Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

Dichloridobis(2-phenylpyridine-κN)-zinc(II)

Sivanesan Dharmalingam,[a] Ha-Jin Lee[b] and Sungho Yoon[a]*

[a]Department of Bio & Nano Chemistry, College of Natural Sciences, Kookmin University, 861-1 Jeongneung-dong, Seongbuk-gu, Seoul 136-702, Republic of Korea, and [b]Jeonju Center, Korea Basic Science Institute (KBSI), 664-14 Dukjin dong 1-ga, Dukjin-gu, Jeonju 561-756, Republic of Korea
Correspondence e-mail: yoona@kookmin.ac.kr

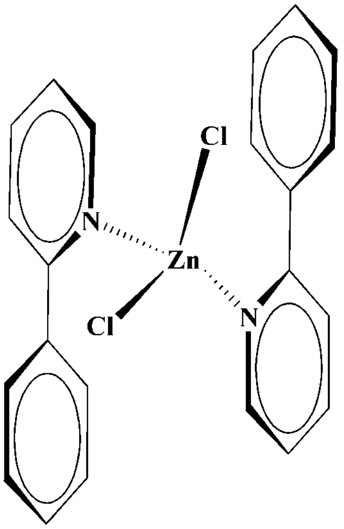
Received 3 March 2012; accepted 10 March 2012

Key indicators: single-crystal X-ray study; T = 200 K; mean σ(C–C) = 0.004 Å; R factor = 0.031; wR factor = 0.074; data-to-parameter ratio = 18.1.

In the title compound, $[ZnCl_2(C_{11}H_9N)_2]$, the Zn^{2+} cation lies on a twofold axis and is coordinated by two Cl^- anions and the N atoms of two 2-phenylpyridine ligands, forming a ZnN_2Cl_2 polyhedron with a slightly distorted tetrahedral coordination geometry. The dihedral angle between the phenyl ring and the metal-bound pyridine ring is 50.3 (4)° for each 2-phenylpyridine ligand. This arranges the phenyl ring from one ligand in the complex above the pyridine ring of the other resulting in an intramolecular π–π interaction, with a centroid–centroid distance of 3.6796 (17) Å. Weak C—H⋯Cl hydrogen bonds stabilize the crystal packing, linking molecules into chains along the c axis.

Related literature

For background to metal complexes with 2-phenylpyridine ligands, see: Samha *et al.* (1993); Yoshinari *et al.* (2010); Zhao *et al.* (2008). For those involving substituted 2-phenylpyridine ligands, see: Santoro *et al.* (2011).



Experimental

Crystal data

$[ZnCl_2(C_{11}H_9N)_2]$
M_r = 446.67
Tetragonal, $I4_1cd$
a = 15.2803 (3) Å
c = 16.4339 (7) Å
V = 3837.1 (2) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 1.57 mm^{-1}
T = 200 K
0.31 × 0.29 × 0.14 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.814, T_{max} = 1.00
13165 measured reflections
2231 independent reflections
1754 reflections with $I > 2\sigma(I)$
R_{int} = 0.047

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.074
S = 1.09
2231 reflections
123 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}
Absolute structure: Flack (1983), 997 Friedel pairs
Flack parameter: 0.02 (2)

Table 1
Selected bond lengths (Å).

Zn1—N1	2.097 (2)	Zn1—Cl1	2.2432 (11)

Table 2
Hydrogen-bond geometry (Å, °).

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
C11—H11⋯Cl1^i	0.95	2.90	3.666 (3)	138

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics:

SHELXTL (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

This research was supported by the Basic Science Research program through the National Research Foundation of Korea (NRF) funded by the Ministry of Education, Science and Technology (MEST) (KRF-2008-C00146).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ5207).

References

Bruker (2000). *SMART*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.

Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.

Samha, H. A., Martinez, T. J. & Armond, M. K. D. (1993). *Inorg. Chem.* **32**, 2583–2586.

Santoro, A., Prokhorov, A. M., Kozhevnikov, V. N., Whitwood, A. C., Donnio, B., Williams, J. A. G. & Bruce, D. W. (2011). *J. Am. Chem. Soc.* **133**, 5248–5251.

Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

Yoshinari, N., Kitani, N. & Konno, T. (2010). *Acta Cryst.* E**66**, m1499.

Zhao, Q., Lei Li, L., Li, F., Yu, M., Liu, Z., Yi, T. & Huang, C. (2008). *Chem. Commun.* pp. 685–687.

supplementary materials

Acta Cryst. (2012). E**68**, m431–m432   [doi:10.1107/S1600536812010616]

Dichloridobis(2-phenylpyridine-*κN*)zinc(II)

Sivanesan Dharmalingam, Ha-Jin Lee and Sungho Yoon

Comment

2-Phenylpyridine coordinated metal complexes of Ir^{III} and Pt^{II} are well known for their intense photoluminescence (Samha *et al.*, 1993; Yoshinari *et al.*, 2010; Zhao *et al.*, 2008). A four coordinate Pt^{II} square planar metal complex has also been reported with two 2-phenylpyridine and two Cl$^-$ ligands (Yoshinari *et al.* 2010). Complexes with substituted 2-phenylpyridine ligands have also been reported (Santoro *et al.*, 2011). Here, we report the structure of a tetrahedrally coordinated Zn^{2+} complex which crystallizes in the tetragonal space group $I4_1cd$ with one half molecule in the asymmetric unit. Bond distances to the metal are given in Table 1 with the structure of the molecule shown in Fig 1 and its crystal packing involving weak intermolecular C—H···Cl interactions detailed in Fig 2 and Table 2.

Experimental

To a solution of 2-phenylpyridine (1.56 ml, 11.0 mmol) in 30 mL of acetonitrile, $ZnCl_2$ (0.50 g, 3.6 mmol) was added at room temperature. After three hours, acetonitrile was removed under reduced pressure and crystals were collected from a dichloromethane and pentane layering system. Colorless block-like crystals. Yield = 90%, (1.45 g).

Refinement

The H atoms were placed at calculated positions and refined as riding with C–H = 0.95 Å [Uiso(H) = 1.2 Ueq(C)].

Computing details

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT* (Bruker, 2000); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

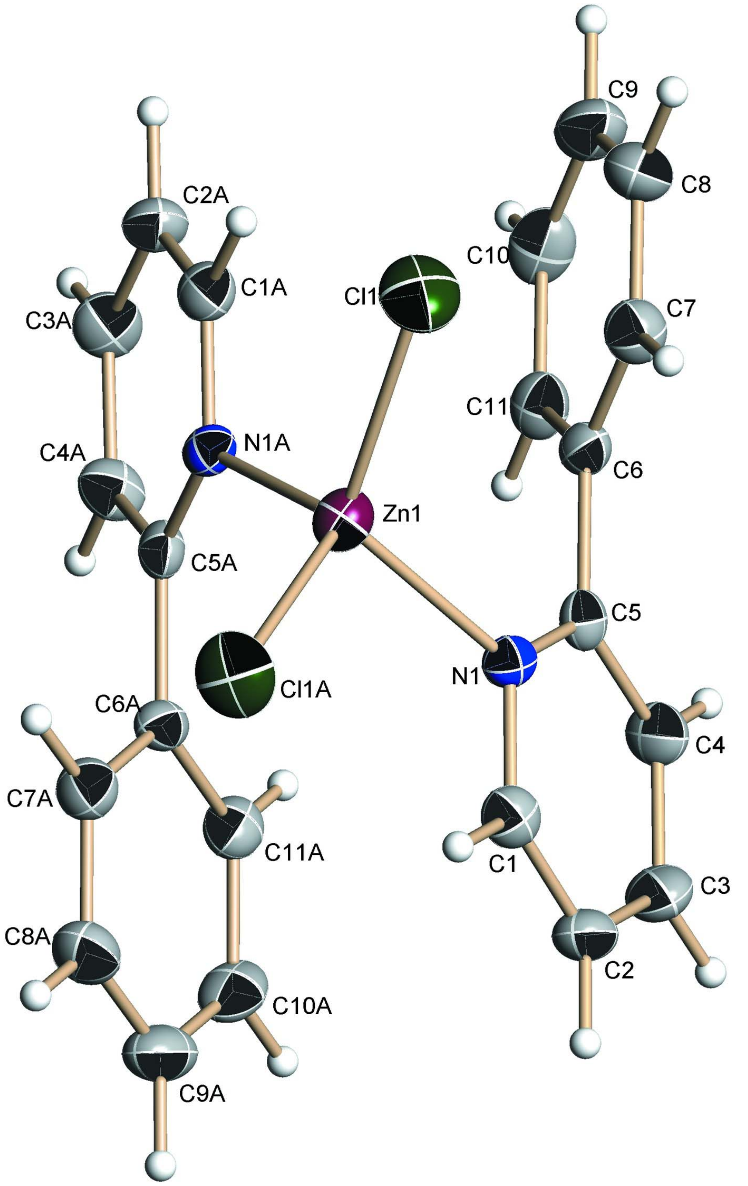


Figure 1

The molecular structure of the title compound, showing the atom-numbering and with displacement ellipsoids drawn at the 50% probability level.

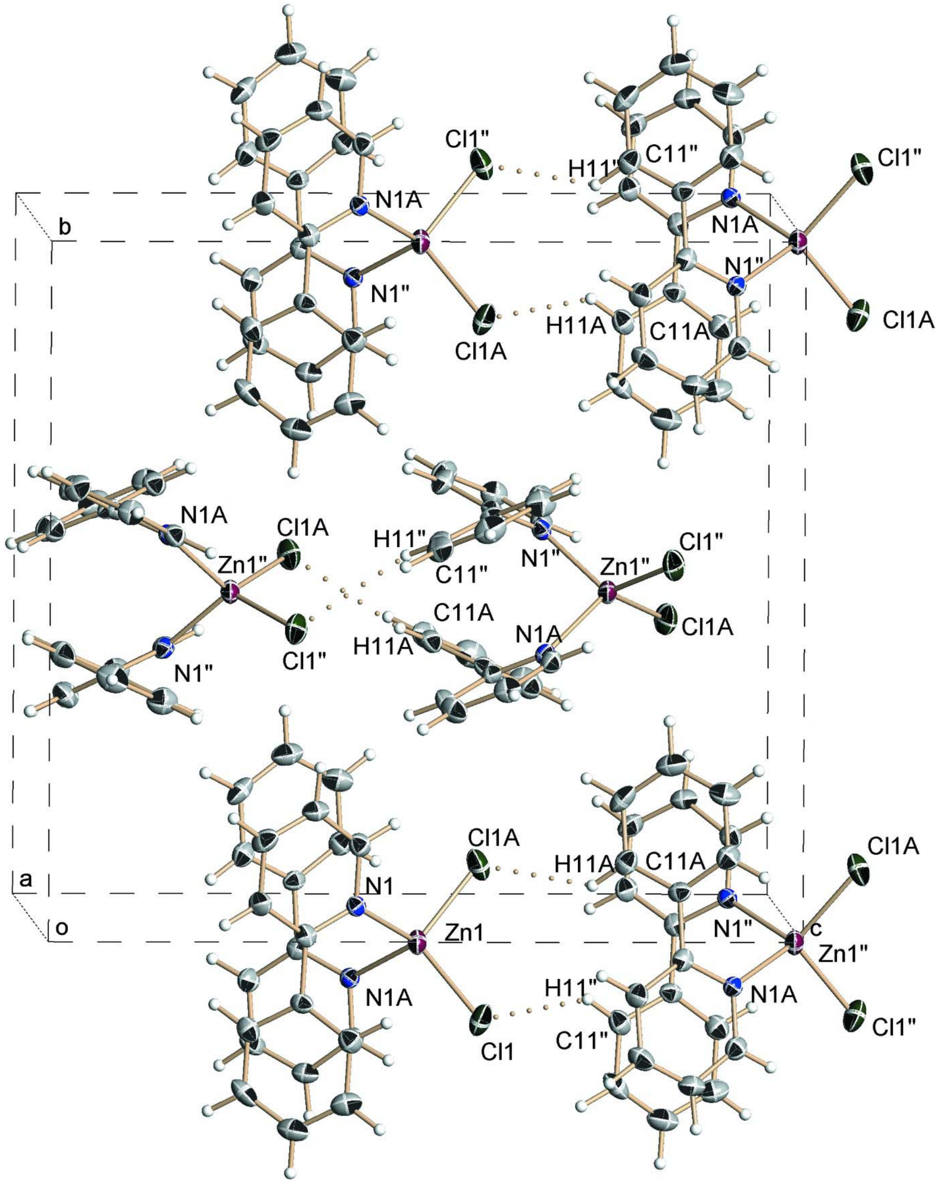


Figure 2

A crystal packing diagram of the title compound, viewed along the *a* axis.

Dichloridobis(2-phenylpyridine-*κN*)zinc(II)

Crystal data

$[ZnCl_2(C_{11}H_9N)_2]$
$M_r = 446.67$
Tetragonal, $I4_1cd$
Hall symbol: I 4bw -2c
$a = 15.2803$ (3) Å
$c = 16.4339$ (7) Å
$V = 3837.1$ (2) Å^3
$Z = 8$
$F(000) = 1824$

$D_x = 1.546$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4803 reflections
$\theta = 2.7–28.1°$
$\mu = 1.57$ mm^{-1}
$T = 200$ K
Block, colorless
0.31 × 0.29 × 0.14 mm

Data collection

Bruker SMART CCD area-detector diffractometer	13165 measured reflections
Radiation source: fine-focus sealed tube	2231 independent reflections
Graphite monochromator	1754 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{\text{int}} = 0.047$
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)	$\theta_{\text{max}} = 28.3°$, $\theta_{\text{min}} = 2.7°$
$T_{\text{min}} = 0.814$, $T_{\text{max}} = 1.00$	$h = -18 \rightarrow 20$
	$k = -20 \rightarrow 20$
	$l = -21 \rightarrow 16$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.031$	$w = 1/[\sigma^2(F_o^2) + (0.0275P)^2 + 1.0418P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.074$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.09$	$\Delta\rho_{\text{max}} = 0.37$ e Å^{-3}
2231 reflections	$\Delta\rho_{\text{min}} = -0.36$ e Å^{-3}
123 parameters	Absolute structure: Flack (1983), 997 Friedel pairs
1 restraint	Flack parameter: 0.02 (2)
Primary atom site location: structure-invariant direct methods	
Secondary atom site location: difference Fourier map	

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}
Zn1	0.0000	0.0000	0.48912 (7)	0.02540 (12)
N1	0.08480 (15)	−0.05713 (15)	0.40397 (14)	0.0207 (5)
C1	0.08984 (19)	−0.14499 (19)	0.40824 (18)	0.0265 (6)
H1	0.0670	−0.1733	0.4551	0.032*
C2	0.12652 (19)	−0.19583 (19)	0.34786 (19)	0.0298 (7)
H2	0.1299	−0.2576	0.3536	0.036*
C3	0.1581 (2)	−0.1554 (2)	0.27923 (19)	0.0329 (7)
H3	0.1834	−0.1888	0.2365	0.039*
C4	0.1525 (2)	−0.0650 (2)	0.27340 (18)	0.0291 (7)
H4	0.1735	−0.0361	0.2261	0.035*
C5	0.11645 (16)	−0.01706 (17)	0.33602 (17)	0.0222 (6)
C6	0.11275 (18)	0.07988 (17)	0.33127 (17)	0.0226 (6)
C7	0.1446 (2)	0.13120 (19)	0.39417 (19)	0.0298 (7)
H7	0.1688	0.1040	0.4411	0.036*
C8	0.1416 (2)	0.2216 (2)	0.3894 (2)	0.0373 (8)

H8	0.1634	0.2564	0.4328	0.045*
C9	0.1067 (2)	0.2607 (2)	0.3209 (2)	0.0389 (8)
H9	0.1040	0.3227	0.3174	0.047*
C10	0.0756 (2)	0.2102 (2)	0.2572 (2)	0.0353 (8)
H10	0.0520	0.2376	0.2102	0.042*
C11	0.0787 (2)	0.1198 (2)	0.26203 (17)	0.0285 (7)
H11	0.0577	0.0851	0.2182	0.034*
Cl1	0.04582 (6)	0.10755 (6)	0.57169 (5)	0.0421 (2)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0278 (3)	0.0310 (3)	0.0174 (2)	0.0033 (2)	0.000	0.000
N1	0.0218 (12)	0.0206 (12)	0.0196 (12)	0.0022 (10)	−0.0029 (10)	0.0004 (10)
C1	0.0260 (17)	0.0283 (16)	0.0253 (15)	0.0001 (13)	−0.0036 (13)	0.0026 (13)
C2	0.0321 (17)	0.0206 (15)	0.0368 (18)	0.0012 (12)	−0.0012 (13)	−0.0022 (13)
C3	0.0350 (18)	0.0287 (18)	0.0350 (18)	0.0024 (14)	0.0066 (15)	−0.0096 (15)
C4	0.0316 (17)	0.0297 (17)	0.0260 (15)	−0.0030 (13)	0.0089 (13)	0.0005 (13)
C5	0.0164 (13)	0.0272 (15)	0.0229 (16)	−0.0006 (11)	−0.0030 (11)	0.0014 (12)
C6	0.0216 (14)	0.0202 (13)	0.0262 (16)	0.0004 (12)	0.0049 (12)	0.0025 (12)
C7	0.0288 (17)	0.0308 (17)	0.0297 (17)	0.0000 (13)	−0.0015 (13)	0.0027 (13)
C8	0.0353 (19)	0.0274 (17)	0.049 (2)	−0.0038 (15)	0.0000 (16)	−0.0047 (15)
C9	0.0400 (18)	0.0252 (15)	0.051 (2)	0.0026 (15)	0.0091 (17)	0.0056 (17)
C10	0.0346 (17)	0.0371 (18)	0.0344 (19)	0.0056 (14)	0.0054 (14)	0.0184 (14)
C11	0.0266 (16)	0.0325 (17)	0.0264 (18)	0.0005 (13)	0.0038 (12)	0.0050 (13)
Cl1	0.0487 (5)	0.0513 (5)	0.0262 (4)	−0.0041 (4)	−0.0028 (4)	−0.0125 (4)

Geometric parameters (Å, º)

Zn1—N1	2.097 (2)	C4—H4	0.9500
Zn1—N1^{i}	2.097 (2)	C5—C6	1.484 (4)
Zn1—Cl1^{i}	2.2432 (11)	C6—C7	1.386 (4)
Zn1—Cl1	2.2432 (11)	C6—C11	1.392 (4)
N1—C1	1.347 (4)	C7—C8	1.384 (4)
N1—C5	1.362 (3)	C7—H7	0.9500
C1—C2	1.379 (4)	C8—C9	1.382 (5)
C1—H1	0.9500	C8—H8	0.9500
C2—C3	1.374 (4)	C9—C10	1.384 (5)
C2—H2	0.9500	C9—H9	0.9500
C3—C4	1.388 (4)	C10—C11	1.384 (4)
C3—H3	0.9500	C10—H10	0.9500
C4—C5	1.378 (4)	C11—H11	0.9500

N1—Zn1—N1^{i}	96.30 (13)	N1—C5—C4	121.0 (2)
N1—Zn1—Cl1^{i}	106.95 (7)	N1—C5—C6	118.6 (2)
N1^{i}—Zn1—Cl1^{i}	121.04 (6)	C4—C5—C6	120.4 (2)
N1—Zn1—Cl1	121.04 (6)	C7—C6—C11	119.6 (3)
N1^{i}—Zn1—Cl1	106.95 (7)	C7—C6—C5	120.8 (2)
Cl1^{i}—Zn1—Cl1	105.55 (7)	C11—C6—C5	119.6 (3)
C1—N1—C5	118.1 (2)	C8—C7—C6	120.7 (3)

C1—N1—Zn1	114.56 (19)	C8—C7—H7	119.6
C5—N1—Zn1	125.39 (18)	C6—C7—H7	119.6
N1—C1—C2	123.2 (3)	C9—C8—C7	119.3 (3)
N1—C1—H1	118.4	C9—C8—H8	120.3
C2—C1—H1	118.4	C7—C8—H8	120.3
C3—C2—C1	118.7 (3)	C8—C9—C10	120.5 (3)
C3—C2—H2	120.6	C8—C9—H9	119.7
C1—C2—H2	120.6	C10—C9—H9	119.7
C2—C3—C4	118.8 (3)	C9—C10—C11	120.1 (3)
C2—C3—H3	120.6	C9—C10—H10	120.0
C4—C3—H3	120.6	C11—C10—H10	120.0
C5—C4—C3	120.2 (3)	C10—C11—C6	119.8 (3)
C5—C4—H4	119.9	C10—C11—H11	120.1
C3—C4—H4	119.9	C6—C11—H11	120.1

Symmetry code: (i) −*x*, −*y*, *z*.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C11—H11···Cl1^{ii}	0.95	2.90	3.666 (3)	138

Symmetry code: (ii) −*x*, *y*, *z*−1/2.