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{2-[(2,5-Dimethylphenyl)iminomethyl]-pyridine-κ^2N,N'}diiodidozinc(II)

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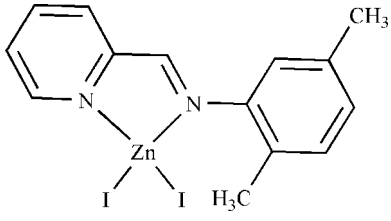
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.009 Å; R factor = 0.072; wR factor = 0.230; data-to-parameter ratio = 26.2.

In the molecule of the title compound, $[ZnI_2(C_{14}H_{14}N_2)]$, the Zn atom is four-coordinated in a distorted tetrahedral geometry by two N atoms of the Schiff base ligand and by two I atoms. The benzene and pyridine rings are oriented at a dihedral angle of 70.75 (3)°. The five-membered ring has an envelope conformation. There is a weak π–π interaction between benzene rings, with a centroid-to-centroid distance of 3.975 (4) Å.

Related literature

For general background, see: Gibson *et al.* (2007); Ittel *et al.* (2000); Gibson & Spitzmesser (2003); Bart *et al.* (2004); Sugiyama *et al.* (2004); Kooistra *et al.* (2004); Bouwkamp *et al.* (2006). For related literature, see: Dehghanpour *et al.* (2007).



Experimental

Crystal data

$[ZnI_2(C_{14}H_{14}N_2)]$
M_r = 529.46
Monoclinic, $P2_1/c$
a = 11.467 (5) Å
b = 9.627 (4) Å
c = 15.868 (6) Å
β = 103.88 (3)°
V = 1700.6 (12) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 5.06 mm^{-1}
T = 298 (2) K
0.5 × 0.4 × 0.25 mm

Data collection

Stoe IPDSII diffractometer
Absorption correction: numerical [*X-RED32* and *X-SHAPE* (Stoe & Cie, 2005)]
T_{min} = 0.100, T_{max} = 0.280
10947 measured reflections
4498 independent reflections
4035 reflections with $I > 2\sigma(I)$
R_{int} = 0.098

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.071
$wR(F^2)$ = 0.230
S = 1.12
4498 reflections
172 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.97 e Å^{-3}
$\Delta\rho_{min}$ = −1.66 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—I1	2.5201 (11)	Zn1—N1	2.059 (5)
Zn1—I2	2.5517 (12)	Zn1—N2	2.104 (5)
I1—Zn1—I2	120.26 (4)	N2—Zn1—I1	107.27 (13)
N1—Zn1—N2	80.16 (19)	N1—Zn1—I2	107.58 (15)
N1—Zn1—I1	112.45 (14)	N2—Zn1—I2	121.99 (13)

Data collection: *X-AREA* (Stoe & Cie, 2005); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2005); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); 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: HK2486).

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supplementary materials

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{2-[(2,5-Dimethylphenyl)iminomethyl]pyridine-κ^2N,N'}diiodidozinc(II)

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Comment

Transition metal compounds containing Schiff base ligands have been of great interest for many years. These compounds play an important role in the development of coordination chemistry (Gibson *et al.*, 2007). Aryl-substituted iminopyridine complexes have emerged as a powerful class of catalysts for a host of important bond-forming reactions including olefin polymerization (Ittel *et al.*, 2000; Gibson & Spitzmesser, 2003), hydrogenation and hydrosilation (Bart *et al.*, 2004). It is also now well established that iminopyridines are both redox (Sugiyama *et al.*, 2004) and chemically active ligands (Kooistra *et al.*, 2004) participating in electron transfer, addition reactions and deprotonation chemistry (Bouwkamp *et al.*, 2006). We report herein the crystal structure of the title compound.

In the molecule of the title compound (Fig. 1), the Zn atom is four-coordinated in distorted tetrahedral geometry (Table 1) by two N atoms of the Schiff base ligand, and two I atoms. The bond angles around the Zn atom deviate from the ideal tetrahedral geometry (Dehghanpour *et al.*, 2007). Rings A (N1/C1–C5) and B (C7/C8/C10/C11/C12/C14) are, of course, planar, and they are oriented at a dihedral angle of 70.75 (3)°. Ring C (Zn1/N1/N2/C5/C6) has envelope conformation, with N2 atom displaced by 0.104 (3) Å from the plane of the other ring atoms. The weak π–π interaction between B rings $CgB\cdots CgB^{i}$ [symmetry code: (iv) 1 - x, 1 - y, 1 - z] may stabilize the structure, with a centroid–centroid distance of 3.975 (4) Å.

Experimental

For the preparation of the title compound, (2,5-dimethyl-N-phenyl)(pyridine-2-yl)methanimine (21.0 mg, 0.1 mmol), and ZnI_2 (31.9 mg, 0.1 mmol) were dissolved in acetonitrile (50 ml). The mixture was stirred for 10 min at room temperature. The resulting solution was left in air for a few days, giving yellow crystals of the title compound (yield; 79%). Calc.: C 31.75 H 2.67, N 5.29%, found: C 31.79, H 2.49, N 5.31%.

Refinement

H atoms were positioned geometrically, with C—H = 0.93 and 0.96 Å for aromatic and methyl H, and constrained to ride on their parent atoms, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures

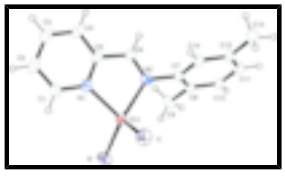

Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

{2-[(2,5-Dimethylphenyl)iminomethyl]pyridine-κ^2N,N'}diiodidozinc(II)

Crystal data

$[ZnI_2(C_{14}H_{14}N_2)]$	F_{000} = 992
M_r = 529.46	D_x = 2.068 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 2112 reflections
a = 11.467 (5) Å	θ = 2.5–29.4º
b = 9.627 (4) Å	μ = 5.06 mm^{-1}
c = 15.868 (6) Å	T = 298 (2) K
β = 103.88 (3)º	Block, yellow
V = 1700.6 (12) Å^3	0.5 × 0.4 × 0.25 mm
Z = 4	

Data collection

Stoe IPDSII diffractometer	R_{int} = 0.098
rotation method scans	θ_{max} = 29.4º
Absorption correction: numerical [X-RED and X-SHAPE (Stoe & Cie, 2005)]	θ_{min} = 2.5º
T_{min} = 0.100, T_{max} = 0.280	h = −15→11
10947 measured reflections	k = −11→13
4498 independent reflections	l = −21→21
4035 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.1439P)^2 + 2.419P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.071	$(\Delta/\sigma)_{max}$ = 0.007
$wR(F^2)$ = 0.230	$\Delta\rho_{max}$ = 1.97 e Å^{-3}
S = 1.12	$\Delta\rho_{min}$ = −1.66 e Å^{-3}
4498 reflections	Extinction correction: none
172 parameters	

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.83553 (6)	0.25679 (7)	0.02157 (4)	0.0406 (2)
I1	0.69958 (5)	0.45620 (5)	0.03661 (4)	0.0622 (2)
I2	0.87622 (5)	0.19974 (6)	−0.12580 (3)	0.0617 (2)
N1	0.9989 (4)	0.2665 (5)	0.1106 (3)	0.0400 (9)
N2	0.8103 (4)	0.1007 (5)	0.1083 (3)	0.0366 (8)
C1	1.0919 (6)	0.3467 (9)	0.1080 (5)	0.0524 (14)
H1	1.086	0.4083	0.062	0.063*
C2	1.1962 (6)	0.3412 (9)	0.1712 (5)	0.0590 (18)
H2	1.2614	0.3967	0.1681	0.071*
C3	1.2026 (6)	0.2495 (9)	0.2411 (5)	0.0596 (19)
H3	1.2721	0.2453	0.2856	0.072*
C4	1.1071 (5)	0.1665 (8)	0.2440 (4)	0.0498 (13)
H4	1.1104	0.1042	0.2893	0.06*
C5	1.0055 (5)	0.1786 (6)	0.1771 (4)	0.0411 (11)
C6	0.8989 (5)	0.0951 (6)	0.1752 (4)	0.0412 (11)
H6	0.8952	0.0384	0.2219	0.049*
C7	0.7036 (5)	0.0265 (5)	0.1120 (3)	0.0356 (9)
C8	0.6663 (5)	−0.0814 (6)	0.0540 (3)	0.0377 (10)
C9	0.7345 (7)	−0.1256 (8)	−0.0114 (5)	0.0531 (14)
H9A	0.8136	−0.1554	0.0183	0.064*
H9B	0.7404	−0.0488	−0.0487	0.064*
H9C	0.693	−0.201	−0.0455	0.064*
C10	0.5634 (5)	−0.1522 (6)	0.0595 (4)	0.0440 (12)
H10	0.5352	−0.2247	0.0213	0.053*
C11	0.5023 (5)	−0.1160 (7)	0.1214 (5)	0.0495 (13)
H11	0.4335	−0.1652	0.1241	0.059*
C12	0.5402 (5)	−0.0092 (8)	0.1791 (4)	0.0491 (13)
C13	0.4725 (8)	0.0300 (13)	0.2483 (7)	0.076 (3)
H13A	0.4453	0.1244	0.2396	0.091*
H13B	0.5253	0.0207	0.305	0.091*
H13C	0.4047	−0.0304	0.2435	0.091*
C14	0.6415 (5)	0.0638 (6)	0.1732 (4)	0.0416 (11)
H14	0.668	0.138	0.2104	0.05*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0414 (4)	0.0406 (4)	0.0392 (4)	−0.0024 (2)	0.0082 (3)	0.0058 (2)
I1	0.0607 (3)	0.0455 (3)	0.0819 (4)	0.00774 (18)	0.0200 (3)	0.0016 (2)
I2	0.0745 (4)	0.0713 (4)	0.0442 (3)	0.0013 (2)	0.0239 (2)	0.00481 (18)
N1	0.036 (2)	0.038 (2)	0.047 (2)	−0.0030 (17)	0.0124 (18)	−0.0020 (18)
N2	0.041 (2)	0.033 (2)	0.0357 (19)	0.0000 (16)	0.0107 (16)	0.0014 (16)
C1	0.048 (3)	0.060 (4)	0.052 (3)	−0.015 (3)	0.019 (3)	−0.006 (3)
C2	0.039 (3)	0.076 (5)	0.064 (4)	−0.011 (3)	0.016 (3)	−0.030 (4)

C3	0.039 (3)	0.079 (5)	0.055 (4)	0.001 (3)	0.001 (3)	−0.032 (4)
C4	0.040 (3)	0.054 (3)	0.050 (3)	0.003 (2)	0.001 (2)	−0.006 (3)
C5	0.041 (2)	0.040 (3)	0.041 (2)	0.000 (2)	0.006 (2)	−0.007 (2)
C6	0.040 (2)	0.037 (2)	0.044 (3)	0.0001 (19)	0.005 (2)	0.006 (2)
C7	0.036 (2)	0.031 (2)	0.037 (2)	0.0000 (17)	0.0042 (17)	0.0039 (17)
C8	0.045 (2)	0.033 (2)	0.034 (2)	0.0013 (19)	0.0083 (19)	0.0027 (18)
C9	0.066 (4)	0.048 (3)	0.050 (3)	−0.003 (3)	0.023 (3)	−0.011 (3)
C10	0.040 (2)	0.036 (2)	0.051 (3)	−0.005 (2)	0.002 (2)	0.001 (2)
C11	0.037 (2)	0.050 (3)	0.060 (3)	−0.002 (2)	0.008 (2)	0.006 (3)
C12	0.033 (2)	0.064 (4)	0.051 (3)	0.002 (2)	0.010 (2)	0.001 (3)
C13	0.054 (4)	0.105 (7)	0.077 (5)	0.010 (4)	0.031 (4)	−0.010 (5)
C14	0.042 (3)	0.042 (3)	0.040 (2)	−0.002 (2)	0.008 (2)	−0.006 (2)

Geometric parameters (Å, °)

Zn1—I1	2.5201 (11)	C7—C8	1.387 (7)
Zn1—I2	2.5517 (12)	C7—N2	1.430 (7)
Zn1—N1	2.059 (5)	C8—C10	1.384 (8)
Zn1—N2	2.104 (5)	C8—C9	1.502 (9)
C1—N1	1.326 (8)	C9—H9A	0.96
C1—C2	1.365 (10)	C9—H9B	0.96
C1—H1	0.93	C9—H9C	0.96
C2—C3	1.406 (13)	C10—C11	1.381 (10)
C2—H2	0.93	C10—H10	0.93
C3—C4	1.365 (11)	C11—C12	1.377 (10)
C3—H3	0.93	C11—H11	0.93
C4—C5	1.380 (8)	C12—C14	1.380 (9)
C4—H4	0.93	C12—C13	1.535 (11)
C5—N1	1.341 (8)	C13—H13A	0.96
C5—C6	1.457 (8)	C13—H13B	0.96
C6—N2	1.283 (7)	C13—H13C	0.96
C6—H6	0.93	C14—H14	0.93
C7—C14	1.382 (8)		
I1—Zn1—I2	120.26 (4)	C14—C7—C8	122.2 (5)
N1—Zn1—N2	80.16 (19)	C14—C7—N2	119.3 (5)
N1—Zn1—I1	112.45 (14)	C8—C7—N2	118.5 (5)
N2—Zn1—I1	107.27 (13)	C10—C8—C7	117.3 (5)
N1—Zn1—I2	107.58 (15)	C10—C8—C9	119.8 (6)
N2—Zn1—I2	121.99 (13)	C7—C8—C9	122.9 (5)
C1—N1—C5	119.8 (6)	C8—C9—H9A	109.5
C1—N1—Zn1	127.7 (5)	C8—C9—H9B	109.5
C5—N1—Zn1	112.4 (4)	H9A—C9—H9B	109.5
C6—N2—C7	117.4 (5)	C8—C9—H9C	109.5
C6—N2—Zn1	111.5 (4)	H9A—C9—H9C	109.5
C7—N2—Zn1	129.6 (3)	H9B—C9—H9C	109.5
N1—C1—C2	121.7 (7)	C11—C10—C8	120.4 (6)
N1—C1—H1	119.2	C11—C10—H10	119.8
C2—C1—H1	119.2	C8—C10—H10	119.8
C1—C2—C3	118.3 (7)	C12—C11—C10	121.9 (6)

C1—C2—H2	120.8	C12—C11—H11	119
C3—C2—H2	120.8	C10—C11—H11	119
C4—C3—C2	120.2 (6)	C11—C12—C14	118.1 (6)
C4—C3—H3	119.9	C11—C12—C13	121.8 (7)
C2—C3—H3	119.9	C14—C12—C13	120.1 (7)
C3—C4—C5	117.4 (7)	C12—C13—H13A	109.5
C3—C4—H4	121.3	C12—C13—H13B	109.5
C5—C4—H4	121.3	H13A—C13—H13B	109.5
N1—C5—C4	122.5 (6)	C12—C13—H13C	109.5
N1—C5—C6	116.3 (5)	H13A—C13—H13C	109.5
C4—C5—C6	121.2 (6)	H13B—C13—H13C	109.5
N2—C6—C5	119.2 (5)	C12—C14—C7	120.0 (6)
N2—C6—H6	120.4	C12—C14—H14	120
C5—C6—H6	120.4	C7—C14—H14	120
N1—C1—C2—C3	−1.3 (11)	C4—C5—N1—C1	−0.7 (9)
C1—C2—C3—C4	1.4 (11)	C6—C5—N1—C1	179.5 (6)
C2—C3—C4—C5	−1.1 (10)	C4—C5—N1—Zn1	179.3 (5)
C3—C4—C5—N1	0.8 (10)	C6—C5—N1—Zn1	−0.5 (6)
C3—C4—C5—C6	−179.5 (6)	N2—Zn1—N1—C1	177.4 (6)
N1—C5—C6—N2	5.8 (8)	I1—Zn1—N1—C1	−77.9 (6)
C4—C5—C6—N2	−174.0 (6)	I2—Zn1—N1—C1	56.8 (6)
C14—C7—C8—C10	−0.2 (8)	N2—Zn1—N1—C5	−2.6 (4)
N2—C7—C8—C10	179.5 (5)	I1—Zn1—N1—C5	102.1 (4)
C14—C7—C8—C9	−178.4 (6)	I2—Zn1—N1—C5	−123.2 (4)
N2—C7—C8—C9	1.3 (8)	C5—C6—N2—C7	−174.8 (5)
C7—C8—C10—C11	−0.6 (8)	C5—C6—N2—Zn1	−7.7 (7)
C9—C8—C10—C11	177.6 (6)	C14—C7—N2—C6	62.5 (7)
C8—C10—C11—C12	0.3 (10)	C8—C7—N2—C6	−117.1 (6)
C10—C11—C12—C14	0.9 (10)	C14—C7—N2—Zn1	−101.8 (6)
C10—C11—C12—C13	−179.5 (7)	C8—C7—N2—Zn1	78.6 (6)
C11—C12—C14—C7	−1.7 (9)	N1—Zn1—N2—C6	5.6 (4)
C13—C12—C14—C7	178.7 (7)	I1—Zn1—N2—C6	−105.0 (4)
C8—C7—C14—C12	1.4 (9)	I2—Zn1—N2—C6	110.3 (4)
N2—C7—C14—C12	−178.3 (5)	N1—Zn1—N2—C7	170.6 (5)
C2—C1—N1—C5	0.9 (10)	I1—Zn1—N2—C7	60.0 (5)
C2—C1—N1—Zn1	−179.0 (5)	I2—Zn1—N2—C7	−84.7 (5)

Fig. 1