

Trichlorido(6-methyl-2,2'-bipyridine- κ^2N,N')(dimethylsulfoxide- κO)-indium(III)

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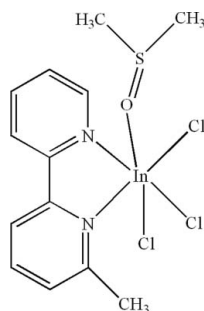
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Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(C-C) = 0.006$ Å; R factor = 0.033; wR factor = 0.076; data-to-parameter ratio = 18.2.

In the title compound, $[In(C_{11}H_{10}N_2)Cl_3(C_2H_6OS)]$, the In^{III} cation is six-coordinated in a distorted octahedral configuration by two N atoms from the chelating 6-methyl-2,2'-bipyridine ligand, one O atom from a dimethylsulfoxide group and three Cl⁻ anions. Weak intermolecular C—H \cdots O and C—H \cdots Cl hydrogen bonds and intramolecular C—H \cdots Cl hydrogen bonds are present in the structure.

Related literature

For related structures, see: Abedi *et al.* (2012*a,b*); Ahmadi *et al.* (2008*a,b,c*, 2009); Amani *et al.* (2009); Ilyukhin *et al.* (1994); Kalateh *et al.* (2008, 2010); Malyarick *et al.* (1992); Nan *et al.* (1987); Newkome *et al.* (1982); Onggo *et al.* (1990, 2005); Shirvan & Haydari Dezfuli (2012*a,b*); Shirvan *et al.* (2012).



Experimental

Crystal data

$[In(C_{11}H_{10}N_2)Cl_3(C_2H_6OS)]$

$M_r = 469.52$

Monoclinic, $P2_1/c$

$a = 13.0169$ (6) Å

$b = 8.5548$ (3) Å

$c = 15.9964$ (8) Å

$\beta = 93.393$ (4)°

$V = 1778.19$ (14) Å³

$Z = 4$

Mo $K\alpha$ radiation

$\mu = 1.90$ mm⁻¹

$T = 298$ K

0.40 × 0.25 × 0.20 mm

Data collection

Bruker APEXII CCD area detector
diffractometer

Absorption correction: multi-scan
(*SADABS*; Bruker, 2001)

$T_{\min} = 0.581$, $T_{\max} = 0.701$

14275 measured reflections

3496 independent reflections

2831 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.053$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.033$

$wR(F^2) = 0.076$

$S = 1.04$

3496 reflections

192 parameters

H-atom parameters constrained

$\Delta\rho_{\text{max}} = 0.65$ e Å⁻³

$\Delta\rho_{\text{min}} = -0.54$ e Å⁻³

Table 1

Selected bond lengths (Å).

In1—Cl1	2.4330 (10)	In1—O1	2.227 (2)
In1—Cl2	2.4468 (11)	In1—N1	2.270 (3)
In1—Cl3	2.4309 (9)	In1—N2	2.398 (3)

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 Cl2	0.93	2.75	3.348 (5)	123
C11—H11B \cdots Cl3	0.96	2.56	3.358 (6)	140
C13—H13A \cdots O1 ⁱ	0.96	2.47	3.419 (6)	169
C13—H13C \cdots Cl2 ⁱⁱ	0.96	2.82	3.612 (5)	141

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); 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: XU5625).

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supplementary materials

Acta Cryst. (2012). E68, m1327–m1328 [doi:10.1107/S1600536812041049]

Trichlorido(6-methyl-2,2'-bipyridine- κ^2N,N')(dimethylsulfoxide- κO)indium(III)**Sadif A. Shirvan, Sara Haydari Dezfuli, Elyas Golabi and Mohammad Amin Gholamzadeh****Comment**

Recently, we reported the synthesis and crystal structure of [In(4,4'-dmbipy)Cl₃(MeOH)].MeOH, (II), (Shirvan & Haydari Dezfuli, 2012a) and [In{NH(py)₂}Cl₃(DMSO)], (III), (Shirvan & Haydari Dezfuli, 2012b) [where 4,4'-dmbpy is 4,4'-dimethyl-2,2'-bipyridine and NH(py)₂ is di-2-pyridylamine]. There are several In^{III} complexes, with formula, [In(N—N)Cl₃(L)], (L = DMSO, H₂O, MeOH and EtOH), such as [In(bipy)Cl₃(H₂O)], (IV), [In(bipy)Cl₃(EtOH)], (V) and [In(bipy)Cl₃(H₂O)].H₂O, (VI), (Malyarick *et al.*, 1992), [In(phen)Cl₃(DMSO)], (VII), (Nan *et al.*, 1987), [In(phen)Cl₃(H₂O)], (VIII) and [In(phen)Cl₃(EtOH)].EtOH, (IX), (Ilyukhin & Malyarik, 1994), [In(4,4'-dmbipy)Cl₃(DMSO)], (X), (Ahmadi *et al.*, 2008a), [In(5,5'-dmbipy)Cl₃(MeOH)], (XI), (Kalateh *et al.*, 2008), [In(4,4'-dtbipy)Cl₃(MeOH)].0.5MeOH, (XII), (Abedi *et al.*, 2012a), [In(4 b t)Cl₃(MeOH)], (XIII) and [In(4 b t)Cl₃(DMSO)], (XIV), (Abedi *et al.*, 2012b) [where bipy is 2,2'-bipyridine, phen is 1,10-phenanthroline, DMSO is dimethyl sulfoxide, 4,4'-dmbpy is 4,4'-dimethyl-2,2'-bipyridine, 5,5'-dmbpy is 5,5'-dimethyl-2,2'-bipyridine, 4,4'-dtbipy is 4,4'-di-tert-butyl-2,2'-bipyridine and 4 b t is 4,4'-bithiazole] have been synthesized and characterized by single-crystal X-ray diffraction methods. 6-Methyl-2,2'-bipyridine (6-mbipy) is a good ligand and a few complexes with 6-mbipy have been prepared, such as that of [Hg(6-mbipy)Cl₂], (XV), (Ahmadi *et al.*, 2008b), [Pt(6-mbipy)Cl₄], (XVI), (Amani *et al.*, 2009), [Pb₄(NO₃)₈(6-mbipy)₄], (XVII), (Ahmadi *et al.*, 2009), [Zn(6-mbipy)Br₂], (XVIII), (Kalateh *et al.*, 2010), [Zn(6-mbipy)Cl₂], (IXX), (Ahmadi *et al.*, 2008c), [Pd(6-mbipy)Cl₂], (XX), (Newkome *et al.*, 1982), [Ru(6-mbipy)₃][BF₄]₂, (XXI), (Onggo *et al.*, 2005), [Fe(6-mbipy)₃][ClO₄]₂.6-mbipy, (XXII), (Onggo *et al.*, 1990), and [Cd(6-mbipy)Br₂(DMSO)], (XXIII), (Shirvan *et al.*, 2012). We report herein the synthesis and crystal structure of the title compound (I).

In the title compound, (Fig. 1), the In^{III} atom is six-coordinated in a distorted octahedral configuration by two N atoms from the chelating 6-methyl-2,2'-bipyridine ligand, one O atom from a dimethyl sulfoxide and three Cl atoms. The In—Cl, In—N and In—O bond lengths and angles are collected in Table 1.

In the crystal structure, intermolecular C—H...O and C—H...Cl hydrogen bonds and π - π contact (Table 2 & Fig. 2) between the pyridine rings, Cg3—Cg3ⁱ [symmetry cods: (i) -X,2-Y,-Z, where Cg3 is centroid of the ring (N2/C6—C10)] may stabilize the structure, with centroid-centroid distance 3.774 (2) Å.

Experimental

For the preparation of the title compound, (I), a solution of 6-methyl-2,2'-bipyridine (0.28 g, 0.26 ml, 1.65 mmol) in methanol (10 ml) was added to a solution of InCl₃.4H₂O (0.48 g, 1.65 mmol) in methanol (10 ml) at room temperature. The suitable crystals for X-ray diffraction experiment were obtained by methanol diffusion to a colorless solution in DMSO. Suitable crystals were isolated after one week (yield; 0.56 g, 72.3%).

Refinement

All H atoms were positioned geometrically with C—H = 0.93 and 0.96 Å and constrained to ride on their parent atoms with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for methyl H atoms and $1.2U_{\text{eq}}(\text{C})$ for the others.

Computing details

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT* (Bruker, 2007); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

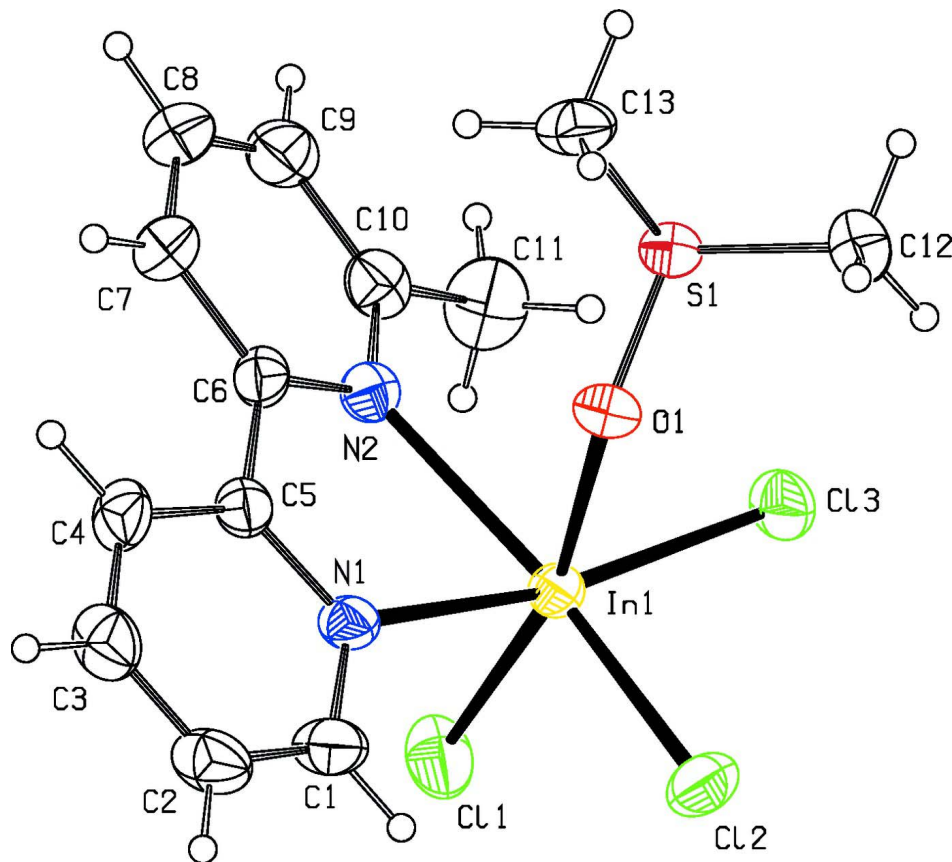


Figure 1

The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

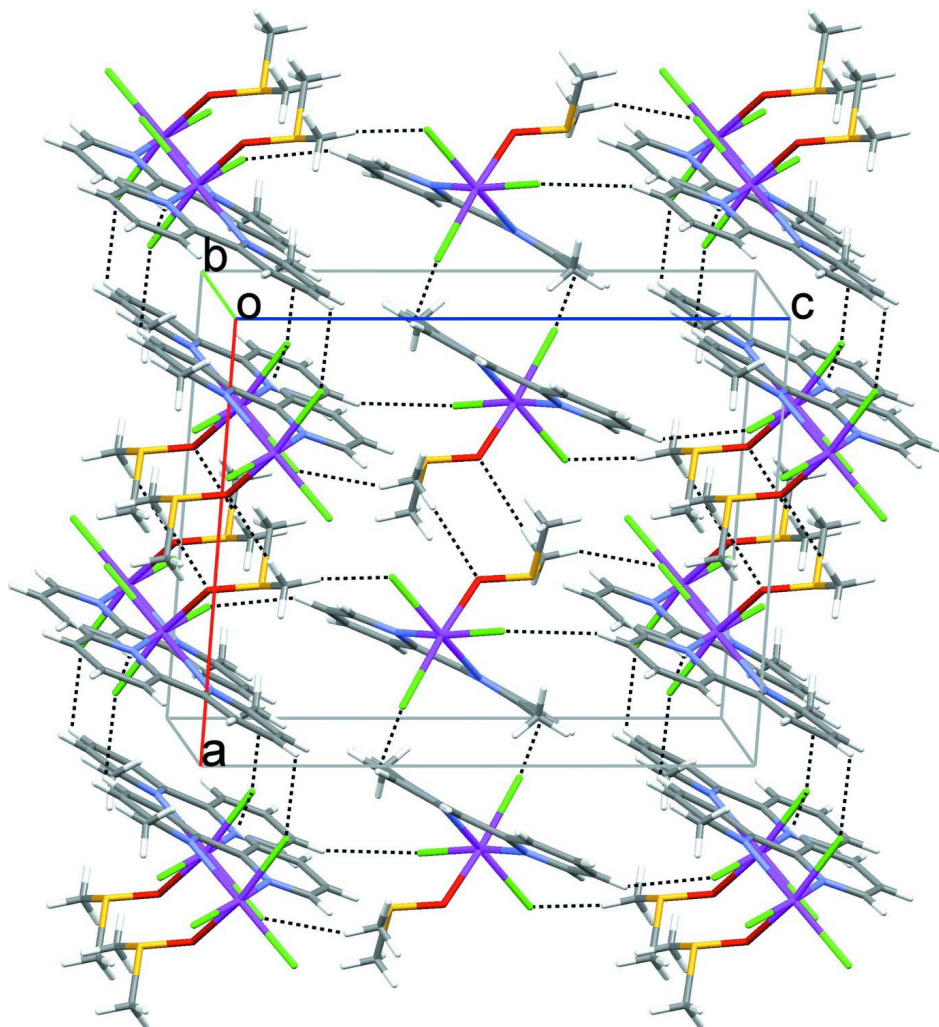


Figure 2

Unit-cell packing diagram for title molecule. Hydrogen bonds are shown as dashed lines.

Trichlorido(6-methyl-2,2'-bipyridine- κ^2N,N')(dimethyl sulfoxide- κO)indium (III)

Crystal data

[In(C₁₁H₁₀N₂)Cl₃(C₂H₆OS)]

$M_r = 469.52$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 13.0169$ (6) Å

$b = 8.5548$ (3) Å

$c = 15.9964$ (8) Å

$\beta = 93.393$ (4)°

$V = 1778.19$ (14) Å³

$Z = 4$

$F(000) = 928$

$D_x = 1.754$ Mg m⁻³

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

Cell parameters from 14275 reflections

$\theta = 1.6$ – 26.0 °

$\mu = 1.90$ mm⁻¹

$T = 298$ K

Prism, colorless

$0.40 \times 0.25 \times 0.20$ mm

Data collection

Bruker APEXII CCD area detector diffractometer	14275 measured reflections 3496 independent reflections
Radiation source: fine-focus sealed tube	2831 reflections with $I > 2\sigma(I)$
Graphite monochromator	$R_{\text{int}} = 0.053$
ω scans	$\theta_{\text{max}} = 26.0^\circ$, $\theta_{\text{min}} = 1.6^\circ$
Absorption correction: multi-scan (SADABS; Bruker, 2001)	$h = -16 \rightarrow 15$ $k = -10 \rightarrow 10$ $l = -17 \rightarrow 19$
$T_{\text{min}} = 0.581$, $T_{\text{max}} = 0.701$	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.033$	H-atom parameters constrained
$wR(F^2) = 0.076$	$w = 1/[\sigma^2(F_o^2) + (0.042P)^2]$
$S = 1.04$	where $P = (F_o^2 + 2F_c^2)/3$
3496 reflections	$(\Delta/\sigma)_{\text{max}} = 0.013$
192 parameters	$\Delta\rho_{\text{max}} = 0.65 \text{ e } \text{\AA}^{-3}$
0 restraints	$\Delta\rho_{\text{min}} = -0.54 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
N1	0.2514 (2)	0.9449 (3)	0.13539 (18)	0.0467 (7)
Cl1	0.12219 (10)	0.60548 (12)	0.13692 (9)	0.0801 (4)
C11	0.0925 (4)	0.6719 (6)	-0.1127 (4)	0.0878 (16)
H11A	0.0557	0.6185	-0.0709	0.105*
H11B	0.1589	0.6247	-0.1165	0.105*
H11C	0.0545	0.6644	-0.1658	0.105*
Cl2	0.40731 (9)	0.63682 (14)	0.17190 (7)	0.0715 (3)
N2	0.1563 (2)	0.8750 (3)	-0.01655 (19)	0.0455 (7)
C5	0.2065 (3)	1.0631 (4)	0.0914 (2)	0.0453 (8)
C2	0.2834 (4)	1.1141 (5)	0.2520 (3)	0.0704 (12)
H2	0.3095	1.1284	0.3069	0.084*
C3	0.2403 (4)	1.2359 (5)	0.2066 (3)	0.0676 (12)
H3	0.2373	1.3349	0.2304	0.081*
In1	0.269337 (19)	0.71247 (3)	0.069351 (15)	0.04247 (9)
C6	0.1608 (3)	1.0271 (4)	0.0064 (2)	0.0458 (8)
Cl3	0.30194 (9)	0.49559 (11)	-0.02363 (7)	0.0630 (3)
S1	0.38648 (7)	0.84709 (11)	-0.09440 (5)	0.0444 (2)

C9	0.0639 (3)	0.9526 (7)	-0.1425 (3)	0.0697 (12)
H9	0.0300	0.9247	-0.1932	0.084*
C12	0.5099 (4)	0.7693 (6)	-0.1071 (3)	0.0766 (13)
H12C	0.5248	0.7738	-0.1651	0.092*
H12B	0.5121	0.6626	-0.0885	0.092*
H12A	0.5602	0.8292	-0.0745	0.092*
C10	0.1050 (3)	0.8364 (5)	-0.0894 (3)	0.0572 (10)
C13	0.4079 (4)	1.0435 (5)	-0.1239 (3)	0.0660 (11)
H13A	0.4648	1.0855	-0.0902	0.079*
H13B	0.3473	1.1042	-0.1157	0.079*
H13C	0.4232	1.0472	-0.1819	0.079*
C8	0.0727 (4)	1.1049 (7)	-0.1215 (3)	0.0752 (13)
H8	0.0467	1.1820	-0.1579	0.090*
C1	0.2870 (4)	0.9711 (5)	0.2141 (2)	0.0635 (11)
H1	0.3156	0.8878	0.2448	0.076*
C7	0.1207 (3)	1.1444 (5)	-0.0456 (3)	0.0668 (11)
H7	0.1262	1.2486	-0.0293	0.080*
O1	0.37807 (18)	0.8589 (3)	0.00075 (14)	0.0470 (6)
C4	0.2017 (3)	1.2113 (4)	0.1264 (3)	0.0581 (10)
H4	0.1722	1.2935	0.0954	0.070*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0648 (19)	0.0362 (15)	0.0397 (16)	-0.0001 (13)	0.0090 (13)	0.0021 (13)
Cl1	0.0865 (8)	0.0494 (6)	0.1099 (9)	-0.0006 (5)	0.0514 (7)	0.0107 (6)
C11	0.080 (3)	0.086 (4)	0.093 (4)	-0.007 (3)	-0.024 (3)	-0.025 (3)
Cl2	0.0945 (8)	0.0633 (6)	0.0549 (6)	0.0203 (6)	-0.0109 (5)	0.0082 (5)
N2	0.0420 (15)	0.0475 (17)	0.0473 (17)	-0.0019 (13)	0.0036 (13)	0.0010 (13)
C5	0.0477 (19)	0.0385 (18)	0.051 (2)	-0.0012 (15)	0.0133 (16)	0.0036 (15)
C2	0.105 (3)	0.059 (3)	0.048 (2)	-0.010 (2)	0.010 (2)	-0.010 (2)
C3	0.088 (3)	0.044 (2)	0.072 (3)	-0.004 (2)	0.018 (2)	-0.013 (2)
In1	0.05532 (16)	0.03124 (13)	0.04150 (14)	0.00100 (11)	0.00834 (10)	0.00223 (10)
C6	0.0443 (18)	0.0391 (18)	0.055 (2)	0.0020 (14)	0.0118 (16)	0.0051 (16)
Cl3	0.0866 (7)	0.0446 (5)	0.0588 (6)	0.0033 (5)	0.0124 (5)	-0.0110 (4)
S1	0.0469 (5)	0.0475 (5)	0.0386 (4)	-0.0044 (4)	0.0013 (4)	0.0013 (4)
C9	0.053 (2)	0.102 (4)	0.053 (2)	0.010 (2)	-0.0027 (19)	0.002 (3)
C12	0.072 (3)	0.092 (3)	0.067 (3)	0.027 (3)	0.017 (2)	0.000 (3)
C10	0.046 (2)	0.069 (3)	0.056 (2)	-0.0017 (18)	0.0019 (18)	-0.007 (2)
C13	0.094 (3)	0.056 (2)	0.048 (2)	-0.006 (2)	0.004 (2)	0.0128 (19)
C8	0.079 (3)	0.088 (4)	0.058 (3)	0.024 (3)	0.000 (2)	0.017 (2)
C1	0.099 (3)	0.050 (2)	0.042 (2)	-0.002 (2)	0.006 (2)	0.0023 (17)
C7	0.079 (3)	0.057 (2)	0.065 (3)	0.016 (2)	0.009 (2)	0.014 (2)
O1	0.0514 (14)	0.0532 (14)	0.0367 (13)	-0.0085 (11)	0.0046 (10)	0.0020 (11)
C4	0.067 (2)	0.0359 (18)	0.073 (3)	0.0062 (18)	0.010 (2)	-0.0004 (19)

Geometric parameters (\AA , $^\circ$)

In1—Cl1	2.4330 (10)	C3—H3	0.9300
In1—Cl2	2.4468 (11)	C6—C7	1.385 (5)

In1—C13	2.4309 (9)	S1—O1	1.536 (2)
In1—O1	2.227 (2)	S1—C12	1.762 (4)
In1—N1	2.270 (3)	S1—C13	1.772 (4)
In1—N2	2.398 (3)	C9—C8	1.348 (7)
N1—C1	1.335 (5)	C9—C10	1.394 (6)
N1—C5	1.346 (4)	C9—H9	0.9300
C11—C10	1.462 (6)	C12—H12C	0.9600
C11—H11A	0.9600	C12—H12B	0.9600
C11—H11B	0.9600	C12—H12A	0.9600
C11—H11C	0.9600	C13—H13A	0.9600
N2—C10	1.349 (5)	C13—H13B	0.9600
N2—C6	1.353 (4)	C13—H13C	0.9600
C5—C4	1.390 (5)	C8—C7	1.376 (7)
C5—C6	1.483 (5)	C8—H8	0.9300
C2—C1	1.368 (6)	C1—H1	0.9300
C2—C3	1.371 (7)	C7—H7	0.9300
C2—H2	0.9300	C4—H4	0.9300
C3—C4	1.367 (7)		
C1—N1—C5	118.9 (3)	N2—C6—C5	117.2 (3)
C1—N1—In1	123.2 (3)	C7—C6—C5	121.1 (3)
C5—N1—In1	117.9 (2)	O1—S1—C12	104.9 (2)
C10—C11—H11A	109.5	O1—S1—C13	102.90 (18)
C10—C11—H11B	109.5	C12—S1—C13	99.7 (2)
H11A—C11—H11B	109.5	C8—C9—C10	120.9 (4)
C10—C11—H11C	109.5	C8—C9—H9	119.6
H11A—C11—H11C	109.5	C10—C9—H9	119.6
H11B—C11—H11C	109.5	S1—C12—H12C	109.5
C10—N2—C6	118.8 (3)	S1—C12—H12B	109.5
C10—N2—In1	127.5 (3)	H12C—C12—H12B	109.5
C6—N2—In1	112.8 (2)	S1—C12—H12A	109.5
N1—C5—C4	120.2 (4)	H12C—C12—H12A	109.5
N1—C5—C6	117.5 (3)	H12B—C12—H12A	109.5
C4—C5—C6	122.2 (3)	N2—C10—C9	120.3 (4)
C1—C2—C3	117.9 (4)	N2—C10—C11	119.8 (4)
C1—C2—H2	121.0	C9—C10—C11	119.9 (4)
C3—C2—H2	121.0	S1—C13—H13A	109.5
C4—C3—C2	119.8 (4)	S1—C13—H13B	109.5
C4—C3—H3	120.1	H13A—C13—H13B	109.5
C2—C3—H3	120.1	S1—C13—H13C	109.5
O1—In1—N1	79.77 (10)	H13A—C13—H13C	109.5
O1—In1—N2	77.17 (9)	H13B—C13—H13C	109.5
N1—In1—N2	71.48 (10)	C9—C8—C7	119.0 (4)
O1—In1—C13	89.36 (7)	C9—C8—H8	120.5
N1—In1—C13	168.44 (8)	C7—C8—H8	120.5
N2—In1—C13	102.44 (8)	N1—C1—C2	123.3 (4)
O1—In1—C11	166.02 (7)	N1—C1—H1	118.3
N1—In1—C11	91.00 (8)	C2—C1—H1	118.3
N2—In1—C11	90.00 (7)	C8—C7—C6	119.2 (4)

Cl3—In1—Cl1	98.93 (4)	C8—C7—H7	120.4
O1—In1—Cl2	90.94 (7)	C6—C7—H7	120.4
N1—In1—Cl2	90.64 (8)	S1—O1—In1	122.40 (14)
N2—In1—Cl2	159.89 (8)	C3—C4—C5	119.7 (4)
Cl3—In1—Cl2	93.47 (4)	C3—C4—H4	120.1
Cl1—In1—Cl2	99.71 (5)	C5—C4—H4	120.1
N2—C6—C7	121.7 (4)		
C1—N1—C5—C4	2.8 (5)	In1—N2—C6—C5	-17.8 (4)
In1—N1—C5—C4	-174.4 (3)	N1—C5—C6—N2	7.9 (5)
C1—N1—C5—C6	-175.5 (3)	C4—C5—C6—N2	-170.3 (3)
In1—N1—C5—C6	7.3 (4)	N1—C5—C6—C7	-174.6 (3)
C1—C2—C3—C4	0.6 (7)	C4—C5—C6—C7	7.1 (5)
C1—N1—In1—O1	-109.3 (3)	C6—N2—C10—C9	4.4 (5)
C5—N1—In1—O1	67.8 (2)	In1—N2—C10—C9	-163.4 (3)
C1—N1—In1—N2	170.9 (3)	C6—N2—C10—C11	-175.5 (4)
C5—N1—In1—N2	-12.0 (2)	In1—N2—C10—C11	16.7 (5)
C1—N1—In1—Cl3	-129.4 (4)	C8—C9—C10—N2	-1.3 (6)
C5—N1—In1—Cl3	47.8 (6)	C8—C9—C10—C11	178.6 (5)
C1—N1—In1—Cl1	81.2 (3)	C10—C9—C8—C7	-1.7 (7)
C5—N1—In1—Cl1	-101.6 (2)	C5—N1—C1—C2	-2.3 (6)
C1—N1—In1—Cl2	-18.5 (3)	In1—N1—C1—C2	174.8 (3)
C5—N1—In1—Cl2	158.7 (2)	C3—C2—C1—N1	0.6 (7)
C10—N2—In1—O1	100.7 (3)	C9—C8—C7—C6	1.5 (7)
C6—N2—In1—O1	-67.7 (2)	N2—C6—C7—C8	1.7 (6)
C10—N2—In1—N1	-176.0 (3)	C5—C6—C7—C8	-175.6 (4)
C6—N2—In1—N1	15.6 (2)	C12—S1—O1—In1	-112.8 (2)
C10—N2—In1—Cl3	14.2 (3)	C13—S1—O1—In1	143.3 (2)
C6—N2—In1—Cl3	-154.2 (2)	N1—In1—O1—S1	-139.25 (18)
C10—N2—In1—Cl1	-84.9 (3)	N2—In1—O1—S1	-66.10 (17)
C6—N2—In1—Cl1	106.7 (2)	Cl3—In1—O1—S1	36.81 (16)
C10—N2—In1—Cl2	155.7 (2)	Cl1—In1—O1—S1	-89.9 (3)
C6—N2—In1—Cl2	-12.7 (4)	Cl2—In1—O1—S1	130.27 (16)
C10—N2—C6—C7	-4.7 (5)	C2—C3—C4—C5	-0.1 (7)
In1—N2—C6—C7	164.9 (3)	N1—C5—C4—C3	-1.7 (6)
C10—N2—C6—C5	172.7 (3)	C6—C5—C4—C3	176.5 (4)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C1—H1...Cl2	0.93	2.75	3.348 (5)	123
C11—H11 <i>B</i> ...Cl3	0.96	2.56	3.358 (6)	140
C13—H13 <i>A</i> ...O1 ⁱ	0.96	2.47	3.419 (6)	169
C13—H13 <i>C</i> ...Cl2 ⁱⁱ	0.96	2.82	3.612 (5)	141

Symmetry codes: (i) $-x+1, -y+2, -z$; (ii) $x, -y+3/2, z-1/2$.