

Dichlorido(5,5'-dimethyl-2,2'-bipyridine- κ^2N,N')zinc(II)

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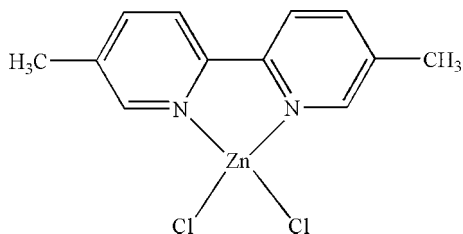
Received 22 August 2008; accepted 22 August 2008

Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(C-C) = 0.013$ Å; R factor = 0.066; wR factor = 0.150; data-to-parameter ratio = 23.3.

The asymmetric unit of the title compound, $[ZnCl_2 \cdot (C_{12}H_{12}N_2)]$, contains two independent molecules. The Zn^{II} atoms are four-coordinated in distorted tetrahedral configurations by two N atoms from 5,5'-dimethyl-2,2'-bipyridine and two terminal Cl atoms. In the crystal structure, intermolecular $C-H \cdots Cl$ hydrogen bonds link the molecules. There are $C-H \cdots \pi$ contacts between the methyl groups and the pyridine and five-membered rings containing Zn^{II} atoms; $\pi-\pi$ contacts also exist between the pyridine rings [centroid-centroid distances = 3.665 (5) and 3.674 (5) Å].

Related literature

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



Experimental

Crystal data

$[ZnCl_2(C_{12}H_{12}N_2)]$

$M_r = 320.53$

Orthorhombic, $Pna2_1$

$a = 16.267$ (2) Å

$b = 11.1704$ (16) Å

$c = 14.9328$ (14) Å

$V = 2713.4$ (6) Å³

$Z = 8$

Mo $K\alpha$ radiation

$\mu = 2.18$ mm⁻¹

$T = 298$ (2) K

$0.28 \times 0.20 \times 0.07$ mm

Data collection

Bruker SMART CCD area-detector diffractometer

Absorption correction: multi-scan (*SADABS*; Sheldrick, 1998)

$T_{\min} = 0.612$, $T_{\max} = 0.860$

14309 measured reflections

7167 independent reflections

4463 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.066$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.066$

$wR(F^2) = 0.150$

$S = 1.07$

7167 reflections

307 parameters

1 restraint

H-atom parameters constrained

$\Delta\rho_{\text{max}} = 0.29$ e Å⁻³

$\Delta\rho_{\text{min}} = -0.30$ e Å⁻³

Absolute structure: Flack (1983),

3320 Friedel pairs

Flack parameter: 0.07 (3)

Table 1

Selected geometric parameters (Å, °).

Zn1—Cl1	2.206 (2)	Zn1—N1	2.058 (6)
Zn1—Cl2	2.215 (2)	Zn1—N2	2.057 (6)
Zn2—Cl3	2.211 (2)	Zn2—N3	2.063 (6)
Zn2—Cl4	2.207 (3)	Zn2—N4	2.066 (6)
N1—Zn1—N2	80.5 (2)	N3—Zn2—N4	79.7 (3)
N1—Zn1—Cl1	112.2 (2)	N3—Zn2—Cl3	112.09 (18)
N1—Zn1—Cl2	117.23 (18)	N3—Zn2—Cl4	114.47 (17)
N2—Zn1—Cl1	115.64 (18)	N4—Zn2—Cl4	112.8 (2)
N2—Zn1—Cl2	111.4 (2)	N4—Zn2—Cl3	115.01 (18)
Cl1—Zn1—Cl2	115.28 (10)	Cl4—Zn2—Cl3	117.19 (9)

Table 2

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
C1—H1 \cdots Cl3 ⁱ	0.93	2.82	3.516 (8)	132
C16—H16 \cdots Cl3 ⁱⁱ	0.93	2.83	3.638 (10)	146
C3—H3A \cdots Cg5	0.96	3.10	3.719 (6)	124
C11—H11A \cdots Cg2 ⁱⁱⁱ	0.96	2.83	3.688 (5)	150
C15—H15C \cdots Cg1 ^{iv}	0.96	2.84	3.704 (6)	150
C23—H23C \cdots Cg4	0.96	3.11	3.690 (6)	120

Symmetry codes: (i) $x + \frac{1}{2}, -y - \frac{3}{2}, z$; (ii) $x + \frac{1}{2}, -y - \frac{5}{2}, z$; (iii) $x, y + 1, z$; (iv) $x, y - 1, z$. Cg1, Cg2, Cg4 and Cg5 are the centroids of atoms Zn1/N1/C6/C7/N2, N1/C1/C2/C4—C6, Zn2/N3/C18/C19/N4 and N3/C13/C14/C16—C18, respectively.

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).

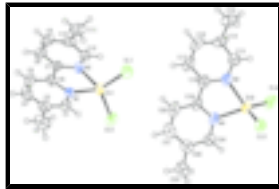
We are grateful to the Islamic Azad University, Shahr-e-Rey Branch, for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2517).

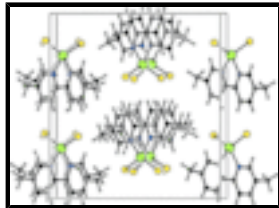
References

- Bruker (1998). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Flack, H. D. (1983). *Acta Cryst.* **A39**, 876–881.

- Gruia, L. M., Rochon, F. D. & Beauchamp, A. L. (2007). *Inorg. Chim. Acta*, **360**, 1825–1840.
- Khan, M. A. & Tuck, D. G. (1984). *Acta Cryst. C* **40**, 60–62.
- Khavasi, H. R., Abedi, A., Amani, V., Notash, B. & Safari, N. (2008). *Polyhedron*, **27**, 1848–1854.
- Kozhevnikov, D. N., Shabunina, O. V., Kopchuk, D. S., Slepukhin, P. A. & Kozhevnikov, V. N. (2006). *Tetrahedron Lett.* **47**, 7025–7029.
- Liu, Q. D., Wang, R. & Wang, S. (2004). *Dalton Trans.* pp. 2073–2079.
- Lundberg, B. K. S. (1966). *Acta Cryst.* **21**, 901–909.
- Preston, H. S. & Kennard, C. H. L. (1969). *J. Chem. Soc. A*, pp. 1965–1968.
- Qin, J., Su, N., Dai, C., Yang, C., Liu, D., Day, M. W., Wu, B. & Chen, C. (1999). *Polyhedron*, **18**, 3461–3464.
- Reimann, C. W., Block, S. & Perloff, A. (1966). *Inorg. Chem.* **5**, 1185–1189.
- Sheldrick, G. M. (1998). *SADABS*. Bruker AXS, Madison, Wisconsin, USA.
- Sheldrick, G. M. (2008). *Acta Cryst. A* **64**, 112–122.
- Steffen, W. L. & Palenik, G. J. (1976). *Acta Cryst. B* **32**, 298–300.
- Steffen, W. L. & Palenik, G. J. (1977). *Inorg. Chem.* **16**, 1119–1127.



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