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A three-dimensional tin(II) phosphonatobenzenesulfonate with Sn_4O_{12} clusters. Corrigendum

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An error in the scattering factors in the paper by Maniam & Stock [*Acta Cryst.* (2011), C**67**, m73–m76] is corrected.

In the paper by Maniam & Stock (2011), the S and P atoms were inadvertently refined using the scattering factors of the other element. A corrected CIF and structure factors are now available. Minor changes in the geometric parameters reported in the paper have occurred as a consequence, but all of the conclusions about the structure remain unchanged.

References

Maniam, P. & Stock, N. (2011). *Acta Cryst.* C**67**, m73–m76.

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supporting information

Acta Cryst. (2011). C**67**, e14 [https://doi.org/10.1107/S0108270111016076]

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Computing details

Data collection: *X-AREA* (Stoe & Cie, 2008); cell refinement: *X-AREA* (Stoe & Cie, 2008); data reduction: *X-AREA* (Stoe & Cie, 2008); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2010); software used to prepare material for publication: XCIF in *SHELXTL* (Sheldrick, 2008).

Poly[μ-hydroxido-(μ7–4-phosphonatobenzenesulfonato)ditin(II)]

Crystal data

$[Sn_2(C_6H_4O_6PS)(OH)]$
M_r = 489.56
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 7.0045 (14) Å
b = 8.487 (2) Å
c = 10.0570 (17) Å
α = 81.10 (2)°
β = 86.17 (2)°
γ = 75.25 (3)°
V = 571.0 (2) Å^3
Z = 2
$F(000)$ = 456
D_x = 2.847 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1556 reflections
θ = 1.9–28.2°
μ = 4.72 mm^{-1}
T = 293 K
Plate, colourless
0.14 × 0.10 × 0.07 mm

Data collection

Stoe IPDS-1 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ scans
Absorption correction: numerical (XRED rev 1.19 and X-SHAPE rev 1.06)
T_{min} = 0.380, T_{max} = 0.581
6691 measured reflections
2550 independent reflections
2146 reflections with $I > 2\sigma(I)$
R_{int} = 0.048
θ_{max} = 28.1°, θ_{min} = 2.5°
h = −9→9
k = −11→11
l = −13→13

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.066
S = 1.02
2550 reflections
155 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0397P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.79$ e Å^{-3}
$\Delta\rho_{min} = -1.08$ e Å^{-3}
Extinction correction: SHELXL97 (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0121 (9)

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}
Sn1	−0.18614 (4)	0.83666 (3)	0.57934 (2)	0.01832 (10)
Sn2	−0.35359 (4)	0.61742 (3)	0.35282 (2)	0.01956 (10)
P1	0.12971 (14)	0.57551 (11)	0.34654 (8)	0.01184 (19)
S1	0.37171 (15)	0.93625 (12)	−0.21627 (8)	0.0192 (2)
O1	−0.0710 (4)	0.6751 (3)	0.3976 (2)	0.0150 (5)
O2	0.1080 (4)	0.4085 (3)	0.3189 (2)	0.0178 (5)
O3	0.2898 (4)	0.5661 (3)	0.4465 (2)	0.0173 (5)
O4	0.2573 (5)	0.9067 (4)	−0.3215 (3)	0.0323 (7)
O5	0.5823 (5)	0.8540 (4)	−0.2319 (3)	0.0270 (7)
O6	0.3415 (5)	1.1096 (4)	−0.2013 (3)	0.0290 (7)
O7	−0.4330 (4)	0.7917 (3)	0.4877 (2)	0.0164 (5)
H7	−0.5508	0.8395	0.5044	0.025*
C1	0.1893 (6)	0.6797 (4)	0.1859 (3)	0.0158 (7)
C2	0.2372 (10)	0.5963 (6)	0.0754 (4)	0.0482 (16)
H2	0.2351	0.4861	0.0837	0.058*
C3	0.2879 (12)	0.6763 (6)	−0.0469 (5)	0.057 (2)
H3	0.3180	0.6203	−0.1211	0.069*
C4	0.2942 (6)	0.8397 (5)	−0.0594 (3)	0.0213 (8)
C5	0.2430 (7)	0.9258 (5)	0.0479 (4)	0.0253 (9)
H5	0.2455	1.0359	0.0389	0.030*
C6	0.1875 (7)	0.8459 (5)	0.1701 (4)	0.0260 (9)
H6	0.1487	0.9044	0.2423	0.031*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.02088 (18)	0.01538 (14)	0.01944 (15)	−0.00646 (11)	−0.00125 (10)	−0.00118 (9)
Sn2	0.01846 (18)	0.02484 (16)	0.01551 (14)	−0.00269 (12)	−0.00038 (9)	−0.00787 (10)
P1	0.0122 (5)	0.0145 (4)	0.0075 (4)	−0.0030 (4)	0.0025 (3)	0.0007 (3)
S1	0.0209 (5)	0.0235 (5)	0.0096 (4)	−0.0031 (4)	0.0045 (3)	0.0022 (3)
O1	0.0129 (14)	0.0192 (12)	0.0121 (11)	−0.0036 (11)	0.0035 (9)	−0.0019 (9)

O2	0.0247 (17)	0.0140 (12)	0.0138 (11)	−0.0049 (11)	−0.0020 (10)	0.0012 (9)
O3	0.0147 (15)	0.0226 (13)	0.0135 (11)	−0.0051 (11)	−0.0016 (9)	0.0020 (10)
O4	0.032 (2)	0.050 (2)	0.0148 (13)	−0.0133 (16)	−0.0001 (11)	0.0001 (13)
O5	0.0213 (18)	0.0370 (17)	0.0170 (13)	0.0009 (14)	0.0059 (11)	−0.0030 (12)
O6	0.039 (2)	0.0227 (15)	0.0184 (13)	−0.0017 (14)	0.0080 (12)	0.0043 (11)
O7	0.0104 (15)	0.0216 (13)	0.0161 (11)	−0.0012 (11)	0.0031 (9)	−0.0049 (9)
C1	0.017 (2)	0.0190 (17)	0.0106 (14)	−0.0047 (15)	0.0027 (12)	0.0000 (13)
C2	0.103 (5)	0.022 (2)	0.021 (2)	−0.023 (3)	0.026 (2)	−0.0072 (17)
C3	0.126 (6)	0.027 (2)	0.020 (2)	−0.025 (3)	0.032 (3)	−0.0093 (18)
C4	0.024 (2)	0.0267 (19)	0.0105 (15)	−0.0062 (17)	0.0060 (14)	0.0015 (14)
C5	0.041 (3)	0.0223 (19)	0.0143 (17)	−0.0131 (19)	0.0088 (16)	−0.0033 (14)
C6	0.046 (3)	0.0216 (19)	0.0125 (16)	−0.0136 (19)	0.0103 (16)	−0.0051 (14)

Geometric parameters (Å, º)

Sn1—O1	2.427 (3)	S1—C4	1.780 (3)
Sn1—O2^{i}	2.124 (2)	O2—Sn1^{i}	2.124 (2)
Sn1—O5^{ii}	2.410 (3)	O3—Sn2^{i}	2.344 (2)
Sn1—O7	2.155 (3)	O5—Sn1^{v}	2.410 (3)
Sn2—O1	2.246 (3)	O7—H7	0.8400
Sn2—O3^{i}	2.344 (2)	C1—C2	1.386 (5)
Sn2—O3^{iii}	2.726 (3)	C1—C6	1.391 (5)
Sn2—O6^{iv}	2.586 (3)	C2—C3	1.381 (6)
Sn2—O7	2.108 (3)	C2—H2	0.9300
P1—O1	1.545 (3)	C3—C4	1.384 (6)
P1—O2	1.532 (3)	C3—H3	0.9300
P1—O3	1.535 (3)	C4—C5	1.373 (6)
P1—C1	1.795 (3)	C5—C6	1.391 (5)
S1—O4	1.460 (4)	C5—H5	0.9300
S1—O5	1.472 (3)	C6—H6	0.9300
S1—O6	1.462 (4)		

O2^{i}—Sn1—O7	91.85 (10)	P1—O1—Sn1	136.42 (15)
O2^{i}—Sn1—O5^{ii}	78.75 (11)	Sn2—O1—Sn1	99.92 (10)
O7—Sn1—O5^{ii}	80.68 (10)	P1—O2—Sn1^{i}	135.22 (15)
O2^{i}—Sn1—O1	76.93 (9)	P1—O3—Sn2^{i}	126.01 (14)
O7—Sn1—O1	69.83 (10)	S1—O5—Sn1^{v}	133.80 (16)
O5^{ii}—Sn1—O1	140.72 (10)	Sn2—O7—Sn1	114.23 (12)
O1—Sn2—O3^{i}	83.17 (9)	Sn2—O7—H7	122.9
O3^{i}—Sn2—O3^{iii}	74.26 (8)	Sn1—O7—H7	122.9
O3^{iii}—Sn2—O6^{iv}	119.16 (10)	C2—C1—C6	118.8 (3)
O6^{iv}—Sn2—O1	73.59 (10)	C2—C1—P1	120.6 (3)
O7—Sn2—O1	74.32 (9)	C6—C1—P1	120.5 (3)
O6^{iv}—Sn2—O3^{i}	152.18 (9)	C3—C2—C1	120.2 (4)
O1—Sn2—O3^{iii}	147.71 (10)	C3—C2—H2	119.9
O2—P1—O3	114.80 (16)	C1—C2—H2	119.9
O2—P1—O1	109.26 (16)	C2—C3—C4	120.2 (4)
O3—P1—O1	109.44 (15)	C2—C3—H3	119.9

O2—P1—C1	105.37 (16)	C4—C3—H3	119.9
O3—P1—C1	109.46 (16)	C5—C4—C3	120.6 (3)
O1—P1—C1	108.27 (16)	C5—C4—S1	120.4 (3)
O4—S1—O6	114.6 (2)	C3—C4—S1	119.1 (3)
O4—S1—O5	110.96 (19)	C4—C5—C6	119.1 (4)
O6—S1—O5	112.1 (2)	C4—C5—H5	120.5
O4—S1—C4	107.95 (19)	C6—C5—H5	120.5
O6—S1—C4	105.61 (18)	C1—C6—C5	121.0 (4)
O5—S1—C4	104.99 (19)	C1—C6—H6	119.5
P1—O1—Sn2	120.56 (15)	C5—C6—H6	119.5
O2—P1—O1—Sn2	−22.08 (19)	O3^{i}—Sn2—O7—Sn1	73.83 (12)
O3—P1—O1—Sn2	−148.56 (14)	O2^{i}—Sn1—O7—Sn2	−64.68 (13)
C1—P1—O1—Sn2	92.19 (18)	O5^{ii}—Sn1—O7—Sn2	−142.96 (13)
O2—P1—O1—Sn1	133.51 (19)	O1—Sn1—O7—Sn2	10.67 (10)
O3—P1—O1—Sn1	7.0 (2)	O2—P1—C1—C2	−10.4 (5)
C1—P1—O1—Sn1	−112.2 (2)	O3—P1—C1—C2	113.5 (4)
O7—Sn2—O1—P1	172.42 (17)	O1—P1—C1—C2	−127.2 (4)
O3^{i}—Sn2—O1—P1	88.70 (16)	O2—P1—C1—C6	169.4 (4)
O7—Sn2—O1—Sn1	9.22 (9)	O3—P1—C1—C6	−66.7 (4)
O3^{i}—Sn2—O1—Sn1	−74.49 (10)	O1—P1—C1—C6	52.6 (4)
O2^{i}—Sn1—O1—P1	−71.2 (2)	C6—C1—C2—C3	1.9 (9)
O7—Sn1—O1—P1	−168.1 (2)	P1—C1—C2—C3	−178.3 (5)
O5^{ii}—Sn1—O1—P1	−124.3 (2)	C1—C2—C3—C4	1.0 (11)
O2^{i}—Sn1—O1—Sn2	87.68 (11)	C2—C3—C4—C5	−2.5 (10)
O7—Sn1—O1—Sn2	−9.25 (9)	C2—C3—C4—S1	177.0 (5)
O5^{ii}—Sn1—O1—Sn2	34.56 (19)	O4—S1—C4—C5	−129.6 (4)
O3—P1—O2—Sn1^{i}	20.6 (3)	O6—S1—C4—C5	−6.6 (4)
O1—P1—O2—Sn1^{i}	−102.7 (2)	O5—S1—C4—C5	112.0 (4)
C1—P1—O2—Sn1^{i}	141.1 (2)	O4—S1—C4—C3	51.0 (5)
O2—P1—O3—Sn2^{i}	−42.0 (2)	O6—S1—C4—C3	174.0 (5)
O1—P1—O3—Sn2^{i}	81.3 (2)	O5—S1—C4—C3	−67.4 (5)
C1—P1—O3—Sn2^{i}	−160.22 (18)	C3—C4—C5—C6	0.9 (8)
O4—S1—O5—Sn1^{v}	46.6 (3)	S1—C4—C5—C6	−178.5 (4)
O6—S1—O5—Sn1^{v}	−82.9 (3)	C2—C1—C6—C5	−3.5 (7)
C4—S1—O5—Sn1^{v}	163.0 (2)	P1—C1—C6—C5	176.7 (4)
O1—Sn2—O7—Sn1	−11.25 (10)	C4—C5—C6—C1	2.0 (7)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O7—H7···O4^{ii}	0.84	2.19	2.878 (4)	139

Symmetry code: (ii) *x*−1, *y*, *z*+1.