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Dichlorido{2-[(4-iodophenyl)iminomethyl]pyridine-κ^2N,N'}zinc(II)

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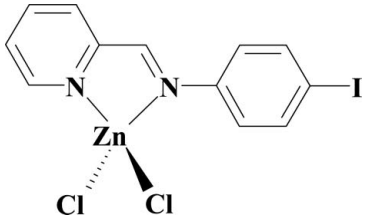
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.009 Å; R factor = 0.061; wR factor = 0.144; data-to-parameter ratio = 22.8.

In the title complex, $[ZnCl_2(C_{12}H_9IN_2)]$, the Zn^{II} atom has a distorted tetrahedral coordination. The organic ligand is bidentate, coordinating the Zn^{II} atom *via* the two N atoms.

Related literature

For related literature, see: Amirnasr *et al.* (2002); Ittel *et al.* (2000); Yamada (1999); Britovsek *et al.* (1999); Small *et al.* (1998).



Experimental

Crystal data

$[ZnCl_2(C_{12}H_9IN_2)]$
M_r = 444.38
Triclinic, $P\overline{1}$
a = 7.5680 (6) Å
b = 8.5363 (6) Å
c = 10.8772 (8) Å
α = 89.790 (2)°
β = 72.613 (2)°
γ = 88.926 (2)°
V = 670.47 (9) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 4.51 mm^{-1}
T = 296 (2) K
0.30 × 0.20 × 0.15 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*APEX2*; Bruker, 2005)
T_{min} = 0.345, T_{max} = 0.551
(expected range = 0.318–0.508)
7690 measured reflections
3470 independent reflections
2895 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.061
$wR(F^2)$ = 0.144
S = 0.97
3470 reflections
152 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.20 e Å^{-3}
$\Delta\rho_{min}$ = −1.12 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—N1	2.089 (5)	Zn1—Cl1	2.1992 (15)
Zn1—N2	2.064 (5)	Zn1—Cl2	2.2167 (17)
N1—Zn1—N2	80.22 (19)	N2—Zn1—Cl2	110.03 (15)
N2—Zn1—Cl1	119.49 (14)	N1—Zn1—Cl2	109.22 (14)
N1—Zn1—Cl1	118.63 (14)	Cl1—Zn1—Cl2	114.51 (6)

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *APEX2*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); 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: SJ2381).

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supplementary materials

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Dichlorido{2-[(4-iodophenyl)iminomethyl]pyridine-κ^2N,N'}zinc(II)

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Comment

Metal complexes with diimines as ligands have played an important role in development of coordination chemistry (Yamada, 1999). Complexes of iminopyridines with late transition metals have recently found a renewal of interest (Small *et al.*, 2003). The unexpected and recent discovery that such complexes, in particular iminopyridine iron(II) and cobalt (II) complexes, may act as active catalysts for olefin polymerization render them more attractive to chemists (Ittel *et al.*, 2000; Britovsek *et al.*, 1999). The title complex, (I), Fig. 1, was prepared by the reaction of $ZnCl_2$ with the bidentate ligand (4-iodo-phenyl)-pyridin-2-ylmethylene- amine.

Molecular structure of complex (I), as well as the atom-numbering scheme are shown in Fig. 1. A s one might expect for a four-coordinated zinc(II) complex, the metal center has a tetrahedral coordination. It shows signficant distortions mainly due to the presence of the 5-membered chelate cycle: the endocyclic N1—Zn1—N2 angle [80.22 (19)°] is much narrower than the ideal tetrahedral angle of 109.5°, whereas the N2—Zn1—Cl1 angle [119.49 (14)°] is much wider than the ideal angle in the tetrahedron. The Zn—Cl and Zn—N bond dimensions compare well with the values found in other tetrahedral diimine complexes of zinc chloride (Amirnasr *et al.*, 2002).

Experimental

The title complex was prepared by the reaction of $ZnCl_2$ with 4-iodo-phenyl)-pyridin-2-ylmethylene-amine (molar ratio 1:1) in acetonitrile at room temperature. The solution was then concentrated under vacuum, and diffusion of diethyl ether vapor into the concentrated solution gave colourless crystals of (I) in 78% yield. Calc. for $C_{12}H_9Cl_2IN_2Zn$: C 32.43, H 2.04, N 6.30%; found: C 32.42, H 2.05, N 6.33%.

Refinement

The H(C) atom positions were calculated and were refined in isotropic approximation in riding model with the U_{iso}(H) parameters equal to 1.2 U_{eq}(Ci) where U_{eq}(Ci) are the equivalent thermal parameters of the atoms to which corresponding H atoms are bonded. There is a high positive residual density peak of 1.20 e Å^{-3} near the I1 center (distance 0.96%A) due to considerable absorption effects which could not be completely corrected.

Figures

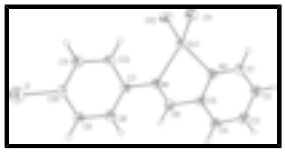

Fig. 1. Molecular structure of (I) showing the atom-labelling scheme with thermal ellipsoids drawn at the 50% probability level.

Dichlorido{2-[(4-iodophenyl)iminomethyl]pyridine- κ^2N,N'}zinc(II)

Crystal data

$[ZnCl_2(C_{12}H_9IN_2)]$	$Z = 2$
$M_r = 444.38$	$F_{000} = 424$
Triclinic, $P\overline{1}$	$D_x = 2.201$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 7.5680$ (6) Å	Cell parameters from 3201 reflections
$b = 8.5363$ (6) Å	$\theta = 2.4$–$31.9°$
$c = 10.8772$ (8) Å	$\mu = 4.51$ mm^{-1}
$\alpha = 89.790$ (2)°	$T = 296$ (2) K
$\beta = 72.613$ (2)°	Plate, colourless
$\gamma = 88.926$ (2)°	0.30 × 0.20 × 0.15 mm
$V = 670.47$ (9) Å^3	

Data collection

Bruker APEXII CCD area-detector diffractometer	3470 independent reflections
Radiation source: fine-focus sealed tube	2895 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.025$
$T = 296(2)$ K	$\theta_{max} = 29.6°$
φ and ω scans	$\theta_{min} = 10.0°$
Absorption correction: multi-scan (APEX2; Bruker, 2005)	$h = -10 \rightarrow 10$
$T_{min} = 0.345$, $T_{max} = 0.551$	$k = -11 \rightarrow 11$
7690 measured reflections	$l = -15 \rightarrow 15$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.061$	H-atom parameters constrained
$wR(F^2) = 0.144$	$w = 1/[\sigma^2(F_o^2) + (0.0347P)^2 + 10.4724P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.97$	$(\Delta/\sigma)_{max} < 0.001$
3470 reflections	$\Delta\rho_{max} = 1.20$ e Å^{-3}
152 parameters	$\Delta\rho_{min} = -1.12$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
I1	0.34217 (8)	0.81139 (7)	1.53276 (6)	0.04453 (19)
Zn1	0.89413 (9)	0.69620 (7)	0.84072 (6)	0.01995 (17)
Cl1	1.1228 (2)	0.84010 (16)	0.85933 (14)	0.0245 (3)
Cl2	0.6921 (2)	0.82264 (17)	0.76324 (17)	0.0303 (3)
N1	0.7512 (7)	0.5596 (6)	0.9973 (5)	0.0195 (9)
N2	0.9510 (7)	0.4763 (6)	0.7586 (5)	0.0220 (9)
C1	1.0571 (8)	0.4354 (7)	0.6413 (6)	0.0240 (11)
H1A	1.1226	0.5129	0.5872	0.029*
C2	1.0743 (9)	0.2816 (7)	0.5963 (6)	0.0260 (11)
H2A	1.1506	0.2572	0.5141	0.031*
C3	0.9757 (9)	0.1648 (7)	0.6761 (6)	0.0253 (11)
H3A	0.9841	0.0612	0.6484	0.030*
C4	0.8634 (9)	0.2074 (7)	0.7993 (6)	0.0242 (11)
H4A	0.7959	0.1328	0.8557	0.029*
C5	0.8554 (8)	0.3655 (7)	0.8353 (6)	0.0216 (10)
C6	0.7421 (8)	0.4166 (7)	0.9652 (6)	0.0217 (10)
H6A	0.6663	0.3468	1.0220	0.026*
C7	0.6558 (5)	0.6143 (4)	1.1248 (3)	0.0192 (10)
C8	0.5653 (5)	0.5138 (3)	1.2234 (3)	0.0230 (11)
H8A	0.5674	0.4065	1.2084	0.028*
C9	0.4715 (5)	0.5737 (4)	1.3445 (3)	0.0226 (10)
H9A	0.4109	0.5065	1.4105	0.027*
C10	0.4684 (5)	0.7341 (4)	1.3669 (3)	0.0214 (10)
C11	0.5589 (6)	0.8346 (3)	1.2683 (3)	0.0234 (11)
H11A	0.5568	0.9419	1.2833	0.028*
C12	0.6527 (5)	0.7746 (4)	1.1472 (3)	0.0225 (10)
H12A	0.7133	0.8418	1.0812	0.027*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.0478 (3)	0.0436 (3)	0.0397 (3)	−0.0029 (2)	−0.0092 (2)	−0.0029 (2)

Zn1	0.0212 (3)	0.0172 (3)	0.0206 (3)	−0.0020 (2)	−0.0048 (2)	0.0012 (2)
Cl1	0.0243 (6)	0.0225 (6)	0.0270 (6)	−0.0045 (5)	−0.0079 (5)	0.0019 (5)
Cl2	0.0307 (7)	0.0220 (6)	0.0428 (8)	−0.0022 (5)	−0.0178 (6)	0.0054 (6)
N1	0.019 (2)	0.020 (2)	0.020 (2)	−0.0002 (16)	−0.0063 (17)	0.0007 (16)
N2	0.018 (2)	0.023 (2)	0.023 (2)	−0.0009 (17)	−0.0039 (18)	−0.0010 (18)
C1	0.024 (3)	0.024 (3)	0.022 (3)	−0.002 (2)	−0.003 (2)	0.003 (2)
C2	0.026 (3)	0.026 (3)	0.023 (3)	−0.001 (2)	−0.004 (2)	−0.005 (2)
C3	0.029 (3)	0.021 (3)	0.026 (3)	0.002 (2)	−0.008 (2)	−0.003 (2)
C4	0.030 (3)	0.018 (2)	0.025 (3)	−0.003 (2)	−0.008 (2)	0.002 (2)
C5	0.022 (2)	0.021 (2)	0.023 (3)	0.0023 (19)	−0.007 (2)	−0.001 (2)
C6	0.019 (2)	0.022 (2)	0.024 (3)	−0.0007 (19)	−0.006 (2)	0.002 (2)
C7	0.018 (2)	0.020 (2)	0.018 (2)	0.0002 (18)	−0.0026 (18)	0.0013 (18)
C8	0.023 (3)	0.019 (2)	0.026 (3)	−0.001 (2)	−0.006 (2)	0.003 (2)
C9	0.024 (3)	0.018 (2)	0.024 (3)	−0.0022 (19)	−0.005 (2)	0.002 (2)
C10	0.020 (2)	0.025 (3)	0.018 (2)	0.001 (2)	−0.0032 (19)	−0.0024 (19)
C11	0.025 (3)	0.021 (2)	0.024 (3)	−0.003 (2)	−0.006 (2)	0.001 (2)
C12	0.024 (3)	0.019 (2)	0.023 (3)	−0.003 (2)	−0.004 (2)	0.0026 (19)

Geometric parameters (Å, °)

Zn1—N1	2.089 (5)	C4—C5	1.402 (8)
Zn1—N2	2.064 (5)	C4—H4A	0.9300
Zn1—Cl1	2.1992 (15)	C5—C6	1.480 (8)
Zn1—Cl2	2.2167 (17)	C6—H6A	0.9300
I1—C10	1.886 (3)	C7—C8	1.3900
N1—C6	1.279 (8)	C7—C12	1.3900
N1—C7	1.434 (5)	C8—C9	1.3900
N2—C5	1.331 (8)	C8—H8A	0.9300
N2—C1	1.332 (8)	C9—C10	1.3900
C1—C2	1.393 (9)	C9—H9A	0.9300
C1—H1A	0.9300	C10—C11	1.3900
C2—C3	1.392 (9)	C11—C12	1.3900
C2—H2A	0.9300	C11—H11A	0.9300
C3—C4	1.400 (9)	C12—H12A	0.9300
C3—H3A	0.9300		
N1—Zn1—N2	80.22 (19)	N2—C5—C4	123.1 (5)
N2—Zn1—Cl1	119.49 (14)	N2—C5—C6	116.3 (5)
N1—Zn1—Cl1	118.63 (14)	C4—C5—C6	120.5 (5)
N2—Zn1—Cl2	110.03 (15)	N1—C6—C5	118.2 (5)
N1—Zn1—Cl2	109.22 (14)	N1—C6—H6A	120.9
Cl1—Zn1—Cl2	114.51 (6)	C5—C6—H6A	120.9
C6—N1—C7	121.1 (5)	C8—C7—C12	120.0
C6—N1—Zn1	112.0 (4)	C8—C7—N1	122.5 (3)
C7—N1—Zn1	126.6 (3)	C12—C7—N1	117.5 (3)
C5—N2—C1	118.4 (5)	C9—C8—C7	120.0
C5—N2—Zn1	112.1 (4)	C9—C8—H8A	120.0
C1—N2—Zn1	129.3 (4)	C7—C8—H8A	120.0
N2—C1—C2	122.8 (6)	C8—C9—C10	120.0
N2—C1—H1A	118.6	C8—C9—H9A	120.0

C2—C1—H1A	118.6	C10—C9—H9A	120.0
C3—C2—C1	119.1 (6)	C11—C10—C9	120.0
C3—C2—H2A	120.4	C11—C10—I1	121.07 (19)
C1—C2—H2A	120.4	C9—C10—I1	118.93 (19)
C2—C3—C4	118.2 (5)	C10—C11—C12	120.0
C2—C3—H3A	120.9	C10—C11—H11A	120.0
C4—C3—H3A	120.9	C12—C11—H11A	120.0
C3—C4—C5	118.2 (6)	C11—C12—C7	120.0
C3—C4—H4A	120.9	C11—C12—H12A	120.0
C5—C4—H4A	120.9	C7—C12—H12A	120.0
N2—Zn1—N1—C6	−9.7 (4)	C3—C4—C5—N2	−0.8 (9)
Cl1—Zn1—N1—C6	−128.1 (4)	C3—C4—C5—C6	−178.7 (6)
Cl2—Zn1—N1—C6	98.2 (4)	C7—N1—C6—C5	−175.3 (5)
N2—Zn1—N1—C7	176.1 (4)	Zn1—N1—C6—C5	10.1 (6)
Cl1—Zn1—N1—C7	57.8 (4)	N2—C5—C6—N1	−3.8 (8)
Cl2—Zn1—N1—C7	−75.9 (4)	C4—C5—C6—N1	174.3 (6)
N1—Zn1—N2—C5	7.7 (4)	C6—N1—C7—C8	6.8 (6)
Cl1—Zn1—N2—C5	125.1 (4)	Zn1—N1—C7—C8	−179.5 (2)
Cl2—Zn1—N2—C5	−99.4 (4)	C6—N1—C7—C12	−171.8 (4)
N1—Zn1—N2—C1	−176.8 (6)	Zn1—N1—C7—C12	1.9 (5)
Cl1—Zn1—N2—C1	−59.3 (6)	C12—C7—C8—C9	0.0
Cl2—Zn1—N2—C1	76.2 (5)	N1—C7—C8—C9	−178.6 (4)
C5—N2—C1—C2	−0.9 (9)	C7—C8—C9—C10	0.0
Zn1—N2—C1—C2	−176.2 (5)	C8—C9—C10—C11	0.0
N2—C1—C2—C3	0.6 (10)	C8—C9—C10—I1	−179.3 (3)
C1—C2—C3—C4	−0.3 (9)	C9—C10—C11—C12	0.0
C2—C3—C4—C5	0.4 (9)	I1—C10—C11—C12	179.3 (3)
C1—N2—C5—C4	1.0 (9)	C10—C11—C12—C7	0.0
Zn1—N2—C5—C4	177.1 (5)	C8—C7—C12—C11	0.0
C1—N2—C5—C6	179.1 (5)	N1—C7—C12—C11	178.6 (4)
Zn1—N2—C5—C6	−4.9 (6)		

Fig. 1