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[2,6-Bis(1*H*-benzimidazol-2-yl)pyridine]dichlorozinc(II) *N*,*N*-dimethylformamide solvate

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Key indicators

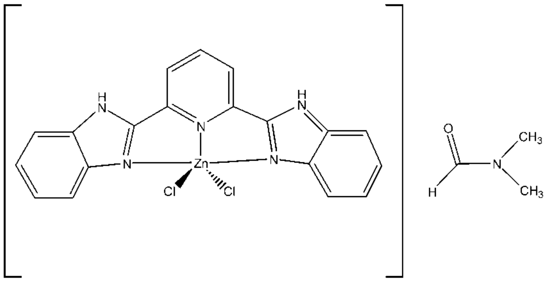
Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.007 Å
R factor = 0.050
wR factor = 0.126
Data-to-parameter ratio = 11.5

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

In the title compound, $[ZnCl_2(C_{19}H_{13}N_5)]\cdot C_3H_7NO$, the Zn^{II} cation shows distorted trigonal–bipyramidal coordination by three N atoms and two Cl atoms, the latter occupying equatorial sites. N—H···O and N—H···Cl hydrogen bonds help to stabilize the crystal packing.

Comment

Imidazole is a ligand that plays an important role in biological systems, since the imidazole moiety of the histidine residues in a large number of metalloproteins constitutes all or some of the binding sites of various transition metal ions (Colacio *et al.*, 2000). Imidazole can force the resultant metal complexes into special geometries (Balamurugan *et al.*, 2001) and the change in molecular structure may influence molecular properties, such as thermal stability (Yu *et al.*, 2003) and photoluminescence (Ho *et al.*, 1999). Therefore, we have prepared the title compound, (I), to evaluate the role of the N coordination in this ligand to Zn.



(I)

Fig. 1 and Table 1 show that the geometry of (I) about the Zn^{II} ion is distorted trigonal–bipyramidal; the N1—Zn—N4 bond angle [144.38 (14)°] is much larger than the N1—Zn—N3 [72.94 (13)°] and N3—Zn—N4 [73.57 (14)°] angles. The entire 2,6-bis(benzimidazol-2-yl)pyridine ligand is approximately planar; the dihedral angles between the benzimidazole moieties and the pyridine ring are 4.3 (2) and 4.8 (3)°.

The crystal structure of (I) is stabilized by hydrogen bonds involving the imidazole N—H groups and a possible C—H···O interaction (Table 2). The first type of hydrogen bond, N—H···Cl, connects two molecules of (I) to construct a stacking structure, with interplanar distances in the range 3.4–3.6 Å, indicating a π–π stacking interaction between adjacent molecules (Ho *et al.*, 1998). The second type of hydrogen bond, N—H···O, exists between the imidazole N atoms of the metal complex and the O atom of the solvent (*N*,*N*-dimethylformamide, DMF). Fig. 2 shows a packing diagram for (I).

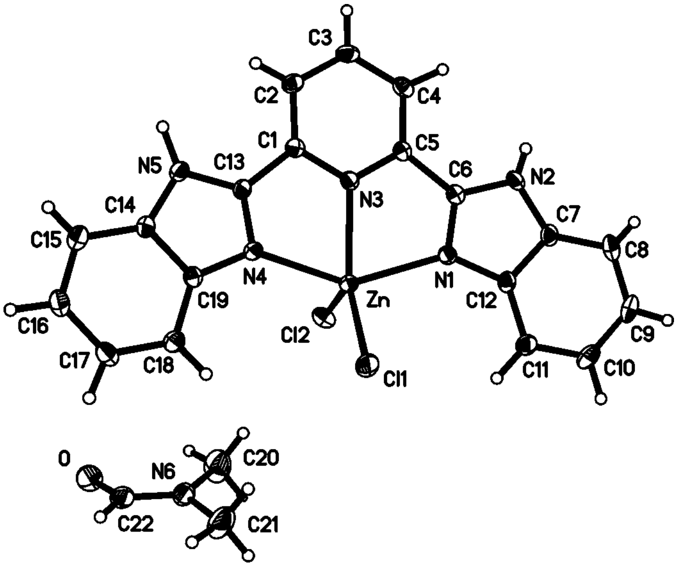


Figure 1
A view of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii.

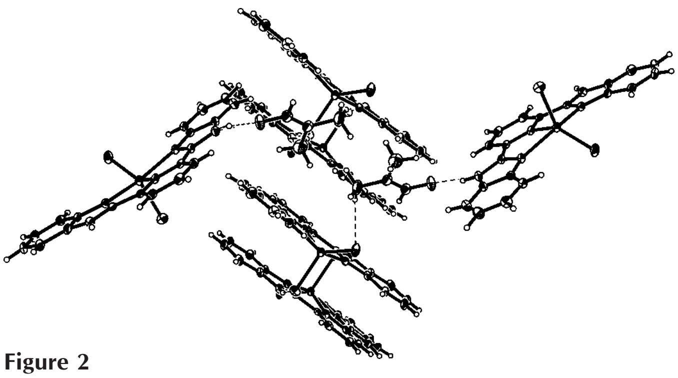


Figure 2
A fragment of the molecular packing of (I), showing how hydrogen bonds (dashed lines) and π–π stacking cooperate to generate an extended structure.

Experimental

Light-brown crystals of (I) were obtained from the diffusion of a zinc chloride solution in *N*,*N*-dimethylformamide into an ethanolic solution of 2,6-bis(benzimidazol-2-yl)pyridine, prepared by heating a mixture of 1,2-phenylenediamine and pyridine-2,6-dicarboxylic acid in polyphosphoric acid (Rüttimann *et al.*, 1992).

Crystal data

$[ZnCl_2(C_{19}H_{13}N_5)]\cdot C_3H_7NO$
$M_r = 520.71$
Monoclinic, $P2_1/n$
$a = 14.594$ (3) Å
$b = 7.889$ (2) Å
$c = 19.811$ (4) Å
$\beta = 102.640$ (8)°
$V = 2225.6$ (9) Å^3
$Z = 4$
$D_x = 1.554$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 28 reflections
$\theta = 5.0$–12.5°
$\mu = 1.37$ mm^{-1}
$T = 295$ (2) K
Rod, light brown
0.80 × 0.20 × 0.20 mm

Data collection

Bruker *P*4 diffractometer
ω scans
Absorption correction: multi-scan (*XEMP* in *XSCANS*; Siemens, 1996)
$T_{min} = 0.723$, $T_{max} = 0.760$
5087 measured reflections
3910 independent reflections
2705 reflections with $I > 2\sigma(I)$
$R_{int} = 0.039$
$\theta_{max} = 25.0°$
$h = -1 \rightarrow 17$
$k = -1 \rightarrow 9$
$l = -23 \rightarrow 23$
3 standard reflections every 97 reflections intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.050$
$wR(F^2) = 0.126$
$S = 1.05$
3910 reflections
341 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0475P)^2 + 3.1157P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.51$ e Å^{-3}
$\Delta\rho_{min} = -0.73$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn—N1	2.179 (4)	Zn—Cl1	2.2571 (13)
Zn—N4	2.187 (4)	Zn—Cl2	2.2933 (16)
Zn—N2	2.201 (4)		
N1—Zn—N4	73.57 (14)	N2—Zn—Cl1	97.85 (10)
N1—Zn—N2	72.94 (13)	N1—Zn—Cl2	106.19 (11)
N4—Zn—N2	144.38 (14)	N4—Zn—Cl2	99.29 (11)
N1—Zn—Cl1	139.64 (11)	N2—Zn—Cl2	101.33 (11)
N4—Zn—Cl1	99.76 (11)	Cl1—Zn—Cl2	114.16 (6)

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3N···Cl2^{i}	0.77 (4)	2.41 (4)	3.142 (5)	163 (5)
N5—H5N···O^{ii}	0.98 (6)	1.74 (6)	2.706 (6)	167 (5)
C20—H20*A*···O	0.96	2.37	2.783 (9)	105

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

All H atoms were initially located in a difference Fourier map. The methyl H atoms were then constrained to an ideal geometry, with C—H distances of 0.98 Å and $U_{iso}(H) = 1.5U_{eq}(C)$, but each group was allowed to rotate freely about its C—C bond. The H atom on DMF atom C22 was also placed in an idealized position and treated as riding, with C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$. The positions of the amine H atoms were refined freely, along with their isotropic displacement parameters. The positions of all other H atoms were refined freely [C—H = 0.78 (4)–0.98 (4) Å] with the constraint $U_{iso}(H) = 1.2U_{eq}(C)$ applied.

Data collection: *XSCANS* (Siemens, 1996); cell refinement: *XSCANS*; data reduction: *SHELXTL* (Bruker, 1997); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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References

Balamurugan, R., Palaniandavar, M. & Gopalan, R. S. (2001). *Inorg. Chem.* **40**, 2246–2255.

Bruker (1997). *SHELXTL*. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.

Colacio, E., Ghazi, M., Kivekäs, R., Klinga, M., Lloret, F. & Moreno, J. M. (2000). *Inorg. Chem.* **39**, 2770–2776.

Ho, K.-Y., Yu, W.-Y., Cheung, K.-K. & Che, C.-M. (1998). *Chem. Commun.* pp. 2101–2102.

Ho, K.-Y., Yu, W.-Y., Cheung, K.-K. & Che, C.-M. (1999). *J. Chem. Soc. Dalton Trans.* pp. 1581–1586.

Rüttimann, S., Moreau, C. M., Williams, A. F., Bernardinelli, G. & Addison, A. W. (1992). *Polyhedron*, **11**, 635–646.

Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.

Siemens (1996). *XSCANS*. Version 2.21. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.

Yu, G., Yin, S., Liu, Y., Shuai, Z. & Zhu, D. (2003). *J. Am. Chem. Soc.* **125**, 14816–14842.