

# Trichlorido(5,5'-dimethyl-2,2'-bipyridine- $\kappa^2N,N'$ )(methanol- $\kappa O$ )indium(III)

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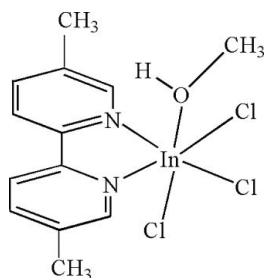
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Key indicators: single-crystal X-ray study;  $T = 120$  K; mean  $\sigma(C-C) = 0.003$  Å;  $R$  factor = 0.029;  $wR$  factor = 0.062; data-to-parameter ratio = 22.6.

In the molecule of the title compound,  $[InCl_3(C_{12}H_{12}N_2)(CH_4O)]$ , the  $In^{III}$  atom is six-coordinated in a distorted octahedral configuration by two N atoms from the chelating 5,5'-dimethyl-2,2'-bipyridine ligand, one O atom from a methanol molecule and three Cl atoms. In the crystal structure, intermolecular  $O-H \cdots Cl$  hydrogen bonds link the molecules into chains parallel to  $[001]$ .

## Related literature

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



## Experimental

### Crystal data

$[InCl_3(C_{12}H_{12}N_2)(CH_4O)]$   
 $M_r = 437.45$   
 Monoclinic,  $P2_1/c$   
 $a = 10.9080$  (6) Å  
 $b = 11.2087$  (7) Å  
 $c = 13.3584$  (8) Å  
 $\beta = 107.211$  (4)°  
 $V = 1560.12$  (16) Å<sup>3</sup>

$Z = 4$

Mo  $K\alpha$  radiation

$\mu = 2.02$  mm<sup>-1</sup>

### Data collection

Bruker SMART CCD area-detector diffractometer

Absorption correction: multi-scan

(*SADABS*; Sheldrick, 1998)

$T_{min} = 0.729$ ,  $T_{max} = 0.820$

$T = 120$  (2) K

$0.17 \times 0.15 \times 0.10$  mm

12144 measured reflections

4185 independent reflections

3716 reflections with  $I > 2\sigma(I)$

$R_{int} = 0.043$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.029$

$wR(F^2) = 0.062$

$S = 1.15$

4185 reflections

185 parameters

H atoms treated by a mixture of independent and constrained refinement

$\Delta\rho_{max} = 0.92$  e Å<sup>-3</sup>

$\Delta\rho_{min} = -0.68$  e Å<sup>-3</sup>

**Table 1**

Selected geometric parameters (Å, °).

In1—Cl1	2.5015 (6)	In1—O1	2.2991 (19)
In1—Cl2	2.4262 (6)	In1—N1	2.279 (2)
In1—Cl3	2.4080 (6)	In1—N2	2.284 (2)
Cl2—In1—Cl1	96.05 (2)	N1—In1—Cl3	162.82 (6)
Cl3—In1—Cl1	100.89 (2)	N1—In1—O1	80.51 (7)
Cl3—In1—Cl2	99.22 (2)	N1—In1—N2	72.73 (7)
O1—In1—Cl1	169.20 (5)	N2—In1—Cl1	87.68 (5)
O1—In1—Cl2	88.30 (5)	N2—In1—Cl2	165.54 (5)
O1—In1—Cl3	88.11 (5)	N2—In1—Cl3	93.76 (5)
N1—In1—Cl1	89.35 (5)	N2—In1—O1	85.77 (7)
N1—In1—Cl2	93.30 (5)		

**Table 2**

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O1—H1B $\cdots$ Cl1 <sup>i</sup>	0.83 (5)	2.29 (5)	3.115 (2)	174 (4)

Symmetry code: (i)  $x, -y + \frac{1}{2}, z + \frac{1}{2}$ .

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINTE* (Bruker, 1998); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); 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: HK2541).

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**supplementary materials**

*Acta Cryst.* (2008). E64, m1353-m1354 [ doi:10.1107/S160053680803119X ]

## Trichlorido(5,5'-dimethyl-2,2'-bipyridine- $\kappa^2N,N'$ )(methanol- $\kappa O$ )indium(III)

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### 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), [HgI<sub>2</sub>(4,4'-dmbpy)], (IV), (Yousefi, Tadayon Pour *et al.*, 2008), [Cd(5,5'-dmbpy)( $\mu$ -Cl)<sub>2</sub>]<sub>n</sub>, (V), (Ahmadi, Khalighi *et al.*, 2008), [Hg(5,5'-dmbpy)I<sub>2</sub>], (VI), (Tadayon Pour *et al.*, 2008), [Cu(5,5'-dcbpy)(en)(H<sub>2</sub>O)<sub>2</sub>].2.5H<sub>2</sub>O, (VII), (Yousefi, Khalighi *et al.*, 2008), [Hg(dmphen)I<sub>2</sub>], (VIII), (Yousefi, Rashidi Vahid *et al.*, 2008), and {[HgCl(dm4bt)]<sub>2</sub>( $\mu$ -Cl)<sub>2</sub>}, (IX), (Khavasi *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, en is ethylene-diamine, dmphen is 4,7-diphenyl-1,10-phenanthroline and dm4bt is 2,2'-dimethyl-4,4'-bithiazole]. We have also reported the syntheses and crystal structures of iron(III) complexes of [Fe(bipy)Cl<sub>3</sub>(DMSO)], (X) and [Fe(phen)Cl<sub>3</sub>(DMSO)], (XI), (Amani *et al.*, 2007) and [Fe(phen)Cl<sub>3</sub>(CH<sub>3</sub>OH)].CH<sub>3</sub>OH, (XII), (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)], (XIII), [In(bipy)Cl<sub>3</sub>(EtOH)], (XIV) and [In(bipy)Cl<sub>3</sub>(H<sub>2</sub>O)].H<sub>2</sub>O, (XV), (Malyarick *et al.*, 1992), [In(phen)Cl<sub>3</sub>(DMSO)], (XVI), (Nan *et al.*, 1987), [In(4,4'-dmbpy)Cl<sub>3</sub>(DMSO)], (XVII), (Ahmadi, Kalateh, Abedi *et al.*, 2008), [In(phen)Cl<sub>3</sub>(H<sub>2</sub>O)], (XVIII), and [In(phen)Cl<sub>3</sub>(EtOH)].EtOH, (XIX), (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 the chelating 5,5'-dimethyl-2,2'-bipyridine ligand, one O atom from one methanol and three Cl atoms. The In—Cl and In—N bond lengths and angles (Table 1) are within normal ranges, as in (XIII), (XIV), (XV) and (XVII).

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

### Experimental

For the preparation of the title compound, (I), a solution of 5,5'-dimethyl-2,2'-bipyridine (0.20 g, 1.10 mmol) in methanol (20 ml) was added to a solution of InCl<sub>3</sub>.4H<sub>2</sub>O (0.16 g, 0.55 mmol) in methanol (50 ml) and the resulting colorless solution was stirred for 20 min at 313 K. This solution was left to evaporate slowly at room temperature. After one week, colorless block crystals of the title compound were isolated (yield; 0.18 g, 74.8%, m.p. <573 K).

## Refinement

H1B atom (for OH) was located in difference synthesis and refined isotropically [O-H = 0.83 (5) Å;  $U_{\text{iso}}(\text{H}) = 0.036 (11) \text{ \AA}^2$ ]. The remaining 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  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .

## Figures

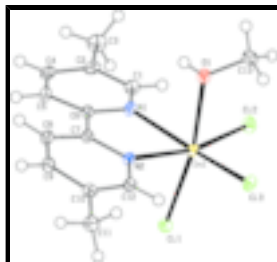


Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

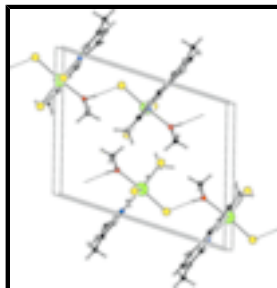


Fig. 2. A partial packing diagram of the title compound. Hydrogen bonds are shown as dashed lines.

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### Crystal data

[InCl<sub>3</sub>(C<sub>12</sub>H<sub>12</sub>N<sub>2</sub>)(CH<sub>4</sub>O)]

$M_r = 437.45$

Monoclinic,  $P2_1/c$

Hall symbol: -P 2ybc

$a = 10.9080 (6) \text{ \AA}$

$b = 11.2087 (7) \text{ \AA}$

$c = 13.3584 (8) \text{ \AA}$

$\beta = 107.211 (4)^\circ$

$V = 1560.12 (16) \text{ \AA}^3$

$Z = 4$

$F_{000} = 864$

$D_x = 1.862 \text{ Mg m}^{-3}$

Mo  $K\alpha$  radiation

$\lambda = 0.71073 \text{ \AA}$

Cell parameters from 1324 reflections

$\theta = 2.0\text{--}29.2^\circ$

$\mu = 2.02 \text{ mm}^{-1}$

$T = 120 (2) \text{ K}$

Block, colorless

$0.17 \times 0.15 \times 0.10 \text{ mm}$

### Data collection

Bruker SMART CCD area-detector  
diffractometer

4185 independent reflections

Radiation source: fine-focus sealed tube	3716 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.043$
$T = 120(2)$ K	$\theta_{\text{max}} = 29.2^\circ$
$\varphi$ and $\omega$ scans	$\theta_{\text{min}} = 2.0^\circ$
Absorption correction: multi-scan (SADABS; Sheldrick, 1998)	$h = -14 \rightarrow 14$
$T_{\text{min}} = 0.729$ , $T_{\text{max}} = 0.820$	$k = -15 \rightarrow 15$
12144 measured reflections	$l = -14 \rightarrow 18$

### Refinement

Refinement on $F^2$	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.029$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.062$	$w = 1/[\sigma^2(F_o^2) + (0.0209P)^2 + 1.9934P]$
$S = 1.15$	where $P = (F_o^2 + 2F_c^2)/3$
4185 reflections	$(\Delta/\sigma)_{\text{max}} = 0.017$
185 parameters	$\Delta\rho_{\text{max}} = 0.92 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\text{min}} = -0.68 \text{ e } \text{\AA}^{-3}$
	Extinction correction: none

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

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
In1	0.773908 (15)	0.320581 (14)	-0.004168 (13)	0.01003 (5)
Cl1	0.87230 (6)	0.29569 (5)	-0.14993 (5)	0.01500 (11)
Cl2	0.55271 (5)	0.31788 (6)	-0.11430 (5)	0.01766 (12)
Cl3	0.79945 (6)	0.53204 (5)	0.02679 (5)	0.01588 (11)
O1	0.69912 (19)	0.30834 (17)	0.13936 (16)	0.0178 (4)
H1B	0.740 (4)	0.280 (4)	0.197 (4)	0.036 (11)*
N1	0.7811 (2)	0.11891 (18)	0.01880 (17)	0.0126 (4)
N2	0.97004 (19)	0.27552 (18)	0.10949 (16)	0.0109 (4)
C1	0.6867 (2)	0.0450 (2)	-0.0335 (2)	0.0152 (5)

## supplementary materials

H1	0.6098	0.0782	-0.0740	0.018*
C2	0.6982 (3)	-0.0788 (2)	-0.0299 (2)	0.0160 (5)
C3	0.5882 (3)	-0.1568 (2)	-0.0885 (2)	0.0222 (5)
H3A	0.5655	-0.1386	-0.1619	0.027*
H3B	0.5158	-0.1426	-0.0632	0.027*
H3C	0.6132	-0.2391	-0.0777	0.027*
C4	0.8152 (3)	-0.1254 (2)	0.0288 (2)	0.0172 (5)
H4	0.8282	-0.2075	0.0310	0.021*
C5	0.9129 (2)	-0.0502 (2)	0.0843 (2)	0.0161 (5)
H5	0.9908	-0.0815	0.1247	0.019*
C6	0.8929 (2)	0.0732 (2)	0.07869 (19)	0.0123 (4)
C7	0.9932 (2)	0.1588 (2)	0.13432 (19)	0.0117 (4)
C8	1.1071 (2)	0.1235 (2)	0.2067 (2)	0.0154 (5)
H8	1.1202	0.0440	0.2269	0.018*
C9	1.2017 (2)	0.2081 (2)	0.2486 (2)	0.0151 (5)
H9	1.2782	0.1852	0.2974	0.018*
C10	1.1821 (2)	0.3271 (2)	0.21787 (19)	0.0136 (4)
C11	1.2857 (2)	0.4191 (2)	0.2546 (2)	0.0171 (5)
H11A	1.2565	0.4812	0.2914	0.020*
H11B	1.3060	0.4525	0.1952	0.020*
H11C	1.3610	0.3824	0.3006	0.020*
C12	1.0617 (2)	0.3568 (2)	0.15016 (19)	0.0137 (4)
H12	1.0442	0.4365	0.1324	0.016*
C13	0.6145 (3)	0.3950 (2)	0.1646 (2)	0.0186 (5)
H13A	0.5359	0.3991	0.1083	0.022*
H13B	0.6552	0.4718	0.1744	0.022*
H13C	0.5963	0.3715	0.2278	0.022*

### Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
In1	0.00974 (8)	0.00875 (8)	0.00997 (8)	0.00064 (6)	0.00040 (5)	0.00051 (6)
Cl1	0.0161 (3)	0.0161 (3)	0.0129 (3)	0.0011 (2)	0.0044 (2)	-0.0003 (2)
Cl2	0.0119 (2)	0.0182 (3)	0.0186 (3)	0.0012 (2)	-0.0019 (2)	0.0003 (2)
Cl3	0.0203 (3)	0.0100 (2)	0.0166 (3)	-0.0002 (2)	0.0043 (2)	-0.0008 (2)
O1	0.0205 (9)	0.0188 (9)	0.0152 (9)	0.0059 (7)	0.0071 (7)	0.0035 (7)
N1	0.0118 (9)	0.0110 (9)	0.0136 (10)	-0.0003 (7)	0.0015 (8)	0.0011 (7)
N2	0.0111 (9)	0.0103 (8)	0.0102 (9)	-0.0003 (7)	0.0017 (7)	0.0009 (7)
C1	0.0161 (11)	0.0140 (11)	0.0152 (12)	-0.0024 (9)	0.0038 (9)	-0.0015 (9)
C2	0.0211 (12)	0.0132 (11)	0.0154 (11)	-0.0040 (9)	0.0080 (10)	-0.0008 (9)
C3	0.0250 (13)	0.0181 (12)	0.0230 (14)	-0.0078 (10)	0.0062 (11)	-0.0056 (10)
C4	0.0246 (13)	0.0096 (10)	0.0204 (13)	-0.0005 (9)	0.0112 (10)	0.0004 (9)
C5	0.0177 (11)	0.0128 (10)	0.0181 (12)	0.0048 (9)	0.0059 (10)	0.0038 (9)
C6	0.0125 (11)	0.0128 (10)	0.0116 (11)	0.0017 (8)	0.0035 (9)	0.0016 (8)
C7	0.0124 (10)	0.0124 (10)	0.0106 (10)	0.0012 (8)	0.0037 (8)	0.0019 (8)
C8	0.0147 (11)	0.0136 (11)	0.0166 (12)	0.0030 (9)	0.0025 (9)	0.0033 (9)
C9	0.0119 (10)	0.0189 (11)	0.0127 (11)	0.0020 (9)	0.0006 (9)	0.0022 (9)
C10	0.0131 (10)	0.0164 (11)	0.0111 (10)	-0.0009 (9)	0.0033 (8)	-0.0015 (9)

C11	0.0124 (11)	0.0211 (12)	0.0149 (12)	-0.0022 (9)	-0.0004 (9)	0.0005 (10)
C12	0.0139 (11)	0.0150 (10)	0.0117 (11)	0.0010 (8)	0.0030 (9)	0.0023 (9)
C13	0.0183 (12)	0.0173 (11)	0.0227 (13)	0.0012 (9)	0.0098 (10)	-0.0030 (10)

*Geometric parameters (Å, °)*

In1—C11	2.5015 (6)	C6—N1	1.347 (3)
In1—C12	2.4262 (6)	C6—C7	1.479 (3)
In1—C13	2.4080 (6)	C7—N2	1.355 (3)
In1—O1	2.2991 (19)	C7—C8	1.387 (3)
In1—N1	2.279 (2)	C8—C9	1.391 (4)
In1—N2	2.284 (2)	C8—H8	0.9300
O1—H1B	0.83 (5)	C9—C10	1.394 (4)
C1—N1	1.345 (3)	C9—H9	0.9300
C1—C2	1.393 (3)	C10—C12	1.397 (3)
C1—H1	0.9300	C10—C11	1.501 (3)
C2—C4	1.387 (4)	C11—H11A	0.9600
C2—C3	1.504 (4)	C11—H11B	0.9600
C3—H3A	0.9600	C11—H11C	0.9600
C3—H3B	0.9600	C12—N2	1.343 (3)
C3—H3C	0.9600	C12—H12	0.9300
C4—C5	1.389 (4)	C13—O1	1.447 (3)
C4—H4	0.9300	C13—H13A	0.9600
C5—C6	1.399 (3)	C13—H13B	0.9600
C5—H5	0.9300	C13—H13C	0.9600
C12—In1—C11	96.05 (2)	C2—C4—C5	120.4 (2)
C13—In1—C11	100.89 (2)	C2—C4—H4	119.8
C13—In1—C12	99.22 (2)	C5—C4—H4	119.8
O1—In1—C11	169.20 (5)	C4—C5—C6	119.2 (2)
O1—In1—C12	88.30 (5)	C4—C5—H5	120.4
O1—In1—C13	88.11 (5)	C6—C5—H5	120.4
N1—In1—C11	89.35 (5)	N1—C6—C5	120.5 (2)
N1—In1—C12	93.30 (5)	N1—C6—C7	117.2 (2)
N1—In1—C13	162.82 (6)	C5—C6—C7	122.3 (2)
N1—In1—O1	80.51 (7)	N2—C7—C8	120.6 (2)
N1—In1—N2	72.73 (7)	N2—C7—C6	116.6 (2)
N2—In1—C11	87.68 (5)	C8—C7—C6	122.8 (2)
N2—In1—C12	165.54 (5)	C7—C8—C9	119.4 (2)
N2—In1—C13	93.76 (5)	C7—C8—H8	120.3
N2—In1—O1	85.77 (7)	C9—C8—H8	120.3
In1—O1—H1B	125 (3)	C8—C9—C10	120.2 (2)
C13—O1—In1	124.22 (16)	C8—C9—H9	119.9
C13—O1—H1B	104 (3)	C10—C9—H9	119.9
C1—N1—In1	123.41 (17)	C9—C10—C12	116.8 (2)
C1—N1—C6	119.6 (2)	C9—C10—C11	121.8 (2)
C6—N1—In1	116.52 (16)	C12—C10—C11	121.4 (2)
C7—N2—In1	116.51 (16)	C10—C11—H11A	109.5
C12—N2—In1	123.91 (16)	C10—C11—H11B	109.5
C12—N2—C7	119.6 (2)	H11A—C11—H11B	109.5



## supplementary materials

N1—C1—C2	123.3 (3)	C10—C11—H11C	109.5
N1—C1—H1	118.4	H11A—C11—H11C	109.5
C2—C1—H1	118.4	H11B—C11—H11C	109.5
C4—C2—C1	116.9 (2)	N2—C12—C10	123.1 (2)
C4—C2—C3	122.3 (2)	N2—C12—H12	118.5
C1—C2—C3	120.8 (3)	C10—C12—H12	118.5
C2—C3—H3A	109.5	O1—C13—H13A	109.5
C2—C3—H3B	109.5	O1—C13—H13B	109.5
H3A—C3—H3B	109.5	H13A—C13—H13B	109.5
C2—C3—H3C	109.5	O1—C13—H13C	109.5
H3A—C3—H3C	109.5	H13A—C13—H13C	109.5
H3B—C3—H3C	109.5	H13B—C13—H13C	109.5
N1—In1—O1—C13	-152.9 (2)	N1—C1—C2—C3	178.8 (2)
N2—In1—O1—C13	133.9 (2)	C1—C2—C4—C5	2.5 (4)
C13—In1—O1—C13	40.01 (19)	C3—C2—C4—C5	-178.0 (2)
C12—In1—O1—C13	-59.27 (19)	C2—C4—C5—C6	-1.2 (4)
C11—In1—O1—C13	-173.3 (2)	C4—C5—C6—N1	-1.2 (4)
N2—In1—N1—C1	-175.9 (2)	C4—C5—C6—C7	-179.1 (2)
O1—In1—N1—C1	95.6 (2)	C5—C6—N1—C1	2.0 (4)
C13—In1—N1—C1	144.79 (17)	C7—C6—N1—C1	-180.0 (2)
C12—In1—N1—C1	7.9 (2)	C5—C6—N1—In1	-170.21 (19)
C11—In1—N1—C1	-88.11 (19)	C7—C6—N1—In1	7.8 (3)
N2—In1—N1—C6	-3.99 (17)	N1—C6—C7—N2	-8.3 (3)
O1—In1—N1—C6	-92.48 (18)	C5—C6—C7—N2	169.6 (2)
C13—In1—N1—C6	-43.3 (3)	N1—C6—C7—C8	173.2 (2)
C12—In1—N1—C6	179.80 (17)	C5—C6—C7—C8	-8.9 (4)
C11—In1—N1—C6	83.78 (17)	C8—C7—N2—C12	4.4 (4)
N1—In1—N2—C12	178.2 (2)	C6—C7—N2—C12	-174.2 (2)
O1—In1—N2—C12	-100.4 (2)	C8—C7—N2—In1	-176.82 (18)
C13—In1—N2—C12	-12.60 (19)	C6—C7—N2—In1	4.6 (3)
C12—In1—N2—C12	-166.46 (16)	N2—C7—C8—C9	-4.3 (4)
C11—In1—N2—C12	88.17 (19)	C6—C7—C8—C9	174.2 (2)
N1—In1—N2—C7	-0.55 (16)	C7—C8—C9—C10	-0.2 (4)
O1—In1—N2—C7	80.81 (17)	C8—C9—C10—C12	4.4 (4)
C13—In1—N2—C7	168.64 (17)	C8—C9—C10—C11	-174.9 (2)
C12—In1—N2—C7	14.8 (3)	C9—C10—C12—N2	-4.5 (4)
C11—In1—N2—C7	-90.59 (17)	C11—C10—C12—N2	174.9 (2)
C2—C1—N1—C6	-0.5 (4)	C10—C12—N2—C7	0.1 (4)
C2—C1—N1—In1	171.1 (2)	C10—C12—N2—In1	-178.61 (18)
N1—C1—C2—C4	-1.7 (4)		

### Hydrogen-bond geometry ( $\text{\AA}$ , $^\circ$ )

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1—H1B $\cdots$ C11 <sup>i</sup>	0.83 (5)	2.29 (5)	3.115 (2)	174 (4)

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

Fig. 1

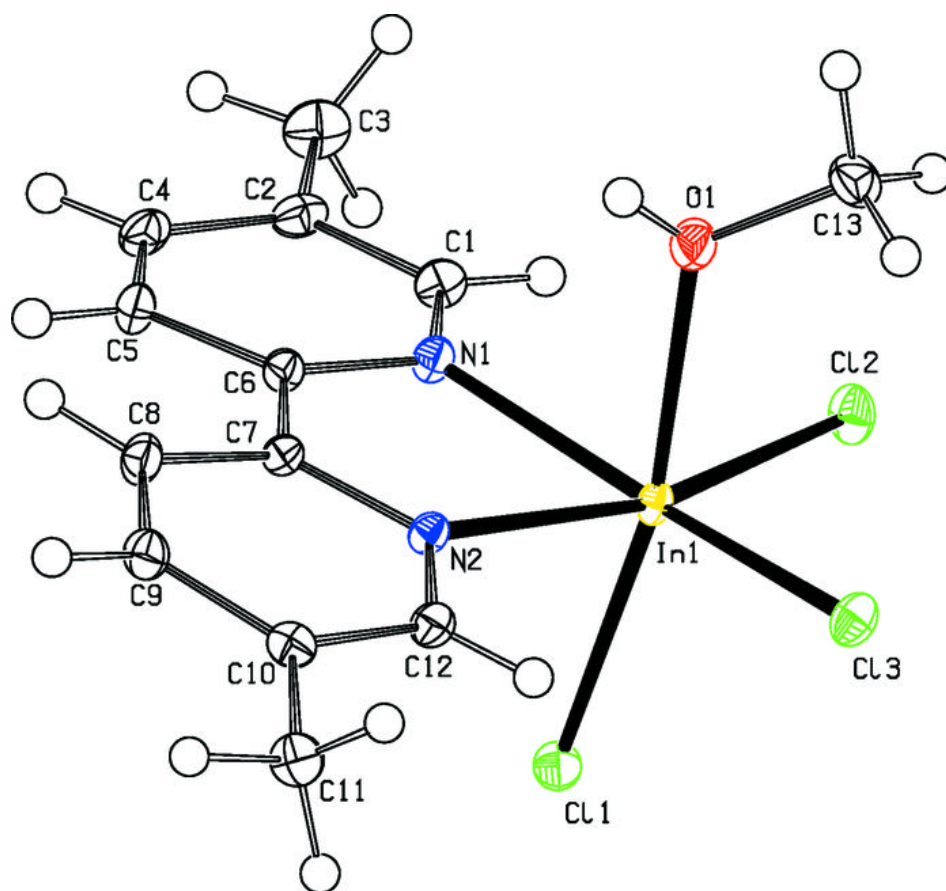


Fig. 2

