Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# Dichlorido(*N*,*N*-dimethylpropane-1,3-diamine-$\kappa^2N,N'$)zinc(II)

**Juan-Lan Huang and Yun-Long Feng***

Zhejiang Key Laboratory for Reactive Chemistry on Solid Surfaces, Institute of Physical Chemistry, Zhejiang Normal University, Jinhua, Zhejiang 321004, People's Republic of China
Correspondence e-mail: sky37@zjnu.cn

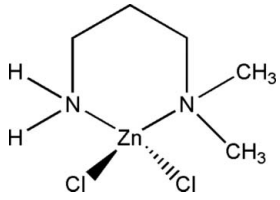
Received 29 March 2007; accepted 3 April 2007

Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.026; $wR$ factor = 0.064; data-to-parameter ratio = 25.4.

The title compound, $[ZnCl_2(C_5N_2H_{14})]$, crystallizes with two discrete mononuclear complex molecules in the the asymmetric unit, with an intermolecular Zn···Zn separation of 5.271 (7) Å. Each $Zn^{II}$ ion is in a distorted tetrahedral coordination geometry formed by two Cl atoms and two N atoms. In the crystal structure, molecules are connected by N—H···Cl hydrogen bonds into tetrameric clusters separated by normal van der Waals distances.

## Related literature

For related literature, see: Johansson & Håkansson (2004).




## Experimental

### Crystal data

$[ZnCl_2(C_5H_{14}N_2)]$
$M_r$ = 238.45
Monoclinic, $P2_1/c$
$a$ = 12.033 (4) Å
$b$ = 11.816 (4) Å
$c$ = 15.113 (4) Å
$\beta$ = 111.817 (3)°
$V$ = 1995.0 (10) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 2.94 mm$^{-1}$
$T$ = 293 (2) K
0.45 × 0.38 × 0.24 mm

### Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.277, $T_{max}$ = 0.494
12998 measured reflections
4701 independent reflections
3625 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.022

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.064
$S$ = 0.99
4701 reflections
185 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.30 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.47 e Å$^{-3}$

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| Zn1—N1 | 2.0176 (16) | Zn2—N3 | 2.0251 (18) |
| Zn1—N2 | 2.0551 (16) | Zn2—N4 | 2.0754 (17) |
| Zn1—Cl2 | 2.2254 (7) | Zn2—Cl3 | 2.2236 (9) |
| Zn1—Cl1 | 2.2419 (7) | Zn2—Cl4 | 2.2319 (7) |
| N1—Zn1—N2 | 99.04 (6) | N3—Zn2—N4 | 96.32 (7) |
| N1—Zn1—Cl2 | 116.63 (5) | N3—Zn2—Cl3 | 107.75 (5) |
| N2—Zn1—Cl2 | 113.75 (5) | N4—Zn2—Cl3 | 110.16 (5) |
| N1—Zn1—Cl1 | 107.11 (6) | N3—Zn2—Cl4 | 116.08 (5) |
| N2—Zn1—Cl1 | 106.50 (5) | N4—Zn2—Cl4 | 107.89 (5) |
| Cl2—Zn1—Cl1 | 112.55 (3) | Cl3—Zn2—Cl4 | 116.68 (3) |

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N3—H3$C$···Cl1$^{i}$ | 0.90 | 2.57 | 3.3106 (19) | 140 |
| N3—H3$D$···Cl2 | 0.90 | 2.58 | 3.481 (2) | 177 |
| N1—H1$C$···Cl1$^{i}$ | 0.90 | 2.90 | 3.5509 (19) | 131 |
| N1—H1$D$···Cl4 | 0.90 | 2.47 | 3.365 (2) | 173 |

Symmetry code: (i) $-x+1, -y+2, -z$.

Data collection: *SMART* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2002); software used to prepare material for publication: *SHELXL97*.

This work was financially supported by the Foundation of Zhejiang Key Laboratory for Reactive Chemistry on Solid Surfaces.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2357).

## References

Bruker (2002). *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2004). *SAINT* and *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.
Johansson, A. & Håkansson, M. (2004). *Acta Cryst.* E**60**, m955–m957.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

 doi:10.1107/S1600536807016583 © 2007 International Union of Crystallography 

# supplementary materials

*Acta Cryst.* (2007). E**63**, m1395 [ **doi:10.1107/S1600536807016583** ]

# Dichlorido(*N*,*N*-dimethylpropane-1,3-diamine-$\kappa^2$*N*,*N*')zinc(II)

**J.-L. Huang and Y.-L. Feng**

## Comment

Fig. 1 shows the two independent molecules in the asymmetric unit of the title compound. In each molecule, a $Zn^{II}$ ion is coordinated by an *N*,*N*-dimethyl-1,3-propylenediamine ligand and two Cl atoms. The average Zn—N bond length is 2.0433 Å and the average Zn—Cl length is 2.2307 Å. Each $Zn^{II}$ ion displays a distorted tetrahedral coordination geometry, as observed in the structure of dichloro (*N*,*N*,*N*'-trimethylethylenediamine)zinc(II) (Johansson & Håkansson, 2004).

The six-membered chelate rings (Zn1/N1/C1/C2/C3/N2 and Zn2/N3/C6/C7/C8/N4) adopt chair-configurations. The dihedral angles between the N1/C1/C3/N2 plane and the C1/C2/C3 and N1/N2/Zn1 planes are 118.70 (4) and 137.46 (7)°, respectively. The dihedral angles between the N3/C6/C8/N4 plane and the C6/C7/C8 and N3/N4/Zn2/ planes are 119.89 (3) and 135.96 (7)°, respectively.

In the crystal structure, N—H···Cl hydrogen bonds link the molecules to form terameric clusters which are separated by the normal van der Waals distances (Fig. 2).

## Experimental

To an ethanolic solution (15 ml) of biacetyl monoxime (0.101 g, 1.0 mmol), *N*,*N*-dimethylpropylenediamine (0.126 ml, 1.0 mmol) was added dropwise with stirring for 10 min. $ZnCl_2$ (0.136 g, 1 mmol) was then added and the mixture was refluxed for 3 h. A small amount of a precipitate appeared and this was filtered off. Colourless crystals of the title compound suitable for X-ray analysis were separated after 3 d (yield 78%).

## Refinement

All H atoms were positioned geometrically and refined using a riding model, with C—H = 0.97 Å and N—H = 0.90 Å, and with $U_{iso}$(H) = 1.2$U_{eq}$(C,*N*),

and methyl groups were allowed to rotate to fit the electron density [methyl C—H = 0.96 Å and $U_{iso}$(H) = 1.5$U_{eq}$(C)].

## Figures

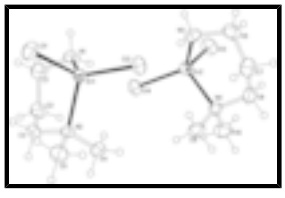
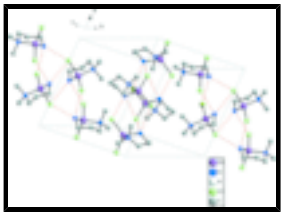


Fig. 1. The asymmetric unit of (I), with displacement ellipsoids drawn at the 30% probability level and H atoms shown as spheres of arbitrary radii.
Fig. 2. A partial packing plot for (I), with hydrogen bonds indicated by dashed lines.



## Dichlorido(*N*,*N*-dimethylpropane-1,3-diamine-κ$^2$*N*,*N*')zinc(II)

*Crystal data*

| | |
|---|---|
| $[ZnCl_2(C_5H_{14}N_2)]$ | $F_{000}$ = 976 |
| $M_r$ = 238.45 | $D_x$ = 1.588 Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation<br>λ = 0.71073 Å |
| Hall symbol: -P 2ybc | Cell parameters from 3925 reflections |
| $a$ = 12.033 (4) Å | θ = 1.8–27.8º |
| $b$ = 11.816 (4) Å | μ = 2.94 mm$^{-1}$ |
| $c$ = 15.113 (4) Å | $T$ = 293 (2) K |
| β = 111.817 (3)º | Block, colourless |
| $V$ = 1995.0 (10) Å$^3$ | 0.45 × 0.38 × 0.24 mm |
| $Z$ = 8 | |

*Data collection*

| | |
|---|---|
| Bruker APEXII area-detector diffractometer | 4701 independent reflections |
| Radiation source: fine-focus sealed tube | 3625 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int}$ = 0.022 |
| $T$ = 293(2) K | $\theta_{max}$ = 27.8º |
| ω scans | $\theta_{min}$ = 1.8º |
| Absorption correction: multi-scan (SADABS; Sheldrick, 1996) | $h$ = −15→15 |
| $T_{min}$ = 0.277, $T_{max}$ = 0.494 | $k$ = −14→15 |
| 12998 measured reflections | $l$ = −14→19 |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)]$ = 0.026 | H-atom parameters constrained |
| $wR(F^2)$ = 0.064 | $w = 1/[\sigma^2(F_o^2) + (0.0354P)^2]$<br>where $P = (F_o^2 + 2F_c^2)/3$ |
| $S$ = 0.99 | $(\Delta/\sigma)_{max}$ = 0.001 |
| 4701 reflections | $\Delta\rho_{max}$ = 0.30 e Å$^{-3}$ |
| 185 parameters | $\Delta\rho_{min}$ = −0.47 e Å$^{-3}$ |

Primary atom site location: structure-invariant direct methods

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 (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Zn1 | 0.411849 (19) | 0.857901 (19) | 0.046947 (15) | 0.03807 (7) |
| Zn2 | 0.863280 (19) | 0.73098 (2) | 0.201793 (15) | 0.04190 (8) |
| N1 | 0.49646 (15) | 0.82785 (14) | −0.04360 (12) | 0.0469 (4) |
| H1C | 0.5200 | 0.8940 | −0.0604 | 0.056* |
| H1D | 0.5623 | 0.7859 | −0.0138 | 0.056* |
| N2 | 0.33563 (13) | 0.70150 (13) | 0.04345 (11) | 0.0390 (4) |
| N3 | 0.82874 (15) | 0.89004 (15) | 0.23443 (12) | 0.0501 (4) |
| H3C | 0.8433 | 0.9395 | 0.1947 | 0.060* |
| H3D | 0.7509 | 0.8957 | 0.2262 | 0.060* |
| N4 | 0.84928 (14) | 0.65333 (14) | 0.32039 (12) | 0.0452 (4) |
| Cl1 | 0.26121 (5) | 0.97769 (5) | −0.02651 (4) | 0.05660 (15) |
| Cl2 | 0.52522 (4) | 0.91528 (5) | 0.19295 (3) | 0.05169 (14) |
| Cl3 | 1.05195 (5) | 0.72640 (6) | 0.21087 (5) | 0.06741 (17) |
| Cl4 | 0.72616 (5) | 0.65413 (5) | 0.07219 (4) | 0.05821 (15) |
| C1 | 0.4183 (2) | 0.76772 (19) | −0.13034 (15) | 0.0559 (6) |
| H1A | 0.4627 | 0.7532 | −0.1711 | 0.067* |
| H1B | 0.3508 | 0.8157 | −0.1652 | 0.067* |
| C2 | 0.3727 (2) | 0.65750 (19) | −0.10731 (16) | 0.0580 (6) |
| H2A | 0.4410 | 0.6136 | −0.0672 | 0.070* |
| H2B | 0.3355 | 0.6158 | −0.1663 | 0.070* |
| C3 | 0.28377 (18) | 0.66473 (18) | −0.05791 (15) | 0.0504 (5) |
| H3A | 0.2208 | 0.7173 | −0.0929 | 0.061* |
| H3B | 0.2472 | 0.5910 | −0.0608 | 0.061* |
| C4 | 0.42189 (19) | 0.61736 (19) | 0.10245 (16) | 0.0558 (6) |
| H4A | 0.3843 | 0.5444 | 0.0938 | 0.084* |
| H4B | 0.4478 | 0.6388 | 0.1683 | 0.084* |
| H4C | 0.4898 | 0.6141 | 0.0837 | 0.084* |
| C5 | 0.23779 (19) | 0.7116 (2) | 0.07969 (17) | 0.0638 (7) |
| H5A | 0.1981 | 0.6399 | 0.0739 | 0.096* |
| H5B | 0.1814 | 0.7675 | 0.0433 | 0.096* |
| H5C | 0.2702 | 0.7339 | 0.1455 | 0.096* |

| | | | | |
|---|---|---|---|---|
| C6 | 0.9032 (2) | 0.9189 (2) | 0.33350 (16) | 0.0621 (6) |
| H6A | 0.8891 | 0.9972 | 0.3457 | 0.075* |
| H6B | 0.9870 | 0.9112 | 0.3427 | 0.075* |
| C7 | 0.8754 (3) | 0.8430 (2) | 0.40354 (17) | 0.0717 (7) |
| H7A | 0.9134 | 0.8749 | 0.4668 | 0.086* |
| H7B | 0.7896 | 0.8445 | 0.3882 | 0.086* |
| C8 | 0.9139 (2) | 0.7215 (2) | 0.40676 (16) | 0.0632 (6) |
| H8A | 0.9986 | 0.7201 | 0.4177 | 0.076* |
| H8B | 0.9039 | 0.6854 | 0.4609 | 0.076* |
| C9 | 0.72181 (19) | 0.6399 (2) | 0.30731 (18) | 0.0631 (6) |
| H9A | 0.7164 | 0.6092 | 0.3644 | 0.095* |
| H9B | 0.6835 | 0.5895 | 0.2550 | 0.095* |
| H9C | 0.6829 | 0.7123 | 0.2940 | 0.095* |
| C10 | 0.9048 (2) | 0.5398 (2) | 0.3337 (2) | 0.0721 (7) |
| H10A | 0.8920 | 0.5019 | 0.3853 | 0.108* |
| H10B | 0.9892 | 0.5473 | 0.3482 | 0.108* |
| H10C | 0.8693 | 0.4965 | 0.2763 | 0.108* |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Zn1 | 0.04375 (13) | 0.03581 (13) | 0.03561 (12) | −0.00228 (9) | 0.01585 (10) | −0.00326 (9) |
| Zn2 | 0.03857 (13) | 0.05028 (15) | 0.04007 (13) | −0.00125 (10) | 0.01835 (10) | −0.00226 (10) |
| N1 | 0.0553 (10) | 0.0405 (10) | 0.0537 (10) | −0.0088 (8) | 0.0303 (8) | −0.0044 (8) |
| N2 | 0.0353 (8) | 0.0411 (9) | 0.0400 (9) | −0.0024 (7) | 0.0133 (7) | 0.0058 (7) |
| N3 | 0.0524 (10) | 0.0493 (11) | 0.0555 (11) | 0.0074 (8) | 0.0280 (9) | 0.0109 (8) |
| N4 | 0.0376 (8) | 0.0502 (11) | 0.0465 (9) | 0.0036 (7) | 0.0140 (7) | 0.0114 (8) |
| Cl1 | 0.0651 (3) | 0.0514 (3) | 0.0478 (3) | 0.0160 (3) | 0.0146 (2) | 0.0050 (2) |
| Cl2 | 0.0492 (3) | 0.0604 (3) | 0.0407 (3) | −0.0019 (2) | 0.0112 (2) | −0.0115 (2) |
| Cl3 | 0.0457 (3) | 0.0857 (5) | 0.0820 (4) | −0.0041 (3) | 0.0366 (3) | −0.0138 (3) |
| Cl4 | 0.0550 (3) | 0.0658 (4) | 0.0502 (3) | −0.0061 (3) | 0.0153 (2) | −0.0133 (3) |
| C1 | 0.0718 (15) | 0.0623 (15) | 0.0411 (12) | −0.0046 (12) | 0.0294 (11) | −0.0081 (10) |
| C2 | 0.0743 (16) | 0.0499 (14) | 0.0501 (13) | −0.0081 (11) | 0.0233 (12) | −0.0179 (10) |
| C3 | 0.0482 (12) | 0.0461 (13) | 0.0495 (12) | −0.0150 (9) | 0.0095 (10) | −0.0061 (9) |
| C4 | 0.0513 (12) | 0.0487 (14) | 0.0602 (14) | 0.0028 (10) | 0.0123 (10) | 0.0165 (10) |
| C5 | 0.0463 (12) | 0.0861 (19) | 0.0657 (15) | −0.0035 (12) | 0.0285 (11) | 0.0110 (13) |
| C6 | 0.0755 (16) | 0.0502 (14) | 0.0658 (15) | −0.0056 (12) | 0.0321 (13) | −0.0141 (11) |
| C7 | 0.095 (2) | 0.081 (2) | 0.0464 (13) | −0.0072 (15) | 0.0353 (13) | −0.0140 (12) |
| C8 | 0.0597 (14) | 0.0829 (19) | 0.0405 (12) | −0.0020 (13) | 0.0110 (11) | 0.0093 (11) |
| C9 | 0.0443 (12) | 0.0783 (18) | 0.0704 (16) | −0.0019 (11) | 0.0256 (11) | 0.0249 (13) |
| C10 | 0.0646 (15) | 0.0552 (16) | 0.096 (2) | 0.0122 (12) | 0.0285 (14) | 0.0187 (14) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Zn1—N1 | 2.0176 (16) | C2—H2A | 0.9700 |
| Zn1—N2 | 2.0551 (16) | C2—H2B | 0.9700 |
| Zn1—Cl2 | 2.2254 (7) | C3—H3A | 0.9700 |
| Zn1—Cl1 | 2.2419 (7) | C3—H3B | 0.9700 |
| Zn2—N3 | 2.0251 (18) | C4—H4A | 0.9600 |

| | | | |
|---|---|---|---|
| Zn2—N4 | 2.0754 (17) | C4—H4B | 0.9600 |
| Zn2—Cl3 | 2.2236 (9) | C4—H4C | 0.9600 |
| Zn2—Cl4 | 2.2319 (7) | C5—H5A | 0.9600 |
| N1—C1 | 1.481 (3) | C5—H5B | 0.9600 |
| N1—H1C | 0.9000 | C5—H5C | 0.9600 |
| N1—H1D | 0.9000 | C6—C7 | 1.516 (3) |
| N2—C4 | 1.474 (2) | C6—H6A | 0.9700 |
| N2—C5 | 1.476 (3) | C6—H6B | 0.9700 |
| N2—C3 | 1.488 (2) | C7—C8 | 1.504 (4) |
| N3—C6 | 1.471 (3) | C7—H7A | 0.9700 |
| N3—H3C | 0.9000 | C7—H7B | 0.9700 |
| N3—H3D | 0.9000 | C8—H8A | 0.9700 |
| N4—C10 | 1.479 (3) | C8—H8B | 0.9700 |
| N4—C9 | 1.480 (3) | C9—H9A | 0.9600 |
| N4—C8 | 1.485 (3) | C9—H9B | 0.9600 |
| C1—C2 | 1.503 (3) | C9—H9C | 0.9600 |
| C1—H1A | 0.9700 | C10—H10A | 0.9600 |
| C1—H1B | 0.9700 | C10—H10B | 0.9600 |
| C2—C3 | 1.518 (3) | C10—H10C | 0.9600 |
| N1—Zn1—N2 | 99.04 (6) | N2—C3—C2 | 114.85 (17) |
| N1—Zn1—Cl2 | 116.63 (5) | N2—C3—H3A | 108.6 |
| N2—Zn1—Cl2 | 113.75 (5) | C2—C3—H3A | 108.6 |
| N1—Zn1—Cl1 | 107.11 (6) | N2—C3—H3B | 108.6 |
| N2—Zn1—Cl1 | 106.50 (5) | C2—C3—H3B | 108.6 |
| Cl2—Zn1—Cl1 | 112.55 (3) | H3A—C3—H3B | 107.5 |
| N3—Zn2—N4 | 96.32 (7) | N2—C4—H4A | 109.5 |
| N3—Zn2—Cl3 | 107.75 (5) | N2—C4—H4B | 109.5 |
| N4—Zn2—Cl3 | 110.16 (5) | H4A—C4—H4B | 109.5 |
| N3—Zn2—Cl4 | 116.08 (5) | N2—C4—H4C | 109.5 |
| N4—Zn2—Cl4 | 107.89 (5) | H4A—C4—H4C | 109.5 |
| Cl3—Zn2—Cl4 | 116.68 (3) | H4B—C4—H4C | 109.5 |
| C1—N1—Zn1 | 111.73 (13) | N2—C5—H5A | 109.5 |
| C1—N1—H1C | 109.3 | N2—C5—H5B | 109.5 |
| Zn1—N1—H1C | 109.3 | H5A—C5—H5B | 109.5 |
| C1—N1—H1D | 109.3 | N2—C5—H5C | 109.5 |
| Zn1—N1—H1D | 109.3 | H5A—C5—H5C | 109.5 |
| H1C—N1—H1D | 107.9 | H5B—C5—H5C | 109.5 |
| C4—N2—C5 | 108.02 (16) | N3—C6—C7 | 111.4 (2) |
| C4—N2—C3 | 110.94 (17) | N3—C6—H6A | 109.3 |
| C5—N2—C3 | 108.57 (16) | C7—C6—H6A | 109.3 |
| C4—N2—Zn1 | 112.57 (13) | N3—C6—H6B | 109.3 |
| C5—N2—Zn1 | 109.13 (14) | C7—C6—H6B | 109.3 |
| C3—N2—Zn1 | 107.54 (11) | H6A—C6—H6B | 108.0 |
| C6—N3—Zn2 | 111.15 (13) | C8—C7—C6 | 116.2 (2) |
| C6—N3—H3C | 109.4 | C8—C7—H7A | 108.2 |
| Zn2—N3—H3C | 109.4 | C6—C7—H7A | 108.2 |
| C6—N3—H3D | 109.4 | C8—C7—H7B | 108.2 |
| Zn2—N3—H3D | 109.4 | C6—C7—H7B | 108.2 |
| H3C—N3—H3D | 108.0 | H7A—C7—H7B | 107.4 |

| | | | |
|---|---|---|---|
| C10—N4—C9 | 108.31 (18) | N4—C8—C7 | 115.82 (19) |
| C10—N4—C8 | 108.07 (17) | N4—C8—H8A | 108.3 |
| C9—N4—C8 | 110.72 (18) | C7—C8—H8A | 108.3 |
| C10—N4—Zn2 | 109.96 (14) | N4—C8—H8B | 108.3 |
| C9—N4—Zn2 | 110.16 (12) | C7—C8—H8B | 108.3 |
| C8—N4—Zn2 | 109.58 (13) | H8A—C8—H8B | 107.4 |
| N1—C1—C2 | 112.16 (18) | N4—C9—H9A | 109.5 |
| N1—C1—H1A | 109.2 | N4—C9—H9B | 109.5 |
| C2—C1—H1A | 109.2 | H9A—C9—H9B | 109.5 |
| N1—C1—H1B | 109.2 | N4—C9—H9C | 109.5 |
| C2—C1—H1B | 109.2 | H9A—C9—H9C | 109.5 |
| H1A—C1—H1B | 107.9 | H9B—C9—H9C | 109.5 |
| C1—C2—C3 | 116.71 (19) | N4—C10—H10A | 109.5 |
| C1—C2—H2A | 108.1 | N4—C10—H10B | 109.5 |
| C3—C2—H2A | 108.1 | H10A—C10—H10B | 109.5 |
| C1—C2—H2B | 108.1 | N4—C10—H10C | 109.5 |
| C3—C2—H2B | 108.1 | H10A—C10—H10C | 109.5 |
| H2A—C2—H2B | 107.3 | H10B—C10—H10C | 109.5 |
| N2—Zn1—N1—C1 | 45.48 (15) | N3—Zn2—N4—C9 | 77.48 (15) |
| Cl2—Zn1—N1—C1 | 167.90 (12) | Cl3—Zn2—N4—C9 | −170.96 (13) |
| Cl1—Zn1—N1—C1 | −65.00 (14) | Cl4—Zn2—N4—C9 | −42.56 (15) |
| N1—Zn1—N2—C4 | 78.10 (15) | N3—Zn2—N4—C8 | −44.57 (15) |
| Cl2—Zn1—N2—C4 | −46.37 (14) | Cl3—Zn2—N4—C8 | 66.99 (14) |
| Cl1—Zn1—N2—C4 | −170.94 (13) | Cl4—Zn2—N4—C8 | −164.61 (13) |
| N1—Zn1—N2—C5 | −161.99 (13) | Zn1—N1—C1—C2 | −57.4 (2) |
| Cl2—Zn1—N2—C5 | 73.54 (13) | N1—C1—C2—C3 | 68.8 (3) |
| Cl1—Zn1—N2—C5 | −51.02 (13) | C4—N2—C3—C2 | −65.1 (2) |
| N1—Zn1—N2—C3 | −44.40 (13) | C5—N2—C3—C2 | 176.39 (19) |
| Cl2—Zn1—N2—C3 | −168.87 (11) | Zn1—N2—C3—C2 | 58.4 (2) |
| Cl1—Zn1—N2—C3 | 66.57 (12) | C1—C2—C3—N2 | −71.8 (3) |
| N4—Zn2—N3—C6 | 49.49 (15) | Zn2—N3—C6—C7 | −63.2 (2) |
| Cl3—Zn2—N3—C6 | −64.07 (15) | N3—C6—C7—C8 | 70.0 (3) |
| Cl4—Zn2—N3—C6 | 162.96 (13) | C10—N4—C8—C7 | 175.9 (2) |
| N3—Zn2—N4—C10 | −163.22 (14) | C9—N4—C8—C7 | −65.6 (3) |
| Cl3—Zn2—N4—C10 | −51.66 (15) | Zn2—N4—C8—C7 | 56.1 (2) |
| Cl4—Zn2—N4—C10 | 76.74 (14) | C6—C7—C8—N4 | −67.7 (3) |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N3—H3C···Cl1$^{i}$ | 0.90 | 2.57 | 3.3106 (19) | 140 |
| N3—H3D···Cl2 | 0.90 | 2.58 | 3.481 (2) | 177 |
| N1—H1C···Cl1$^{i}$ | 0.90 | 2.90 | 3.5509 (19) | 131 |
| N1—H1D···Cl4 | 0.90 | 2.47 | 3.365 (2) | 173 |

Symmetry codes: (i) −*x*+1, −*y*+2, −*z*.

**Fig. 1**

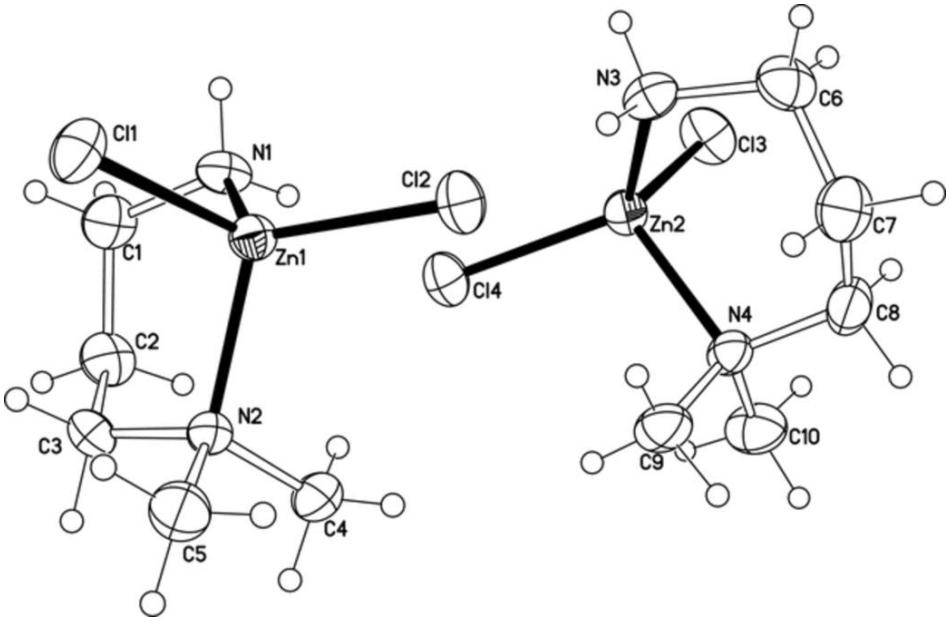


**Fig. 2**