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Poly[hemi(ethylenediammonium) [di-μ-oxalato-indium(III)] dihydrate]

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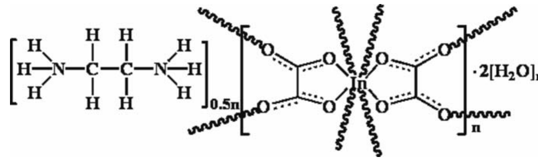
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.006 Å; disorder in solvent or counterion; R factor = 0.018; wR factor = 0.046; data-to-parameter ratio = 10.5.

In title compound, $\{(C_2H_{10}N_2)_{0.5}[In(C_2O_4)_2]\cdot 2H_2O\}_n$, the unique In^{III} ion is coordinated by eight O atoms from four oxalate ligands in a distorted square-antiprismatic environment. The doubly bis-chelating oxalate ligands act as bridging ligands connecting symmetry-related In^{III} ions and forming a three-dimensional open framework structure. Ethylenediammonium cations and water molecules occupy the voids within the structure. The unique ethylenediammonium cation and one water molecule both lie on a twofold rotation axis. One of the other two water molecules residing on general crystallographic sites was refined as disordered with half occupancy. In the crystal structure, cations and water molecules are linked to the anionic framework *via* intermolecular O—H···O and N—H···O hydrogen bonds.

Related literature

For background information on open-framework materials, see: Fang *et al.* (2004); Li *et al.* (2008); Serre *et al.* (2006); Sun *et al.* (2006). For related materials containing the oxalate ligand, see: Audebrand *et al.* (2001, 2004); Kokunov *et al.* (2004); Stock *et al.* (2000); Chakrabarti & Natarajan (2002); Evans & Lin (2001); Vaidhyanathan *et al.* (2001); Gavilan *et al.* (2007); Bataille *et al.* (2000); Trombe *et al.* (2001); Yuan *et al.* (2004). For indium oxaltes, see: Audebrand *et al.* (2003); Bulc *et al.* (1983); Bulc & Golič (1983); Chen *et al.* (2003); Huang & Lii (1998); Jeanneau *et al.* (2003); Yang *et al.* (2005); For the bond-valence method, see: Brown (1996). For bond distances and angles for bridging bidentate oxalate groups, see: Hann (1957).



Experimental

Crystal data

$(C_2H_{10}N_2)_{0.5}[In(C_2O_4)_2]\cdot 2H_2O$
M_r = 357.95
Orthorhombic, $Fdd2$
a = 15.8498 (4) Å
b = 31.1643 (8) Å
c = 8.6618 (2) Å
V = 4278.48 (18) Å^3
Z = 16
Mo $K\alpha$ radiation
μ = 2.26 mm^{-1}
T = 293 K
0.40 × 0.38 × 0.38 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.426, T_{max} = 0.467 (expected range = 0.387–0.424)
7189 measured reflections
1679 independent reflections
1673 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.018
$wR(F^2)$ = 0.046
S = 1.06
1679 reflections
160 parameters
13 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.71 e Å^{-3}
Absolute structure: Flack (1983), 668 Friedel pairs
Flack parameter: 0.00 (3)

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1C···OW1^{i}	0.89	2.35	2.880 (8)	118
N1—H1B···O7^{ii}	0.89	2.47	2.956 (5)	115
N1—H1B···OW3	0.89	2.21	2.825 (8)	126
N1—H1C···O4^{i}	0.89	2.44	3.140 (6)	136
N1—H1C···O5^{iii}	0.89	2.38	3.166 (5)	147
OW1—HW1A···O2^{iv}	0.85	2.04	2.889 (5)	180
OW2—HW2B···O1^{iii}	0.85	2.46	3.241 (15)	153
OW2—HW2A···O3	0.85	2.39	3.12 (3)	145
OW3—HW3B···O8^{v}	0.85	2.19	2.870 (6)	137
OW3—HW3A···O7	0.85	2.26	2.971 (7)	141
OW3—HW3A···O3^{ii}	0.85	2.40	2.962 (6)	124

Symmetry codes: (i) $x, y, z-1$; (ii) $x+\frac{1}{4}, -y+\frac{3}{4}, z-\frac{1}{4}$; (iii) $-x, -y+\frac{1}{2}, z-\frac{1}{2}$; (iv) $-x+\frac{1}{2}, -y+\frac{1}{2}, z$; (v) $x-\frac{1}{4}, -y+\frac{3}{4}, z-\frac{3}{4}$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2779).

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supporting information

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Poly[hemi(ethylenediammonium) [di-μ-oxalato-indium(III)] dihydrate]

Qiaozhen Sun, Yang Liu, Hongwu Li and Zhi Luo

S1. Comment

The synthesis of open-framework materials has emerged as an important area of research because of their potential applications in separation processes, ion exchange and catalysis. In the past few years, there has been considerable effort in designing open-framework structures formed by metal organic carboxylates because of its interesting structural features and the quality for apt design (Fang *et al.*, 2004; Li *et al.*, 2008; Serre *et al.*, 2006; Sun *et al.*, 2006) of which the oxalate ligand plays a major role in the assembly of metal-organic porous frameworks. Many metal oxalate structures are reported such as tin (Audebrand *et al.*, 2001; Kokunov *et al.*, 2004; Stock *et al.*, 2000), zinc (Chakrabarti & Natarajan, 2002; Rvans & Lin, 2001; Vaidhyanathan *et al.*, 2001), zirconium (Audebrand *et al.*, 2004; Gavilan *et al.*, 2007), rare earth (Bataille *et al.*, 2000; Trombe *et al.*, 2001; Yuan *et al.*, 2004). The structures of these compounds vary from monomers, dimmers, chains, layered honeycomb networks to three dimensional frameworks. In this paper, we selected indium and synthesized the three-dimensional indium oxalate compound $[(C_2N_2H_{10})_{0.5}In(C_2O_4)_2.2H_2O]_n$ (Fig. 1). Although many indium oxalates have been reported (Audebrand *et al.*, 2003; Bulc *et al.*, 1983; Chen *et al.*, 2003; Huang & Lii, 1998; Jeanneau *et al.*, 2003; Yang *et al.*, 2005), relatively a few of them are three dimensional open frameworks (Chen *et al.*, 2003; Huang & Lii, 1998; Yang *et al.*, 2005).

In the title structure, the In ion is coordinated by eight O atoms from four tetradentate oxalate groups, forming a distorted square antiprismatic arrangement (Fig. 2) in which atoms O1, O2, O5A and O6A (Symmetry code A: -*x*, 0.5 - *y*, 1/2 + *z*) are approximately in the same plane with a deviation of ca. 0.01 Å, while the other plane (formed by atoms O3, O4, O7B and O8B; Symmetry code B: *x* - 1/4, 0.75 - *y*, 1/4 + *z*) is significantly distorted, with a deviation of ca. 0.24 Å. The eight In—O bond distances vary between 2.168 (3) and 2.423 (3) Å (average 2.279 Å), which agrees well with the value 2.265 Å calculated for an eightfold coordinated indium atom with the bond valence method using the program VALENCE (Brown, 1996).

The indium ions are linked by the oxygen atoms of oxalate, giving rise to a three-dimensional interdependent porous framework (Fig. 3). The protonated ethylenediammonium and water molecules occupy the voids, interacting with oxalate anions through N—H···O and O—H···O hydrogen bonds. Without water molecules and cations, the framework exhibits voids possessing approximate dimensions of 6.9×14.5 Å along the crystallographic *c* axis and an analysis of the void shows that *ca* 44% of the space is empty. Thus, the ethylenediammonium and water molecules assigned to these cavities act as not only charge-compensating cations but also organic templates. The bond distances and angles for the bridging bidentate oxalate groups are in good agreement with the mean values reported by Hann (1957) for oxalate compounds, *i.e.*, 1.24 and 1.52 Å, 118 and 123° for the C1—O1 and C1—C2 bond lengths and O1—C1—C2 and O1—C1—O5 angles, respectively.

S2. Experimental

A mixture of $Ti(SO_4)_2$ (0.2 g, 0.84 mmol), $H_2C_2O_4.2H_2O$ (1.0 g, 7.93 mmol), $InCl_3.4H_2O$ (2 ml, 0.5 mol/*L*) and $H_2N(CH_2)_2NH_2$ (0.2 ml, CR) in H_2O (5.0 ml) was sealed in a 20 ml stainless-steal reactor with Teflon liner and heated at 393 K for 2 days under autogenously pressure. Colorless crystals were isolated after the reaction solution was cooled gradually and washed with water.

S3. Refinement

H atoms bonded to C and N atoms were inlcuded in calcluated positions with C-H = 0.97 and N-H = 0.89Å and $U_{iso}(H)$ = $1.2U_{eq}(C)$ or $1.5U_{eq}(N)$. The H atoms bonded to O atoms were either included in calculated positions [O-H = 0.85Å] based on 'as found' locations or based on the most efficient H-bonding location and with $U_{iso}(H)$= 1.0-1.2$U_{eq}(C)$.

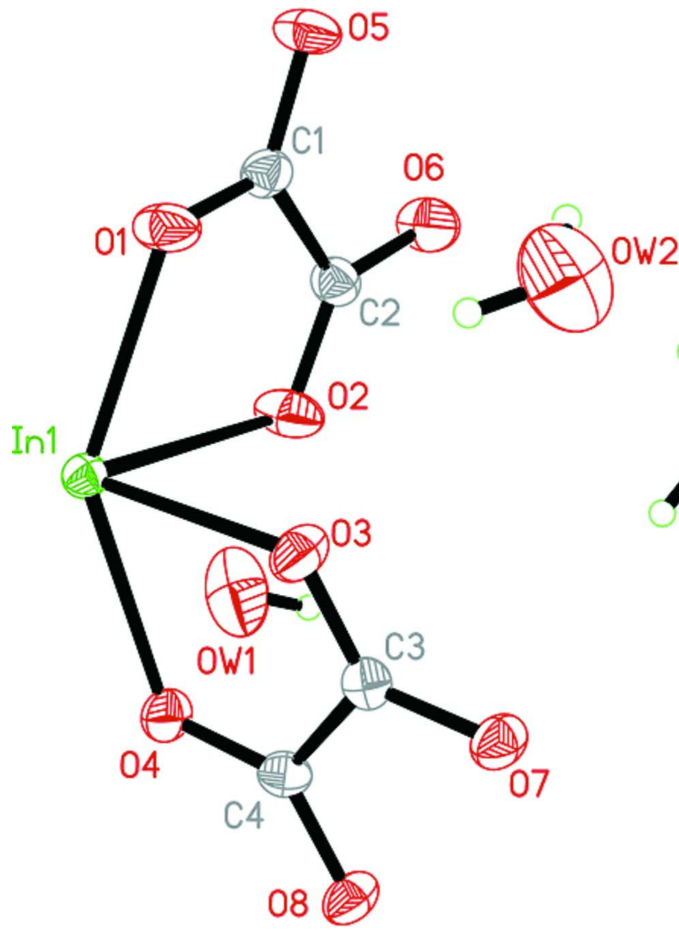

Figure 1

The asymmetric unit showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

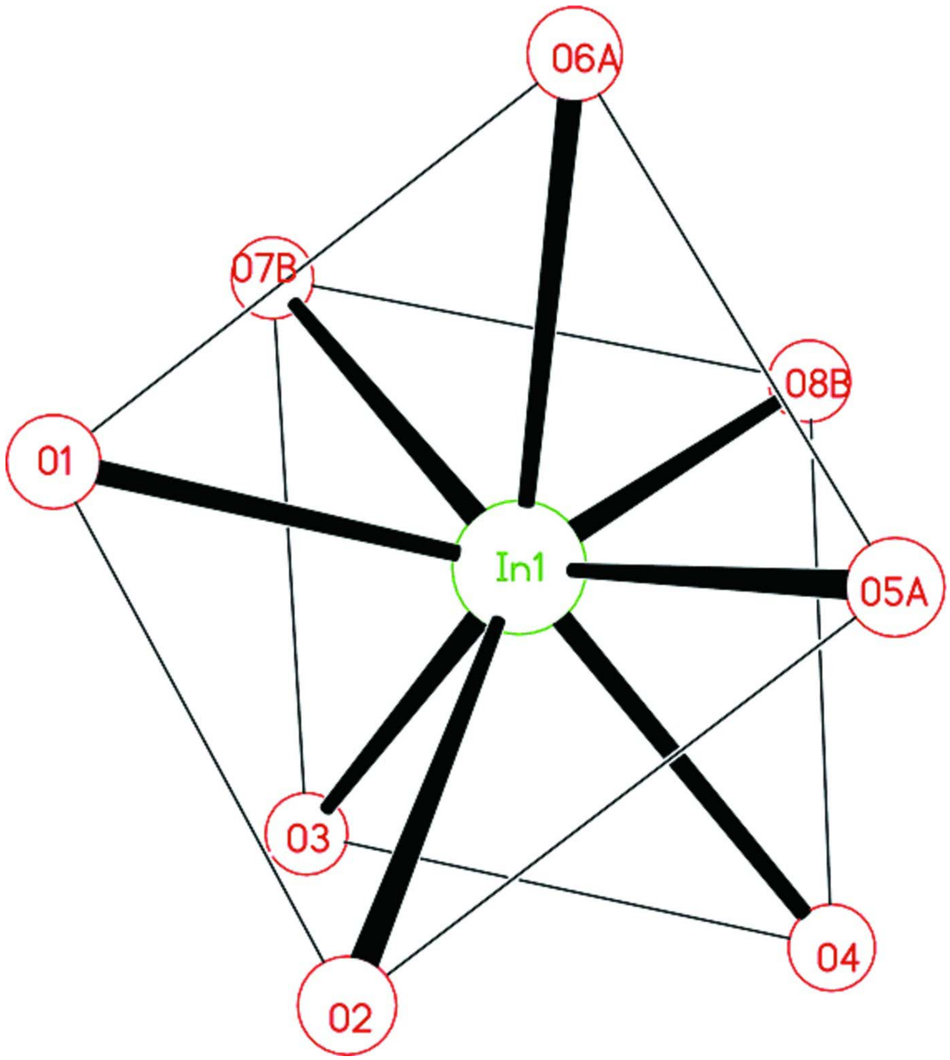

Figure 2

The distorted square antiprismatic environment of Indium. Symmetry codes A: -*x*, 0.5 - *y*, 1/2 + *z*; B: *x* - 1/4, 0.75 - *y*, 1/4 + *z*.

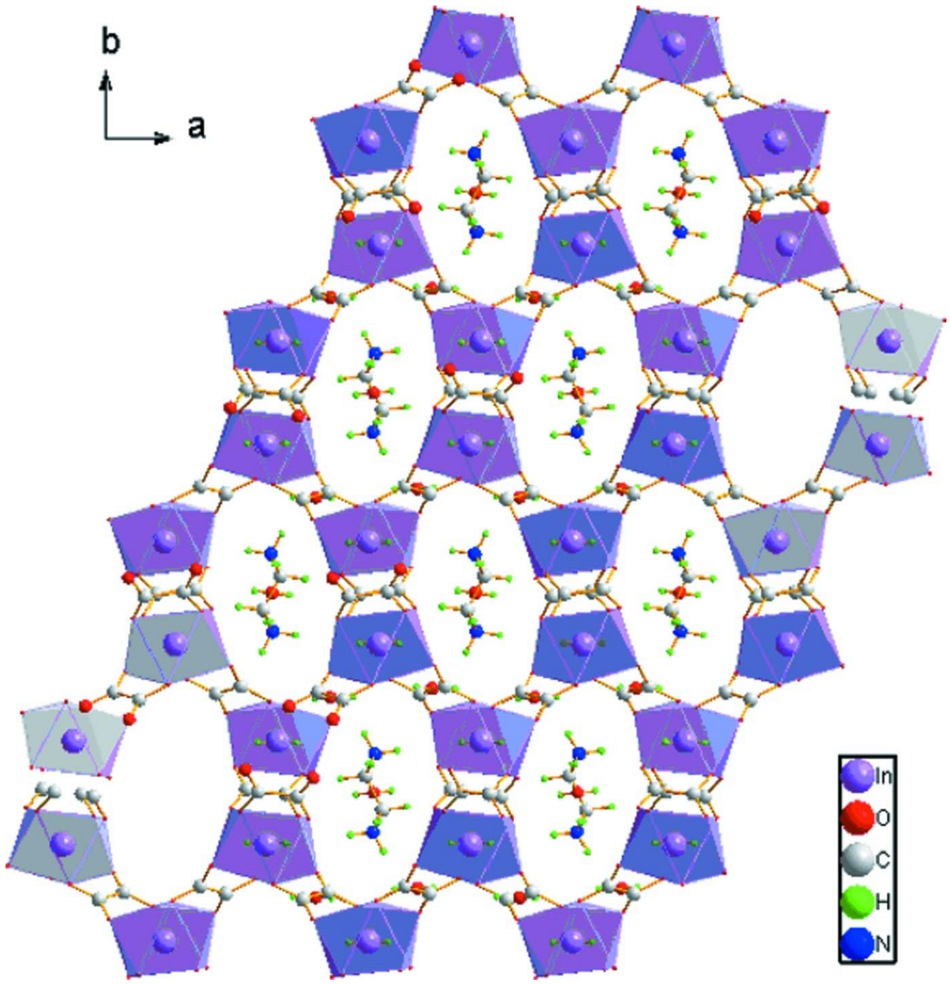

Figure 3

Part of the crystal structure viewed crystal along the *c* axis, the ethylenediammonium and water molecules reside in the voids.

Poly[hemi(ethylenediammonium) [di-μ-oxalato-indium(III)] dihydrate]

Crystal data

$(C_2H_{10}N_2)_{0.5}[In(C_2O_4)_2]\cdot 2H_2O$
M_r = 357.95
Orthorhombic, *Fdd*2
Hall symbol: F 2 -2d
a = 15.8498 (4) Å
b = 31.1643 (8) Å
c = 8.6618 (2) Å
V = 4278.48 (18) Å^3
Z = 16
$F(000)$ = 2800
D_x = 2.223 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 7228 reflections
θ = 2.6–27.9°
μ = 2.26 mm^{-1}
T = 293 K
Block, colourless
0.4 × 0.38 × 0.38 mm

Data collection

Bruker SMART CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans

Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.426, T_{max} = 0.467
7189 measured reflections
1679 independent reflections
1673 reflections with $I > 2\sigma(I)$
R_{int} = 0.025
θ_{max} = 25.0°, θ_{min} = 2.6°
$h = -18 \rightarrow 18$
$k = -36 \rightarrow 36$
$l = -10 \rightarrow 10$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.018
$wR(F^2)$ = 0.046
S = 1.06
1679 reflections
160 parameters
13 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
$w = 1/[\sigma^2(F_o^2) + (0.0322P)^2 + 7.4478P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.71 e Å^{-3}
Extinction correction: *SHELXTL* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.00087 (5)
Absolute structure: Flack (1983), 668 Friedel pairs
Absolute structure parameter: 0.00 (3)

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 (Å²)

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
In1	0.013694 (15)	0.314689 (7)	0.33266 (6)	0.01510 (11)	
O1	−0.06449 (17)	0.27864 (9)	0.1683 (4)	0.0277 (6)	
O2	0.10165 (19)	0.26861 (9)	0.1750 (4)	0.0290 (7)	
O3	0.04152 (19)	0.35822 (9)	0.1416 (3)	0.0241 (6)	
O4	0.14920 (17)	0.34173 (8)	0.3713 (3)	0.0220 (6)	
C1	−0.0334 (2)	0.25113 (11)	0.0817 (7)	0.0194 (7)	
C2	0.0620 (2)	0.24552 (11)	0.0823 (7)	0.0204 (7)	
C3	0.1128 (2)	0.37559 (10)	0.1357 (4)	0.0165 (7)	
C4	0.1740 (2)	0.36645 (11)	0.2696 (5)	0.0180 (8)	
O5	−0.07692 (18)	0.22769 (9)	−0.0061 (3)	0.0259 (7)	
O6	0.09025 (18)	0.21856 (9)	−0.0112 (4)	0.0302 (7)	
O7	0.13838 (16)	0.39927 (8)	0.0302 (3)	0.0223 (6)	
O8	0.24530 (18)	0.38498 (9)	0.2625 (4)	0.0231 (6)	
C5	0.2294 (3)	0.2715 (2)	−0.2277 (8)	0.0535 (16)	
H5C	0.1687	0.2676	−0.2275	0.064*	
H5A	0.2444	0.2864	−0.1332	0.064*	

N1	0.2527 (3)	0.29883 (17)	−0.3608 (6)	0.0502 (12)	
H1A	0.3035	0.2913	−0.3949	0.075*	
H1B	0.2534	0.3262	−0.3316	0.075*	
H1C	0.2150	0.2954	−0.4360	0.075*	
OW1	0.2500	0.2500	0.3570 (7)	0.0504 (16)	
HW1A	0.2938	0.2445	0.3040	0.050*	
OW2	0.0119 (6)	0.3117 (3)	−0.173 (3)	0.069 (2)	0.50
HW2B	0.0188	0.2848	−0.1847	0.083*	0.50
HW2A	0.0010	0.3173	−0.0793	0.083*	0.50
OW3	0.1418 (3)	0.36723 (19)	−0.2928 (7)	0.1000 (17)	
HW3B	0.1123	0.3788	−0.3632	0.120*	
HW3A	0.1542	0.3857	−0.2244	0.120*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
In1	0.01446 (16)	0.01545 (14)	0.01540 (15)	−0.00012 (8)	−0.00093 (14)	0.00069 (11)
O1	0.0185 (13)	0.0268 (13)	0.0378 (17)	−0.0013 (11)	0.0018 (14)	−0.0157 (13)
O2	0.0224 (15)	0.0289 (15)	0.0358 (17)	0.0008 (12)	−0.0078 (14)	−0.0104 (13)
O3	0.0187 (14)	0.0299 (14)	0.0237 (15)	−0.0058 (12)	−0.0031 (12)	0.0086 (11)
O4	0.0264 (15)	0.0220 (12)	0.0176 (15)	−0.0037 (10)	−0.0021 (11)	0.0065 (10)
C1	0.0209 (18)	0.0154 (15)	0.0218 (17)	−0.0017 (14)	0.001 (2)	0.0002 (16)
C2	0.0220 (19)	0.0194 (16)	0.0199 (17)	0.0002 (14)	0.000 (2)	−0.0018 (17)
C3	0.0177 (19)	0.0139 (15)	0.0179 (17)	0.0038 (13)	0.0005 (15)	0.0001 (14)
C4	0.019 (2)	0.0132 (15)	0.0214 (17)	0.0010 (14)	−0.0015 (16)	−0.0011 (14)
O5	0.0193 (15)	0.0251 (13)	0.0333 (17)	−0.0004 (11)	−0.0037 (13)	−0.0135 (13)
O6	0.0213 (15)	0.0324 (15)	0.0369 (19)	0.0024 (12)	0.0032 (14)	−0.0131 (14)
O7	0.0224 (13)	0.0229 (12)	0.0217 (14)	−0.0042 (10)	−0.0032 (11)	0.0066 (10)
O8	0.0180 (13)	0.0273 (15)	0.0239 (15)	−0.0057 (11)	−0.0039 (13)	0.0084 (12)
C5	0.031 (3)	0.080 (4)	0.049 (4)	−0.020 (2)	0.006 (3)	−0.016 (3)
N1	0.028 (2)	0.074 (3)	0.049 (3)	−0.006 (2)	−0.011 (2)	−0.001 (2)
OW1	0.026 (2)	0.086 (4)	0.039 (4)	0.024 (2)	0.000	0.000
OW2	0.084 (4)	0.067 (4)	0.055 (4)	0.013 (4)	−0.002 (5)	−0.006 (4)
OW3	0.083 (3)	0.146 (4)	0.072 (3)	0.016 (3)	−0.030 (3)	−0.045 (3)

Geometric parameters (Å, º)

In1—O5^{i}	2.168 (3)	C4—O8	1.270 (5)
In1—O3	2.185 (3)	O5—In1^{iii}	2.168 (3)
In1—O1	2.196 (3)	O6—In1^{iii}	2.370 (3)
In1—O8^{ii}	2.230 (3)	O7—In1^{iv}	2.327 (3)
In1—O7^{ii}	2.327 (3)	O8—In1^{iv}	2.230 (3)
In1—O4	2.331 (3)	C5—N1	1.480 (8)
In1—O6^{i}	2.370 (3)	C5—C5^{v}	1.492 (12)
In1—O2	2.423 (3)	C5—H5C	0.9700
O1—C1	1.242 (5)	C5—H5A	0.9700
O2—C2	1.248 (6)	N1—H1A	0.8900
O3—C3	1.253 (5)	N1—H1B	0.8900

O4—C4	1.235 (5)	N1—H1C	0.8900
C1—O5	1.260 (6)	OW1—HW1A	0.8500
C1—C2	1.522 (6)	OW2—HW2B	0.8502
C2—O6	1.250 (6)	OW2—HW2A	0.8500
C3—O7	1.243 (4)	OW3—HW3B	0.8498
C3—C4	1.539 (5)	OW3—HW3A	0.8500
O5^{i}—In1—O3	140.63 (11)	C4—O4—In1	114.7 (2)
O5^{i}—In1—O1	111.52 (10)	O1—C1—O5	123.2 (4)
O3—In1—O1	86.60 (12)	O1—C1—C2	118.2 (4)
O5^{i}—In1—O8^{ii}	92.22 (11)	O5—C1—C2	118.7 (4)
O3—In1—O8^{ii}	96.82 (11)	O2—C2—O6	128.6 (4)
O1—In1—O8^{ii}	137.63 (10)	O2—C2—C1	115.8 (4)
O5^{i}—In1—O7^{ii}	144.54 (11)	O6—C2—C1	115.5 (4)
O3—In1—O7^{ii}	74.02 (11)	O7—C3—O3	125.5 (4)
O1—In1—O7^{ii}	68.82 (10)	O7—C3—C4	117.2 (3)
O8^{ii}—In1—O7^{ii}	71.65 (10)	O3—C3—C4	117.3 (3)
O5^{i}—In1—O4	72.66 (9)	O4—C4—O8	127.0 (4)
O3—In1—O4	72.43 (9)	O4—C4—C3	116.8 (3)
O1—In1—O4	142.91 (10)	O8—C4—C3	116.1 (3)
O8^{ii}—In1—O4	76.46 (10)	C1—O5—In1^{iii}	119.2 (3)
O7^{ii}—In1—O4	129.79 (9)	C2—O6—In1^{iii}	114.5 (3)
O5^{i}—In1—O6^{i}	71.78 (10)	C3—O7—In1^{iv}	115.0 (2)
O3—In1—O6^{i}	147.56 (11)	C4—O8—In1^{iv}	118.0 (3)
O1—In1—O6^{i}	75.75 (11)	N1—C5—C5^{v}	114.0 (4)
O8^{ii}—In1—O6^{i}	79.52 (11)	N1—C5—H5C	108.7
O7^{ii}—In1—O6^{i}	74.28 (10)	C5^{v}—C5—H5C	108.7
O4—In1—O6^{i}	135.78 (10)	N1—C5—H5A	108.7
O5^{i}—In1—O2	74.70 (10)	C5^{v}—C5—H5A	108.7
O3—In1—O2	79.93 (11)	H5C—C5—H5A	107.6
O1—In1—O2	69.90 (11)	C5—N1—H1A	109.5
O8^{ii}—In1—O2	152.36 (10)	C5—N1—H1B	109.5
O7^{ii}—In1—O2	131.86 (10)	H1A—N1—H1B	109.5
O4—In1—O2	76.41 (9)	C5—N1—H1C	109.5
O6^{i}—In1—O2	117.54 (10)	H1A—N1—H1C	109.5
C1—O1—In1	121.4 (3)	H1B—N1—H1C	109.5
C2—O2—In1	114.5 (3)	HW2B—OW2—HW2A	109.8
C3—O3—In1	118.7 (2)	HW3B—OW3—HW3A	109.8

Symmetry codes: (i) −*x*, −*y*+1/2, *z*+1/2; (ii) *x*−1/4, −*y*+3/4, *z*+1/4; (iii) −*x*, −*y*+1/2, *z*−1/2; (iv) *x*+1/4, −*y*+3/4, *z*−1/4; (v) −*x*+1/2, −*y*+1/2, *z*.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*C*···O*W*1^{vi}	0.89	2.35	2.880 (8)	118
N1—H1*B*···O7^{iv}	0.89	2.47	2.956 (5)	115
N1—H1*B*···O*W*3	0.89	2.21	2.825 (8)	126
N1—H1*C*···O4^{vi}	0.89	2.44	3.140 (6)	136

N1—H1*C*···O5[iii]	0.89	2.38	3.166 (5)	147
O*W*1—H*W*1*A*···O2[v]	0.85	2.04	2.889 (5)	180
O*W*2—H*W*2*B*···O1[iii]	0.85	2.46	3.241 (15)	153
O*W*2—H*W*2*A*···O3	0.85	2.39	3.12 (3)	145
O*W*3—H*W*3*B*···O8[vii]	0.85	2.19	2.870 (6)	137
O*W*3—H*W*3*A*···O7	0.85	2.26	2.971 (7)	141
O*W*3—H*W*3*A*···O3[iv]	0.85	2.40	2.962 (6)	124

Symmetry codes: (iii) −*x*, −*y*+1/2, *z*−1/2; (iv) *x*+1/4, −*y*+3/4, *z*−1/4; (v) −*x*+1/2, −*y*+1/2, *z*; (vi) *x*, *y*, *z*−1; (vii) *x*−1/4, −*y*+3/4, *z*−3/4.