

Tri- μ -sulfato- κ^6 O:O'-bis[aqua(1,10-phenanthroline- κ^2 N,N')indium(III)] dihydrate

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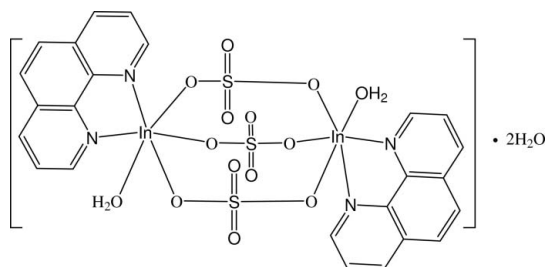
Received 5 September 2010; accepted 10 September 2010

 Key indicators: single-crystal X-ray study; $T = 295$ K; mean $\sigma(\text{C}-\text{C}) = 0.026$ Å; R factor = 0.082; wR factor = 0.224; data-to-parameter ratio = 13.0.

In the title dinuclear In^{III} compound, $[\text{In}_2(\text{SO}_4)_3(\text{C}_{12}\text{H}_8\text{N}_2)_2(\text{H}_2\text{O})_2] \cdot 2\text{H}_2\text{O}$, each In^{III} cation is coordinated by a 1,10-phenanthroline (phen) ligand, a water molecule and three sulfate O atoms in a distorted InN_2O_4 octahedral geometry. Three sulfate anions bridge two In^{III} cations, forming the dinuclear entities. $\text{O}-\text{H} \cdots \text{O}$ and weak $\text{C}-\text{H} \cdots \text{O}$ hydrogen bonding is observed in the crystal structure. The crystal structure is further consolidated by $\pi-\pi$ stacking between nearly parallel phen ring systems [dihedral angle = $4.2(4)^\circ$], the centroid-centroid distance between benzene rings of adjacent phen ligands being $3.528(9)$ Å.

Related literature

For structures of indium complexes with Lewis base ligands, see: Ahmadi *et al.* (2008); Kalateh *et al.* (2008); Xiao & Zhan (2010). For the crystal structure of an indium compound with a sulfonate bridging ligand, see: Ramezanipour *et al.* (2005).



Experimental

Crystal data

$[\text{In}_2(\text{SO}_4)_3(\text{C}_{12}\text{H}_8\text{N}_2)_2(\text{H}_2\text{O})_2] \cdot 2\text{H}_2\text{O}$
 $M_r = 950.32$
 Triclinic, $P\bar{1}$

$a = 10.5909(2)$ Å
 $b = 12.0354(2)$ Å
 $c = 13.3593(3)$ Å
 $\alpha = 79.904(1)^\circ$

$\beta = 79.606(1)^\circ$
 $\gamma = 64.727(1)^\circ$
 $V = 1505.32(5)$ Å³
 $Z = 2$

Mo $K\alpha$ radiation
 $\mu = 1.83$ mm⁻¹
 $T = 295$ K
 $0.18 \times 0.12 \times 0.04$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
 Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
 $T_{\text{min}} = 0.789$, $T_{\text{max}} = 0.850$
 14402 measured reflections
 5277 independent reflections
 4377 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.079$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.082$
 $wR(F^2) = 0.224$
 $S = 1.17$
 5277 reflections

406 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 3.41$ e Å⁻³
 $\Delta\rho_{\text{min}} = -1.32$ e Å⁻³

Table 1
 Selected bond lengths (Å).

In1—N1	2.240 (11)	In2—N3	2.247 (12)
In1—N2	2.228 (11)	In2—N4	2.246 (11)
In1—O1	2.109 (9)	In2—O2	2.109 (9)
In1—O5	2.187 (9)	In2—O6	2.103 (10)
In1—O9	2.075 (10)	In2—O10	2.146 (9)
In1—O13	2.206 (9)	In2—O14	2.159 (9)

Table 2
 Hydrogen-bond geometry (Å, °).

$D-\text{H} \cdots A$	$D-\text{H}$	$\text{H} \cdots A$	$D \cdots A$	$D-\text{H} \cdots A$
O13—H13A \cdots O4 ⁱ	0.81	1.94	2.602 (15)	138
O13—H13B \cdots O12 ⁱⁱ	0.84	1.94	2.637 (16)	139
O14—H14A \cdots O8 ⁱⁱⁱ	0.82	1.85	2.667 (17)	173
O14—H14B \cdots O16	0.87	1.76	2.565 (19)	152
O15—H15A \cdots O12	0.90	1.99	2.841 (18)	156
O15—H15B \cdots O7	0.89	2.12	2.887 (19)	143
O16—H16A \cdots O4 ⁱⁱⁱ	0.82	2.01	2.808 (19)	165
O16—H16B \cdots O15 ^{iv}	0.85	1.88	2.72 (2)	166
C8—H8 \cdots O10 ^v	0.93	2.53	3.27 (2)	137
C9—H9 \cdots O12 ^v	0.93	2.54	3.425 (19)	158
C11—H11 \cdots O11 ⁱ	0.93	2.41	3.24 (2)	148
C15—H15 \cdots O15 ^{vi}	0.93	2.56	3.28 (2)	135

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 1999); 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* (Farrugia, 1997); software used to prepare material for publication: *PLATON* (Spek, 2009).

This work was supported financially by Yuanpei University, Taiwan.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5026).

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supplementary materials

Acta Cryst. (2010). E66, m1260-m1261 [doi:10.1107/S1600536810036330]

Tri- μ -sulfato- $\kappa^6 O:O'$ -bis[aqua(1,10-phenanthroline- $\kappa^2 N,N'$)]indium(III) dihydrate

F. M. Shen and S. F. Lush

Comment

There are several reports on coordination of Lewis base to indium metal, such as tris(benzimidazol-2-ylmethyl)amine, [InCl₂(C₂₄H₂₁N₇)]Cl (Xiao & Zhan, 2010), 5,5'-dimethyl-2,2'-bipyridine, [InCl₃(C₁₂H₁₂N₂)(CH₄O)] (Kalateh *et al.*, 2008) and 4,4'-dimethyl-2,2'-bipyridine, [InCl₃(C₁₂H₁₂N₂)(C₂H₆OS)] (Ahmadi *et al.*, 2008). The sulfonato ligand exhibits a bridging mode in a In^(III) compound (Ramezanipour *et al.*, 2005).

In the structure, the In^{III} atom is six-coordinated within a slightly distorted octahedral coordination geometry defined by 1,10-phenanthroline-N atoms, three sulfate-O atoms and aqua molecule as shown in Fig. 1 and Table 1). In the crystal structure, there are several O—H...O and C—H...O hydrogen bonds (Table 2 and Fig. 2). The supra-molecular structure is consolidated by π - π stacking between nearly parallel phen rings systems [dihedral angle 4.2 (4)°], the centroids distance between benzene rings Cg7 (C4—C9)...Cg8 (C16—C21) of adjacent phen ligands is 3.528 (9) Å [symmetry code: $x, -1+y, z$].

Experimental

The reaction of benzoic acid (0.176 g, 1.0 mmol) and sodium hydroxide (0.04 g, 1.0 mmol) in methanol/water (1:1, 10 ml) at room temperature for one hour produced a colorless solutions, to which 1,10-phenanthroline (0.218 g, 1 mmol) and In₂(SO₄)₃·6H₂O (91.0 mg, 0.50 mmol) in water (5 ml) was added. The resulting solution was stirred for one hour at 323 K and the precipitate was filtered. Colorless crystals were obtained by slow evaporation of the filtrate for more than five days.

Refinement

The water H atoms were placed in chemical sensible positions and refined in riding mode with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$. The remaining H atoms were positioned geometrically and refined using a riding model with C—H = 0.93 Å (aromatic) and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. The precise of the structure is low.

Figures

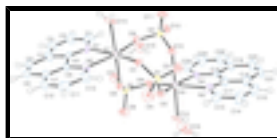


Fig. 1. View of the title compound with the atom numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 50% probability level.

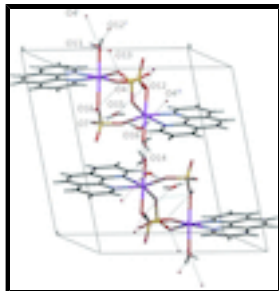


Fig. 2. The molecular packing for the title compound. Hydrogen-bonding associations are shown as dotted lines.

Tri- μ -sulfato- κ^6 O:O'-bis[aqua(1,10-phenanthroline- κ^2 N,N')]indium(III) dihydrate

Crystal data

$[\text{In}_2(\text{SO}_4)_3(\text{C}_{12}\text{H}_8\text{N}_2)_2(\text{H}_2\text{O})_2] \cdot 2\text{H}_2\text{O}$

$M_r = 950.32$

Triclinic, $P\bar{1}$

Hall symbol: -P 1

$a = 10.5909(2) \text{ \AA}$

$b = 12.0354(2) \text{ \AA}$

$c = 13.3593(3) \text{ \AA}$

$\alpha = 79.904(1)^\circ$

$\beta = 79.606(1)^\circ$

$\gamma = 64.727(1)^\circ$

$V = 1505.32(5) \text{ \AA}^3$

$Z = 2$

$F(000) = 940$

$D_x = 2.097 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 10717 reflections

$\theta = 2.0\text{--}25.0^\circ$

$\mu = 1.83 \text{ mm}^{-1}$

$T = 295 \text{ K}$

Prism, colorless

$0.18 \times 0.12 \times 0.04 \text{ mm}$

Data collection

Bruker SMART CCD area-detector diffractometer

Radiation source: fine-focus sealed tube graphite

Detector resolution: 9 pixels mm^{-1}

ω scan

Absorption correction: multi-scan (SADABS; Bruker, 2000)

$T_{\min} = 0.789$, $T_{\max} = 0.850$

14402 measured reflections

5277 independent reflections

4377 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.079$

$\theta_{\max} = 25.0^\circ$, $\theta_{\min} = 2.3^\circ$

$h = -12 \rightarrow 12$

$k = -13 \rightarrow 14$

$l = -15 \rightarrow 15$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.082$

$wR(F^2) = 0.224$

$S = 1.17$

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

$w = 1/[\sigma^2(F_o^2) + (0.0492P)^2 + 58.7561P]$

5277 reflections
406 parameters
0 restraints

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.003$
 $\Delta\rho_{\max} = 3.41 \text{ e } \text{Å}^{-3}$
 $\Delta\rho_{\min} = -1.32 \text{ e } \text{Å}^{-3}$

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.

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted R -factors wR and all goodnesses 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 observed criterion of $F^2 > \sigma(F^2)$ is used only for calculating $-R$ -factor-obs *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)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
In1	0.23687 (10)	0.37849 (8)	0.12705 (7)	0.0204 (3)
In2	0.15197 (10)	0.63043 (9)	0.34430 (7)	0.0205 (3)
S1	-0.0558 (3)	0.6360 (3)	0.1863 (3)	0.0227 (7)
S2	0.2944 (4)	0.3255 (3)	0.3720 (3)	0.0226 (7)
S3	0.3709 (3)	0.5796 (3)	0.1245 (3)	0.0225 (7)
O1	0.0541 (10)	0.5445 (9)	0.1186 (7)	0.030 (2)
O2	-0.0126 (9)	0.6094 (9)	0.2926 (7)	0.0259 (12)
O3	-0.0774 (11)	0.7586 (10)	0.1424 (8)	0.037 (3)
O4	-0.1878 (11)	0.6163 (11)	0.1984 (8)	0.037 (3)
O5	0.1989 (9)	0.3469 (9)	0.2939 (7)	0.0259 (12)
O6	0.3012 (10)	0.4480 (9)	0.3727 (8)	0.029 (2)
O7	0.4358 (11)	0.2357 (10)	0.3495 (8)	0.035 (2)
O8	0.2261 (10)	0.2921 (10)	0.4705 (8)	0.032 (2)
O9	0.3816 (10)	0.4486 (9)	0.1378 (8)	0.031 (2)
O10	0.2435 (9)	0.6503 (9)	0.1889 (7)	0.0259 (12)
O11	0.3554 (11)	0.6339 (10)	0.0190 (8)	0.041 (3)
O12	0.4971 (11)	0.5716 (10)	0.1598 (8)	0.035 (2)
O13	0.2881 (10)	0.4015 (10)	-0.0407 (7)	0.0319 (17)
H13A	0.2306	0.4310	-0.0813	0.048*
H13B	0.3722	0.3720	-0.0684	0.048*
O14	0.0542 (10)	0.6127 (10)	0.4992 (7)	0.0319 (17)
H14A	-0.0315	0.6365	0.5110	0.048*
H14B	0.0906	0.6270	0.5466	0.048*
N1	0.4033 (12)	0.1854 (10)	0.1249 (9)	0.026 (3)
N2	0.1239 (12)	0.2648 (11)	0.1099 (9)	0.024 (2)
N3	0.0258 (13)	0.8347 (11)	0.3484 (9)	0.029 (3)
N4	0.2974 (13)	0.7026 (11)	0.3855 (9)	0.027 (3)

supplementary materials

C1	0.5403 (15)	0.1495 (15)	0.1316 (12)	0.036 (4)
H1	0.5755	0.2084	0.1308	0.043*
C2	0.6308 (16)	0.0235 (15)	0.1399 (13)	0.039 (4)
H2	0.7252	-0.0002	0.1458	0.047*
C3	0.5828 (18)	-0.0640 (14)	0.1396 (12)	0.038 (4)
H3	0.6439	-0.1472	0.1440	0.046*
C4	0.4372 (17)	-0.0271 (13)	0.1323 (12)	0.035 (4)
C5	0.3541 (15)	0.0995 (13)	0.1217 (10)	0.025 (3)
C6	0.2044 (13)	0.1400 (13)	0.1147 (10)	0.023 (3)
C7	0.1516 (18)	0.0558 (15)	0.1097 (11)	0.034 (2)
C8	0.241 (2)	-0.0743 (14)	0.1168 (13)	0.043 (3)
H8	0.2051	-0.1314	0.1128	0.051*
C9	0.377 (2)	-0.1128 (15)	0.1294 (13)	0.043 (3)
H9	0.4334	-0.1971	0.1365	0.051*
C10	0.0089 (18)	0.1022 (15)	0.0970 (11)	0.034 (2)
H10	-0.0299	0.0478	0.0907	0.041*
C11	-0.0732 (17)	0.2247 (17)	0.0936 (13)	0.043 (4)
H11	-0.1684	0.2547	0.0869	0.051*
C12	-0.0121 (15)	0.3057 (14)	0.1005 (12)	0.033 (3)
H12	-0.0681	0.3900	0.0985	0.040*
C13	-0.1113 (17)	0.8982 (16)	0.3400 (12)	0.038 (4)
H13	-0.1635	0.8547	0.3339	0.046*
C14	-0.181 (2)	1.0270 (15)	0.3400 (14)	0.049 (5)
H14	-0.2748	1.0686	0.3295	0.059*
C15	-0.106 (2)	1.0893 (16)	0.3558 (12)	0.045 (4)
H15	-0.1511	1.1744	0.3579	0.054*
C16	0.0386 (19)	1.0274 (15)	0.3690 (12)	0.040 (4)
C17	0.0940 (16)	0.9010 (14)	0.3676 (11)	0.030 (3)
C18	0.2413 (15)	0.8307 (13)	0.3847 (10)	0.026 (3)
C19	0.3237 (18)	0.8895 (14)	0.3983 (12)	0.035 (4)
C20	0.260 (2)	1.0237 (17)	0.3947 (13)	0.049 (5)
H20	0.3137	1.0650	0.4022	0.058*
C21	0.126 (2)	1.0879 (15)	0.3809 (14)	0.048 (5)
H21	0.0869	1.1736	0.3789	0.057*
C22	0.4654 (19)	0.8164 (19)	0.4137 (14)	0.048 (3)
H22	0.5225	0.8539	0.4233	0.057*
C23	0.5219 (19)	0.6850 (19)	0.4148 (14)	0.048 (3)
H23	0.6148	0.6349	0.4253	0.057*
C24	0.4313 (16)	0.6369 (16)	0.3995 (12)	0.035 (4)
H24	0.4665	0.5517	0.3989	0.042*
O15	0.6347 (12)	0.3469 (12)	0.2823 (12)	0.059 (4)
H15A	0.5690	0.4170	0.2546	0.089*
H15B	0.6100	0.2850	0.3113	0.089*
O16	0.1901 (16)	0.5776 (15)	0.6508 (10)	0.069 (5)
H16A	0.2024	0.5127	0.6878	0.104*
H16B	0.2324	0.6122	0.6739	0.104*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
In1	0.0203 (5)	0.0179 (5)	0.0237 (5)	-0.0076 (4)	-0.0032 (4)	-0.0041 (4)
In2	0.0198 (5)	0.0197 (5)	0.0224 (5)	-0.0078 (4)	-0.0016 (4)	-0.0048 (4)
S1	0.0180 (16)	0.0237 (17)	0.0250 (17)	-0.0057 (13)	-0.0037 (13)	-0.0053 (13)
S2	0.0238 (17)	0.0209 (17)	0.0225 (17)	-0.0089 (14)	-0.0027 (13)	-0.0015 (13)
S3	0.0217 (17)	0.0234 (17)	0.0238 (17)	-0.0114 (14)	-0.0011 (13)	-0.0022 (13)
O1	0.024 (5)	0.028 (5)	0.028 (5)	0.002 (4)	-0.006 (4)	-0.011 (4)
O2	0.020 (3)	0.034 (3)	0.023 (3)	-0.015 (2)	-0.004 (2)	0.008 (2)
O3	0.038 (6)	0.026 (6)	0.034 (6)	-0.002 (5)	-0.003 (5)	-0.003 (5)
O4	0.033 (6)	0.049 (7)	0.036 (6)	-0.020 (5)	-0.016 (5)	-0.003 (5)
O5	0.020 (3)	0.034 (3)	0.023 (3)	-0.015 (2)	-0.004 (2)	0.008 (2)
O6	0.031 (5)	0.023 (5)	0.031 (5)	-0.010 (4)	-0.004 (4)	0.002 (4)
O7	0.027 (5)	0.028 (6)	0.041 (6)	-0.004 (5)	-0.004 (5)	-0.002 (5)
O8	0.025 (5)	0.038 (6)	0.030 (5)	-0.012 (5)	-0.003 (4)	0.002 (5)
O9	0.030 (6)	0.027 (5)	0.037 (6)	-0.013 (5)	0.000 (4)	-0.008 (4)
O10	0.020 (3)	0.034 (3)	0.023 (3)	-0.015 (2)	-0.004 (2)	0.008 (2)
O11	0.039 (6)	0.038 (6)	0.023 (5)	-0.006 (5)	0.014 (5)	0.008 (5)
O12	0.027 (5)	0.036 (6)	0.046 (6)	-0.018 (5)	0.002 (5)	-0.006 (5)
O13	0.023 (4)	0.052 (5)	0.022 (4)	-0.025 (4)	0.003 (3)	0.009 (3)
O14	0.023 (4)	0.052 (5)	0.022 (4)	-0.025 (4)	0.003 (3)	0.009 (3)
N1	0.030 (7)	0.020 (6)	0.024 (6)	-0.005 (5)	-0.008 (5)	-0.004 (5)
N2	0.023 (6)	0.026 (6)	0.026 (6)	-0.013 (5)	-0.006 (5)	0.002 (5)
N3	0.030 (7)	0.027 (7)	0.029 (7)	-0.009 (5)	-0.004 (5)	-0.011 (5)
N4	0.036 (7)	0.026 (6)	0.024 (6)	-0.018 (6)	-0.010 (5)	-0.001 (5)
C1	0.017 (7)	0.039 (9)	0.040 (9)	0.001 (6)	-0.006 (6)	-0.005 (7)
C2	0.020 (7)	0.035 (9)	0.046 (10)	0.004 (7)	-0.005 (7)	-0.002 (7)
C3	0.044 (10)	0.023 (8)	0.034 (9)	0.004 (7)	-0.015 (7)	0.000 (6)
C4	0.039 (9)	0.018 (7)	0.042 (9)	-0.006 (7)	-0.007 (7)	0.004 (6)
C5	0.035 (8)	0.023 (7)	0.016 (6)	-0.011 (6)	0.001 (6)	-0.007 (5)
C6	0.015 (6)	0.026 (7)	0.025 (7)	-0.007 (6)	0.005 (5)	-0.010 (6)
C7	0.051 (7)	0.041 (6)	0.026 (5)	-0.033 (6)	0.001 (5)	-0.008 (5)
C8	0.059 (7)	0.022 (6)	0.044 (7)	-0.018 (6)	0.010 (6)	-0.007 (5)
C9	0.059 (7)	0.022 (6)	0.044 (7)	-0.018 (6)	0.010 (6)	-0.007 (5)
C10	0.051 (7)	0.041 (6)	0.026 (5)	-0.033 (6)	0.001 (5)	-0.008 (5)
C11	0.027 (8)	0.056 (11)	0.047 (10)	-0.019 (8)	0.000 (7)	-0.009 (8)
C12	0.022 (7)	0.027 (8)	0.047 (9)	-0.008 (6)	-0.007 (7)	0.002 (7)
C13	0.034 (9)	0.039 (9)	0.032 (8)	-0.005 (7)	-0.006 (7)	-0.008 (7)
C14	0.053 (11)	0.026 (9)	0.050 (11)	0.006 (8)	-0.022 (9)	0.000 (8)
C15	0.057 (11)	0.031 (9)	0.032 (9)	-0.002 (8)	0.000 (8)	-0.013 (7)
C16	0.057 (11)	0.028 (8)	0.032 (9)	-0.014 (8)	-0.007 (8)	-0.003 (7)
C17	0.034 (8)	0.024 (7)	0.031 (8)	-0.010 (6)	-0.005 (6)	-0.004 (6)
C18	0.030 (8)	0.030 (8)	0.015 (6)	-0.014 (6)	0.009 (5)	-0.002 (6)
C19	0.048 (10)	0.028 (8)	0.035 (8)	-0.022 (7)	-0.004 (7)	-0.004 (7)
C20	0.084 (15)	0.038 (10)	0.040 (10)	-0.039 (11)	-0.008 (9)	-0.006 (8)
C21	0.075 (14)	0.019 (8)	0.053 (11)	-0.025 (9)	0.000 (10)	-0.005 (7)

supplementary materials

C22	0.042 (7)	0.066 (8)	0.048 (7)	-0.029 (7)	-0.012 (6)	-0.013 (7)
C23	0.042 (7)	0.066 (8)	0.048 (7)	-0.029 (7)	-0.012 (6)	-0.013 (7)
C24	0.030 (8)	0.040 (9)	0.037 (9)	-0.015 (7)	-0.013 (7)	0.003 (7)
O15	0.028 (6)	0.042 (7)	0.107 (12)	-0.014 (6)	-0.023 (7)	0.009 (7)
O16	0.086 (11)	0.102 (12)	0.050 (8)	-0.071 (10)	-0.044 (8)	0.038 (8)

Geometric parameters (Å, °)

In1—N1	2.240 (11)	C3—C4	1.43 (2)
In1—N2	2.228 (11)	C3—H3	0.9300
In1—O1	2.109 (9)	C4—C5	1.39 (2)
In1—O5	2.187 (9)	C4—C9	1.43 (2)
In1—O9	2.075 (10)	C5—C6	1.462 (19)
In1—O13	2.206 (9)	C6—C7	1.37 (2)
In2—N3	2.247 (12)	C7—C10	1.40 (2)
In2—N4	2.246 (11)	C7—C8	1.44 (2)
In2—O2	2.109 (9)	C8—C9	1.34 (3)
In2—O6	2.103 (10)	C8—H8	0.9300
In2—O10	2.146 (9)	C9—H9	0.9300
In2—O14	2.159 (9)	C10—C11	1.35 (2)
S1—O3	1.425 (11)	C10—H10	0.9300
S1—O4	1.491 (11)	C11—C12	1.40 (2)
S1—O1	1.504 (10)	C11—H11	0.9300
S1—O2	1.509 (10)	C12—H12	0.9300
S2—O7	1.440 (10)	C13—C14	1.40 (2)
S2—O8	1.461 (10)	C13—H13	0.9300
S2—O5	1.497 (10)	C14—C15	1.36 (3)
S2—O6	1.509 (10)	C14—H14	0.9300
S3—O11	1.451 (10)	C15—C16	1.42 (3)
S3—O12	1.456 (11)	C15—H15	0.9300
S3—O10	1.464 (10)	C16—C17	1.38 (2)
S3—O9	1.512 (10)	C16—C21	1.44 (2)
O13—H13A	0.8112	C17—C18	1.46 (2)
O13—H13B	0.8450	C18—C19	1.39 (2)
O14—H14A	0.8198	C19—C22	1.41 (2)
O14—H14B	0.8726	C19—C20	1.46 (2)
N1—C1	1.341 (19)	C20—C21	1.33 (3)
N1—C5	1.351 (18)	C20—H20	0.9300
N2—C12	1.331 (18)	C21—H21	0.9300
N2—C6	1.371 (18)	C22—C23	1.43 (3)
N3—C13	1.34 (2)	C22—H22	0.9300
N3—C17	1.362 (19)	C23—C24	1.37 (2)
N4—C24	1.326 (19)	C23—H23	0.9300
N4—C18	1.394 (19)	C24—H24	0.9300
C1—C2	1.40 (2)	O15—H15A	0.9033
C1—H1	0.9300	O15—H15B	0.8951
C2—C3	1.35 (2)	O16—H16A	0.8201
C2—H2	0.9300	O16—H16B	0.8501
O9—In1—O1	99.7 (4)	N1—C1—H1	119.8

O9—In1—O5	91.1 (4)	C2—C1—H1	119.8
O1—In1—O5	93.0 (4)	C3—C2—C1	121.0 (15)
O9—In1—O13	87.6 (4)	C3—C2—H2	119.5
O1—In1—O13	90.4 (4)	C1—C2—H2	119.5
O5—In1—O13	176.5 (4)	C2—C3—C4	119.2 (14)
O9—In1—N2	167.3 (4)	C2—C3—H3	120.4
O1—In1—N2	92.8 (4)	C4—C3—H3	120.4
O5—In1—N2	90.8 (4)	C5—C4—C3	116.8 (14)
O13—In1—N2	89.8 (4)	C5—C4—C9	119.8 (15)
O9—In1—N1	92.2 (4)	C3—C4—C9	123.3 (14)
O1—In1—N1	167.8 (4)	N1—C5—C4	123.0 (14)
O5—In1—N1	89.7 (4)	N1—C5—C6	118.8 (12)
O13—In1—N1	87.2 (4)	C4—C5—C6	118.0 (13)
N2—In1—N1	75.3 (4)	C7—C6—N2	123.0 (13)
O6—In2—O2	103.9 (4)	C7—C6—C5	120.3 (13)
O6—In2—O10	93.0 (4)	N2—C6—C5	116.6 (12)
O2—In2—O10	90.0 (3)	C6—C7—C10	117.1 (15)
O6—In2—O14	88.1 (4)	C6—C7—C8	120.3 (15)
O2—In2—O14	88.6 (4)	C10—C7—C8	122.6 (14)
O10—In2—O14	178.4 (4)	C9—C8—C7	119.7 (16)
O6—In2—N4	90.1 (4)	C9—C8—H8	120.2
O2—In2—N4	165.7 (4)	C7—C8—H8	120.2
O10—In2—N4	86.4 (4)	C8—C9—C4	121.6 (15)
O14—In2—N4	94.7 (4)	C8—C9—H9	119.2
O6—In2—N3	162.6 (4)	C4—C9—H9	119.2
O2—In2—N3	92.0 (4)	C11—C10—C7	121.1 (14)
O10—In2—N3	93.8 (4)	C11—C10—H10	119.5
O14—In2—N3	85.4 (4)	C7—C10—H10	119.5
N4—In2—N3	74.4 (4)	C10—C11—C12	118.7 (15)
O3—S1—O4	111.4 (7)	C10—C11—H11	120.6
O3—S1—O1	109.8 (6)	C12—C11—H11	120.6
O4—S1—O1	108.3 (6)	N2—C12—C11	121.7 (15)
O3—S1—O2	111.8 (6)	N2—C12—H12	119.2
O4—S1—O2	105.6 (6)	C11—C12—H12	119.2
O1—S1—O2	109.9 (6)	N3—C13—C14	123.5 (17)
O7—S2—O8	112.4 (6)	N3—C13—H13	118.2
O7—S2—O5	114.4 (6)	C14—C13—H13	118.2
O8—S2—O5	106.6 (6)	C15—C14—C13	118.1 (17)
O7—S2—O6	107.7 (6)	C15—C14—H14	121.0
O8—S2—O6	109.7 (6)	C13—C14—H14	121.0
O5—S2—O6	105.9 (6)	C14—C15—C16	121.5 (16)
O11—S3—O12	113.5 (7)	C14—C15—H15	119.3
O11—S3—O10	108.3 (6)	C16—C15—H15	119.3
O12—S3—O10	111.7 (6)	C17—C16—C15	114.6 (16)
O11—S3—O9	110.9 (7)	C17—C16—C21	120.9 (16)
O12—S3—O9	105.8 (6)	C15—C16—C21	124.5 (16)
O10—S3—O9	106.5 (6)	N3—C17—C16	126.2 (15)
S1—O1—In1	140.6 (6)	N3—C17—C18	116.2 (13)
S1—O2—In2	129.8 (5)	C16—C17—C18	117.6 (14)

supplementary materials

S2—O5—In1	128.9 (5)	C19—C18—N4	120.9 (13)
S2—O6—In2	131.2 (6)	C19—C18—C17	121.2 (14)
S3—O9—In1	131.6 (6)	N4—C18—C17	118.0 (13)
S3—O10—In2	136.9 (6)	C18—C19—C22	118.4 (15)
In1—O13—H13A	124.8	C18—C19—C20	118.3 (16)
In1—O13—H13B	121.1	C22—C19—C20	123.3 (16)
H13A—O13—H13B	113.7	C21—C20—C19	120.9 (16)
In2—O14—H14A	120.1	C21—C20—H20	119.5
In2—O14—H14B	116.0	C19—C20—H20	119.5
H14A—O14—H14B	112.8	C20—C21—C16	121.1 (15)
C1—N1—C5	119.4 (13)	C20—C21—H21	119.4
C1—N1—In1	126.4 (11)	C16—C21—H21	119.4
C5—N1—In1	114.1 (9)	C19—C22—C23	120.3 (16)
C12—N2—C6	118.5 (12)	C19—C22—H22	119.8
C12—N2—In1	126.6 (10)	C23—C22—H22	119.8
C6—N2—In1	114.9 (8)	C24—C23—C22	116.3 (17)
C13—N3—C17	115.7 (13)	C24—C23—H23	121.9
C13—N3—In2	127.4 (11)	C22—C23—H23	121.9
C17—N3—In2	116.7 (9)	N4—C24—C23	125.0 (16)
C24—N4—C18	119.1 (13)	N4—C24—H24	117.5
C24—N4—In2	126.0 (10)	C23—C24—H24	117.5
C18—N4—In2	114.5 (9)	H15A—O15—H15B	118.7
N1—C1—C2	120.4 (16)	H16A—O16—H16B	106.6

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O13—H13A \cdots O4 ⁱ	0.81	1.94	2.602 (15)	138
O13—H13B \cdots O12 ⁱⁱ	0.84	1.94	2.637 (16)	139
O14—H14A \cdots O8 ⁱⁱⁱ	0.82	1.85	2.667 (17)	173
O14—H14B \cdots O16	0.87	1.76	2.565 (19)	152
O15—H15A \cdots O12	0.90	1.99	2.841 (18)	156
O15—H15B \cdots O7	0.89	2.12	2.887 (19)	143
O16—H16A \cdots O4 ⁱⁱⁱ	0.82	2.01	2.808 (19)	165
O16—H16B \cdots O15 ^{iv}	0.85	1.88	2.72 (2)	166
C8—H8 \cdots O10 ^v	0.93	2.53	3.27 (2)	137
C9—H9 \cdots O12 ^v	0.93	2.54	3.425 (19)	158
C11—H11 \cdots O11 ⁱ	0.93	2.41	3.24 (2)	148
C15—H15 \cdots O15 ^{vi}	0.93	2.56	3.28 (2)	135

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

Fig. 1

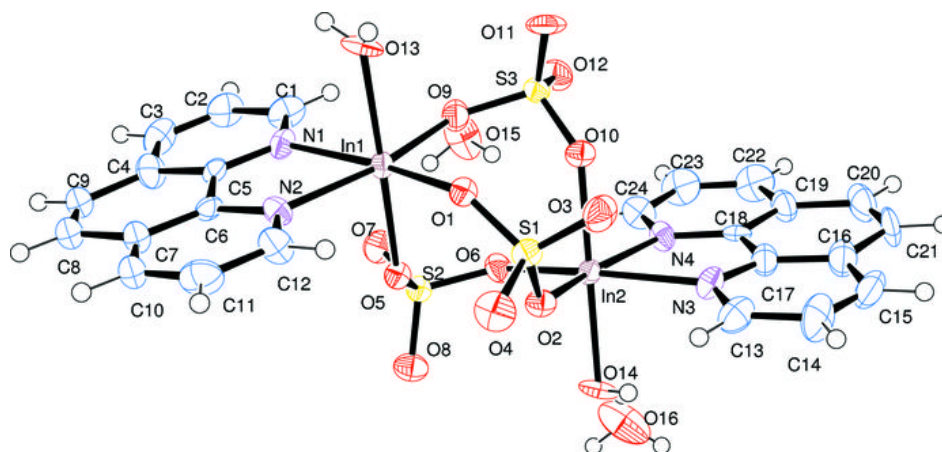


Fig. 2

