.04 (4)
O4^{ii}—In1—O3	172.86 (5)	O4^{ii}—Ag1—O6^{vii}	119.79 (4)
O2^{iii}—In1—O3	89.55 (5)	O2^{vi}—Ag1—O6^{vii}	148.46 (4)
O5^{iv}—In1—O3	87.43 (5)	O7^{ii}—Ag1—O6^{vii}	119.64 (4)
O1^{i}—In1—O6	173.56 (5)	O5^{vii}—Ag1—O6^{vii}	50.65 (4)
O4^{ii}—In1—O6	82.94 (5)	O1—P1—O2	111.17 (8)
O2^{iii}—In1—O6	92.62 (5)	O1—P1—O3	113.17 (8)
O5^{iv}—In1—O6	92.35 (5)	O2—P1—O3	113.16 (8)
O3—In1—O6	89.98 (5)	O1—P1—O7	104.17 (8)
O3^{v}—Ag1—O6	134.04 (4)	O2—P1—O7	107.40 (8)
O3^{v}—Ag1—O4^{ii}	155.99 (4)	O3—P1—O7	107.10 (7)
O6—Ag1—O4^{ii}	69.47 (4)	O4—P2—O5	115.20 (8)
O3^{v}—Ag1—O2^{vi}	85.86 (5)	O4—P2—O6	113.76 (8)
O6—Ag1—O2^{vi}	91.29 (4)	O5—P2—O6	109.65 (8)
O4^{ii}—Ag1—O2^{vi}	89.15 (5)	O4—P2—O7	100.90 (8)
O3^{v}—Ag1—O7^{ii}	102.17 (4)	O5—P2—O7	109.63 (8)
O6—Ag1—O7^{ii}	123.47 (4)	O6—P2—O7	107.01 (7)
O4^{ii}—Ag1—O7^{ii}	54.04 (4)	P1—O7—P2	137.27 (9)
O2^{vi}—Ag1—O7^{ii}	86.57 (4)		

Symmetry codes: (i) −*x*+1, *y*−1/2, −*z*+1/2; (ii) −*x*, *y*−1/2, −*z*+1/2; (iii) −*x*+1, −*y*+1, −*z*+1; (iv) *x*, −*y*+3/2, *z*−1/2; (v) *x*−1, *y*, *z*; (vi) *x*−1, −*y*+3/2, *z*−1/2; (vii) −*x*, −*y*+1, −*z*+1.

Fig. 1

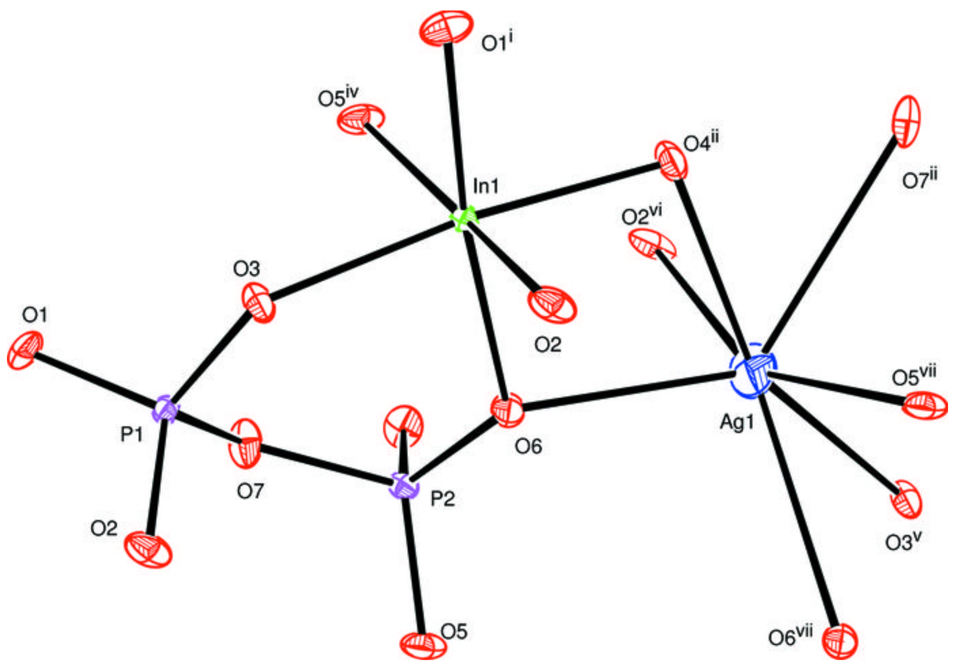

Fig. 2