

# Trichlorido(4,4'-dimethyl-2,2'-bipyridine- $\kappa^2N,N'$ )(dimethyl sulfoxide- $\kappa O$ )-indium(III)

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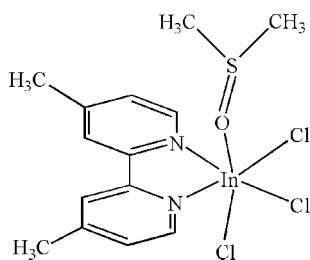
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Key indicators: single-crystal X-ray study;  $T = 298$  K; mean  $\sigma(C-C) = 0.004$  Å;  $R$  factor = 0.036;  $wR$  factor = 0.086; data-to-parameter ratio = 25.1.

In the molecule of the title compound,  $[InCl_3(C_{12}H_{12}N_2)(C_2H_6OS)]$ , the  $In^{III}$  atom is six-coordinated in a distorted octahedral configuration by two N atoms from the chelating 4,4'-dimethyl-2,2'-bipyridine ligand, one O atom from dimethyl sulfoxide and three Cl atoms. In the crystal structure, intermolecular  $C-H \cdots Cl$  hydrogen bonds link the molecules into centrosymmetric dimers.

## Related literature

For related literature, see: Ahmadi, Kalateh *et al.* (2008); Ahmadi, Khalighi *et al.* (2008); Amani *et al.* (2007); Ilyukhin & Malyarick (1994); Khavasi *et al.* (2007); Khalighi *et al.* (2008); Malyarick *et al.* (1992); Nan *et al.* (1987); Yousefi, Khalighi *et al.* (2008); Yousefi, Tadayon Pour *et al.* (2008).



## Experimental

### Crystal data

$[InCl_3(C_{12}H_{12}N_2)(C_2H_6OS)]$   $V = 1884.7$  (7) Å<sup>3</sup>  
 $M_r = 483.54$   $Z = 4$   
 Monoclinic,  $P2_1/n$  Mo  $K\alpha$  radiation  
 $a = 8.2565$  (17) Å  $\mu = 1.79$  mm<sup>-1</sup>  
 $b = 23.456$  (5) Å  $T = 298$  (2) K  
 $c = 10.121$  (2) Å  $0.49 \times 0.46 \times 0.44$  mm  
 $\beta = 105.95$  (3)°

### Data collection

Bruker SMART CCD area-detector diffractometer 13791 measured reflections  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1998) 5046 independent reflections  
 $T_{min} = 0.404$ ,  $T_{max} = 0.455$  4804 reflections with  $I > 2\sigma(I)$   
 $R_{int} = 0.038$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.035$  201 parameters  
 $wR(F^2) = 0.085$  H-atom parameters constrained  
 $S = 1.16$   $\Delta\rho_{max} = 0.86$  e Å<sup>-3</sup>  
 5046 reflections  $\Delta\rho_{min} = -0.69$  e Å<sup>-3</sup>

Table 1

Selected geometric parameters (Å, °).

Cl1—In1	2.4180 (12)	O1—In1	2.233 (2)
Cl2—In1	2.4592 (10)	N1—In1	2.293 (2)
Cl3—In1	2.4398 (9)	N2—In1	2.294 (2)
Cl1—In1—Cl2	99.03 (4)	N1—In1—Cl1	93.59 (7)
Cl1—In1—Cl3	98.15 (3)	N1—In1—Cl2	89.72 (7)
Cl3—In1—Cl2	96.15 (3)	N1—In1—Cl3	165.87 (6)
O1—In1—Cl1	90.56 (7)	N2—In1—Cl1	162.86 (7)
O1—In1—Cl2	168.67 (6)	N2—In1—Cl2	89.26 (7)
O1—In1—Cl3	88.39 (6)	N2—In1—Cl3	95.83 (7)
O1—In1—N1	83.64 (9)	N1—In1—N2	71.34 (9)
O1—In1—N2	79.94 (9)		

Table 2

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
Cl1—H1 $\cdots$ Cl1	0.93	2.77	3.427 (4)	128
Cl10—H10C $\cdots$ Cl2 <sup>i</sup>	0.96	2.80	3.700 (4)	156

Symmetry code: (i)  $-x + 2, -y, -z + 2$ .

Data collection: SMART (Bruker, 1998); cell refinement: SAINT (Bruker, 1998); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Sheldrick, 2008); program(s) used to refine structure: SHELXTL; molecular graphics: ORTEP-3 for Windows (Farrugia, 1997) and PLATON (Spek, 2003); 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: HK2532).

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## supporting information

*Acta Cryst.* (2008). E64, m1306–m1307 [doi:10.1107/S1600536808029553]

## Trichlorido(4,4'-dimethyl-2,2'-bipyridine- $\kappa^2N,N'$ )(dimethyl sulfoxide- $\kappa O$ )indium(III)

Roya Ahmadi, Khadijeh Kalateh, Anita Abedi, Vahid Amani and Hamid Reza Khavasi

### S1. Comment

Recently, we reported the syntheses and crystal structures of [Zn(5,5'-dmbpy)Cl<sub>2</sub>], (II), (Khalighi *et al.*, 2008), [Zn(6-mbpy)Cl<sub>2</sub>], (III), (Ahmadi, Kalateh *et al.*, 2008), [Cd(5,5'-dmbpy)( $\mu$ -Cl)<sub>2</sub>]<sub>n</sub>, (IV), (Ahmadi, Khalighi *et al.*, 2008), (Hg(4,4'-dmbpy)I<sub>2</sub>), (V), (Yousefi, Tadayon Pour *et al.*, 2008) and [Cu(5,5'-dcbpy)(en)(H<sub>2</sub>O)<sub>2</sub>].2.5H<sub>2</sub>O, (VI), (Yousefi, Khalighi *et al.*, 2008) [where 5,5'-dmbpy is 5,5'-dimethyl-2,2'-bipyridine, 6-mbpy is 6-methyl-2,2'-bipyridine, 4,4'-dmbpy is 4,4'-dimethyl-2,2'-bipyridine, 5,5'-dcbpy is 2,2'-bipyridine-5,5'-dicarboxylate and en is ethylenediamine]. We have also reported the synthesis and crystal structures of iron(III) complexes of [Fe(bipy)Cl<sub>3</sub>(DMSO)], (VII) and [Fe(phen)Cl<sub>3</sub>(DMSO)], (VIII), (Amani *et al.*, 2007) and [Fe(phen)Cl<sub>3</sub>(CH<sub>3</sub>OH)].CH<sub>3</sub>OH, (IX), (Khavasi *et al.*, 2007) [where bipy is 2,2'-bipyridine, DMSO is dimethyl sulfoxide and phen is 1,10-phenanthroline]. There are several In<sup>III</sup> complexes, with formula, [In(N—N)Cl<sub>3</sub>(L)], (L = DMSO, H<sub>2</sub>O and EtOH), such as [In(bipy)Cl<sub>3</sub>(H<sub>2</sub>O)], (X), [In(bipy)Cl<sub>3</sub>(EtOH)], (XI) and [In(bipy)Cl<sub>3</sub>(H<sub>2</sub>O)].H<sub>2</sub>O, (XII), (Malyarick *et al.*, 1992), [In(phen)Cl<sub>3</sub>(DMSO)], (XIII), (Nan *et al.*, 1987), [In(phen)Cl<sub>3</sub>(H<sub>2</sub>O)], (XIV) and [In(phen)Cl<sub>3</sub>(EtOH)].EtOH, (XV), (Ilyukhin & Malyarick, 1994) have been synthesized and characterized by single-crystal X-ray diffraction methods. We report herein the synthesis and crystal structure of the title compound, (I).

In the title compound, (Fig. 1), the In<sup>III</sup> atom is six-coordinated in a distorted octahedral configuration by two N atoms from 4,4'-dimethyl-2,2'-bipyridine, one O atom from dimethyl sulfoxide and three Cl atoms. The In—Cl and In—N bond lengths and angles (Table 1) are within normal ranges, as in (XI), (XII), (XIII) and (XV).

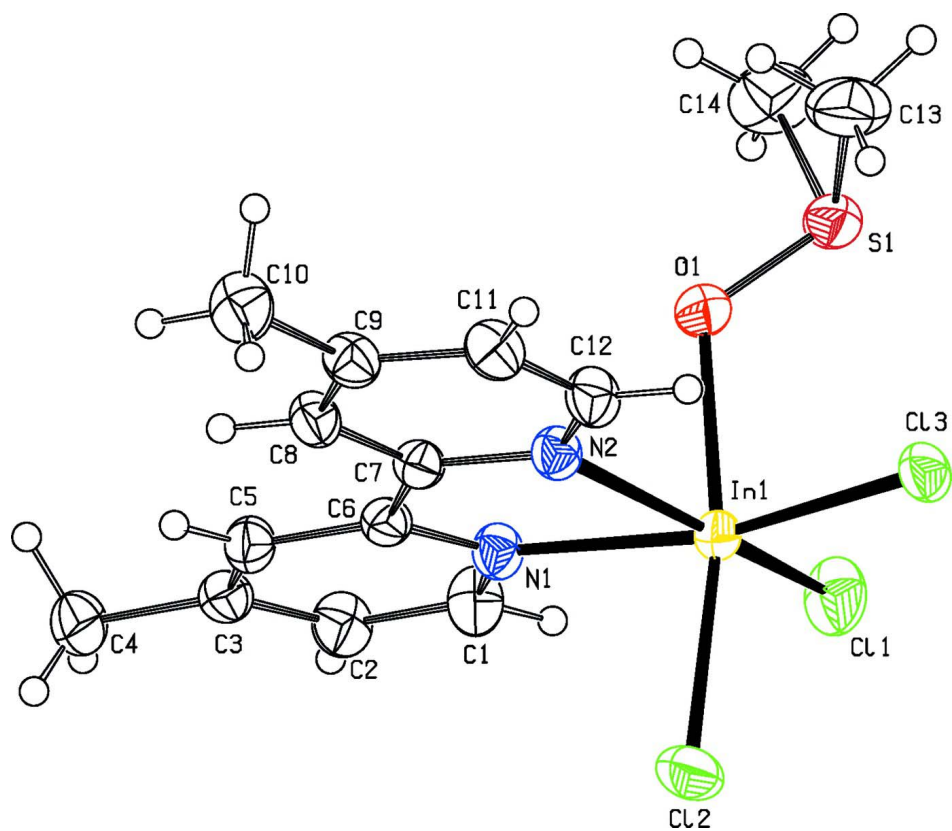
In the crystal structure, intermolecular C—H...O hydrogen bonds (Table 2) link the molecules into centrosymmetric dimers (Fig. 2), in which they may be effective in the stabilization of the structure.

### S2. Experimental

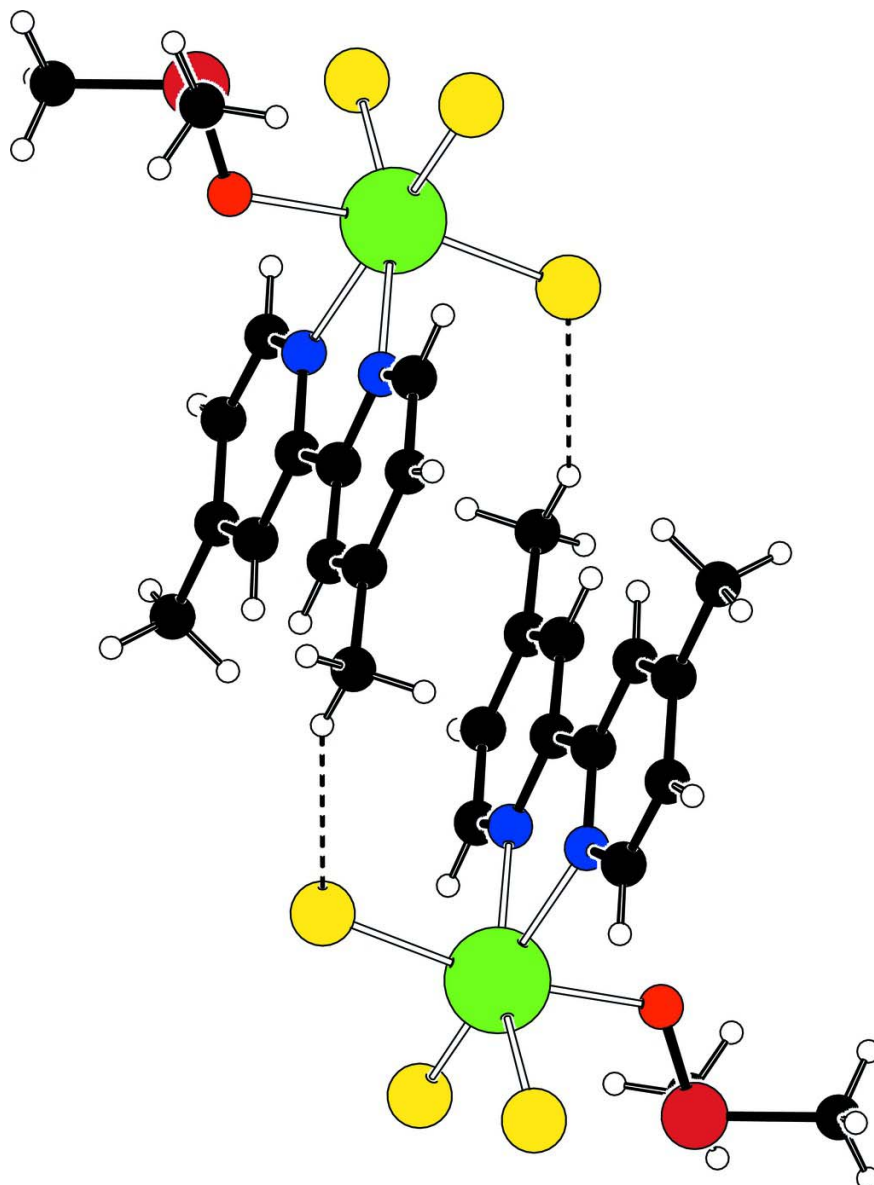
For the preparation of the title compound, (I), a solution of 4,4'-dimethyl-2,2'-bipyridine (0.20 g, 1.10 mmol) in methanol (10 ml) was added to a solution of InCl<sub>3</sub>.4H<sub>2</sub>O (0.16 g, 0.55 mmol) in methanol (5 ml) at room temperature. The suitable crystals for X-ray analysis were isolated after one week by methanol diffusion to a colorless solution in DMSO (yield; 0.19 g, 71.4%).

### S3. Refinement

H atoms were positioned geometrically, with C—H = 0.93 and 0.96 Å for aromatic and methyl H, respectively, and constrained to ride on their parent atoms with U<sub>iso</sub>(H) = 1.2U<sub>eq</sub>(C).

**Figure 1**

The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 40% probability level.



**Figure 2**

A partial packing diagram of the title compound. Hydrogen bonds are shown as dashed lines.

**Trichlorido(4,4'-dimethyl-2,2'-bipyridine- $\kappa^2N,N'$ )(dimethyl sulfoxide- $\kappa O$ )indium(III)**

*Crystal data*

[InCl<sub>3</sub>(C<sub>12</sub>H<sub>12</sub>N<sub>2</sub>)(C<sub>2</sub>H<sub>6</sub>OS)]

$M_r = 483.54$

Monoclinic,  $P2_1/n$

Hall symbol:  $-P\ 2_1n$

$a = 8.2565$  (17) Å

$b = 23.456$  (5) Å

$c = 10.121$  (2) Å

$\beta = 105.95$  (3)°

$V = 1884.7$  (7) Å<sup>3</sup>

$Z = 4$

$F(000) = 960$

$D_x = 1.704$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 2052 reflections

$\theta = 1.7$ – $29.3$ °

$\mu = 1.79$  mm<sup>-1</sup>

$T = 298$  K

Prism, colorless

$0.49 \times 0.46 \times 0.44$  mm

*Data collection*

Bruker SMART CCD area-detector  
diffractometer  
Radiation source: fine-focus sealed tube  
Graphite monochromator  
 $\varphi$  and  $\omega$  scans  
Absorption correction: multi-scan  
(*SADABS*; Sheldrick, 1998)  
 $T_{\min} = 0.404$ ,  $T_{\max} = 0.455$

13791 measured reflections  
5046 independent reflections  
4804 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.038$   
 $\theta_{\max} = 29.3^\circ$ ,  $\theta_{\min} = 1.7^\circ$   
 $h = -11 \rightarrow 11$   
 $k = -28 \rightarrow 32$   
 $l = -13 \rightarrow 12$

*Refinement*

Refinement on  $F^2$   
Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.036$   
 $wR(F^2) = 0.085$   
 $S = 1.16$   
5046 reflections  
201 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  
 $w = 1/[\sigma^2(F_o^2) + (0.0263P)^2 + 2.6542P]$   
where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.018$   
 $\Delta\rho_{\max} = 0.86 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -0.69 \text{ e } \text{\AA}^{-3}$

*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 ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
In1	0.67799 (2)	0.143868 (8)	0.722848 (19)	0.03114 (7)
Cl1	0.46060 (14)	0.15508 (4)	0.50881 (9)	0.0586 (2)
Cl2	0.89844 (14)	0.10102 (4)	0.63344 (12)	0.0620 (3)
Cl3	0.78999 (10)	0.24070 (3)	0.74202 (8)	0.04094 (16)
S1	0.41807 (11)	0.23105 (4)	0.82159 (9)	0.04457 (18)
O1	0.4998 (3)	0.17216 (10)	0.8405 (2)	0.0410 (5)
N1	0.5893 (3)	0.05448 (10)	0.7626 (2)	0.0345 (5)
N2	0.8245 (3)	0.11591 (10)	0.9400 (2)	0.0329 (5)
C1	0.4701 (4)	0.02601 (15)	0.6694 (3)	0.0443 (7)
H1	0.4125	0.0447	0.5892	0.053*
C2	0.4290 (4)	-0.03006 (14)	0.6877 (3)	0.0440 (7)
H2	0.3452	-0.0484	0.6207	0.053*
C3	0.5131 (4)	-0.05872 (13)	0.8059 (3)	0.0378 (6)
C4	0.4753 (5)	-0.12005 (14)	0.8289 (4)	0.0501 (8)
H4A	0.4398	-0.1232	0.9113	0.060*
H4B	0.5747	-0.1426	0.8378	0.060*

H4C	0.3872	-0.1335	0.7522	0.060*
C5	0.6370 (4)	-0.02882 (13)	0.9026 (3)	0.0369 (6)
H5	0.6968	-0.0468	0.9832	0.044*
C6	0.6714 (3)	0.02770 (12)	0.8790 (3)	0.0308 (5)
C7	0.8006 (3)	0.06232 (12)	0.9795 (3)	0.0311 (5)
C8	0.8859 (4)	0.04184 (13)	1.1078 (3)	0.0359 (6)
H8	0.8674	0.0047	1.1325	0.043*
C9	1.0000 (4)	0.07688 (13)	1.2006 (3)	0.0374 (6)
C10	1.0914 (5)	0.05639 (17)	1.3414 (4)	0.0530 (9)
H10A	1.0620	0.0799	1.4089	0.064*
H10B	1.2106	0.0585	1.3532	0.064*
H10C	1.0601	0.0176	1.3524	0.064*
C11	1.0221 (4)	0.13209 (14)	1.1568 (3)	0.0403 (6)
H11	1.0970	0.1569	1.2147	0.048*
C12	0.9325 (4)	0.14978 (13)	1.0270 (3)	0.0400 (6)
H12	0.9482	0.1867	0.9995	0.048*
C13	0.5259 (7)	0.2699 (2)	0.9695 (5)	0.0731 (13)
H13A	0.6407	0.2757	0.9686	0.088*
H13B	0.5234	0.2489	1.0504	0.088*
H13C	0.4720	0.3061	0.9699	0.088*
C14	0.2249 (5)	0.2199 (2)	0.8626 (5)	0.0722 (13)
H14A	0.2464	0.2014	0.9503	0.087*
H14B	0.1527	0.1963	0.7935	0.087*
H14C	0.1711	0.2559	0.8661	0.087*

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
In1	0.03794 (11)	0.02645 (10)	0.03083 (10)	-0.00110 (7)	0.01249 (7)	0.00088 (7)
C11	0.0729 (6)	0.0538 (5)	0.0380 (4)	-0.0016 (4)	-0.0033 (4)	0.0062 (3)
C12	0.0772 (6)	0.0409 (4)	0.0877 (7)	0.0027 (4)	0.0561 (6)	-0.0066 (4)
C13	0.0448 (4)	0.0282 (3)	0.0536 (4)	-0.0030 (3)	0.0197 (3)	0.0006 (3)
S1	0.0475 (4)	0.0469 (4)	0.0438 (4)	0.0125 (3)	0.0200 (3)	0.0068 (3)
O1	0.0441 (11)	0.0412 (12)	0.0434 (11)	0.0053 (9)	0.0216 (9)	0.0042 (9)
N1	0.0379 (12)	0.0297 (12)	0.0350 (11)	-0.0049 (9)	0.0085 (9)	-0.0006 (9)
N2	0.0326 (11)	0.0296 (11)	0.0373 (12)	-0.0019 (9)	0.0111 (9)	0.0009 (9)
C1	0.0473 (17)	0.0394 (16)	0.0392 (15)	-0.0067 (14)	0.0002 (13)	0.0022 (12)
C2	0.0460 (17)	0.0384 (16)	0.0441 (16)	-0.0122 (13)	0.0067 (13)	-0.0062 (13)
C3	0.0455 (15)	0.0313 (14)	0.0406 (14)	-0.0055 (12)	0.0183 (12)	-0.0046 (11)
C4	0.068 (2)	0.0322 (16)	0.0527 (19)	-0.0109 (15)	0.0213 (17)	-0.0040 (14)
C5	0.0446 (15)	0.0312 (14)	0.0354 (13)	-0.0030 (12)	0.0116 (12)	0.0015 (11)
C6	0.0335 (12)	0.0290 (13)	0.0311 (12)	-0.0019 (10)	0.0109 (10)	-0.0028 (10)
C7	0.0329 (12)	0.0294 (13)	0.0321 (12)	0.0000 (10)	0.0109 (10)	-0.0018 (10)
C8	0.0405 (14)	0.0284 (13)	0.0382 (14)	-0.0002 (11)	0.0095 (11)	-0.0007 (11)
C9	0.0377 (14)	0.0364 (15)	0.0356 (14)	0.0029 (12)	0.0059 (11)	-0.0030 (11)
C10	0.061 (2)	0.051 (2)	0.0391 (16)	0.0022 (17)	-0.0007 (15)	0.0011 (14)
C11	0.0388 (15)	0.0365 (15)	0.0424 (15)	-0.0051 (12)	0.0058 (12)	-0.0067 (12)
C12	0.0416 (15)	0.0314 (14)	0.0478 (16)	-0.0073 (12)	0.0136 (13)	-0.0020 (12)

C13	0.091 (3)	0.064 (3)	0.079 (3)	-0.017 (2)	0.048 (3)	-0.028 (2)
C14	0.042 (2)	0.100 (4)	0.079 (3)	0.017 (2)	0.025 (2)	0.007 (3)

*Geometric parameters (Å, °)*

C11—In1	2.4180 (12)	C7—N2	1.350 (4)
C12—In1	2.4592 (10)	C7—C8	1.382 (4)
C13—In1	2.4398 (9)	C8—C9	1.400 (4)
O1—In1	2.233 (2)	C8—H8	0.9300
O1—S1	1.526 (2)	C9—C11	1.397 (4)
N1—In1	2.293 (2)	C9—C10	1.497 (4)
N2—In1	2.294 (2)	C10—H10A	0.9600
C1—N1	1.339 (4)	C10—H10B	0.9600
C1—C2	1.383 (5)	C10—H10C	0.9600
C1—H1	0.9300	C11—C12	1.382 (5)
C2—C3	1.382 (5)	C11—H11	0.9300
C2—H2	0.9300	C12—N2	1.331 (4)
C3—C5	1.395 (4)	C12—H12	0.9300
C3—C4	1.504 (4)	C13—S1	1.770 (5)
C4—H4A	0.9600	C13—H13A	0.9600
C4—H4B	0.9600	C13—H13B	0.9600
C4—H4C	0.9600	C13—H13C	0.9600
C5—C6	1.390 (4)	C14—S1	1.775 (4)
C5—H5	0.9300	C14—H14A	0.9600
C6—N1	1.343 (4)	C14—H14B	0.9600
C6—C7	1.495 (4)	C14—H14C	0.9600
C11—In1—C12	99.03 (4)	H4B—C4—H4C	109.5
C11—In1—C13	98.15 (3)	C6—C5—C3	120.3 (3)
C13—In1—C12	96.15 (3)	C6—C5—H5	119.9
O1—In1—C11	90.56 (7)	C3—C5—H5	119.9
O1—In1—C12	168.67 (6)	N1—C6—C5	121.3 (3)
O1—In1—C13	88.39 (6)	N1—C6—C7	115.9 (2)
O1—In1—N1	83.64 (9)	C5—C6—C7	122.8 (3)
O1—In1—N2	79.94 (9)	N2—C7—C8	121.6 (3)
N1—In1—C11	93.59 (7)	N2—C7—C6	116.1 (2)
N1—In1—C12	89.72 (7)	C8—C7—C6	122.3 (3)
N1—In1—C13	165.87 (6)	C7—C8—C9	120.1 (3)
N2—In1—C11	162.86 (7)	C7—C8—H8	119.9
N2—In1—C12	89.26 (7)	C9—C8—H8	119.9
N2—In1—C13	95.83 (7)	C11—C9—C8	117.0 (3)
N1—In1—N2	71.34 (9)	C11—C9—C10	121.6 (3)
O1—S1—C13	104.9 (2)	C8—C9—C10	121.4 (3)
O1—S1—C14	103.4 (2)	C9—C10—H10A	109.5
C13—S1—C14	98.8 (2)	C9—C10—H10B	109.5
H14B—C14—H14C	109.5	H10A—C10—H10B	109.5
S1—O1—In1	122.38 (12)	C9—C10—H10C	109.5
C1—N1—C6	118.7 (3)	H10A—C10—H10C	109.5



C1—N1—In1	122.7 (2)	H10B—C10—H10C	109.5
C6—N1—In1	118.26 (18)	C12—C11—C9	119.8 (3)
C12—N2—C7	119.1 (3)	C12—C11—H11	120.1
C12—N2—In1	123.0 (2)	C9—C11—H11	120.1
C7—N2—In1	117.94 (18)	N2—C12—C11	122.4 (3)
N1—C1—C2	122.7 (3)	N2—C12—H12	118.8
N1—C1—H1	118.7	C11—C12—H12	118.8
C2—C1—H1	118.7	S1—C13—H13A	109.5
C3—C2—C1	119.7 (3)	S1—C13—H13B	109.5
C3—C2—H2	120.2	H13A—C13—H13B	109.5
C1—C2—H2	120.2	S1—C13—H13C	109.5
C2—C3—C5	117.4 (3)	H13A—C13—H13C	109.5
C2—C3—C4	121.6 (3)	H13B—C13—H13C	109.5
C5—C3—C4	121.1 (3)	S1—C14—H14A	109.5
C3—C4—H4A	109.5	S1—C14—H14B	109.5
C3—C4—H4B	109.5	H14A—C14—H14B	109.5
H4A—C4—H4B	109.5	S1—C14—H14C	109.5
C3—C4—H4C	109.5	H14A—C14—H14C	109.5
H4A—C4—H4C	109.5		
S1—O1—In1—N1	-154.51 (17)	N1—C1—C2—C3	-0.1 (5)
S1—O1—In1—N2	133.38 (17)	C1—C2—C3—C5	0.2 (5)
S1—O1—In1—Cl1	-60.97 (15)	C1—C2—C3—C4	-178.7 (3)
S1—O1—In1—Cl3	37.17 (15)	C2—C3—C5—C6	0.4 (5)
S1—O1—In1—Cl2	151.0 (2)	C4—C3—C5—C6	179.4 (3)
C1—N1—In1—O1	98.2 (3)	C3—C5—C6—N1	-1.2 (4)
C6—N1—In1—O1	-88.1 (2)	C3—C5—C6—C7	179.0 (3)
C1—N1—In1—N2	179.7 (3)	C5—C6—N1—C1	1.3 (4)
C6—N1—In1—N2	-6.6 (2)	C7—C6—N1—C1	-178.9 (3)
C1—N1—In1—Cl1	8.0 (3)	C5—C6—N1—In1	-172.7 (2)
C6—N1—In1—Cl1	-178.3 (2)	C7—C6—N1—In1	7.1 (3)
C1—N1—In1—Cl3	154.2 (2)	N1—C6—C7—N2	-2.2 (4)
C6—N1—In1—Cl3	-32.1 (4)	C5—C6—C7—N2	177.6 (3)
C1—N1—In1—Cl2	-91.0 (3)	N1—C6—C7—C8	175.1 (3)
C6—N1—In1—Cl2	82.7 (2)	C5—C6—C7—C8	-5.1 (4)
C12—N2—In1—O1	-88.9 (2)	C8—C7—N2—C12	-0.2 (4)
C7—N2—In1—O1	91.9 (2)	C6—C7—N2—C12	177.1 (3)
C12—N2—In1—N1	-175.5 (3)	C8—C7—N2—In1	179.0 (2)
C7—N2—In1—N1	5.30 (19)	C6—C7—N2—In1	-3.7 (3)
C12—N2—In1—Cl1	-146.1 (2)	N2—C7—C8—C9	0.2 (4)
C7—N2—In1—Cl1	34.7 (4)	C6—C7—C8—C9	-177.0 (3)
C12—N2—In1—Cl3	-1.6 (2)	C7—C8—C9—C11	-0.2 (4)
C7—N2—In1—Cl3	179.24 (19)	C7—C8—C9—C10	178.6 (3)
C12—N2—In1—Cl2	94.5 (2)	C8—C9—C11—C12	0.3 (5)
C7—N2—In1—Cl2	-84.65 (19)	C10—C9—C11—C12	-178.5 (3)
In1—O1—S1—C13	-105.2 (2)	C9—C11—C12—N2	-0.3 (5)
In1—O1—S1—C14	151.6 (2)	C11—C12—N2—C7	0.3 (5)
C2—C1—N1—C6	-0.6 (5)	C11—C12—N2—In1	-178.9 (2)

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C2—C1—N1—In1                      173.1 (3)

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*Hydrogen-bond geometry (Å, °)*

<i>D—H...A</i>	<i>D—H</i>	<i>H...A</i>	<i>D...A</i>	<i>D—H...A</i>
C1—H1...C11	0.93	2.77	3.427 (4)	128
C10—H10C...C12 <sup>i</sup>	0.96	2.80	3.700 (4)	156

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Symmetry code: (i)  $-x+2, -y, -z+2$ .