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Dichlorido(6-methyl-2,2'-bipyridine- κ^2N,N')zinc(II)Roya Ahmadi,^a Khadijeh Kalateh,^a Amin Ebadi,^b Vahid Amani^{a*} and Hamid Reza Khavasi^c

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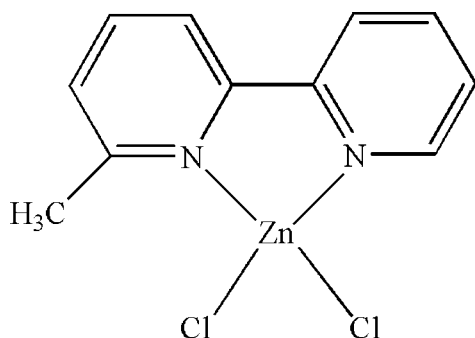
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Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(C-C) = 0.008$ Å; R factor = 0.061; wR factor = 0.130; data-to-parameter ratio = 23.2.

In the molecule of the title compound, $[ZnCl_2(C_{11}H_{10}N_2)]$, the Zn^{II} atom is four-coordinated in a distorted tetrahedral configuration by two N atoms from the 6-methyl-2,2'-bipyridine ligand and by two Cl atoms. There are $\pi-\pi$ contacts between the pyridine ring and the five-membered ring, and also between the pyridine rings, [centroid-centroid distances = 3.685 (3) and 3.757 (3) Å, respectively].

Related literature

For related literature, see: Ahmadi *et al.* (2008); Yousefi *et al.* (2008); Khan & Tuck (1984); Gruia *et al.* (2007); Kozhevnikov *et al.* (2006); Reimann *et al.* (1966); Preston & Kennard (1969); Liu *et al.* (2004); Khavasi *et al.* (2008); Khalighi *et al.* (2008); Steffen & Palenik (1976, 1977); Qin *et al.* (1999); Lundberg (1966).



Experimental

Crystal data

$[ZnCl_2(C_{11}H_{10}N_2)]$
 $M_r = 306.50$
Monoclinic, $P2_1/n$
 $a = 7.4674$ (15) Å
 $b = 9.5105$ (17) Å

$c = 17.656$ (4) Å
 $\beta = 96.551$ (18)°
 $V = 1245.7$ (4) Å³
 $Z = 4$
Mo $K\alpha$ radiation

$\mu = 2.37$ mm⁻¹
 $T = 298$ (2) K

0.30 × 0.15 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (SADABS; Sheldrick, 1998)
 $T_{min} = 0.668$, $T_{max} = 0.802$

14041 measured reflections
3358 independent reflections
2576 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.078$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.060$
 $wR(F^2) = 0.130$
 $S = 1.17$
3358 reflections

145 parameters
H-atom parameters constrained
 $\Delta\rho_{max} = 1.04$ e Å⁻³
 $\Delta\rho_{min} = -0.70$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Zn1—N1	2.066 (4)	Zn1—Cl1	2.2236 (15)
Zn1—N2	2.053 (4)	Zn1—Cl2	2.1995 (13)
N1—Zn1—Cl1	111.08 (11)	N1—Zn1—Cl2	116.84 (11)
N2—Zn1—Cl1	109.16 (11)	N2—Zn1—Cl2	117.28 (10)
Cl2—Zn1—Cl1	116.72 (5)	N2—Zn1—N1	80.31 (15)

Data collection: SMART (Bruker, 1998); cell refinement: SAINT (Bruker, 1998); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Sheldrick, 2008); program(s) used to refine structure: SHELXTL; 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: HK2529).

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supplementary materials

Acta Cryst. (2008). E64, m1266 [doi:10.1107/S1600536808028894]

Dichlorido(6-methyl-2,2'-bipyridine- κ^2N,N')zinc(II)

R. Ahmadi, K. Kalateh, A. Ebadi, V. Amani and H. R. Khavasi

Comment

Recently, we reported the syntheses and crystal structures of [Cd(5,5'-dmbpy)(μ -Cl)₂]_n, (II), (Ahmadi *et al.*, 2008) and [Hg(4,4'-dmbpy)I₂], (III), (Yousefi *et al.*, 2008) [where 5,5'-dmbpy is 5,5'-dimethyl-2,2'-bipyridine and 4,4'-dmbpy is 4,4'-dimethyl-2,2'-bi-pyridine]. There are several Zn^{II} complexes, with formula, [ZnCl₂(N-N)], such as [ZnCl₂(bipy)], (IV), (Khan & Tuck, 1984), [ZnCl₂(biim)], (V), (Gruia *et al.*, 2007), [ZnCl₂(phbipy)], (VI), (Kozhevnikov *et al.*, 2006), [ZnCl₂(phen)], (VII), (Reimann *et al.*, 1966), [ZnCl₂(dmphen)], (VIII), (Preston & Kennard, 1969), [ZnCl₂(dpdmbip)], (IX), (Liu *et al.*, 2004), [ZnCl₂(dm4bt)], (X), (Khavasi *et al.*, 2008) and [Zn(5,5'-dmbpy)Cl₂], (XI), (Khalighi *et al.*, 2008) [where bipy is 2,2'-bipyridine, biim is 2,2'-biimidazole, phbipy is 5-phenyl-2,2'-bipyridine, phen is 1,10-phenanthroline, dmphen is 2,9-dimethyl-1,10-phenanthroline, dpdmbip is 4,4'-diphenyl-6,6'-dimethyl-2,2'-bipyrimidine and dm4bt is 2,2'-dimethyl-4,4'-bithiazole] have been synthesized and characterized by single-crystal X-ray diffraction methods.

There are several Zn^{II} complexes, with formula, [ZnCl₂L₂], such as [ZnCl₂(py)₂], (XII), (Steffen & Palenik, 1976), [ZnCl₂(4-cypy)₂], (XIII), (Steffen & Palenik, 1977), [ZnCl₂(2-ampy)₂], (XIV), (Qin *et al.*, 1999) and [ZnCl₂(im)₂], (XV), (Lundberg, 1966) [where py is pyridine, 4-cypy is 4-cyanopyridine, 2-ampy is 2-aminopyridine and im is imidazole] have been synthesized and characterized by single-crystal X-ray diffraction methods. We report herein the synthesis and crystal structure of the title compound, (I).

In the title compound, (I), (Fig. 1), the Zn^{II} atom is four-coordinated in a distorted tetrahedral configuration by two N atoms from 6-methyl-2,2'-bi-pyridine and two Cl atoms. The Zn-Cl and Zn-N bond lengths and angles (Table 1) are within normal ranges, as in (IV), (VII), (X) and (XI).

In the crystal structure, the π — π contacts (Fig. 2) between the rings A (Zn1/N1/N2/C5/C6) and C (N2/C6-C10), and also between the pyridine rings B (N1/C1-C5) and C, Cg1...Cg3ⁱ and Cg2...Cg3ⁱⁱ [symmetry codes: (i) -x, -y, -z; (ii) 1 - x, -y, -z, where Cg1, Cg2 and Cg3 are the centroids of the rings A (Zn1/N1/N2/C5/C6), B (N1/C1-C5) and C (N2/C6-C10), respectively] may stabilize the structure, with centroid-centroid distances of 3.685 (3) Å and 3.757 (3) Å, respectively.

Experimental

For the preparation of the title compound, (I), a solution of 6-methyl-2,2'-bipyridine (0.15 g, 0.88 mmol) in methanol (10 ml) was added to a solution of ZnCl₂ (0.12 g, 0.88 mmol) in acetonitrile (30 ml) and the resulting colorless solution was stirred for 20 min at at 313 K, and then it was left to evaporate slowly at room temperature. After one week, colorless block crystals of the title compound were isolated (yield; 0.19 g, 70.4%).

Refinement

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

Figures

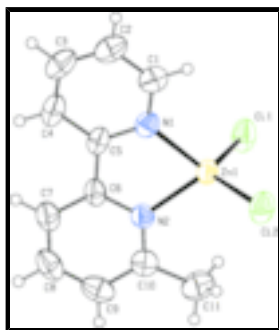


Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 40% probability level.

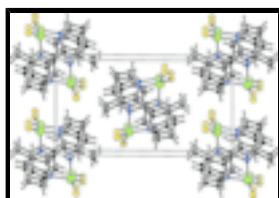


Fig. 2. A packing diagram of the title compound.

Dichlorido(6-methyl-2,2'-bipyridine- $\kappa^2\text{N},\text{N}'$)zinc(II)

Crystal data

$[\text{ZnCl}_2(\text{C}_{11}\text{H}_{10}\text{N}_2)]$

$M_r = 306.50$

Monoclinic, $P2_1/n$

Hall symbol: $-P\ 2_1/n$

$a = 7.4674\ (15)\ \text{\AA}$

$b = 9.5105\ (17)\ \text{\AA}$

$c = 17.656\ (4)\ \text{\AA}$

$\beta = 96.551\ (18)^\circ$

$V = 1245.7\ (4)\ \text{\AA}^3$

$Z = 4$

$F_{000} = 616$

$D_x = 1.634\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation

$\lambda = 0.71073\ \text{\AA}$

Cell parameters from 1987 reflections

$\theta = 2.3\text{--}29.2^\circ$

$\mu = 2.37\ \text{mm}^{-1}$

$T = 298\ (2)\ \text{K}$

Block, colorless

$0.30 \times 0.15 \times 0.10\ \text{mm}$

Data collection

Bruker SMART CCD area-detector
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 298(2)\ \text{K}$

3358 independent reflections

2576 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.078$

$\theta_{\text{max}} = 29.2^\circ$

φ and ω scans	$\theta_{\min} = 2.3^\circ$
Absorption correction: multi-scan (SADABS; Sheldrick, 1998)	$h = -10 \rightarrow 10$
$T_{\min} = 0.668$, $T_{\max} = 0.802$	$k = -12 \rightarrow 13$
10401 measured reflections	$l = -24 \rightarrow 24$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.060$	H-atom parameters constrained
$wR(F^2) = 0.130$	$w = 1/[\sigma^2(F_o^2) + (0.0315P)^2 + 1.9318P]$
$S = 1.17$	where $P = (F_o^2 + 2F_c^2)/3$
3358 reflections	$(\Delta/\sigma)_{\max} = 0.004$
145 parameters	$\Delta\rho_{\max} = 1.05 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\min} = -0.70 \text{ e } \text{\AA}^{-3}$
	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 $F^2 > \sigma(F^2)$ 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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Zn1	0.26730 (7)	0.26879 (5)	0.08829 (3)	0.04730 (16)
Cl1	0.53626 (17)	0.30874 (16)	0.15251 (8)	0.0708 (4)
Cl2	0.04386 (18)	0.40228 (15)	0.11668 (9)	0.0701 (4)
N1	0.2881 (5)	0.2367 (4)	-0.0261 (2)	0.0494 (8)
N2	0.2225 (5)	0.0559 (4)	0.0820 (2)	0.0460 (8)
C1	0.3141 (7)	0.3363 (6)	-0.0782 (3)	0.0619 (12)
H1	0.3145	0.4304	-0.0639	0.074*
C2	0.3400 (8)	0.3028 (7)	-0.1517 (3)	0.0741 (16)
H2	0.3573	0.3733	-0.1867	0.089*
C3	0.3401 (8)	0.1653 (7)	-0.1730 (3)	0.0726 (16)
H3	0.3590	0.1414	-0.2226	0.087*
C4	0.3121 (6)	0.0608 (6)	-0.1210 (3)	0.0626 (13)
H4	0.3120	-0.0335	-0.1350	0.075*

supplementary materials

C5	0.2840 (5)	0.1004 (5)	-0.0466 (2)	0.0465 (9)
C6	0.2434 (5)	-0.0003 (5)	0.0127 (3)	0.0469 (9)
C7	0.2248 (7)	-0.1435 (5)	0.0005 (3)	0.0606 (12)
H7	0.2412	-0.1824	-0.0465	0.073*
C8	0.1819 (7)	-0.2268 (6)	0.0589 (4)	0.0698 (15)
H8	0.1668	-0.3230	0.0512	0.084*
C9	0.1608 (7)	-0.1700 (6)	0.1293 (4)	0.0679 (14)
H9	0.1323	-0.2268	0.1692	0.082*
C10	0.1834 (6)	-0.0254 (5)	0.1392 (3)	0.0566 (11)
C11	0.1652 (11)	0.0450 (7)	0.2132 (3)	0.091 (2)
H11A	0.0699	0.1132	0.2063	0.109*
H11B	0.2763	0.0912	0.2311	0.109*
H11C	0.1376	-0.0239	0.2498	0.109*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0498 (3)	0.0446 (3)	0.0483 (3)	-0.0009 (2)	0.0092 (2)	-0.0117 (2)
Cl1	0.0512 (6)	0.0826 (9)	0.0770 (9)	0.0013 (6)	0.0008 (6)	-0.0358 (7)
Cl2	0.0599 (7)	0.0712 (8)	0.0801 (9)	0.0137 (6)	0.0111 (6)	-0.0207 (7)
N1	0.0449 (18)	0.056 (2)	0.0475 (19)	0.0037 (16)	0.0055 (15)	-0.0037 (17)
N2	0.0411 (18)	0.0465 (18)	0.050 (2)	-0.0016 (14)	0.0053 (15)	-0.0024 (15)
C1	0.060 (3)	0.068 (3)	0.059 (3)	0.005 (2)	0.012 (2)	0.007 (2)
C2	0.078 (4)	0.096 (5)	0.051 (3)	0.004 (3)	0.015 (3)	0.010 (3)
C3	0.068 (3)	0.107 (5)	0.044 (3)	0.010 (3)	0.011 (2)	-0.004 (3)
C4	0.052 (3)	0.077 (3)	0.056 (3)	0.014 (2)	-0.001 (2)	-0.023 (3)
C5	0.0370 (19)	0.058 (2)	0.043 (2)	0.0091 (18)	-0.0018 (16)	-0.0112 (18)
C6	0.0346 (19)	0.048 (2)	0.056 (2)	0.0026 (17)	-0.0032 (17)	-0.0144 (19)
C7	0.057 (3)	0.049 (3)	0.074 (3)	0.001 (2)	0.004 (2)	-0.014 (2)
C8	0.058 (3)	0.043 (2)	0.106 (4)	0.000 (2)	0.001 (3)	-0.009 (3)
C9	0.057 (3)	0.058 (3)	0.088 (4)	-0.003 (2)	0.003 (3)	0.022 (3)
C10	0.050 (2)	0.060 (3)	0.059 (3)	0.002 (2)	0.003 (2)	0.002 (2)
C11	0.129 (6)	0.093 (5)	0.053 (3)	-0.010 (4)	0.025 (4)	0.013 (3)

Geometric parameters (\AA , $^\circ$)

Zn1—N1	2.066 (4)	C5—C6	1.475 (7)
Zn1—N2	2.053 (4)	C6—N2	1.360 (5)
Zn1—Cl1	2.2236 (15)	C6—C7	1.384 (6)
Zn1—Cl2	2.1995 (13)	C7—C8	1.367 (8)
C1—N1	1.350 (6)	C7—H7	0.9300
C1—C2	1.371 (7)	C8—C9	1.381 (8)
C1—H1	0.9300	C8—H8	0.9300
C2—C3	1.361 (9)	C9—C10	1.394 (7)
C2—H2	0.9300	C9—H9	0.9300
C3—C4	1.385 (8)	C10—N2	1.329 (6)
C3—H3	0.9300	C10—C11	1.488 (8)
C4—C5	1.406 (6)	C11—H11A	0.9600
C4—H4	0.9300	C11—H11B	0.9600

C5—N1	1.345 (6)	C11—H11C	0.9600
N1—Zn1—C11	111.08 (11)	N1—C5—C4	120.5 (5)
N2—Zn1—C11	109.16 (11)	N1—C5—C6	115.8 (4)
Cl2—Zn1—C11	116.72 (5)	C4—C5—C6	123.7 (4)
N1—Zn1—Cl2	116.84 (11)	N2—C6—C7	120.5 (5)
N2—Zn1—Cl2	117.28 (10)	N2—C6—C5	115.9 (4)
N2—Zn1—N1	80.31 (15)	C7—C6—C5	123.6 (4)
C1—N1—Zn1	126.6 (3)	C8—C7—C6	118.7 (5)
C5—N1—Zn1	113.8 (3)	C8—C7—H7	120.6
C5—N1—C1	119.6 (4)	C6—C7—H7	120.6
C6—N2—Zn1	113.6 (3)	C7—C8—C9	120.9 (5)
C10—N2—Zn1	125.5 (3)	C7—C8—H8	119.5
C10—N2—C6	120.8 (4)	C9—C8—H8	119.5
N1—C1—C2	121.9 (5)	C8—C9—C10	118.2 (5)
N1—C1—H1	119.0	C8—C9—H9	120.9
C2—C1—H1	119.0	C10—C9—H9	120.9
C3—C2—C1	119.3 (5)	N2—C10—C9	120.9 (5)
C3—C2—H2	120.3	N2—C10—C11	117.1 (5)
C1—C2—H2	120.3	C9—C10—C11	122.1 (5)
C2—C3—C4	120.1 (5)	C10—C11—H11A	109.5
C2—C3—H3	120.0	C10—C11—H11B	109.5
C4—C3—H3	120.0	H11A—C11—H11B	109.5
C3—C4—C5	118.5 (5)	C10—C11—H11C	109.5
C3—C4—H4	120.7	H11A—C11—H11C	109.5
C5—C4—H4	120.7	H11B—C11—H11C	109.5
N2—Zn1—N1—C5	-6.9 (3)	C6—C5—N1—Zn1	7.2 (5)
Cl2—Zn1—N1—C5	-122.7 (3)	C6—C5—N1—C1	-176.3 (4)
Cl1—Zn1—N1—C5	100.0 (3)	N1—C5—C6—N2	-2.7 (5)
N2—Zn1—N1—C1	176.9 (4)	C4—C5—C6—N2	179.1 (4)
Cl2—Zn1—N1—C1	61.1 (4)	N1—C5—C6—C7	176.6 (4)
Cl1—Zn1—N1—C1	-76.2 (4)	C4—C5—C6—C7	-1.6 (7)
Cl1—Zn1—N2—C10	73.8 (4)	C5—C6—N2—Zn1	-3.3 (4)
Cl2—Zn1—N2—C10	-61.8 (4)	C5—C6—N2—C10	179.1 (4)
N1—Zn1—N2—C10	-177.1 (4)	C7—C6—N2—Zn1	177.4 (3)
Cl1—Zn1—N2—C6	-103.7 (3)	C7—C6—N2—C10	-0.2 (6)
Cl2—Zn1—N2—C6	120.7 (3)	N2—C6—C7—C8	1.2 (7)
N1—Zn1—N2—C6	5.4 (3)	C5—C6—C7—C8	-178.1 (4)
C2—C1—N1—C5	-1.2 (7)	C6—C7—C8—C9	-1.2 (8)
C2—C1—N1—Zn1	174.8 (4)	C7—C8—C9—C10	0.3 (8)
N1—C1—C2—C3	-0.2 (9)	C8—C9—C10—N2	0.7 (8)
C1—C2—C3—C4	0.8 (9)	C8—C9—C10—C11	-179.4 (6)
C2—C3—C4—C5	0.0 (8)	C9—C10—N2—Zn1	-178.0 (4)
C3—C4—C5—N1	-1.4 (7)	C9—C10—N2—C6	-0.7 (7)
C3—C4—C5—C6	176.7 (4)	C11—C10—N2—Zn1	2.0 (6)
C4—C5—N1—Zn1	-174.5 (3)	C11—C10—N2—C6	179.3 (5)
C4—C5—N1—C1	2.0 (6)		

Fig. 1

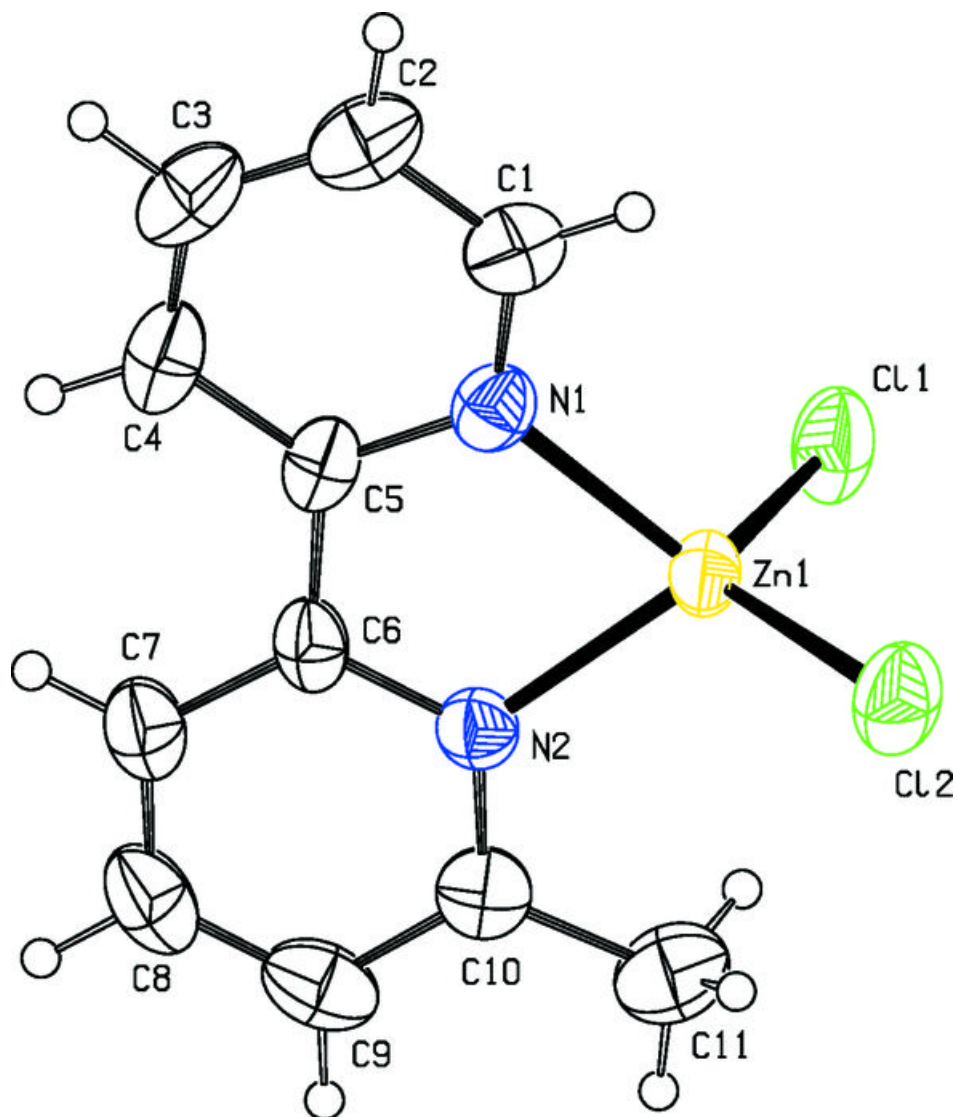


Fig. 2

