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# Bis[4-(dimethylamino)pyridinium] tetrachloridozincate

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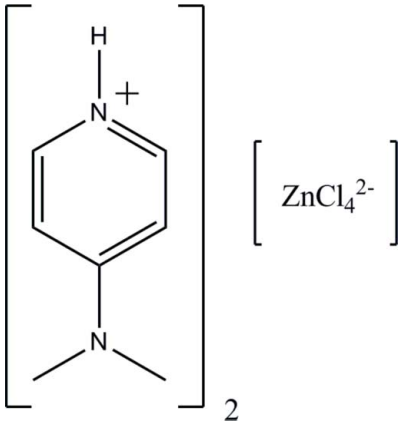
Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.020; $wR$ factor = 0.053; data-to-parameter ratio = 27.4.

In the title compound, $(C_7H_{11}N_2)_2[ZnCl_4]$, $[ZnCl_4]^{2-}$ anions and 4-(dimethylamino)pyridinium cations are held together by various intermolecular interactions including Coulombic attraction, hydrogen bonding and $\pi$–$\pi$ stacking interactions. Three Cl atoms of the $[ZnCl_4]^{2-}$ tetrahedron act as acceptors in N—H···Cl hydrogen bonds. The hydrogen bonds, both of which are bifurcated, lead to the formation of a three-dimensional network. Within the network, intermolecular $\pi$–$\pi$ stacking interactions with a centroid–centroid distance of 3.5911 (7) Å arrange the 4-(dimethylamino)pyridinium cations into antiparallel dimers.

## Related literature

For common applications of organic–inorganic hybrid materials, see: Kobel & Hanack (1986); Pierpont & Jung (1994); Huskins & Robson (1990). For related structures and discussion of geometrical features, see: Albrecht *et al.* (2003); El Glaoui *et al.* (2008).




## Experimental

### Crystal data

$(C_7H_{11}N_2)_2[ZnCl_4]$
$M_r$ = 453.55
Triclinic, $P\overline{1}$
$a$ = 7.7056 (8) Å
$b$ = 8.2159 (8) Å
$c$ = 16.0972 (16) Å
$\alpha$ = 77.422 (1)°
$\beta$ = 79.804 (1)°
$\gamma$ = 75.983 (1)°
$V$ = 956.67 (17) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 1.85 mm$^{-1}$
$T$ = 100 K
0.55 × 0.50 × 0.45 mm

### Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min}$ = 0.602, $T_{max}$ = 0.746
21487 measured reflections
5803 independent reflections
5638 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.019

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.020
$wR(F^2)$ = 0.053
$S$ = 1.07
5803 reflections
212 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.48 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.44 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N3—H3···Cl1$^{i}$ | 0.88 | 2.88 | 3.5090 (11) | 130 |
| N3—H3···Cl3$^{i}$ | 0.88 | 2.46 | 3.2224 (10) | 146 |
| N1—H1*A*···Cl2 | 0.88 | 2.81 | 3.4043 (10) | 126 |
| N1—H1*A*···Cl1 | 0.88 | 2.53 | 3.2066 (10) | 134 |

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RK2262).

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# supporting information

*Acta Cryst.* (2011). E**67**, m343 [doi:10.1107/S1600536811005010]

## Bis[4-(dimethylamino)pyridinium] tetrachloridozincate

**Riadh Kefi, Frederic Lefebvre, Matthias Zeller and Cherif Ben Nasr**

### S1. Comment

Organic–inorganic compounds constitute a vast family of hybrid materials of considerable technological importance (Kobel & Hanack, 1986; Pierpont & Jung, 1994; Huskins & Robson, 1990). In this work, we report the molecular and crystal structures of one such compound, $(C_7H_{11}N_2)_2ZnCl_4$. As shown in Fig. 1, only the nitrogen atom of the aromatic ring of the title compound is protonated, but not the dimethylamine group. Thus, to ensure charge equilibrium, the structure associates each tetrachlorizincate anion with two 4-(dimethylamino)pyridinium cations. Fig.2 shows that the atomic arrangement of the title hybrid material which can be described as inorganic $[ZnCl_4]^{2-}$ units isolated from each other by the organic cations. The different entities are held together by columbic attraction and multiple hydrogen bonds to form a three dimensional network. Previous studies have shown that the presence of hydrogen bonds influences appreciably the geometrical parameters of the tetrachlorozincate anions (Albrecht *et al.*, 2003). Indeed, the fact that the Zn—Cl4 bond lengh is the shortest meets the expectation derived from hydrogen bonding effects, as the atom Cl4 is not involved in a hydrogen bond, while the remaining Cl1, Cl2 and Cl3 are acting as acceptors of hydrogen bonds with concurrently weakened Zn—Cl bonds. Both of the hydrogen bonds are bifurcated, N1—H1···(Cl1, Cl2) and N3—H3···(Cl1$^{i}$, Cl3$^{i}$) (Table 1). Symmetry code: (i) -*x*, -*y*+1, -*z*. The Cl—Zn—Cl bond angles range from 102.25 (1)° to 117.03 (1)°. These values indicate that the coordination geometry of the zinc atom can be regarded as a slightly distorted tetrahedron, similar as in other related compounds such as 4-(2–ammonioethyl)morpholin–4–ium tetrachlorozincate where the corresponding limit angles are 98.90 (4)° to 114.74 (4)° (El Glaoui *et al.*, 2008). Intermolecular *π*–*π* stacking is present between adjacent 4-(dimethylamino)pyridinium cations with a centroid–centroid distance of 3.5911 (7)Å (symmetry code for the second pyridine ring: (i) -*x*, -*y*+1, -*z*).

### S2. Experimental

A mixture of an aqueous solution of 4-(dimethylamino)pyridine (4 mmol, 0.488 g), zinc chloride (2 mmol, 0.396 g) and HCl (10 ml, 0.4 *M*) in a Petri dish was slowly evaporated at room temperature. Crystals of the title compound, which remained stable under normal conditions of temperature and humidity, were isolated after several days and subjected to X–ray diffraction analysis (yield 57%).

### S3. Refinement

Reflection (0 0 1) was obscured by the beamstop and was omitted from the refinement. C—H hydrogen atoms were placed in calculated positions with C—H distances in the range 0.93Å–0.97Å. N—H hydrogen atoms were placed in calculated positions with N—H distances of 0.88Å. The $U_{iso}$(H) values of all H atoms were constrained to 1.2(1.5) times $U_{eq}$ of the respective parent atom.

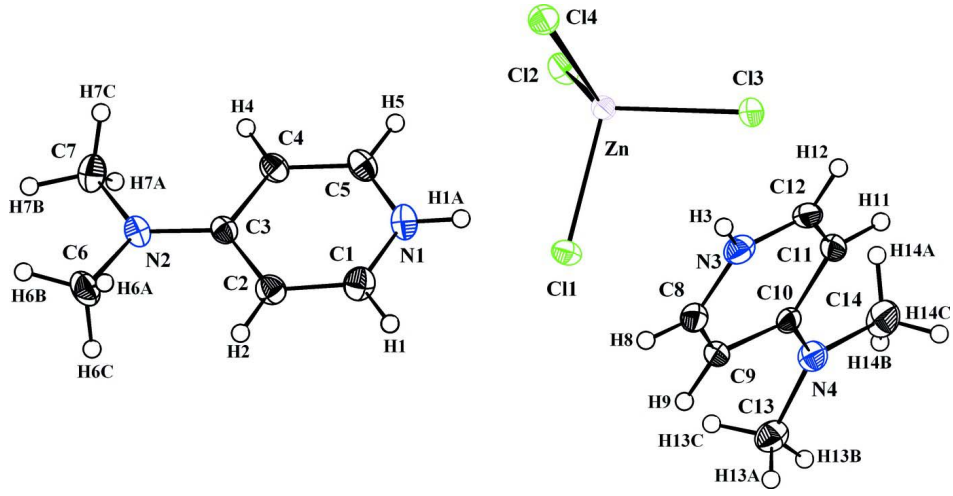


**Figure 1**

A view of the title compound with the atom numbering scheme. Displacement ellipsoids are drawn at 50% probability level. H atoms are presented as a small spheres of arbitrary radius.

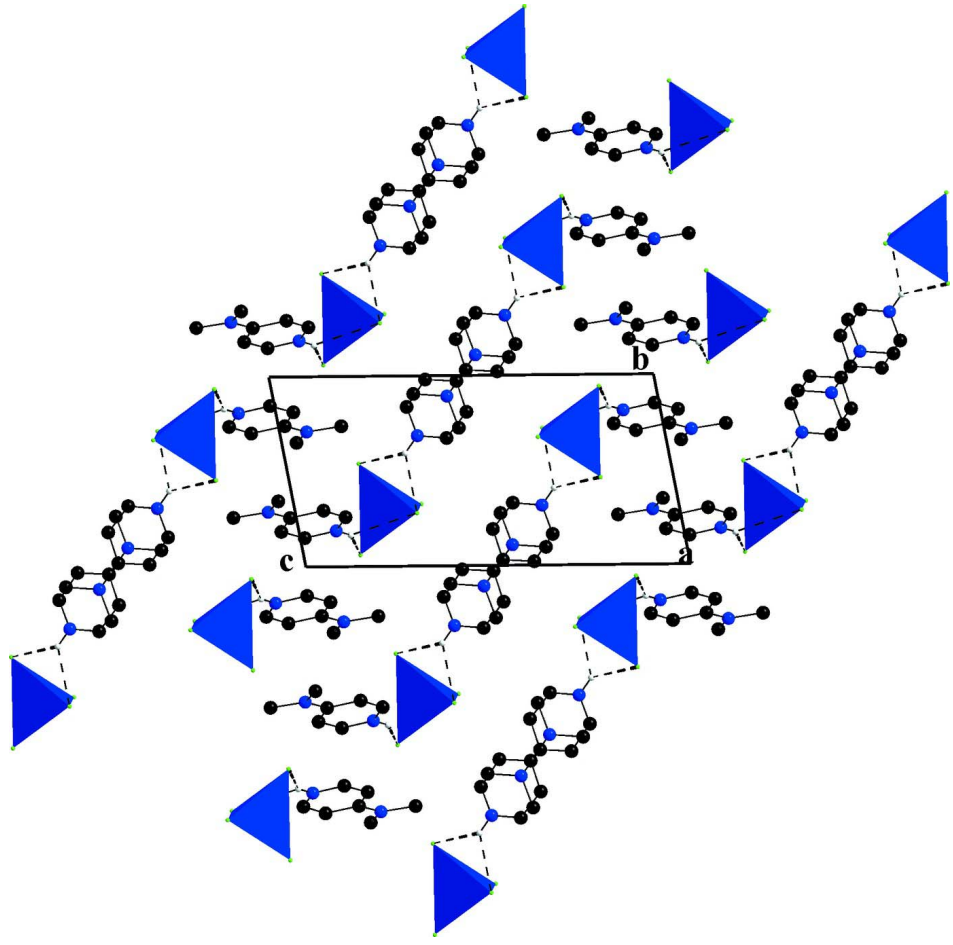


**Figure 2**

The packing of $(C_7H_{11}N_2)_2ZnCl_4$, viewed down the *a* axis. Hydrogen bonds are denoted by dotted lines.

**Bis[4-(dimethylamino)pyridinium] tetrachloridozincatee**

*Crystal data*

$(C_7H_{11}N_2)_2[ZnCl_4]$
$M_r = 453.55$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 7.7056$ (8) Å
$b = 8.2159$ (8) Å
$c = 16.0972$ (16) Å
$\alpha = 77.422$ (1)°
$\beta = 79.804$ (1)°
$\gamma = 75.983$ (1)°
$V = 956.67$ (17) Å$^3$
$Z = 2$
$F(000) = 464$
$D_x = 1.574$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 8289 reflections
$\theta = 2.6$–$31.0°$
$\mu = 1.85$ mm$^{-1}$
$T = 100$ K
Block, colourless
0.55 × 0.50 × 0.45 mm

*Data collection*

Bruker SMART APEX CCD diffractometer
Radiation source: fine–focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min} = 0.602$, $T_{max} = 0.746$
21487 measured reflections
5803 independent reflections
5638 reflections with $I > 2\sigma(I)$
$R_{int} = 0.019$
$\theta_{max} = 31.5°$, $\theta_{min} = 2.6°$
$h = -11 \rightarrow 11$
$k = -11 \rightarrow 11$
$l = -23 \rightarrow 23$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.020$
$wR(F^2) = 0.053$
$S = 1.07$
5803 reflections
212 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0265P)^2 + 0.3664P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.004$
$\Delta\rho_{max} = 0.48$ e Å$^{-3}$
$\Delta\rho_{min} = -0.44$ e Å$^{-3}$

*Special details*

**Geometry**. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.14583 (16) | 0.32828 (15) | 0.43051 (7) | 0.0193 (2) |
| H1 | 0.0707 | 0.4358 | 0.4378 | 0.023* |
| C2 | 0.13978 (15) | 0.19127 (14) | 0.49549 (7) | 0.01699 (19) |

| | | | | |
|---|---|---|---|---|
| H2 | 0.0616 | 0.2037 | 0.5475 | 0.020* |
| C3 | 0.25157 (14) | 0.02905 (13) | 0.48499 (6) | 0.01385 (18) |
| C4 | 0.36177 (14) | 0.01982 (14) | 0.40430 (7) | 0.01539 (18) |
| H4 | 0.4353 | −0.0863 | 0.3935 | 0.018* |
| C5 | 0.36190 (15) | 0.16277 (14) | 0.34264 (7) | 0.01706 (19) |
| H5 | 0.4373 | 0.1555 | 0.2895 | 0.020* |
| C6 | 0.15682 (17) | −0.09487 (17) | 0.63337 (7) | 0.0221 (2) |
| H6A | 0.1832 | 0.0006 | 0.6528 | 0.033* |
| H6B | 0.1952 | −0.2011 | 0.6733 | 0.033* |
| H6C | 0.0269 | −0.0753 | 0.6315 | 0.033* |
| C7 | 0.36088 (17) | −0.27506 (15) | 0.53236 (8) | 0.0217 (2) |
| H7A | 0.3255 | −0.3030 | 0.4825 | 0.033* |
| H7B | 0.3391 | −0.3621 | 0.5830 | 0.033* |
| H7C | 0.4894 | −0.2719 | 0.5215 | 0.033* |
| C8 | −0.02081 (15) | 0.25984 (14) | −0.12815 (7) | 0.01678 (19) |
| H8 | 0.0133 | 0.2852 | −0.1884 | 0.020* |
| C9 | 0.07683 (14) | 0.29557 (13) | −0.07416 (7) | 0.01428 (18) |
| H9 | 0.1783 | 0.3455 | −0.0971 | 0.017* |
| C10 | 0.02760 (14) | 0.25842 (13) | 0.01653 (6) | 0.01374 (18) |
| C11 | −0.12782 (14) | 0.18589 (14) | 0.04599 (7) | 0.01695 (19) |
| H11 | −0.1684 | 0.1612 | 0.1057 | 0.020* |
| C12 | −0.21802 (14) | 0.15207 (14) | −0.01175 (8) | 0.0186 (2) |
| H12 | −0.3199 | 0.1016 | 0.0085 | 0.022* |
| C13 | 0.29355 (16) | 0.34659 (15) | 0.03844 (8) | 0.0207 (2) |
| H13A | 0.3693 | 0.2723 | 0.0000 | 0.031* |
| H13B | 0.3570 | 0.3413 | 0.0869 | 0.031* |
| H13C | 0.2679 | 0.4643 | 0.0070 | 0.031* |
| C14 | 0.06780 (18) | 0.26180 (17) | 0.16320 (7) | 0.0250 (2) |
| H14A | −0.0625 | 0.3053 | 0.1748 | 0.038* |
| H14B | 0.1316 | 0.3219 | 0.1902 | 0.038* |
| H14C | 0.0967 | 0.1394 | 0.1868 | 0.038* |
| Cl1 | 0.21516 (3) | 0.72097 (3) | 0.315840 (16) | 0.01547 (5) |
| Cl2 | 0.55357 (4) | 0.45957 (3) | 0.189582 (16) | 0.01755 (5) |
| Cl3 | 0.49003 (3) | 0.93916 (3) | 0.147680 (17) | 0.01690 (5) |
| Cl4 | 0.72105 (3) | 0.67369 (3) | 0.331637 (17) | 0.01814 (5) |
| N1 | 0.25646 (14) | 0.31464 (12) | 0.35590 (6) | 0.01823 (18) |
| H1A | 0.2598 | 0.4057 | 0.3155 | 0.022* |
| N2 | 0.25439 (13) | −0.10807 (12) | 0.54743 (6) | 0.01678 (17) |
| N3 | −0.16574 (13) | 0.18872 (12) | −0.09693 (6) | 0.01829 (18) |
| H3 | −0.2268 | 0.1661 | −0.1328 | 0.022* |
| N4 | 0.12405 (13) | 0.28980 (13) | 0.07042 (6) | 0.01765 (17) |
| Zn1 | 0.507513 (15) | 0.695820 (15) | 0.249259 (7) | 0.01220 (4) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0226 (5) | 0.0160 (5) | 0.0197 (5) | −0.0029 (4) | −0.0029 (4) | −0.0049 (4) |
| C2 | 0.0179 (5) | 0.0175 (5) | 0.0155 (5) | −0.0035 (4) | 0.0002 (4) | −0.0049 (4) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C3 | 0.0142 (4) | 0.0154 (5) | 0.0132 (4) | −0.0055 (3) | −0.0019 (3) | −0.0026 (3) |
| C4 | 0.0167 (4) | 0.0160 (5) | 0.0142 (4) | −0.0053 (4) | 0.0002 (4) | −0.0042 (4) |
| C5 | 0.0197 (5) | 0.0193 (5) | 0.0135 (4) | −0.0077 (4) | 0.0001 (4) | −0.0037 (4) |
| C6 | 0.0240 (5) | 0.0281 (6) | 0.0127 (5) | −0.0088 (4) | 0.0012 (4) | 0.0001 (4) |
| C7 | 0.0281 (6) | 0.0148 (5) | 0.0211 (5) | −0.0040 (4) | −0.0051 (4) | −0.0001 (4) |
| C8 | 0.0165 (5) | 0.0172 (5) | 0.0147 (4) | −0.0016 (4) | −0.0020 (4) | −0.0012 (4) |
| C9 | 0.0128 (4) | 0.0148 (4) | 0.0130 (4) | −0.0019 (3) | 0.0005 (3) | −0.0010 (3) |
| C10 | 0.0134 (4) | 0.0119 (4) | 0.0130 (4) | 0.0012 (3) | −0.0006 (3) | −0.0013 (3) |
| C11 | 0.0155 (4) | 0.0145 (5) | 0.0163 (5) | −0.0004 (4) | 0.0023 (4) | 0.0000 (4) |
| C12 | 0.0121 (4) | 0.0147 (5) | 0.0255 (5) | −0.0011 (3) | 0.0002 (4) | −0.0005 (4) |
| C13 | 0.0186 (5) | 0.0194 (5) | 0.0249 (5) | −0.0028 (4) | −0.0066 (4) | −0.0041 (4) |
| C14 | 0.0288 (6) | 0.0295 (6) | 0.0129 (5) | 0.0024 (5) | −0.0037 (4) | −0.0043 (4) |
| Cl1 | 0.01256 (10) | 0.01683 (11) | 0.01659 (11) | −0.00351 (8) | 0.00141 (8) | −0.00440 (8) |
| Cl2 | 0.02090 (12) | 0.01512 (11) | 0.01719 (11) | −0.00582 (9) | 0.00273 (9) | −0.00613 (9) |
| Cl3 | 0.01644 (11) | 0.01347 (11) | 0.01837 (11) | −0.00359 (8) | −0.00078 (9) | 0.00147 (8) |
| Cl4 | 0.01623 (11) | 0.02174 (12) | 0.01760 (11) | −0.00576 (9) | −0.00483 (9) | −0.00201 (9) |
| N1 | 0.0245 (5) | 0.0151 (4) | 0.0156 (4) | −0.0066 (3) | −0.0036 (4) | −0.0004 (3) |
| N2 | 0.0188 (4) | 0.0170 (4) | 0.0137 (4) | −0.0056 (3) | −0.0005 (3) | −0.0004 (3) |
| N3 | 0.0154 (4) | 0.0178 (4) | 0.0218 (5) | −0.0020 (3) | −0.0059 (3) | −0.0027 (3) |
| N4 | 0.0183 (4) | 0.0202 (4) | 0.0134 (4) | −0.0017 (3) | −0.0024 (3) | −0.0032 (3) |
| Zn1 | 0.01192 (6) | 0.01210 (6) | 0.01234 (6) | −0.00284 (4) | −0.00084 (4) | −0.00200 (4) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—N1 | 1.3533 (15) | C9—C10 | 1.4263 (14) |
| C1—C2 | 1.3634 (16) | C9—H9 | 0.9500 |
| C1—H1 | 0.9500 | C10—N4 | 1.3378 (14) |
| C2—C3 | 1.4274 (15) | C10—C11 | 1.4268 (15) |
| C2—H2 | 0.9500 | C11—C12 | 1.3635 (17) |
| C3—N2 | 1.3352 (13) | C11—H11 | 0.9500 |
| C3—C4 | 1.4266 (14) | C12—N3 | 1.3476 (15) |
| C4—C5 | 1.3627 (15) | C12—H12 | 0.9500 |
| C4—H4 | 0.9500 | C13—N4 | 1.4633 (15) |
| C5—N1 | 1.3513 (15) | C13—H13A | 0.9800 |
| C5—H5 | 0.9500 | C13—H13B | 0.9800 |
| C6—N2 | 1.4658 (14) | C13—H13C | 0.9800 |
| C6—H6A | 0.9800 | C14—N4 | 1.4631 (15) |
| C6—H6B | 0.9800 | C14—H14A | 0.9800 |
| C6—H6C | 0.9800 | C14—H14B | 0.9800 |
| C7—N2 | 1.4641 (15) | C14—H14C | 0.9800 |
| C7—H7A | 0.9800 | Cl1—Zn1 | 2.2983 (3) |
| C7—H7B | 0.9800 | Cl2—Zn1 | 2.2747 (3) |
| C7—H7C | 0.9800 | Cl3—Zn1 | 2.2831 (3) |
| C8—N3 | 1.3530 (14) | Cl4—Zn1 | 2.2409 (3) |
| C8—C9 | 1.3628 (15) | N1—H1A | 0.8800 |
| C8—H8 | 0.9500 | N3—H3 | 0.8800 |
| | | | |
| N1—C1—C2 | 121.51 (10) | C12—C11—C10 | 119.87 (10) |

| | | | |
|---|---|---|---|
| N1—C1—H1 | 119.2 | C12—C11—H11 | 120.1 |
| C2—C1—H1 | 119.2 | C10—C11—H11 | 120.1 |
| C1—C2—C3 | 119.63 (10) | N3—C12—C11 | 121.40 (10) |
| C1—C2—H2 | 120.2 | N3—C12—H12 | 119.3 |
| C3—C2—H2 | 120.2 | C11—C12—H12 | 119.3 |
| N2—C3—C4 | 121.16 (10) | N4—C13—H13A | 109.5 |
| N2—C3—C2 | 122.02 (10) | N4—C13—H13B | 109.5 |
| C4—C3—C2 | 116.81 (9) | H13A—C13—H13B | 109.5 |
| C5—C4—C3 | 120.18 (10) | N4—C13—H13C | 109.5 |
| C5—C4—H4 | 119.9 | H13A—C13—H13C | 109.5 |
| C3—C4—H4 | 119.9 | H13B—C13—H13C | 109.5 |
| N1—C5—C4 | 121.05 (10) | N4—C14—H14A | 109.5 |
| N1—C5—H5 | 119.5 | N4—C14—H14B | 109.5 |
| C4—C5—H5 | 119.5 | H14A—C14—H14B | 109.5 |
| N2—C6—H6A | 109.5 | N4—C14—H14C | 109.5 |
| N2—C6—H6B | 109.5 | H14A—C14—H14C | 109.5 |
| H6A—C6—H6B | 109.5 | H14B—C14—H14C | 109.5 |
| N2—C6—H6C | 109.5 | C5—N1—C1 | 120.78 (10) |
| H6A—C6—H6C | 109.5 | C5—N1—H1A | 119.6 |
| H6B—C6—H6C | 109.5 | C1—N1—H1A | 119.6 |
| N2—C7—H7A | 109.5 | C3—N2—C7 | 120.52 (9) |
| N2—C7—H7B | 109.5 | C3—N2—C6 | 121.19 (10) |
| H7A—C7—H7B | 109.5 | C7—N2—C6 | 118.25 (9) |
| N2—C7—H7C | 109.5 | C12—N3—C8 | 121.00 (10) |
| H7A—C7—H7C | 109.5 | C12—N3—H3 | 119.5 |
| H7B—C7—H7C | 109.5 | C8—N3—H3 | 119.5 |
| N3—C8—C9 | 120.80 (10) | C10—N4—C14 | 121.26 (10) |
| N3—C8—H8 | 119.6 | C10—N4—C13 | 120.79 (9) |
| C9—C8—H8 | 119.6 | C14—N4—C13 | 117.89 (10) |
| C8—C9—C10 | 120.37 (10) | Cl4—Zn1—Cl2 | 111.223 (12) |
| C8—C9—H9 | 119.8 | Cl4—Zn1—Cl3 | 110.797 (11) |
| C10—C9—H9 | 119.8 | Cl2—Zn1—Cl3 | 111.809 (13) |
| N4—C10—C9 | 121.08 (10) | Cl4—Zn1—Cl1 | 117.034 (13) |
| N4—C10—C11 | 122.37 (10) | Cl2—Zn1—Cl1 | 103.260 (10) |
| C9—C10—C11 | 116.54 (10) | Cl3—Zn1—Cl1 | 102.256 (10) |

| | | | |
|---|---|---|---|
| N1—C1—C2—C3 | −0.32 (17) | C4—C5—N1—C1 | −0.92 (17) |
| C1—C2—C3—N2 | 178.17 (10) | C2—C1—N1—C5 | 1.62 (17) |
| C1—C2—C3—C4 | −1.56 (15) | C4—C3—N2—C7 | −4.66 (16) |
| N2—C3—C4—C5 | −177.50 (10) | C2—C3—N2—C7 | 175.62 (10) |
| C2—C3—C4—C5 | 2.24 (15) | C4—C3—N2—C6 | 173.16 (10) |
| C3—C4—C5—N1 | −1.05 (16) | C2—C3—N2—C6 | −6.56 (16) |
| N3—C8—C9—C10 | 0.00 (16) | C11—C12—N3—C8 | 0.33 (16) |
| C8—C9—C10—N4 | 178.74 (10) | C9—C8—N3—C12 | 0.33 (16) |
| C8—C9—C10—C11 | −0.90 (15) | C9—C10—N4—C14 | 176.17 (10) |
| N4—C10—C11—C12 | −178.11 (10) | C11—C10—N4—C14 | −4.20 (16) |
| C9—C10—C11—C12 | 1.53 (15) | C9—C10—N4—C13 | −6.40 (16) |
| C10—C11—C12—N3 | −1.29 (16) | C11—C10—N4—C13 | 173.22 (10) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N3—H3···Cl1$^{i}$ | 0.88 | 2.88 | 3.5090 (11) | 130 |
| N3—H3···Cl3$^{i}$ | 0.88 | 2.46 | 3.2224 (10) | 146 |
| N1—H1*A*···Cl2 | 0.88 | 2.81 | 3.4043 (10) | 126 |
| N1—H1*A*···Cl1 | 0.88 | 2.53 | 3.2066 (10) | 134 |

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