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# {Bis[2-(3,5-dimethylpyrazol-1-yl)ethyl]-amine-$\kappa^2N,N'$}dichloridozinc(II) methanol solvate

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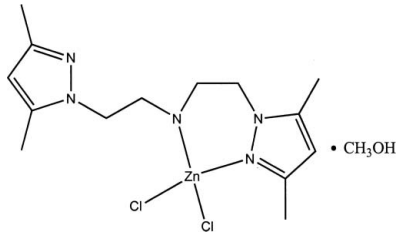
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.028; $wR$ factor = 0.082; data-to-parameter ratio = 16.7.

In the title compound, $[ZnCl_2(C_{14}H_{23}N_5)]\cdot CH_3OH$, the Zn atom is coordinated by two N atoms and two Cl atoms in an approximately tetrahedral arrangement. The dihedral angle between the N—Zn—N and Cl—Zn—Cl planes is 89.69 (5)°. The methanol solvent molecule takes part in the formation of the hydrogen-bond system.

## Related literature

For the synthesis of bis[2–(3,5–dimethylpyrazol–1–yl)-ethyl]amine see: Sorrell & Malachowski, (1983). For related structures see: van Berkel *et al.* (1994); Ajellal *et al.* (2006); Pañella *et al.* (2006); Mendoza *et al.* (2006); Lian *et al.* (2007).




## Experimental

*Crystal data*

$[ZnCl_2(C_{14}H_{23}N_5)]\cdot CH_4O$
$M_r$ = 429.71
Triclinic, $P\overline{1}$
$a$ = 9.3550 (6) Å
$b$ = 9.3562 (4) Å
$c$ = 13.3177 (7) Å
$\alpha$ = 83.362 (4)°
$\beta$ = 72.448 (5)°
$\gamma$ = 65.563 (4)°
$V$ = 1011.77 (10) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 1.49 mm$^{-1}$
$T$ = 293 (2) K
0.45 × 0.40 × 0.35 mm

*Data collection*

Enraf–Nonius CAD-4 diffractometer
Absorption correction: $\psi$ scan (*ABSCALC*; McArdle & Daly, 1999)
$T_{min}$ = 0.517, $T_{max}$ = 0.594
4135 measured reflections
3753 independent reflections
3209 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.008
3 standard reflections
frequency: 60 min
intensity decay: 0.2%

*Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.082
$S$ = 1.04
3753 reflections
225 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.38 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.33 e Å$^{-3}$

**Table 1**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O—H1$O$···N5$^{i}$ | 0.78 (4) | 2.04 (4) | 2.787 (3) | 159 (3) |
| N3—H3$N$···O$^{ii}$ | 0.83 (3) | 2.09 (2) | 2.889 (3) | 163 (2) |

Symmetry codes: (i) $x, y-1, z$; (ii) $-x+1, -y+1, -z+1$.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD* (McArdle, 1999); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEX* (McArdle, 1995); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RK2043).

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# supplementary materials

*Acta Cryst.* (2007). E**63**, m2679 [ **doi:10.1107/S1600536807048179** ]

# {Bis[2-(3,5-dimethylpyrazol-1-yl)ethyl]amine-$\kappa^2N,N'$}dichloridozinc(II) methanol solvate

**R. E. Lee, Y. D. Park and J. H. Jeong**

## Comment

The ligand, bis[2–(3,5–dimethylpyrazol–1–yl)ethyl]amine, synthesized (Sorrell & Malachowski, 1983) and its complex of cobalt, copper or zinc was reported (van Berkel *et al.*, 1994). Nickel complex of the ligand was reported as an efficient catalyst for dimerization of enthylene to 1–butene (Ajellal *et al.*, 2006). Aluminium and zinc alkyl complexes bearing the ligand were synthesized and show the activities on polymerization of methyl methacrylate and lactide (Lian *et al.*, 2007). Also palladium complexes containing the ligand were reported (Pañella *et al.*, 2006; Mendoza *et al.*, 2006). In the title complex, the ligand acts as bidentate though it is a potential tridentate. However, the ligand was $\kappa^3$ bonding mode at zinc from reaction $ZnCl_2$–to–ligand ratio of 2:1 (van Berkel *et al.*, 1994). Herein, we report the crystal structure of Zn(II) complex containing bis[2–(3,5–dimethylpyrazol–1–yl)ethyl]amine as bidentate. The geometry around Zn(II) is an approximately tetrahedron. The dihedral angle between N—Zn—N and Cl—Zn—Cl planes is 89.69 (5)°.

The methanol solvate molecule takes part in the formation of H–bonds system: the hydroxo–group of one is a donor and acceptor in this system - see table of hydrogen–bond geometry.

## Experimental

To bis{2–(3,5–dimethyl–1–pyrazolyl)ethyl}amine (1.67 g, 6.4 mmol) was added dropwise a solution of $ZnCl_2$ (0.87 g, 6.4 mmol) in methanol (20 ml). The mixture was stirred for 1 day at room temperature. The solvent was removed and the residue was washed with ether to give white solids. Colorless crystals was obtained from methanol solution. Yield; 1.63 g (64%). Anal. Calculated for $C_{15}H_{27}Cl_2N_5OZn$: C, 41.93; H, 6.33; N, 16.30. Found: C, 42.09; H, 6.24; N, 16.46%. $^1$H NMR (DMSO–$d_6$); δ 5.97 (s, H-*Pz*), 4.20 (t, $CH_2$-*Pz*, J=6.0, 5.7 Hz), 3.07 (t, $NCH_2$–, J=5.7, 5.4 Hz), 2.25 (s, $CH_3$-*Pz*), 2.18 (s, $CH_3$-*Pz*), where *Pz* - pyrazolyl.

## Refinement

All H atoms, except H atoms of hydroxy and amine groups, which were refined isotropically, were positioned geometrically and refined using a riding model, with C—H = 0.97Å and $U_{iso}$(H) = 1.2$U_{eq}$(C) for $CH_2$, and C—H = 0.96Å and $U_{iso}$(H) = 1.5$U_{eq}$(C) for $CH_3$ H atoms.

## Figures

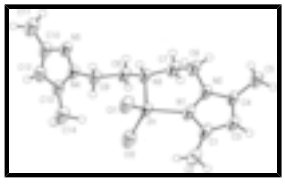


Fig. 1. A view of the dichlorido{bis[2–(3,5–dimethylpyrazol–1–yl)ethyl]amine–$\kappa^2N,N'$}zinc with the numbering scheme. Displacement ellipsoids are drawn at the 40% probability level. H atoms are drawn as a spheres with arbitrary radius.

## {Bis[2-(3,5-dimethylpyrazol-1-yl)ethyl]amine- $\kappa^2N,N'$}dichloridozinc(II) methanol solvate

*Crystal data*

| | |
|---|---|
| $[ZnCl_2(C_{14}H_{23}N_5)]\cdot CH_4O$ | $Z = 2$ |
| $M_r = 429.71$ | $F_{000} = 448$ |
| Triclinic, $P\overline{1}$ | $D_x = 1.411$ Mg m$^{-3}$ |
| Hall symbol: -P 1 | Mo $K\alpha$ radiation<br>$\lambda = 0.71069$ Å |
| $a = 9.3550$ (6) Å | Cell parameters from 25 reflections |
| $b = 9.3562$ (4) Å | $\theta = 10.6$–$13.2°$ |
| $c = 13.3177$ (7) Å | $\mu = 1.49$ mm$^{-1}$ |
| $\alpha = 83.362$ (4)° | $T = 293$ (2) K |
| $\beta = 72.448$ (5)° | Block, colourless |
| $\gamma = 65.563$ (4)° | 0.45 × 0.40 × 0.35 mm |
| $V = 1011.77$ (10) Å$^3$ | |

*Data collection*

| | |
|---|---|
| Enraf–Nonius CAD-4 diffractometer | $R_{int} = 0.008$ |
| Radiation source: Fine–focus sealed tube | $\theta_{max} = 25.5°$ |
| Monochromator: Graphite | $\theta_{min} = 1.6°$ |
| $T = 293$(2) K | $h = 0\rightarrow11$ |
| Scintillation counter scans | $k = -10\rightarrow11$ |
| Absorption correction: ψ scan (ABSCALC; McArdle & Daly, 1999) | $l = -15\rightarrow16$ |
| $T_{min} = 0.517$, $T_{max} = 0.594$ | 3 standard reflections |
| 4135 measured reflections | every 60 min |
| 3753 independent reflections | intensity decay: 0.2% |
| 3209 reflections with $I > 2\sigma(I)$ | |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.028$ | H atoms treated by a mixture of independent and constrained refinement |
| $wR(F^2) = 0.082$ | $w = 1/[\sigma^2(F_o^2) + (0.0529P)^2 + 0.1929P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 1.04$ | $(\Delta/\sigma)_{max} < 0.001$ |
| 3753 reflections | $\Delta\rho_{max} = 0.38$ e Å$^{-3}$ |
| 225 parameters | $\Delta\rho_{min} = -0.33$ e Å$^{-3}$ |
| Primary atom site location: structure-invariant direct methods | Extinction correction: none |

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Zn | 0.50037 (3) | 0.75209 (3) | 0.161235 (17) | 0.04246 (10) |
| Cl1 | 0.53380 (8) | 0.54111 (7) | 0.26152 (5) | 0.06128 (16) |
| Cl2 | 0.27310 (8) | 0.86417 (8) | 0.10889 (5) | 0.06388 (17) |
| N1 | 0.7028 (2) | 0.7171 (2) | 0.03740 (13) | 0.0458 (4) |
| C1 | 0.7535 (3) | 0.6476 (2) | −0.05640 (15) | 0.0455 (4) |
| C2 | 0.6472 (3) | 0.5905 (3) | −0.09021 (19) | 0.0612 (6) |
| H2A | 0.6768 | 0.4810 | −0.0745 | 0.092* |
| H2B | 0.6620 | 0.6053 | −0.1646 | 0.092* |
| H2C | 0.5348 | 0.6486 | −0.0532 | 0.092* |
| C3 | 0.9078 (3) | 0.6424 (2) | −0.10956 (16) | 0.0480 (5) |
| H3 | 0.9703 | 0.5994 | −0.1761 | 0.058* |
| C4 | 0.9508 (2) | 0.7128 (2) | −0.04526 (15) | 0.0426 (4) |
| C5 | 1.0994 (3) | 0.7445 (3) | −0.06226 (18) | 0.0572 (5) |
| H5A | 1.0735 | 0.8541 | −0.0760 | 0.086* |
| H5B | 1.1834 | 0.6837 | −0.1213 | 0.086* |
| H5C | 1.1372 | 0.7163 | −0.0004 | 0.086* |
| N2 | 0.8257 (2) | 0.7571 (2) | 0.04240 (12) | 0.0435 (4) |
| C6 | 0.8102 (3) | 0.8360 (3) | 0.13570 (17) | 0.0573 (6) |
| H6A | 0.8966 | 0.8739 | 0.1202 | 0.069* |
| H6B | 0.8250 | 0.7606 | 0.1921 | 0.069* |
| C7 | 0.6463 (3) | 0.9729 (3) | 0.17301 (18) | 0.0551 (5) |
| H7A | 0.6579 | 1.0460 | 0.2128 | 0.066* |
| H7B | 0.6121 | 1.0276 | 0.1124 | 0.066* |
| N3 | 0.5195 (2) | 0.9201 (2) | 0.23970 (13) | 0.0419 (4) |
| H3N | 0.549 (3) | 0.874 (3) | 0.2914 (18) | 0.039 (6)* |
| C8 | 0.3639 (3) | 1.0539 (2) | 0.28370 (16) | 0.0469 (4) |
| H8A | 0.3140 | 1.1054 | 0.2280 | 0.056* |
| H8B | 0.3842 | 1.1296 | 0.3151 | 0.056* |
| C9 | 0.2496 (3) | 0.9949 (3) | 0.36641 (17) | 0.0493 (5) |
| H9A | 0.2168 | 0.9319 | 0.3324 | 0.059* |
| H9B | 0.3074 | 0.9282 | 0.4151 | 0.059* |
| N4 | 0.1048 (2) | 1.1224 (2) | 0.42467 (13) | 0.0476 (4) |
| N5 | 0.1135 (2) | 1.1900 (2) | 0.50638 (14) | 0.0518 (4) |
| C10 | −0.0371 (3) | 1.2995 (3) | 0.54475 (18) | 0.0545 (5) |
| C11 | −0.0740 (4) | 1.3975 (4) | 0.6380 (2) | 0.0752 (8) |
| H11A | −0.1389 | 1.3647 | 0.6989 | 0.113* |
| H11B | −0.1332 | 1.5059 | 0.6244 | 0.113* |
| H11C | 0.0266 | 1.3848 | 0.6503 | 0.113* |
| C12 | −0.1397 (3) | 1.3013 (3) | 0.4873 (2) | 0.0573 (6) |
| H12 | −0.2497 | 1.3671 | 0.4984 | 0.069* |
| C13 | −0.0471 (3) | 1.1874 (3) | 0.41129 (17) | 0.0500 (5) |
| C14 | −0.0908 (3) | 1.1326 (3) | 0.3282 (2) | 0.0667 (6) |
| H14A | −0.0051 | 1.1154 | 0.2634 | 0.100* |
| H14B | −0.1911 | 1.2109 | 0.3180 | 0.100* |
| H14C | −0.1041 | 1.0363 | 0.3498 | 0.100* |

| | | | | |
|---|---|---|---|---|
| C15 | 0.4334 (4) | 0.2736 (4) | 0.4990 (3) | 0.0890 (9) |
| H151 | 0.3527 | 0.3363 | 0.4636 | 0.134* |
| H152 | 0.5311 | 0.2085 | 0.4486 | 0.134* |
| H153 | 0.4579 | 0.3410 | 0.5342 | 0.134* |
| O | 0.3734 (3) | 0.1799 (3) | 0.57224 (17) | 0.0806 (6) |
| H1O | 0.306 (4) | 0.161 (4) | 0.561 (3) | 0.081 (10)* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Zn | 0.04342 (14) | 0.04865 (15) | 0.03929 (14) | −0.02289 (10) | −0.00885 (10) | −0.00452 (9) |
| Cl1 | 0.0659 (3) | 0.0536 (3) | 0.0568 (3) | −0.0239 (3) | −0.0080 (3) | 0.0041 (2) |
| Cl2 | 0.0606 (3) | 0.0711 (4) | 0.0668 (4) | −0.0204 (3) | −0.0321 (3) | −0.0099 (3) |
| N1 | 0.0505 (9) | 0.0558 (10) | 0.0378 (8) | −0.0310 (8) | −0.0053 (7) | −0.0068 (7) |
| C1 | 0.0583 (12) | 0.0434 (10) | 0.0379 (10) | −0.0248 (9) | −0.0102 (9) | −0.0027 (8) |
| C2 | 0.0751 (16) | 0.0703 (15) | 0.0517 (13) | −0.0436 (13) | −0.0101 (11) | −0.0144 (11) |
| C3 | 0.0528 (11) | 0.0489 (11) | 0.0370 (10) | −0.0184 (9) | −0.0052 (9) | −0.0075 (8) |
| C4 | 0.0410 (10) | 0.0439 (10) | 0.0379 (9) | −0.0133 (8) | −0.0089 (8) | −0.0004 (8) |
| C5 | 0.0402 (11) | 0.0761 (15) | 0.0513 (12) | −0.0205 (10) | −0.0072 (9) | −0.0100 (11) |
| N2 | 0.0427 (9) | 0.0531 (9) | 0.0376 (8) | −0.0223 (7) | −0.0086 (7) | −0.0056 (7) |
| C6 | 0.0487 (12) | 0.0872 (16) | 0.0444 (11) | −0.0358 (11) | −0.0048 (9) | −0.0203 (11) |
| C7 | 0.0607 (13) | 0.0643 (13) | 0.0478 (11) | −0.0389 (11) | 0.0015 (10) | −0.0180 (10) |
| N3 | 0.0440 (9) | 0.0495 (9) | 0.0341 (8) | −0.0211 (7) | −0.0085 (7) | −0.0038 (7) |
| C8 | 0.0506 (11) | 0.0474 (11) | 0.0410 (10) | −0.0201 (9) | −0.0075 (9) | −0.0055 (8) |
| C9 | 0.0449 (11) | 0.0507 (11) | 0.0452 (11) | −0.0157 (9) | −0.0076 (9) | 0.0000 (9) |
| N4 | 0.0407 (9) | 0.0569 (10) | 0.0405 (9) | −0.0157 (8) | −0.0098 (7) | −0.0015 (7) |
| N5 | 0.0438 (9) | 0.0649 (11) | 0.0437 (9) | −0.0197 (8) | −0.0098 (8) | −0.0035 (8) |
| C10 | 0.0470 (11) | 0.0623 (13) | 0.0500 (12) | −0.0243 (10) | −0.0023 (9) | −0.0046 (10) |
| C11 | 0.0654 (16) | 0.0877 (19) | 0.0651 (16) | −0.0284 (14) | −0.0016 (13) | −0.0250 (14) |
| C12 | 0.0377 (10) | 0.0615 (13) | 0.0662 (14) | −0.0155 (10) | −0.0108 (10) | −0.0020 (11) |
| C13 | 0.0426 (11) | 0.0608 (13) | 0.0502 (12) | −0.0249 (10) | −0.0145 (9) | 0.0077 (10) |
| C14 | 0.0623 (15) | 0.0826 (17) | 0.0657 (15) | −0.0330 (13) | −0.0271 (12) | 0.0016 (13) |
| C15 | 0.091 (2) | 0.102 (2) | 0.098 (2) | −0.0493 (19) | −0.0520 (19) | 0.0208 (19) |
| O | 0.0804 (13) | 0.1126 (17) | 0.0730 (13) | −0.0492 (13) | −0.0461 (11) | 0.0182 (11) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Zn—N1 | 2.0349 (16) | N3—H3N | 0.83 (2) |
| Zn—N3 | 2.0787 (17) | C8—C9 | 1.516 (3) |
| Zn—Cl1 | 2.2158 (6) | C8—H8A | 0.9700 |
| Zn—Cl2 | 2.2330 (6) | C8—H8B | 0.9700 |
| N1—C1 | 1.335 (2) | C9—N4 | 1.450 (3) |
| N1—N2 | 1.369 (2) | C9—H9A | 0.9700 |
| C1—C3 | 1.386 (3) | C9—H9B | 0.9700 |
| C1—C2 | 1.497 (3) | N4—C13 | 1.354 (3) |
| C2—H2A | 0.9600 | N4—N5 | 1.359 (3) |
| C2—H2B | 0.9600 | N5—C10 | 1.337 (3) |
| C2—H2C | 0.9600 | C10—C12 | 1.391 (3) |
| C3—C4 | 1.374 (3) | C10—C11 | 1.498 (3) |

| | | | |
|---|---|---|---|
| C3—H3 | 0.9300 | C11—H11A | 0.9600 |
| C4—N2 | 1.338 (2) | C11—H11B | 0.9600 |
| C4—C5 | 1.485 (3) | C11—H11C | 0.9600 |
| C5—H5A | 0.9600 | C12—C13 | 1.366 (3) |
| C5—H5B | 0.9600 | C12—H12 | 0.9300 |
| C5—H5C | 0.9600 | C13—C14 | 1.494 (3) |
| N2—C6 | 1.458 (3) | C14—H14A | 0.9600 |
| C6—C7 | 1.517 (3) | C14—H14B | 0.9600 |
| C6—H6A | 0.9700 | C14—H14C | 0.9600 |
| C6—H6B | 0.9700 | C15—O | 1.383 (4) |
| C7—N3 | 1.479 (3) | C15—H151 | 0.9600 |
| C7—H7A | 0.9700 | C15—H152 | 0.9600 |
| C7—H7B | 0.9700 | C15—H153 | 0.9600 |
| N3—C8 | 1.476 (3) | O—H1O | 0.78 (3) |
| N1—Zn—N3 | 97.10 (6) | C8—N3—H3N | 105.1 (15) |
| N1—Zn—Cl1 | 111.06 (5) | C7—N3—H3N | 108.8 (15) |
| N3—Zn—Cl1 | 107.94 (5) | Zn—N3—H3N | 104.9 (15) |
| N1—Zn—Cl2 | 110.94 (5) | N3—C8—C9 | 109.32 (17) |
| N3—Zn—Cl2 | 108.51 (5) | N3—C8—H8A | 109.8 |
| Cl1—Zn—Cl2 | 118.95 (3) | C9—C8—H8A | 109.8 |
| C1—N1—N2 | 105.84 (16) | N3—C8—H8B | 109.8 |
| C1—N1—Zn | 132.04 (15) | C9—C8—H8B | 109.8 |
| N2—N1—Zn | 121.97 (12) | H8A—C8—H8B | 108.3 |
| N1—C1—C3 | 109.52 (18) | N4—C9—C8 | 112.15 (18) |
| N1—C1—C2 | 120.74 (19) | N4—C9—H9A | 109.2 |
| C3—C1—C2 | 129.74 (19) | C8—C9—H9A | 109.2 |
| C1—C2—H2A | 109.5 | N4—C9—H9B | 109.2 |
| C1—C2—H2B | 109.5 | C8—C9—H9B | 109.2 |
| H2A—C2—H2B | 109.5 | H9A—C9—H9B | 107.9 |
| C1—C2—H2C | 109.5 | C13—N4—N5 | 111.80 (17) |
| H2A—C2—H2C | 109.5 | C13—N4—C9 | 129.17 (19) |
| H2B—C2—H2C | 109.5 | N5—N4—C9 | 119.02 (17) |
| C4—C3—C1 | 106.98 (17) | C10—N5—N4 | 105.05 (18) |
| C4—C3—H3 | 126.5 | N5—C10—C12 | 110.4 (2) |
| C1—C3—H3 | 126.5 | N5—C10—C11 | 119.9 (2) |
| N2—C4—C3 | 106.46 (18) | C12—C10—C11 | 129.6 (2) |
| N2—C4—C5 | 122.74 (19) | C10—C11—H11A | 109.5 |
| C3—C4—C5 | 130.78 (19) | C10—C11—H11B | 109.5 |
| C4—C5—H5A | 109.5 | H11A—C11—H11B | 109.5 |
| C4—C5—H5B | 109.5 | C10—C11—H11C | 109.5 |
| H5A—C5—H5B | 109.5 | H11A—C11—H11C | 109.5 |
| C4—C5—H5C | 109.5 | H11B—C11—H11C | 109.5 |
| H5A—C5—H5C | 109.5 | C13—C12—C10 | 106.5 (2) |
| H5B—C5—H5C | 109.5 | C13—C12—H12 | 126.7 |
| C4—N2—N1 | 111.20 (16) | C10—C12—H12 | 126.7 |
| C4—N2—C6 | 128.46 (17) | N4—C13—C12 | 106.2 (2) |
| N1—N2—C6 | 120.34 (16) | N4—C13—C14 | 122.7 (2) |
| N2—C6—C7 | 113.19 (19) | C12—C13—C14 | 131.1 (2) |
| N2—C6—H6A | 108.9 | C13—C14—H14A | 109.5 |

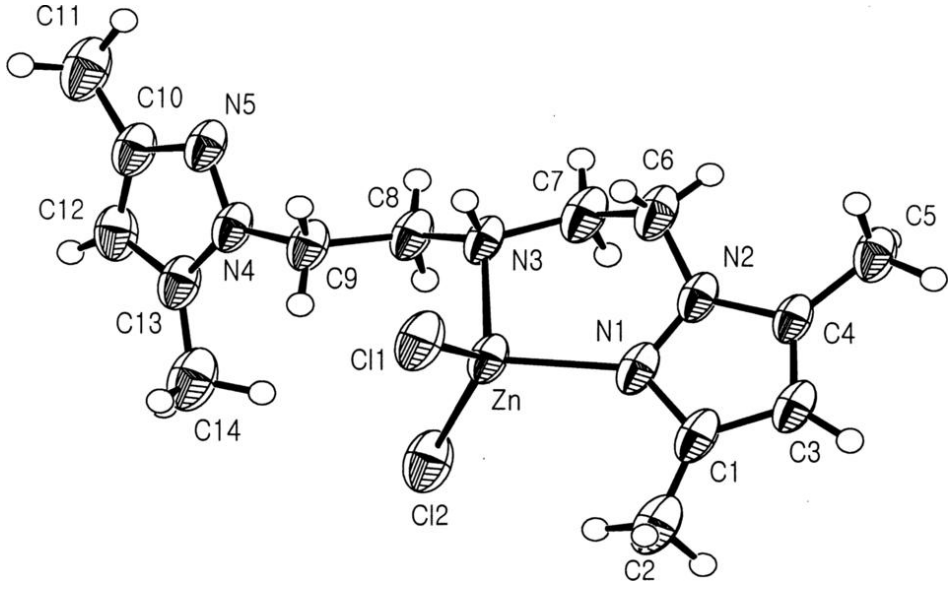
| | | | |
|---|---|---|---|
| C7—C6—H6A | 108.9 | C13—C14—H14B | 109.5 |
| N2—C6—H6B | 108.9 | H14A—C14—H14B | 109.5 |
| C7—C6—H6B | 108.9 | C13—C14—H14C | 109.5 |
| H6A—C6—H6B | 107.8 | H14A—C14—H14C | 109.5 |
| N3—C7—C6 | 111.62 (19) | H14B—C14—H14C | 109.5 |
| N3—C7—H7A | 109.3 | O—C15—H151 | 109.5 |
| C6—C7—H7A | 109.3 | O—C15—H152 | 109.5 |
| N3—C7—H7B | 109.3 | H151—C15—H152 | 109.5 |
| C6—C7—H7B | 109.3 | O—C15—H153 | 109.5 |
| H7A—C7—H7B | 108.0 | H151—C15—H153 | 109.5 |
| C8—N3—C7 | 111.73 (17) | H152—C15—H153 | 109.5 |
| C8—N3—Zn | 114.97 (13) | C15—O—H1O | 116 (2) |
| C7—N3—Zn | 110.82 (12) | | |
| N3—Zn—N1—C1 | −164.96 (19) | C6—C7—N3—C8 | 175.01 (17) |
| Cl1—Zn—N1—C1 | 82.7 (2) | C6—C7—N3—Zn | −55.4 (2) |
| Cl2—Zn—N1—C1 | −52.0 (2) | N1—Zn—N3—C8 | 137.79 (14) |
| N3—Zn—N1—N2 | 20.20 (16) | Cl1—Zn—N3—C8 | −107.31 (13) |
| Cl1—Zn—N1—N2 | −92.17 (15) | Cl2—Zn—N3—C8 | 22.86 (15) |
| Cl2—Zn—N1—N2 | 133.17 (14) | N1—Zn—N3—C7 | 9.90 (16) |
| N2—N1—C1—C3 | 0.6 (2) | Cl1—Zn—N3—C7 | 124.80 (15) |
| Zn—N1—C1—C3 | −174.84 (15) | Cl2—Zn—N3—C7 | −105.03 (15) |
| N2—N1—C1—C2 | −178.83 (19) | C7—N3—C8—C9 | −169.66 (18) |
| Zn—N1—C1—C2 | 5.7 (3) | Zn—N3—C8—C9 | 62.9 (2) |
| N1—C1—C3—C4 | −0.5 (2) | N3—C8—C9—N4 | 170.79 (17) |
| C2—C1—C3—C4 | 178.9 (2) | C8—C9—N4—C13 | 98.9 (3) |
| C1—C3—C4—N2 | 0.1 (2) | C8—C9—N4—N5 | −82.3 (2) |
| C1—C3—C4—C5 | −178.0 (2) | C13—N4—N5—C10 | 0.1 (2) |
| C3—C4—N2—N1 | 0.2 (2) | C9—N4—N5—C10 | −178.89 (19) |
| C5—C4—N2—N1 | 178.60 (19) | N4—N5—C10—C12 | −0.3 (3) |
| C3—C4—N2—C6 | 179.6 (2) | N4—N5—C10—C11 | 179.1 (2) |
| C5—C4—N2—C6 | −2.1 (3) | N5—C10—C12—C13 | 0.3 (3) |
| C1—N1—N2—C4 | −0.5 (2) | C11—C10—C12—C13 | −179.0 (3) |
| Zn—N1—N2—C4 | 175.48 (13) | N5—N4—C13—C12 | 0.0 (2) |
| C1—N1—N2—C6 | −179.9 (2) | C9—N4—C13—C12 | 178.9 (2) |
| Zn—N1—N2—C6 | −3.9 (3) | N5—N4—C13—C14 | −178.8 (2) |
| C4—N2—C6—C7 | 133.5 (2) | C9—N4—C13—C14 | 0.1 (4) |
| N1—N2—C6—C7 | −47.2 (3) | C10—C12—C13—N4 | −0.2 (3) |
| N2—C6—C7—N3 | 83.4 (2) | C10—C12—C13—C14 | 178.5 (2) |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O—H1O···N5$^{i}$ | 0.78 (4) | 2.04 (4) | 2.787 (3) | 159 (3) |
| N3—H3N···O$^{ii}$ | 0.83 (3) | 2.09 (2) | 2.889 (3) | 163 (2) |

Symmetry codes: (i) *x*, *y*−1, *z*; (ii) −*x*+1, −*y*+1, −*z*+1.

**Fig. 1**


C11
C10
N5
C12
N4
C13
C14
C9
C8
C7
C6
N3
N2
C5
C4
N1
Cl1
Zn
Cl2
C1
C3
C2