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Iodido[tris(1-methylbenzimidazol-2-ylmethyl)amine]zinc(II) perchlorate dimethylformamide hemisolvate

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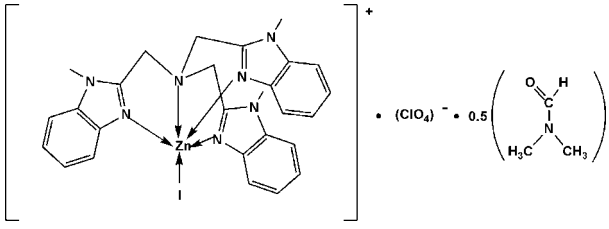
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.016 Å; disorder in solvent or counterion; R factor = 0.068; wR factor = 0.244; data-to-parameter ratio = 16.3.

In the cation of the title compound, $[ZnI(C_{27}H_{27}N_7)]ClO_4\cdot 0.5C_3H_7NO$, the Zn^{II} ion is chelated by a tris(1-methylbenzimidazol-2-ylmethyl)amine (Mentb) ligand with an I atom completing the coordination. The five-coordinate N_4I ligand set may be best described as trigonal–bipyramidal, with approximate C_3 molecular site symmetry.

Related literature

For related literature see: Pandey *et al.* (1992); Addison *et al.* (1981); Wu *et al.* (2006); Athimoolam *et al.* (2005); Cox *et al.* (2003); Mohamed *et al.* (2003); Spek (2003); Stähler *et al.* (2001).



Experimental

Crystal data

$[ZnI(C_{27}H_{27}N_7)]ClO_4\cdot 0.5C_3H_7NO$
M_r = 777.82
Triclinic, $P\overline{1}$
a = 12.743 (2) Å
b = 14.399 (3) Å
c = 14.554 (3) Å
α = 97.562 (2)°
β = 112.766 (2)°
γ = 114.420 (2)°
V = 2102.7 (7) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.42 mm^{-1}
T = 298 (2) K
0.50 × 0.42 × 0.39 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.537, T_{max} = 0.608
(expected range = 0.509–0.575)
10873 measured reflections
7231 independent reflections
4303 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.069
$wR(F^2)$ = 0.245
S = 1.09
7231 reflections
443 parameters
251 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.56 e Å^{-3}

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1996); 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: LH2386).

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supplementary materials

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Iodido[tris(1-methylbenzimidazol-2-ylmethyl)amine]zinc(II) perchlorate dimethylformamide hemisolvate

H.-L. Wu, B. Qi, W.-B. Lv, P. Liu and J.-G. Liu

Comment

The asymmetric unit of the title compound, (Fig. 1), consists of a [Zn(Mentb)(I)] cation, a perchlorate anion and half a DMF molecule. The perchlorate anions is disordered and the DMF solvent is half occupancy. The Zn^{II} ion is five-coordinate with a N_4I ligand set. The Mentb ligand acts as a tetradentate N-donor, and an iodide completes the coordination. The coordination geometry of the Zn^{II} may be best described as trigonal-bipyramidal, with approximate C_3 molecular site symmetry. This geometry is assumed by the Zn^{II} to relieve the steric crowding. The equatorial plane is occupied by three N atoms of three benzimidazolyl groups, while the Zn^{II} atom protrudes towards I and is 0.563 (5) Å from the plane of atoms N2/N4/N6. The axial sites are occupyied by N1 and I1, with Zn1—N1 2.442 (5) Å, Zn1—I1 2.6148 (10) Å and N1—Zn1—I1 is 179.50 (13)°. The three benzimidazole ring arms of the Mentb ligand form a cone-shaped cavity. The angles N2—Zn1—N6, N2—Zn1—N4 and N4—Zn1—N6 are 115.2 (2), 110.7 (2) and 112.9 (2) °, respectively. The N1—Zn1—N2 74.6 (2), N1—Zn1—N4 73.9 (2) and N1—Zn1—N6, 74.2 (2)° angles, which are all *ca* 16 ° less than the ideal value of 90°, are imposed by the geometry of the Mentb ligand. The bond angles and distance in the three benzimidazole groups are equal within experimental error. In the crystal structure, there are weak π···π stacking interactions with a centroid···centroid distance of 3.542 (6)Å bewteen inversion related molecules (see Fig. 2). Some references related to the title compound are Pandey *et al.* (1992), Addison *et al.* (1981) & Wu *et al.*, (2006).

Experimental

To a stired solution of tris(*N*-methylbenzimidazol-2-ylmethyl)amine (0.0899 g, 0.2 mmol) in hot MeOH (10 ml) was added $Zn(ClO_4)_2{\cdot}6(H_2O)$ (0.0745 g, 0.2 mmol), followed by a solution of sodium iodide (0.0301 g, 0.2 mmol) in MeOH (5 ml). A colorless crystalline product formed rapidly. The precipitate was filtered off, washed with MeOH and absolute Et_2O, and dried *in vacuo*. The dried precipitate was dissolved in DMF to form a colorless solution that was allowed to evaporate at room temperature. Colorless crystals suitable for X-ray diffraction studies were obtained after one week. Yield, 0.101 g (65%). (found: C, 44.32; H, 3.77; N,13.58; Zn, 8.23. Calcd. for C28.5 H30.5 C l I N7.5 0O4.50 Zn: C, 44.01; H, 3.95; N, 13.51; Cu, 8.41%)

Refinement

H atoms were placed in calculated positions, with C—H distances ranging from 0.93 to 0.97 Å, and treated as riding, with $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}(C)$ for methyl H atoms. The Atoms O2/O3/O4 of the perchlorate anion are disordered over two sites with refined occupancies 0.562 (17):0.438 (17). The highest peak of 1.18 e $A^{\circ -3}$ is 3.72Å from H27B. The SQUEEZE option in *PLATON* (Spek, 2003) indicated there was a solvent cavity of volume 599 $Å^3$ containing approximately 90 electrons (possibly additional disordered DMF). In the final cycles of refinement, this contribution to the electron density

was removed from the observed data. The density, the F(000) value, the molecular weight and the formula are given without taking into account the results obtained with the SQUEEZE option *PLATON* (Spek, 2003). Similar treatments of disordered solvent molecules were carried out by Stähler *et al.* (2001), Cox *et al.* (2003), Mohamed *et al.* (2003) and Athimoolam *et al.* (2005).

Figures

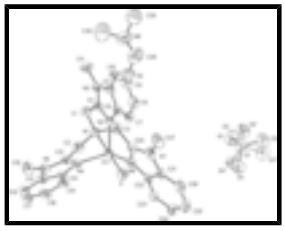


Fig. 1. The asymmetric unit of the title compound. Displacement ellipsoids are drawn at the 30% probabilty level. The major component of disorder is shown with open bonds.

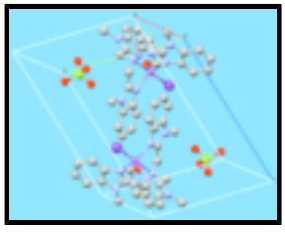


Fig. 2. Partial packing plot of title compound. H atoms are omitted for clarity.

Iodido[tris(1-methylbenzimidazol-2-ylmethyl)amine]zinc(II) perchlorate dimethylformamide hemisolvate

Crystal data

$[ZnI(C_{27}H_{27}N_7)]ClO_4·0.5C_3H_7NO$	$Z = 2$
$M_r = 777.82$	$F_{000} = 780$
Triclinic, $P\overline{1}$	$D_x = 1.229$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 12.743$ (2) Å	Cell parameters from 3637 reflections
$b = 14.399$ (3) Å	$\theta = 2.2$–23.8º
$c = 14.554$ (3) Å	$\mu = 1.42$ mm^{-1}
$\alpha = 97.562$ (2)º	$T = 298$ (2) K
$\beta = 112.766$ (2)º	Block, colourless
$\gamma = 114.420$ (2)º	0.50 × 0.42 × 0.39 mm
$V = 2102.7$ (7) Å^3	

Data collection

Bruker SMART CCD diffractometer	7231 independent reflections
Radiation source: fine-focus sealed tube	4303 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.020$
$T = 298$(2) K	$\theta_{max} = 25.0$º
φ and ω scans	$\theta_{min} = 1.9$º
Absorption correction: multi-scan	$h = -15 \rightarrow 11$

(SADABS; Bruker, 2000)
T_{min} = 0.537, T_{max} = 0.608
10873 measured reflections
k = −17→16
l = −17→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.069
$wR(F^2)$ = 0.245
S = 1.09
7231 reflections
443 parameters
251 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
$w = 1/[\sigma^2(F_o^2) + (0.1343P)^2 + 1.7701P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.56 e Å^{-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 $F^2 > 2$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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Zn1	0.17757 (8)	0.33681 (6)	0.18237 (6)	0.0481 (3)	
I1	0.01595 (6)	0.30635 (5)	0.25900 (5)	0.0818 (3)	
Cl1	0.3784 (3)	0.2727 (2)	0.8325 (2)	0.0851 (7)	
N1	0.3298 (5)	0.3651 (4)	0.1122 (4)	0.0413 (12)	
N2	0.1770 (6)	0.1913 (5)	0.1515 (5)	0.0513 (14)	
N3	0.2031 (7)	0.0727 (5)	0.0621 (6)	0.0651 (18)	
N4	0.0976 (6)	0.3644 (5)	0.0429 (5)	0.0544 (15)	
N5	0.1150 (8)	0.4303 (5)	−0.0832 (5)	0.0645 (18)	
N6	0.3567 (6)	0.4701 (5)	0.2979 (5)	0.0512 (14)	
N7	0.5753 (6)	0.5621 (5)	0.3815 (5)	0.0620 (17)	
N8	0.605 (3)	0.132 (2)	0.163 (2)	0.185 (8)	0.50
O1	0.4358 (8)	0.2947 (6)	0.7669 (6)	0.112 (2)	
O2	0.2766 (19)	0.1658 (11)	0.7939 (17)	0.129 (6)	0.438 (17)
O3	0.4796 (17)	0.293 (2)	0.9358 (12)	0.121 (5)	0.438 (17)

O4	0.338 (2)	0.3502 (16)	0.8425 (17)	0.111 (5)	0.438 (17)
O2'	0.344 (2)	0.1694 (10)	0.8390 (15)	0.126 (5)	0.562 (17)
O3'	0.4773 (15)	0.3486 (14)	0.9443 (9)	0.127 (5)	0.562 (17)
O4'	0.2711 (15)	0.2913 (17)	0.8095 (13)	0.114 (4)	0.562 (17)
O5	0.539 (2)	0.2270 (18)	0.2079 (14)	0.150 (6)	0.50
C1	0.2863 (9)	0.2584 (6)	0.0460 (7)	0.065 (2)	
H1A	0.3614	0.2561	0.0463	0.077*	
H1B	0.2241	0.2435	−0.0266	0.077*	
C2	0.3133 (8)	0.4366 (6)	0.0547 (7)	0.062 (2)	
H2A	0.3392	0.4294	0.0008	0.074*	
H2B	0.3698	0.5114	0.1030	0.074*	
C3	0.4577 (8)	0.4139 (7)	0.2062 (7)	0.065 (2)	
H3A	0.5263	0.4582	0.1912	0.078*	
H3B	0.4735	0.3572	0.2258	0.078*	
C4	0.2216 (7)	0.1737 (6)	0.0867 (6)	0.0548 (18)	
C5	0.1431 (8)	0.0209 (6)	0.1158 (7)	0.064 (2)	
C6	0.1256 (7)	0.0941 (6)	0.1728 (6)	0.058 (2)	
C7	0.0668 (9)	0.0654 (7)	0.2332 (7)	0.071 (2)	
H7	0.0530	0.1132	0.2699	0.085*	
C8	0.0284 (10)	−0.0386 (8)	0.2375 (8)	0.086 (3)	
H8	−0.0109	−0.0611	0.2787	0.104*	
C9	0.0480 (12)	−0.1097 (8)	0.1807 (10)	0.098 (4)	
H9	0.0194	−0.1792	0.1846	0.118*	
C10	0.1049 (10)	−0.0841 (7)	0.1219 (10)	0.090 (3)	
H10	0.1190	−0.1324	0.0864	0.108*	
C11	0.2406 (11)	0.0263 (8)	−0.0060 (8)	0.088 (3)	
H11A	0.3264	0.0361	0.0365	0.133*	
H11B	0.2432	0.0621	−0.0570	0.133*	
H11C	0.1772	−0.0500	−0.0425	0.133*	
C12	0.1750 (8)	0.4097 (6)	0.0041 (6)	0.0538 (18)	
C13	−0.0117 (11)	0.3958 (7)	−0.1021 (7)	0.074 (3)	
C14	−0.0247 (8)	0.3530 (6)	−0.0231 (6)	0.060 (2)	
C15	−0.1424 (9)	0.3112 (7)	−0.0193 (7)	0.070 (2)	
H15	−0.1516	0.2839	0.0333	0.084*	
C16	−0.2467 (11)	0.3130 (9)	−0.1009 (9)	0.095 (3)	
H16	−0.3276	0.2856	−0.1021	0.114*	
C17	−0.2336 (13)	0.3533 (10)	−0.1780 (9)	0.095 (3)	
H17	−0.3059	0.3514	−0.2308	0.114*	
C18	−0.1203 (13)	0.3951 (9)	−0.1793 (8)	0.092 (3)	
H18	−0.1129	0.4240	−0.2314	0.111*	
C19	0.1741 (12)	0.4828 (9)	−0.1429 (8)	0.094 (3)	
H19A	0.1449	0.5325	−0.1621	0.141*	
H19B	0.1480	0.4287	−0.2060	0.141*	
H19C	0.2686	0.5219	−0.1000	0.141*	
C20	0.4631 (8)	0.4824 (6)	0.2959 (6)	0.0554 (18)	
C21	0.5376 (9)	0.6073 (7)	0.4445 (6)	0.062 (2)	
C22	0.4016 (8)	0.5502 (6)	0.3924 (6)	0.0543 (18)	
C23	0.3320 (9)	0.5747 (7)	0.4340 (6)	0.062 (2)	
H23	0.2402	0.5367	0.3995	0.075*	

C24	0.4090 (12)	0.6613 (8)	0.5328 (8)	0.083 (3)	
H24	0.3660	0.6807	0.5637	0.100*	
C25	0.5447 (12)	0.7178 (9)	0.5846 (8)	0.092 (3)	
H25	0.5917	0.7746	0.6490	0.110*	
C26	0.6109 (11)	0.6908 (8)	0.5418 (7)	0.085 (3)	
H26	0.7027	0.7275	0.5770	0.102*	
C27	0.7098 (9)	0.5979 (9)	0.4038 (9)	0.091 (3)	
H27A	0.7384	0.6556	0.3769	0.136*	
H27B	0.7132	0.5381	0.3700	0.136*	
H27C	0.7667	0.6236	0.4791	0.136*	
C28	0.564 (4)	0.158 (3)	0.226 (2)	0.198 (9)	0.50
H28	0.5561	0.1270	0.2766	0.238*	0.50
C29	0.630 (4)	0.044 (3)	0.183 (3)	0.207 (10)	0.50
H29A	0.7233	0.0704	0.2147	0.310*	0.50
H29B	0.5847	−0.0151	0.1169	0.310*	0.50
H29C	0.5988	0.0180	0.2299	0.310*	0.50
C30	0.607 (4)	0.150 (3)	0.066 (3)	0.205 (10)	0.50
H30A	0.6091	0.2173	0.0640	0.308*	0.50
H30B	0.5290	0.0913	0.0042	0.308*	0.50
H30C	0.6838	0.1537	0.0659	0.308*	0.50

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0486 (5)	0.0468 (5)	0.0512 (5)	0.0267 (4)	0.0244 (4)	0.0156 (4)
I1	0.0762 (5)	0.0963 (5)	0.0871 (5)	0.0451 (4)	0.0503 (4)	0.0340 (4)
Cl1	0.0785 (15)	0.0850 (16)	0.1106 (19)	0.0383 (13)	0.0627 (15)	0.0453 (14)
N1	0.040 (3)	0.032 (3)	0.040 (3)	0.015 (2)	0.013 (2)	0.008 (2)
N2	0.051 (3)	0.049 (3)	0.056 (4)	0.030 (3)	0.024 (3)	0.017 (3)
N3	0.059 (4)	0.052 (4)	0.075 (5)	0.032 (3)	0.026 (4)	0.004 (3)
N4	0.059 (4)	0.050 (4)	0.053 (4)	0.032 (3)	0.023 (3)	0.016 (3)
N5	0.086 (5)	0.058 (4)	0.064 (4)	0.044 (4)	0.039 (4)	0.028 (3)
N6	0.052 (4)	0.048 (3)	0.052 (4)	0.028 (3)	0.022 (3)	0.019 (3)
N7	0.050 (4)	0.064 (4)	0.056 (4)	0.025 (3)	0.015 (3)	0.024 (3)
N8	0.165 (12)	0.217 (15)	0.128 (11)	0.135 (11)	0.018 (10)	−0.026 (12)
O1	0.104 (4)	0.131 (5)	0.117 (5)	0.051 (4)	0.076 (4)	0.048 (4)
O2	0.103 (7)	0.116 (7)	0.136 (8)	0.037 (7)	0.047 (7)	0.046 (7)
O3	0.104 (7)	0.127 (8)	0.122 (7)	0.042 (7)	0.058 (6)	0.065 (7)
O4	0.107 (7)	0.109 (7)	0.124 (7)	0.054 (6)	0.065 (6)	0.039 (6)
O2'	0.120 (7)	0.107 (6)	0.134 (7)	0.049 (6)	0.050 (6)	0.061 (6)
O3'	0.110 (6)	0.113 (7)	0.124 (7)	0.025 (6)	0.059 (6)	0.044 (6)
O4'	0.101 (7)	0.121 (7)	0.125 (7)	0.059 (6)	0.056 (6)	0.041 (6)
O5	0.162 (11)	0.178 (13)	0.104 (9)	0.143 (10)	0.014 (9)	−0.002 (9)
C1	0.073 (5)	0.063 (5)	0.072 (5)	0.041 (5)	0.043 (5)	0.020 (4)
C2	0.073 (5)	0.053 (4)	0.069 (5)	0.032 (4)	0.043 (5)	0.026 (4)
C3	0.054 (5)	0.068 (5)	0.079 (6)	0.032 (4)	0.038 (4)	0.026 (4)
C4	0.049 (4)	0.052 (4)	0.063 (5)	0.029 (4)	0.025 (4)	0.016 (4)
C5	0.049 (4)	0.044 (4)	0.072 (5)	0.019 (4)	0.014 (4)	0.005 (4)

C6	0.046 (4)	0.044 (4)	0.058 (5)	0.018 (4)	0.009 (4)	0.013 (4)
C7	0.074 (6)	0.055 (5)	0.064 (5)	0.024 (4)	0.027 (5)	0.017 (4)
C8	0.075 (6)	0.060 (6)	0.087 (7)	0.015 (5)	0.025 (5)	0.030 (5)
C9	0.107 (9)	0.045 (5)	0.113 (9)	0.027 (6)	0.039 (7)	0.031 (6)
C10	0.081 (7)	0.050 (6)	0.119 (9)	0.034 (5)	0.033 (7)	0.024 (6)
C11	0.092 (7)	0.077 (6)	0.091 (7)	0.050 (6)	0.040 (6)	0.002 (5)
C12	0.072 (5)	0.042 (4)	0.052 (4)	0.032 (4)	0.031 (4)	0.016 (3)
C13	0.105 (8)	0.055 (5)	0.058 (5)	0.052 (5)	0.025 (5)	0.019 (4)
C14	0.069 (5)	0.045 (4)	0.058 (5)	0.036 (4)	0.019 (4)	0.008 (4)
C15	0.066 (5)	0.066 (5)	0.080 (6)	0.043 (5)	0.028 (5)	0.019 (4)
C16	0.082 (7)	0.083 (7)	0.102 (8)	0.056 (6)	0.018 (6)	0.016 (6)
C17	0.100 (8)	0.110 (9)	0.093 (8)	0.080 (8)	0.031 (7)	0.045 (7)
C18	0.121 (9)	0.096 (8)	0.070 (6)	0.081 (8)	0.027 (6)	0.027 (5)
C19	0.122 (9)	0.102 (8)	0.085 (7)	0.066 (7)	0.056 (7)	0.059 (6)
C20	0.052 (4)	0.053 (4)	0.066 (5)	0.031 (4)	0.027 (4)	0.028 (4)
C21	0.070 (6)	0.060 (5)	0.049 (5)	0.034 (5)	0.020 (4)	0.025 (4)
C22	0.065 (5)	0.053 (4)	0.046 (4)	0.035 (4)	0.021 (4)	0.023 (3)
C23	0.069 (5)	0.065 (5)	0.048 (4)	0.038 (4)	0.022 (4)	0.016 (4)
C24	0.117 (9)	0.082 (7)	0.064 (6)	0.058 (7)	0.046 (6)	0.030 (5)
C25	0.100 (8)	0.090 (7)	0.050 (5)	0.045 (7)	0.013 (6)	0.010 (5)
C26	0.076 (6)	0.082 (7)	0.056 (6)	0.031 (6)	0.006 (5)	0.023 (5)
C27	0.056 (5)	0.104 (8)	0.093 (7)	0.036 (5)	0.022 (5)	0.041 (6)
C28	0.176 (12)	0.224 (15)	0.124 (11)	0.121 (12)	0.018 (11)	−0.030 (12)
C29	0.186 (13)	0.214 (16)	0.143 (13)	0.125 (13)	0.012 (12)	−0.012 (13)
C30	0.180 (13)	0.219 (16)	0.133 (12)	0.108 (13)	0.014 (13)	−0.002 (13)

Geometric parameters (Å, °)

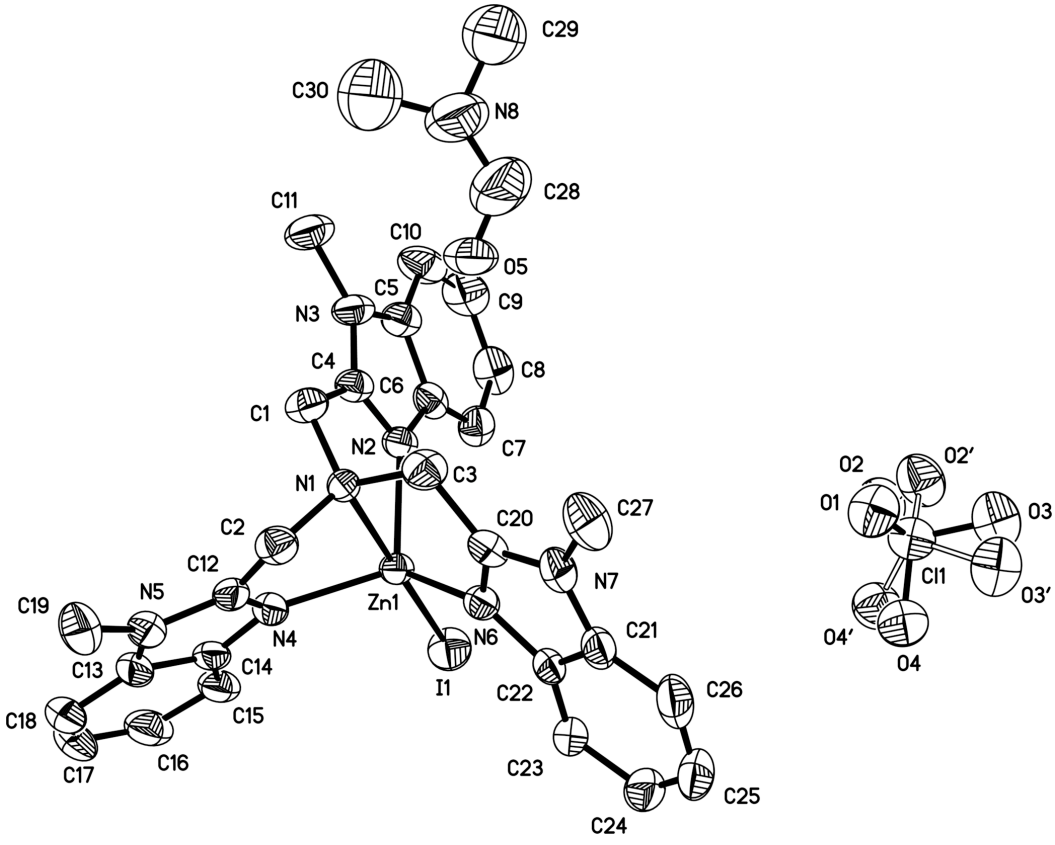
Zn1—N4	2.064 (6)	C6—C7	1.362 (12)
Zn1—N6	2.069 (6)	C7—C8	1.388 (12)
Zn1—N2	2.080 (6)	C7—H7	0.9300
Zn1—N1	2.442 (5)	C8—C9	1.393 (16)
Zn1—I1	2.6148 (10)	C8—H8	0.9300
Cl1—O2	1.387 (11)	C9—C10	1.318 (16)
Cl1—O2'	1.394 (10)	C9—H9	0.9300
Cl1—O1	1.406 (6)	C10—H10	0.9300
Cl1—O4'	1.423 (10)	C11—H11A	0.9600
Cl1—O4	1.426 (12)	C11—H11B	0.9600
Cl1—O3	1.442 (12)	C11—H11C	0.9600
Cl1—O3'	1.495 (11)	C13—C18	1.400 (14)
N1—C2	1.440 (9)	C13—C14	1.407 (12)
N1—C1	1.445 (9)	C14—C15	1.393 (12)
N1—C3	1.448 (9)	C15—C16	1.412 (13)
N2—C4	1.322 (9)	C15—H15	0.9300
N2—C6	1.414 (9)	C16—C17	1.364 (16)
N3—C4	1.347 (9)	C16—H16	0.9300
N3—C5	1.377 (11)	C17—C18	1.323 (16)
N3—C11	1.455 (11)	C17—H17	0.9300
N4—C12	1.308 (10)	C18—H18	0.9300

N4—C14	1.403 (10)	C19—H19A	0.9600
N5—C12	1.350 (10)	C19—H19B	0.9600
N5—C13	1.374 (12)	C19—H19C	0.9600
N5—C19	1.450 (11)	C21—C22	1.377 (11)
N6—C20	1.306 (10)	C21—C26	1.387 (13)
N6—C22	1.405 (9)	C22—C23	1.377 (11)
N7—C20	1.343 (10)	C23—C24	1.417 (12)
N7—C21	1.392 (11)	C23—H23	0.9300
N7—C27	1.450 (11)	C24—C25	1.374 (15)
N8—C28	1.298 (19)	C24—H24	0.9300
N8—C29	1.473 (19)	C25—C26	1.365 (15)
N8—C30	1.474 (19)	C25—H25	0.9300
O5—C28	1.197 (19)	C26—H26	0.9300
C1—C4	1.501 (11)	C27—H27A	0.9600
C1—H1A	0.9700	C27—H27B	0.9600
C1—H1B	0.9700	C27—H27C	0.9600
C2—C12	1.468 (11)	C28—H28	0.9300
C2—H2A	0.9700	C29—H29A	0.9600
C2—H2B	0.9700	C29—H29B	0.9600
C3—C20	1.490 (11)	C29—H29C	0.9600
C3—H3A	0.9700	C30—H30A	0.9600
C3—H3B	0.9700	C30—H30B	0.9600
C5—C6	1.398 (11)	C30—H30C	0.9600
C5—C10	1.411 (12)		
N4—Zn1—N6	112.9 (2)	C6—C7—H7	121.6
N4—Zn1—N2	110.7 (2)	C8—C7—H7	121.6
N6—Zn1—N2	115.2 (2)	C7—C8—C9	120.8 (10)
N4—Zn1—N1	73.9 (2)	C7—C8—H8	119.6
N6—Zn1—N1	74.2 (2)	C9—C8—H8	119.6
N2—Zn1—N1	74.6 (2)	C10—C9—C8	123.7 (9)
N4—Zn1—I1	106.57 (19)	C10—C9—H9	118.2
N6—Zn1—I1	105.53 (17)	C8—C9—H9	118.2
N2—Zn1—I1	105.19 (17)	C9—C10—C5	116.2 (10)
N1—Zn1—I1	179.50 (13)	C9—C10—H10	121.9
O2—Cl1—O2'	34.7 (9)	C5—C10—H10	121.9
O2—Cl1—O1	112.7 (9)	N3—C11—H11A	109.5
O2'—Cl1—O1	112.6 (8)	N3—C11—H11B	109.5
O2—Cl1—O4'	81.0 (10)	H11A—C11—H11B	109.5
O2'—Cl1—O4'	110.6 (9)	N3—C11—H11C	109.5
O1—Cl1—O4'	115.5 (7)	H11A—C11—H11C	109.5
O2—Cl1—O4	113.4 (10)	H11B—C11—H11C	109.5
O2'—Cl1—O4	138.0 (10)	N4—C12—N5	113.1 (7)
O1—Cl1—O4	105.5 (8)	N4—C12—C2	121.8 (7)
O4'—Cl1—O4	32.9 (8)	N5—C12—C2	125.1 (7)
O2—Cl1—O3	108.3 (10)	N5—C13—C18	134.0 (10)
O2'—Cl1—O3	76.0 (10)	N5—C13—C14	107.0 (7)
O1—Cl1—O3	108.1 (9)	C18—C13—C14	119.0 (11)
O4'—Cl1—O3	127.4 (11)	C15—C14—N4	131.5 (8)
O4—Cl1—O3	108.6 (10)	C15—C14—C13	121.6 (8)

O2—Cl1—O3'	130.3 (10)	N4—C14—C13	106.9 (8)
O2'—Cl1—O3'	104.4 (8)	C14—C15—C16	115.4 (10)
O1—Cl1—O3'	109.7 (7)	C14—C15—H15	122.3
O4'—Cl1—O3'	103.1 (9)	C16—C15—H15	122.3
O4—Cl1—O3'	77.8 (10)	C17—C16—C15	122.6 (11)
O3—Cl1—O3'	31.9 (10)	C17—C16—H16	118.7
C2—N1—C1	114.2 (6)	C15—C16—H16	118.7
C2—N1—C3	114.5 (6)	C18—C17—C16	121.4 (10)
C1—N1—C3	113.6 (6)	C18—C17—H17	119.3
C2—N1—Zn1	103.2 (4)	C16—C17—H17	119.3
C1—N1—Zn1	105.8 (4)	C17—C18—C13	120.0 (11)
C3—N1—Zn1	103.9 (4)	C17—C18—H18	120.0
C4—N2—C6	106.1 (6)	C13—C18—H18	120.0
C4—N2—Zn1	117.3 (5)	N5—C19—H19A	109.5
C6—N2—Zn1	136.1 (5)	N5—C19—H19B	109.5
C4—N3—C5	106.7 (7)	H19A—C19—H19B	109.5
C4—N3—C11	127.5 (8)	N5—C19—H19C	109.5
C5—N3—C11	125.8 (7)	H19A—C19—H19C	109.5
C12—N4—C14	106.4 (7)	H19B—C19—H19C	109.5
C12—N4—Zn1	118.0 (5)	N6—C20—N7	113.4 (7)
C14—N4—Zn1	135.4 (6)	N6—C20—C3	122.3 (7)
C12—N5—C13	106.6 (7)	N7—C20—C3	124.3 (7)
C12—N5—C19	126.8 (8)	C22—C21—C26	121.8 (9)
C13—N5—C19	126.5 (8)	C22—C21—N7	106.5 (7)
C20—N6—C22	105.5 (6)	C26—C21—N7	131.7 (9)
C20—N6—Zn1	117.7 (5)	C21—C22—C23	121.3 (7)
C22—N6—Zn1	136.2 (5)	C21—C22—N6	108.3 (7)
C20—N7—C21	106.3 (7)	C23—C22—N6	130.4 (7)
C20—N7—C27	127.6 (8)	C22—C23—C24	115.9 (9)
C21—N7—C27	126.1 (8)	C22—C23—H23	122.0
C28—N8—C29	108 (3)	C24—C23—H23	122.0
C28—N8—C30	138 (3)	C25—C24—C23	122.5 (10)
C29—N8—C30	113 (3)	C25—C24—H24	118.7
N1—C1—C4	110.0 (6)	C23—C24—H24	118.7
N1—C1—H1A	109.7	C26—C25—C24	120.2 (10)
C4—C1—H1A	109.7	C26—C25—H25	119.9
N1—C1—H1B	109.7	C24—C25—H25	119.9
C4—C1—H1B	109.7	C25—C26—C21	118.3 (10)
H1A—C1—H1B	108.2	C25—C26—H26	120.8
N1—C2—C12	110.2 (6)	C21—C26—H26	120.8
N1—C2—H2A	109.6	N7—C27—H27A	109.5
C12—C2—H2A	109.6	N7—C27—H27B	109.5
N1—C2—H2B	109.6	H27A—C27—H27B	109.5
C12—C2—H2B	109.6	N7—C27—H27C	109.5
H2A—C2—H2B	108.1	H27A—C27—H27C	109.5
N1—C3—C20	110.3 (6)	H27B—C27—H27C	109.5
N1—C3—H3A	109.6	O5—C28—N8	109 (3)
C20—C3—H3A	109.6	O5—C28—H28	125.4
N1—C3—H3B	109.6	N8—C28—H28	125.4

C20—C3—H3B	109.6	N8—C29—H29A	109.5
H3A—C3—H3B	108.1	N8—C29—H29B	109.5
N2—C4—N3	112.8 (7)	H29A—C29—H29B	109.5
N2—C4—C1	123.0 (7)	N8—C29—H29C	109.5
N3—C4—C1	124.2 (7)	H29A—C29—H29C	109.5
N3—C5—C6	107.7 (7)	H29B—C29—H29C	109.5
N3—C5—C10	131.2 (9)	N8—C30—H30A	109.5
C6—C5—C10	121.1 (10)	N8—C30—H30B	109.5
C7—C6—C5	121.3 (8)	H30A—C30—H30B	109.5
C7—C6—N2	131.9 (8)	N8—C30—H30C	109.5
C5—C6—N2	106.7 (7)	H30A—C30—H30C	109.5
C6—C7—C8	116.8 (9)	H30B—C30—H30C	109.5

Fig. 1


C29
C30
N8
C28
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C10
O5
C5
C9
N3
C4
C6
C8
C1
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N1
C3
C2
C20
C27
C12
N5
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C14
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C16
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C25
C24
O2
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Cl1
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Fig. 2