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Crystal structure of bis(μ_2 -5-nonanoylquinolin-8-olato)bis[aquadichloridoindium(III)]

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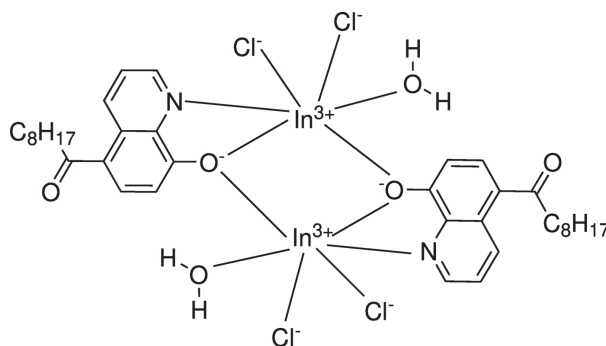
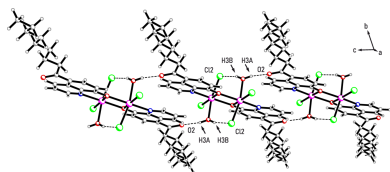
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Crystallization of 5-nonanoyl-8-hydroxyquinoline in the presence of InCl_3 in acetonitrile yields a dinuclear In^{III} complex crystallizing in the space group $P\bar{1}$. In this complex, $[\text{In}_2(\text{C}_{18}\text{H}_{22}\text{NO}_2)_2\text{Cl}_4(\text{H}_2\text{O})_2]$, each indium ion is sixfold coordinated by two chloride ions, one water molecule and two 8-quinolinolate ions. The crystal of the title complex is composed of two-dimensional supramolecular aggregates, resulting from the linkage of the $\text{O}_{\text{water}}-\text{H}\cdots\text{O}=\text{C}$ and $\text{O}_{\text{water}}-\text{H}\cdots\text{Cl}$ hydrogen bonds as well as bifurcated $\text{C}_{\text{arene}}-\text{H}\cdots\text{Cl}$ contacts.

1. Chemical context

As a result of the remarkable complexing properties of 8-hydroxyquinoline and its substituted derivatives towards various metal ions, their use as extracting agents for these ionic substrates has received much attention (for examples, see: Uhlemann *et al.*, 1984; Filik *et al.*, 1994; Gloe *et al.*, 1996; Yamada *et al.*, 2006). In addition, their application in the formation of luminescent coordination compounds has been the subject of intensive research (Matsumura *et al.*, 1996; Montes *et al.*, 2006; Feng *et al.*, 2007, 2008). Furthermore, 8-hydroxyquinoline-based building blocks have been used to construct artificial receptors, such as carbohydrate receptors (Mazik *et al.*, 2011; Geffert *et al.*, 2013), and have formed the basis for the development of various supramolecular architectures (Albrecht *et al.*, 2008).

Our previous studies on the extraction of indium ions by 8-hydroxyquinolines bearing alkanoyl or alkyl groups of different chain lengths showed that the 5-alkanoyl derivatives are more effective indium extractors than the analogues containing 5-alkyl-, 7-alkanoyl- or 7-alkyl substituents (Schulze *et al.*, 2019). The derivative with the *n*-nonanoyl group at the 5-position proved to be a particularly effective extractor for indium ions, showing not only the best selectivity for indium over iron and zinc ions, but also the most favorable extraction kinetics under the chosen experimental conditions.



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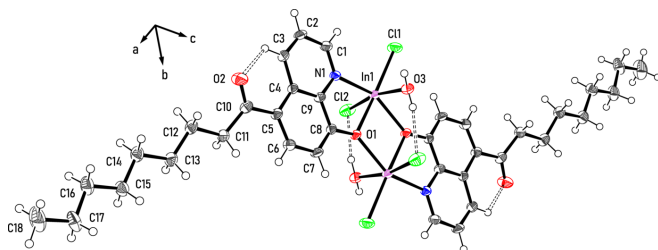


Figure 1
Perspective view of the molecular structure of the title complex including the labeling of atoms in the asymmetric unit. The ellipsoids correspond to the thermal displacement at 50% probability.

In this article we describe the crystal structure of a dinuclear In^{III} complex obtained by crystallization of 5-nonanoyl-8-hydroxyquinoline in the presence of InCl_3 in acetonitrile.

2. Structural commentary

The title complex crystallizes in the centrosymmetric space group $P\bar{1}$ with one half of the complex in the asymmetric unit of the cell. This structural motif is expanded by an inversion center to form a dinuclear complex as depicted in Fig. 1. Within the asymmetric unit, the indium ion is fivefold coordinated *via* one water molecule and two chloride ions as well as the atoms N1 and O1 of the bidentate quinolinolate ligand. The sixth coordination site of the metal center is occupied by the quinolinolate oxygen atom O1 of the inversion-related fragment of the complex, so that each In^{III} center adopts a distorted octahedral coordination geometry of the composition NO_3Cl_2 . The $\text{In}-\text{Y}$ bond lengths ($\text{Y} = \text{N}, \text{O}, \text{Cl}$) are listed in Table 1 and range between 2.17 and 2.43 Å. The nonanoyl fragment of the quinolinolate ligand exists in an elongated conformation. The complex structure is stabilized by intramolecular hydrogen bonds involving the water hydrogen atom H3B and the chloride ion Cl2 [$d(\text{H}\cdots\text{Cl}) = 2.27(4)$ Å, $\text{O}-\text{H}\cdots\text{Cl} = 165(4)^\circ$] as well as $\text{C}-\text{H}\cdots\text{O}$ contacts between the nonanoyl oxygen atom O2 and the arene hydrogen atom H3 [$d(\text{H}\cdots\text{O}) = 2.21$ Å, $\text{C}-\text{H}\cdots\text{O} = 122^\circ$].

3. Supramolecular features

Regarding the packing behavior of the dinuclear complexes, hydrogen bonds play an important role. On one hand, the

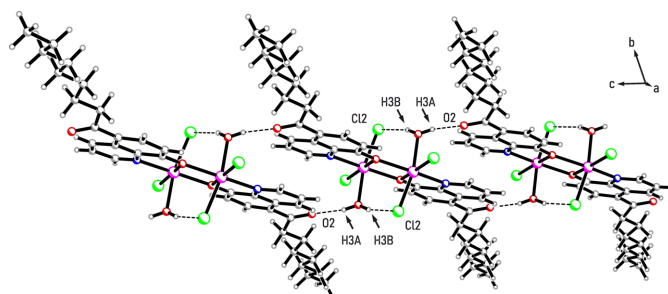


Figure 2
Supramolecular chain formed by strong hydrogen bonds; color code: N – blue, O – red, Cl – green, In – magenta, C/H – gray.

Table 1

Geometric data (Å, °) for short intra- and intermolecular interactions.

CgA is the centroid of the N1/C1–C4/C9 ring.

$\text{In}-\text{Y}$		$\text{In}-\text{Y}$		
$\text{In1}-\text{O1}^{\text{i}}$	2.166 (3)	$\text{In1}-\text{N1}^{\text{ii}}$	2.241 (4)	
$\text{In1}-\text{O1}^{\text{ii}}$	2.209 (3)	$\text{In1}-\text{Cl1}^{\text{ii}}$	2.382 (2)	
$\text{In1}-\text{O3}^{\text{ii}}$	2.227 (4)	$\text{In1}-\text{Cl2}^{\text{ii}}$	2.430 (2)	
$D-\text{H}\cdots A/\text{Cg}$	$D-\text{H}$	$\text{H}\cdots A/\text{Cg}$	$D-A/\text{Cg}$	$D-\text{H}\cdots A/\text{Cg}$
$\text{O3}-\text{H3A}\cdots\text{O2}^{\text{iii}}$	0.84 (4)	1.84 (4)	2.668 (4)	168 (5)
$\text{O3}-\text{H3B}\cdots\text{Cl2}^{\text{i}}$	0.92 (4)	2.27 (4)	3.165 (4)	165 (4)
$\text{C1}-\text{H1}\cdots\text{Cl1}^{\text{iv}}$	0.95	2.76	3.417 (6)	127
$\text{C2}-\text{H2}\cdots\text{Cl1}^{\text{iv}}$	0.95	2.89	3.469 (5)	120
$\text{C3}-\text{H3}\cdots\text{O2}^{\text{ii}}$	0.95	2.21	2.835 (6)	122
$\text{C15}-\text{H15A}\cdots\text{CgA}^{\text{v}}$	0.99	2.94	3.766 (6)	141

Symmetry codes: (i) $x-1, -y+1, -z+1$; (ii) x, y, z ; (iii) $-x+2, -y, -z+1$; (iv) $-x+1, -y, -z+1$; (v) $x+1, y, z$.

observed interaction between the water hydrogen atom H3A and the carbonyl oxygen atom O2 [$d = 1.84(4)$ Å, $\text{C}-\text{H}\cdots\text{O} = 168(5)^\circ$; see Fig. 2] of adjacent molecules leads to the formation of infinite supramolecular chains in the $[10\bar{1}]$ direction. On the other hand, weaker $\text{C}_{\text{arene}}-\text{H}\cdots\text{Cl}$ hydrogen bonds with the chloride ion Cl2 acting as a bifurcated acceptor for H1 and H2 of the neighboring molecule (see Fig. 3a and Table 1) crosslink these chains along the b axis to form a two-dimensional supramolecular network.

The packing structure of the complex shown in Fig. 3b indicates that the parallel orientation of the aliphatic C_8H_{17} units has a strong influence on the cohesion of the crystal structure by van der Waals forces. They are supported by $\text{C}-\text{H}\cdots\pi$ interactions between H15A and the heterocyclic subunit (A) of the quinoline scaffold (see Fig. 3c and Table 1). In addition, the interactions between H17B and C6 of the quinoline ring appear to have a stabilizing effect. Other

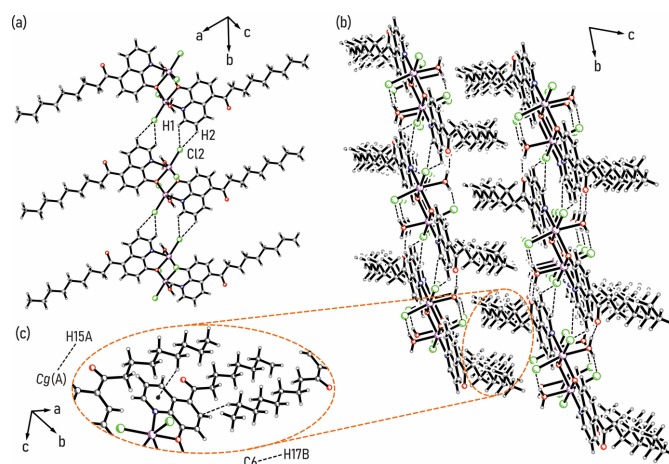


Figure 3

(a) Chain-like association of complex molecules *via* $\text{C}-\text{H}\cdots\text{Cl}$ interactions; color code: N – blue, O – red, Cl – green, In – magenta, C/H – gray. (b) Excerpt of the packing structure showing two supramolecular networks assembled *via* hydrogen bonds (dashed lines). Their mutual interactions are largely restricted to dispersive forces between interlocking aliphatic moieties. (c) Graphical representation of weak interactions in which the aliphatic substituents participate.

contacts involving the aromatic rings are absent in the crystal, as the closest $Cg \cdots Cg$ distances between their centroids amount to about 4.2 Å.

4. Database survey

A search in the Cambridge Structural Database (CSD, Version 5.44, update of September 2023; Groom *et al.*, 2016) for indium complexes with ligands based on 8-hydroxyquinoline yielded 15 hits. The quinolines often occur as individual ligands within the complexes, but sometimes they are also incorporated as a subunit of larger molecules.

Common to all complexes is that the 8-quinolinolate acts as a chelating ligand, complexing the indium ion *via* its oxygen and ring nitrogen atom. The reported indium complexes are predominantly mononuclear. However, three dinuclear complexes are also included in the database entries mentioned above. In the case of the dinuclear chelate complexes, the indium ions possess coordination numbers of six (ALESES; Alexander *et al.*, 2021) or five (SOMYOL, SOMZEC; Kwak *et al.*, 2019). The mononuclear complexes mostly have a coordination number of six, but occasionally the indium ion is coordinated five-, seven- or eightfold.

In the crystal structure with the reference code ALESES, the indium ion adopts a coordination environment of the composition N_2O_3Cl . Since this complex lacks a quinoline-bound keto group and no water molecule is involved, a strand-like association as in the crystal structure of the title complex cannot be observed. Instead, weak $C_{aryl}-H \cdots Cl$ and $C_{aryl}-H \cdots O$ hydrogen bonds as well as $\pi \cdots \pi$ contacts between the quinoline units of adjacent complexes lead to the formation of two-dimensional supramolecular networks. The packing structures of the complexes with the reference codes SOMYOL and SOMZEC, containing NO_2C_2 -coordinated indium ions, consist of an infinite strand-like arrangement of molecules connected by $\pi \cdots \pi$ interactions similar to those mentioned above.

5. Synthesis and crystallization

5-Nonanoyl-8-hydroxyquinoline (50 mg, 0.18 mmol) and indium(III) chloride (116 mg, 0.52 mmol) were stirred in methanol (5 mL) for 30 min at room temperature and the solvent was removed under vacuum. Afterwards the residue was crystallized by slow evaporation from acetonitrile. 5-Nonanoyl-8-hydroxyquinoline was synthesized according to the literature procedure (Uhlemann *et al.*, 1981).

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. All non-hydrogen atoms were refined anisotropically. Both hydrogen atoms of the water molecule (H3A, H3B) were located in difference-Fourier maps and placed accordingly. The remaining hydrogen atoms were positioned geometrically and refined isotropically using a riding model, with C–H bond distances of 0.95 Å (aryl),

Table 2
Experimental details.

Crystal data	
Chemical formula	$[In_2(C_{18}H_{22}NO_2)_2Cl_4(H_2O)_2]$
M_r	976.20
Crystal system, space group	Triclinic, $P\bar{1}$
Temperature (K)	163
a, b, c (Å)	10.297 (4), 10.940 (4), 11.711 (5)
α, β, γ (°)	63.57 (3), 72.47 (3), 62.92 (3)
V (Å ³)	1043.8 (8)
Z	1
Radiation type	Mo $K\alpha$
μ (mm ⁻¹)	1.40
Crystal size (mm)	0.19 × 0.10 × 0.07
Data collection	
Diffractometer	Stoe Stadivari
Absorption correction	Multi-scan (<i>X-RED32</i> ; Stoe & Cie, 2002)
T_{min}, T_{max}	0.766, 0.907
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	62899, 62899, 42801
R_{int}	0.039
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.039, 0.061, 0.88
No. of reflections	62899
No. of parameters	234
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å ⁻³)	0.94, -0.74

Computer programs: *X-AREA*, *X-RED32* and *LANA* (Stoe & Cie, 2002), *SHELXT2018/2* (Sheldrick, 2015a), *SHELXL2018/3* (Sheldrick, 2015b), *OLEX2*

0.98 Å (methylene) and 0.99 Å (methyl). The thermal displacement ellipsoids of all hydrogen atoms were set to $U_{iso}(H) = 1.2U_{eq}(C)$ and $U_{iso}(H) = 1.5U_{eq}(C/O)$, the latter applying to methyl and water moieties.

The crystal was refined as a two-component non-merohedral twin, whereby the main domain makes up 72% of the crystal. The two domains were identified and integrated simultaneously *via* the *Recipe/Index/Refine* and *Integrate* modules, respectively, of the *X-AREA* program suite, followed by absorption correction and scaling of the resulting HKLF5 dataset *via* the modules *X-RED32* and *LANA*, respectively (Stoe & Cie, 2002). The reflection file employed in the subsequent refinement contained reflections from the two individual domains as well as reflections to which both domains contributed.

By recognizing twinning, the *R*-values as well as the maximum residual electron density (Table 2) improved drastically compared to the model based on untreated HKLF4 data ($R_1 = 7.24\%$, $wR_2 = 22.71\%$, maximum electron density = 3.94 e \AA^{-3}).

Acknowledgements

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Crystal structure of bis(μ_2 -5-nonanoylquinolin-8-olato)bis[aqua-dichloridoindium(III)]

Betty Fuhrmann, Eric Meier and Monika Mazik

Computing details

Bis(μ_2 -5-nonanoylquinolin-8-olato)bis[aquadichloridoindium(III)]

Crystal data

[In₂(C₁₈H₂₂NO₂)₂Cl₄(H₂O)₂]

$M_r = 976.20$

Triclinic, $P\bar{1}$

$a = 10.297$ (4) Å

$b = 10.940$ (4) Å

$c = 11.711$ (5) Å

$\alpha = 63.57$ (3)°

$\beta = 72.47$ (3)°

$\gamma = 62.92$ (3)°

$V = 1043.8$ (8) Å³

$Z = 1$

$F(000) = 492$

$D_x = 1.553$ Mg m⁻³

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

Cell parameters from 24127 reflections

$\theta = 2.2$ – 28.7 °

$\mu = 1.40$ mm⁻¹

$T = 163$ K

Plate, colourless

$0.19 \times 0.10 \times 0.07$ mm

Data collection

Stoe Stadivari

diffractometer

Radiation source: Primux 50 Mo

Graded multilayer mirror monochromator

Detector resolution: 5.81 pixels mm⁻¹

rotation method, ω scans

Absorption correction: multi-scan

(X-Red32; Stoe & Cie, 2002)

$T_{\min} = 0.766$, $T_{\max} = 0.907$

62899 measured reflections

62899 independent reflections

42801 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.039$

$\theta_{\max} = 27.5$ °, $\theta_{\min} = 2.2$ °

$h = -13 \rightarrow 13$

$k = -14 \rightarrow 14$

$l = -15 \rightarrow 15$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.039$

$wR(F^2) = 0.061$

$S = 0.88$

62899 reflections

234 parameters

0 restraints

Primary atom site location: dual

Hydrogen site location: mixed

H atoms treated by a mixture of independent

and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0118P)^2]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 0.94$ e Å⁻³

$\Delta\rho_{\min} = -0.74$ e 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. Refined as a 2-component twin.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.7219 (4)	0.0957 (5)	0.3966 (5)	0.0270 (12)
H1	0.6420	0.0662	0.4143	0.032*
C2	0.8613 (4)	0.0088 (5)	0.3551 (4)	0.0284 (12)
H2	0.8760	-0.0788	0.3459	0.034*
C3	0.9763 (4)	0.0515 (5)	0.3279 (4)	0.0260 (12)
H3	1.0710	-0.0055	0.2973	0.031*
C4	0.9562 (4)	0.1795 (5)	0.3447 (4)	0.0202 (11)
C5	1.0678 (4)	0.2360 (5)	0.3187 (4)	0.0226 (11)
C6	1.0297 (4)	0.3609 (5)	0.3417 (5)	0.0266 (12)
H6	1.1039	0.3973	0.3255	0.032*
C7	0.8868 (4)	0.4380 (5)	0.3880 (4)	0.0260 (12)
H7	0.8668	0.5223	0.4053	0.031*
C8	0.7761 (4)	0.3912 (5)	0.4080 (4)	0.0202 (11)
C9	0.8106 (4)	0.2605 (5)	0.3875 (4)	0.0202 (11)
C10	1.2233 (4)	0.1595 (5)	0.2701 (5)	0.0252 (12)
C11	1.3194 (4)	0.2486 (5)	0.2001 (5)	0.0274 (12)
H11A	1.3243	0.2894	0.2584	0.033*
H11B	1.2720	0.3328	0.1255	0.033*
C12	1.4756 (4)	0.1645 (5)	0.1521 (5)	0.0301 (13)
H12A	1.4734	0.1317	0.0866	0.036*
H12B	1.5228	0.0760	0.2244	0.036*
C13	1.5642 (4)	0.2633 (5)	0.0937 (5)	0.0312 (13)
H13A	1.5621	0.2980	0.1595	0.037*
H13B	1.5156	0.3510	0.0216	0.037*
C14	1.7255 (4)	0.1892 (5)	0.0439 (5)	0.0327 (13)
H14A	1.7693	0.0905	0.1089	0.039*
H14B	1.7296	0.1761	-0.0356	0.039*
C15	1.8144 (4)	0.2809 (5)	0.0162 (5)	0.0340 (13)
H15A	1.8062	0.2969	0.0953	0.041*
H15B	1.7710	0.3785	-0.0501	0.041*
C16	1.9767 (4)	0.2114 (5)	-0.0297 (5)	0.0404 (14)
H16A	2.0183	0.1097	0.0320	0.048*
H16B	1.9861	0.2058	-0.1140	0.048*
C17	2.0644 (4)	0.2983 (6)	-0.0424 (5)	0.0453 (15)
H17A	2.0549	0.3039	0.0420	0.054*
H17B	2.0225	0.4001	-0.1039	0.054*
C18	2.2278 (4)	0.2295 (6)	-0.0887 (5)	0.066 (2)
H18A	2.2719	0.1317	-0.0248	0.099*

H18B	2.2781	0.2924	-0.1001	0.099*
H18C	2.2379	0.2203	-0.1707	0.099*
Cl1	0.34019 (11)	0.21319 (13)	0.53300 (14)	0.0374 (4)
Cl2	0.38785 (12)	0.53711 (14)	0.27233 (13)	0.0403 (4)
In1	0.47713 (3)	0.36247 (4)	0.47732 (4)	0.02240 (9)
N1	0.6970 (3)	0.2161 (4)	0.4119 (4)	0.0220 (9)
O1	0.6352 (2)	0.4620 (3)	0.4468 (3)	0.0220 (8)
O2	1.2707 (3)	0.0302 (3)	0.2842 (4)	0.0403 (10)
O3	0.5333 (3)	0.2442 (3)	0.6779 (3)	0.0288 (9)
H3A	0.588 (4)	0.154 (5)	0.700 (5)	0.043*
H3B	0.559 (4)	0.294 (5)	0.707 (4)	0.043*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.026 (3)	0.023 (3)	0.035 (4)	-0.012 (2)	0.000 (2)	-0.013 (3)
C2	0.029 (2)	0.019 (3)	0.040 (4)	-0.007 (2)	0.000 (2)	-0.017 (3)
C3	0.023 (2)	0.019 (3)	0.030 (3)	-0.003 (2)	0.001 (2)	-0.012 (3)
C4	0.021 (2)	0.016 (3)	0.021 (3)	-0.004 (2)	-0.002 (2)	-0.007 (2)
C5	0.018 (2)	0.019 (3)	0.029 (3)	-0.003 (2)	-0.003 (2)	-0.011 (2)
C6	0.016 (2)	0.024 (3)	0.039 (4)	-0.007 (2)	-0.001 (2)	-0.014 (3)
C7	0.023 (2)	0.019 (3)	0.039 (4)	-0.006 (2)	-0.001 (2)	-0.017 (3)
C8	0.019 (2)	0.016 (3)	0.021 (3)	-0.003 (2)	-0.002 (2)	-0.007 (2)
C9	0.019 (2)	0.016 (3)	0.025 (3)	-0.003 (2)	-0.006 (2)	-0.008 (2)
C10	0.021 (2)	0.024 (3)	0.030 (3)	-0.003 (2)	-0.007 (2)	-0.013 (3)
C11	0.021 (2)	0.027 (3)	0.035 (4)	-0.009 (2)	0.002 (2)	-0.015 (3)
C12	0.018 (2)	0.033 (3)	0.039 (4)	-0.004 (2)	-0.001 (2)	-0.020 (3)
C13	0.023 (2)	0.033 (3)	0.037 (4)	-0.009 (2)	0.000 (2)	-0.017 (3)
C14	0.022 (2)	0.037 (3)	0.037 (4)	-0.008 (2)	0.000 (2)	-0.017 (3)
C15	0.026 (3)	0.036 (3)	0.038 (4)	-0.013 (2)	0.000 (2)	-0.013 (3)
C16	0.026 (3)	0.056 (4)	0.040 (4)	-0.018 (3)	0.004 (2)	-0.020 (3)
C17	0.032 (3)	0.068 (4)	0.036 (4)	-0.029 (3)	0.003 (3)	-0.013 (3)
C18	0.033 (3)	0.106 (6)	0.065 (5)	-0.036 (3)	0.008 (3)	-0.035 (4)
Cl1	0.0307 (6)	0.0322 (8)	0.0596 (11)	-0.0178 (6)	0.0014 (6)	-0.0234 (8)
Cl2	0.0544 (8)	0.0296 (8)	0.0394 (10)	-0.0098 (7)	-0.0191 (7)	-0.0124 (7)
In1	0.01802 (15)	0.01785 (17)	0.0336 (2)	-0.00564 (12)	-0.00088 (14)	-0.01387 (16)
N1	0.0185 (18)	0.018 (2)	0.030 (3)	-0.0068 (17)	0.0014 (17)	-0.011 (2)
O1	0.0158 (15)	0.0197 (17)	0.032 (2)	-0.0057 (13)	0.0026 (13)	-0.0154 (17)
O2	0.0220 (17)	0.022 (2)	0.069 (3)	-0.0035 (15)	0.0001 (17)	-0.018 (2)
O3	0.0322 (18)	0.0194 (19)	0.032 (2)	-0.0070 (15)	-0.0026 (16)	-0.0109 (18)

Geometric parameters (Å, °)

C1—N1	1.308 (5)	C13—H13A	0.9900
C1—C2	1.396 (5)	C13—H13B	0.9900
C1—H1	0.9500	C14—C15	1.522 (5)
C2—C3	1.367 (5)	C14—H14A	0.9900
C2—H2	0.9500	C14—H14B	0.9900

C3—C4	1.414 (5)	C15—C16	1.524 (5)
C3—H3	0.9500	C15—H15A	0.9900
C4—C9	1.420 (5)	C15—H15B	0.9900
C4—C5	1.437 (5)	C16—C17	1.522 (6)
C5—C6	1.368 (6)	C16—H16A	0.9900
C5—C10	1.497 (5)	C16—H16B	0.9900
C6—C7	1.402 (5)	C17—C18	1.534 (5)
C6—H6	0.9500	C17—H17A	0.9900
C7—C8	1.372 (5)	C17—H17B	0.9900
C7—H7	0.9500	C18—H18A	0.9800
C8—O1	1.344 (4)	C18—H18B	0.9800
C8—C9	1.421 (6)	C18—H18C	0.9800
C9—N1	1.370 (5)	C11—In1	2.3825 (14)
C10—O2	1.215 (5)	C12—In1	2.4302 (19)
C10—C11	1.511 (5)	In1—O1 ⁱ	2.166 (3)
C11—C12	1.522 (5)	In1—O1	2.209 (3)
C11—H11A	0.9900	In1—O3	2.227 (4)
C11—H11B	0.9900	In1—N1	2.241 (3)
C12—C13	1.528 (5)	O1—In1 ⁱ	2.166 (3)
C12—H12A	0.9900	O3—H3A	0.84 (4)
C12—H12B	0.9900	O3—H3B	0.92 (4)
C13—C14	1.538 (5)		
N1—C1—C2	122.5 (4)	C15—C14—H14B	109.4
N1—C1—H1	118.7	C13—C14—H14B	109.4
C2—C1—H1	118.7	H14A—C14—H14B	108.0
C3—C2—C1	119.0 (4)	C14—C15—C16	114.1 (4)
C3—C2—H2	120.5	C14—C15—H15A	108.7
C1—C2—H2	120.5	C16—C15—H15A	108.7
C2—C3—C4	120.8 (4)	C14—C15—H15B	108.7
C2—C3—H3	119.6	C16—C15—H15B	108.7
C4—C3—H3	119.6	H15A—C15—H15B	107.6
C3—C4—C9	116.0 (4)	C17—C16—C15	112.3 (4)
C3—C4—C5	125.9 (4)	C17—C16—H16A	109.1
C9—C4—C5	118.0 (4)	C15—C16—H16A	109.1
C6—C5—C4	118.3 (4)	C17—C16—H16B	109.1
C6—C5—C10	120.2 (4)	C15—C16—H16B	109.1
C4—C5—C10	121.4 (4)	H16A—C16—H16B	107.9
C5—C6—C7	123.5 (4)	C16—C17—C18	112.7 (4)
C5—C6—H6	118.2	C16—C17—H17A	109.0
C7—C6—H6	118.2	C18—C17—H17A	109.0
C8—C7—C6	119.7 (4)	C16—C17—H17B	109.0
C8—C7—H7	120.2	C18—C17—H17B	109.0
C6—C7—H7	120.2	H17A—C17—H17B	107.8
O1—C8—C7	123.6 (4)	C17—C18—H18A	109.5
O1—C8—C9	117.5 (3)	C17—C18—H18B	109.5
C7—C8—C9	118.9 (4)	H18A—C18—H18B	109.5
N1—C9—C4	121.8 (4)	C17—C18—H18C	109.5

N1—C9—C8	116.8 (4)	H18A—C18—H18C	109.5
C4—C9—C8	121.4 (4)	H18B—C18—H18C	109.5
O2—C10—C5	121.4 (4)	O1 ⁱ —In1—O1	72.65 (11)
O2—C10—C11	120.6 (4)	O1 ⁱ —In1—O3	78.60 (12)
C5—C10—C11	118.0 (4)	O1—In1—O3	84.69 (12)
C10—C11—C12	115.3 (4)	O1 ⁱ —In1—N1	144.79 (11)
C10—C11—H11A	108.5	O1—In1—N1	73.40 (11)
C12—C11—H11A	108.5	O3—In1—N1	89.29 (13)
C10—C11—H11B	108.5	O1 ⁱ —In1—Cl1	112.71 (8)
C12—C11—H11B	108.5	O1—In1—Cl1	169.15 (8)
H11A—C11—H11B	107.5	O3—In1—Cl1	87.16 (9)
C11—C12—C13	109.9 (3)	N1—In1—Cl1	99.38 (10)
C11—C12—H12A	109.7	O1 ⁱ —In1—Cl2	89.09 (9)
C13—C12—H12A	109.7	O1—In1—Cl2	91.53 (9)
C11—C12—H12B	109.7	O3—In1—Cl2	167.69 (9)
C13—C12—H12B	109.7	N1—In1—Cl2	100.88 (11)
H12A—C12—H12B	108.2	Cl1—In1—Cl2	97.88 (6)
C12—C13—C14	114.7 (4)	C1—N1—C9	119.8 (3)
C12—C13—H13A	108.6	C1—N1—In1	124.9 (3)
C14—C13—H13A	108.6	C9—N1—In1	115.3 (3)
C12—C13—H13B	108.6	C8—O1—In1 ⁱ	134.6 (2)
C14—C13—H13B	108.6	C8—O1—In1	117.0 (2)
H13A—C13—H13B	107.6	In1 ⁱ —O1—In1	107.35 (11)
C15—C14—C13	111.3 (4)	In1—O3—H3A	118 (3)
C15—C14—H14A	109.4	In1—O3—H3B	115 (3)
C13—C14—H14A	109.4	H3A—O3—H3B	112 (4)
N1—C1—C2—C3	-0.8 (7)	C4—C5—C10—O2	-20.8 (7)
C1—C2—C3—C4	1.7 (7)	C6—C5—C10—C11	-23.3 (6)
C2—C3—C4—C9	-1.6 (7)	C4—C5—C10—C11	157.9 (4)
C2—C3—C4—C5	-179.6 (4)	O2—C10—C11—C12	-0.7 (7)
C3—C4—C5—C6	-179.3 (5)	C5—C10—C11—C12	-179.4 (4)
C9—C4—C5—C6	2.8 (7)	C10—C11—C12—C13	-175.2 (4)
C3—C4—C5—C10	-0.5 (7)	C11—C12—C13—C14	178.9 (4)
C9—C4—C5—C10	-178.4 (4)	C12—C13—C14—C15	-166.9 (4)
C4—C5—C6—C7	-0.8 (7)	C13—C14—C15—C16	178.2 (4)
C10—C5—C6—C7	-179.6 (4)	C14—C15—C16—C17	-173.9 (4)
C5—C6—C7—C8	-2.3 (7)	C15—C16—C17—C18	-179.9 (4)
C6—C7—C8—O1	-177.0 (4)	C2—C1—N1—C9	-0.3 (7)
C6—C7—C8—C9	3.2 (7)	C2—C1—N1—In1	179.8 (3)
C3—C4—C9—N1	0.5 (6)	C4—C9—N1—C1	0.5 (7)
C5—C4—C9—N1	178.6 (4)	C8—C9—N1—C1	-179.1 (4)
C3—C4—C9—C8	180.0 (4)	C4—C9—N1—In1	-179.6 (3)
C5—C4—C9—C8	-1.8 (7)	C8—C9—N1—In1	0.8 (5)
O1—C8—C9—N1	-1.4 (6)	C7—C8—O1—In1 ⁱ	-12.1 (7)
C7—C8—C9—N1	178.4 (4)	C9—C8—O1—In1 ⁱ	167.7 (3)
O1—C8—C9—C4	179.1 (4)	C7—C8—O1—In1	-178.5 (4)

C7—C8—C9—C4	-1.1 (7)	C9—C8—O1—In1	1.3 (5)
C6—C5—C10—O2	157.9 (5)		

Symmetry code: (i) $-x+1, -y+1, -z+1$.

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>
O3—H3A...O2 ⁱⁱ	0.84 (4)	1.84 (4)	2.668 (4)	168 (5)
O3—H3B...Cl2 ⁱ	0.92 (4)	2.27 (4)	3.165 (4)	165 (4)

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