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# Dichloridobis(1-ethyl-2,6-dimethylpyridinium-4-olate-$\kappa O$)zinc(II)

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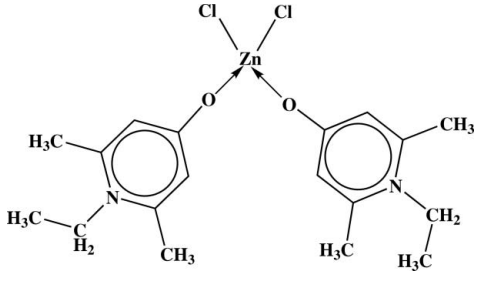
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.031; $wR$ factor = 0.084; data-to-parameter ratio = 21.8.

In the title compound, $[ZnCl_2(C_9H_{13}NO)_2]$, the $Zn^{II}$ ion is coordinated by two $Cl^-$ anions and two O atoms of two zwitterionic organic ligands in a distorted tetrahedral arrangement. In the crystal, molecules are linked into sheets parallel to the $bc$ plane by C—H···Cl and C—H···O hydrogen bonds and weak $\pi$–$\pi$ interactions [centroid–centroid distance = 3.669 (1) Å].

## Related literature

For general background to pyridinium compounds, see: Anwar *et al.* (1997, 1999); Damiano *et al.* (2007); Darensbourg *et al.* (2003); Mootz & Wusson (1981). For hydrogen-bond motifs, see: Bernstein *et al.* (1995). For the preparation of 1-ethyl-2,6-dimethyl-4(1*H*)-pyridinone trihydrate, see: Garratt (1963).




## Experimental

### Crystal data

$[ZnCl_2(C_9H_{13}NO)_2]$
$M_r$ = 438.68
Monoclinic, $C2/c$
$a$ = 30.365 (2) Å
$b$ = 8.5366 (6) Å
$c$ = 15.7982 (12) Å
$\beta$ = 94.281 (4)°
$V$ = 4083.7 (5) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 1.48 mm$^{-1}$
$T$ = 293 K
0.25 × 0.25 × 0.23 mm

### Data collection

Bruker SMART APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*, Bruker, 2008)
$T_{min}$ = 0.709, $T_{max}$ = 0.727
19140 measured reflections
5069 independent reflections
4248 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.042

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.084
$S$ = 0.99
5069 reflections
233 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.61 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.56 e Å$^{-3}$

**Table 1**
Selected bond lengths (Å).

| | | | |
|---|---|---|---|
| Cl1—Zn1 | 2.2292 (5) | O1—Zn1 | 1.9649 (13) |
| Cl2—Zn1 | 2.2349 (6) | O2—Zn1 | 1.9472 (13) |

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C8—H8$A$···O1$^{i}$ | 0.96 | 2.53 | 3.344 (3) | 143 |
| C10—H10$A$···Cl1$^{ii}$ | 0.96 | 2.82 | 3.740 (2) | 162 |
| C10—H10$C$···Cl1$^{iii}$ | 0.96 | 2.82 | 3.745 (2) | 162 |
| C13—H13···Cl2$^{iv}$ | 0.93 | 2.82 | 3.709 (2) | 161 |

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

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI5172).

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# supporting information

*Acta Cryst.* (2010). E**66**, m1448 [https://doi.org/10.1107/S160053681004119X]

## Dichloridobis(1-ethyl-2,6-dimethylpyridinium-4-olate-$\kappa O$)zinc(II)

**M. Thenmozhi, A. Philominal, S. Dhanuskodi and M. N. Ponnuswamy**

### S1. Comment

Organic pyridinium salts have been widely used as guest molecules in the construction of supramolecular architecture in the field of chemistry (Damiano *et al.*, 2007). Pyridinium cations are good candidates for second-harmonic generation (SHG) materials because they possess large hyperpolarizabilities ($\beta$) irrespective of the short cutoff wavelength. Since pyridinium cations are ionic species, they possess an easy tunability into noncentrosymmetric structures by changing counter anions (Anwar *et al.*, 1997, 1999). The zinc halides substituted in pyridines lead to a variety of complexes involving zinc centers and were shown to be catalytically active for the coupling of carbon dioxide and epoxides to provide high molecular weight polycarbonates and cyclic carbonates (Darensbourg *et al.*, 2003). As a part of our interest, we report here the crystal structure of the title pyridinium dichlorozinc(II) complex.

In the title molecule (Fig. 1), the $Zn^{II}$ atom is coordinated by a pair of pyridinium oxide group and terminal halide ions in a distorted tetrahedral arrangement. The organic ligand exists in a zwitterionic structure, involving a conjugated pyridinium fragment. The C atoms of methyl substituents at C2, C6, C12 and C16 lie in the plane of the corresponding pyridinium rings, which are evident from the C9—C2—N1—C6 [176.99 (16)°], C10—C6—N1—C2 [-175.51 (17)°], C19—C12—N11—C16 [178.46 (18)°] and C20—C16—N11—C12 [-178.4 (2)°] torsion angles. The C—C bond of the ethyl groups attached at N1 and N11 are approximately perpendicular to the attached pyridinium ring, which can be seen from the C8—C7—N1—C2 [93.7 (2)°] and C18—C17—N11—C12 [90.0 (2)°] torsion angles. The sum of the bond angles around the protonated nitrogen atoms N1 [360.0°] and N11 [359.99°] of both the pyridinium rings is in accordance with $sp^2$ character. Due to protonation of N1 and N11 atoms of the pyridinium rings, the C2—N1—C6 and C12—N11—C16 angles are widened in comparison with the literature value (Mootz & Wusson, 1981). The pyridinium rings are planar and oriented each other at an angle of 67.79 (8)°.

The packing of the molecules in the unit cell is promoted by the existence of weak C—H···O, C—H···Cl and $\pi\cdots\pi$ types of intermolecular interactions. The C8—H8A···O1 interaction leads to the formation of a centrosymmetric $R_2^2(16)$ dimer (Bernstein *et al.*, 1995). The Cl1 atom acts as an acceptor in a linear fashion for the methyl group hydrogen from the neighbouring molecule [Fig. 2 and Table 2]. The C13—H13···Cl2 intermolecular interaction also contributes to the crystal packing, which form zigzag chains along the *c* axis. The crystal structure is further augmented by $\pi\cdots\pi$ interaction between adjacent pyridinium rings [Cg1(x, y, z)···Cg1(-x, y, 1/2-z) = 3.669 (1) Å; where Cg1 is the centroid of the (N1-C6) ring, Fig.2].

### S2. Experimental

1-Ethyl-2,6-dimethyl-4(1H)pyridinone trihydrate (EDMP.3$H_2O$) was synthesized according to the reported method (Garratt, 1963). The title complex was prepared by the reaction of $ZnCl_2$ with EDMP.3$H_2O$ in a 1:2 molar ratio in aqueous medium. Single crystals were harvested after a typical growth period of 15 days from a saturated aqueous solution at 303 K by slow evaporation of the solvent.

## S3. Refinement

H atoms were positioned geometrically (C-H = 0.93-0.97 Å) and allowed to ride on their parent atoms, with $U_{iso}$(H) = 1.5$U_{eq}$(C) for methyl H and 1.2$U_{eq}$(C) for other H atoms.

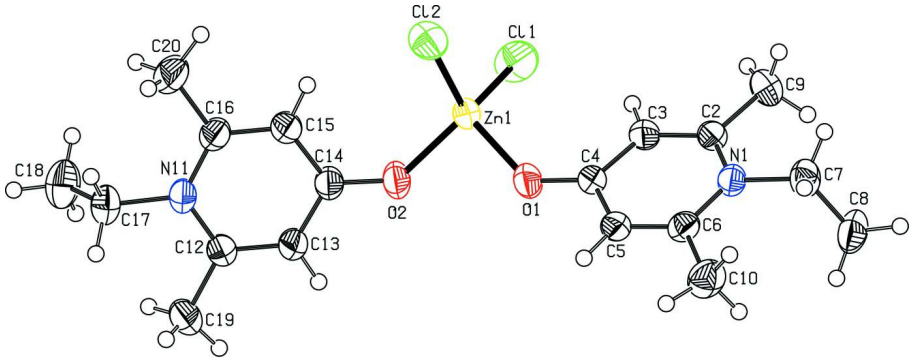


**Figure 1**

The molecular structure of the title compound, showing 50% probability displacement ellipsoids.

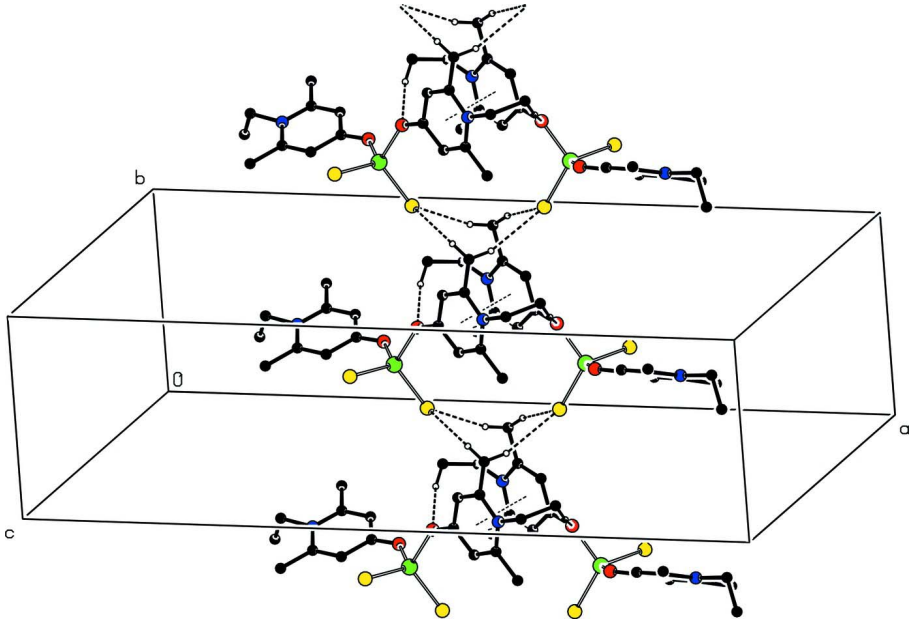


**Figure 2**

The crystal packing of the title compound. H atoms not involved in hydrogen bonding (dashed lines) have been omitted for clarity.

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*Crystal data*

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Monoclinic, *C*2/*c*
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$\beta$ = 94.281 (4)°
*V* = 4083.7 (5) Å$^3$
*Z* = 8
*F*(000) = 1824
$D_x$ = 1.427 Mg m$^{-3}$
Mo *K*$\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 5069 reflections

$\theta$ = 1.3–28.3°
$\mu$ = 1.48 mm$^{-1}$
$T$ = 293 K

Block, yellow
0.25 × 0.25 × 0.23 mm

*Data collection*

Bruker SMART APEXII area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$ and $\varphi$ scans
Absorption correction: multi-scan (*SADABS*, Bruker, 2008)
$T_{min}$ = 0.709, $T_{max}$ = 0.727

19140 measured reflections
5069 independent reflections
4248 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.042
$\theta_{max}$ = 28.3°, $\theta_{min}$ = 1.3°
$h$ = −40→40
$k$ = −11→10
$l$ = −21→20

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.084
$S$ = 0.99
5069 reflections
233 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
$w = 1/[\sigma^2(F_o^2) + (0.0343P)^2 + 3.3394P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.61 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.56 e Å$^{-3}$
Extinction correction: *SHELXL97*, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.00082 (11)

*Special details*

**Geometry**. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2\text{sigma}(F^2)$ 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$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C2 | −0.01906 (5) | 1.0155 (2) | 0.10794 (11) | 0.0359 (4) |
| C3 | 0.01997 (6) | 0.9693 (2) | 0.14837 (11) | 0.0374 (4) |
| H3 | 0.0255 | 0.8629 | 0.1558 | 0.045* |
| C4 | 0.05235 (5) | 1.0787 (2) | 0.17944 (11) | 0.0364 (4) |
| C5 | 0.04059 (5) | 1.2375 (2) | 0.16743 (12) | 0.0383 (4) |
| H5 | 0.0603 | 1.3145 | 0.1880 | 0.046* |
| C6 | 0.00144 (6) | 1.2821 (2) | 0.12668 (11) | 0.0377 (4) |
| C7 | −0.07005 (6) | 1.2200 (3) | 0.04757 (12) | 0.0466 (4) |
| H7A | −0.0797 | 1.1375 | 0.0082 | 0.056* |
| H7B | −0.0646 | 1.3131 | 0.0147 | 0.056* |
| C8 | −0.10658 (6) | 1.2540 (3) | 0.10526 (14) | 0.0568 (5) |
| H8A | −0.1111 | 1.1639 | 0.1399 | 0.085* |

| | | | | |
|---|---|---|---|---|
| H8B | −0.1334 | 1.2777 | 0.0715 | 0.085* |
| H8C | −0.0984 | 1.3419 | 0.1409 | 0.085* |
| C9 | −0.05273 (7) | 0.8962 (3) | 0.07675 (14) | 0.0507 (5) |
| H9A | −0.0810 | 0.9241 | 0.0956 | 0.076* |
| H9B | −0.0442 | 0.7949 | 0.0988 | 0.076* |
| H9C | −0.0545 | 0.8931 | 0.0159 | 0.076* |
| C10 | −0.00998 (7) | 1.4522 (2) | 0.11818 (15) | 0.0554 (5) |
| H10A | −0.0341 | 1.4755 | 0.1520 | 0.083* |
| H10B | −0.0183 | 1.4759 | 0.0598 | 0.083* |
| H10C | 0.0152 | 1.5142 | 0.1374 | 0.083* |
| C12 | 0.26273 (6) | 0.9691 (2) | 0.45067 (12) | 0.0416 (4) |
| C13 | 0.21875 (6) | 0.9588 (2) | 0.42739 (12) | 0.0419 (4) |
| H13 | 0.1987 | 0.9930 | 0.4650 | 0.050* |
| C14 | 0.20270 (6) | 0.8981 (2) | 0.34832 (11) | 0.0391 (4) |
| C15 | 0.23516 (6) | 0.8424 (2) | 0.29655 (13) | 0.0459 (4) |
| H15 | 0.2263 | 0.7964 | 0.2447 | 0.055* |
| C16 | 0.27915 (6) | 0.8540 (2) | 0.32029 (13) | 0.0434 (4) |
| C17 | 0.34104 (6) | 0.9425 (2) | 0.41988 (14) | 0.0468 (4) |
| H17A | 0.3451 | 1.0363 | 0.4542 | 0.056* |
| H17B | 0.3561 | 0.9581 | 0.3686 | 0.056* |
| C18 | 0.36164 (8) | 0.8059 (3) | 0.46811 (18) | 0.0676 (7) |
| H18A | 0.3477 | 0.7925 | 0.5202 | 0.101* |
| H18B | 0.3926 | 0.8254 | 0.4805 | 0.101* |
| H18C | 0.3578 | 0.7127 | 0.4344 | 0.101* |
| C19 | 0.27833 (7) | 1.0377 (3) | 0.53495 (15) | 0.0652 (7) |
| H19A | 0.2934 | 1.1346 | 0.5264 | 0.098* |
| H19B | 0.2981 | 0.9657 | 0.5649 | 0.098* |
| H19C | 0.2534 | 1.0567 | 0.5676 | 0.098* |
| C20 | 0.31287 (8) | 0.7970 (4) | 0.26254 (16) | 0.0698 (7) |
| H20A | 0.2981 | 0.7509 | 0.2127 | 0.105* |
| H20B | 0.3315 | 0.7201 | 0.2916 | 0.105* |
| H20C | 0.3306 | 0.8836 | 0.2463 | 0.105* |
| Cl1 | 0.08868 (2) | 0.63005 (6) | 0.23807 (5) | 0.06526 (17) |
| Cl2 | 0.163428 (18) | 0.86170 (7) | 0.10513 (3) | 0.05362 (14) |
| N1 | −0.02813 (5) | 1.17136 (17) | 0.09508 (9) | 0.0364 (3) |
| N11 | 0.29302 (5) | 0.92018 (19) | 0.39652 (10) | 0.0401 (3) |
| O1 | 0.08947 (4) | 1.04133 (16) | 0.21754 (10) | 0.0509 (3) |
| O2 | 0.16095 (4) | 0.89431 (19) | 0.32761 (9) | 0.0514 (3) |
| Zn1 | 0.126091 (6) | 0.85132 (2) | 0.221676 (13) | 0.03522 (8) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C2 | 0.0331 (8) | 0.0397 (9) | 0.0349 (9) | −0.0027 (7) | 0.0028 (6) | −0.0047 (7) |
| C3 | 0.0367 (8) | 0.0331 (8) | 0.0420 (10) | 0.0009 (7) | 0.0001 (7) | −0.0038 (7) |
| C4 | 0.0311 (8) | 0.0414 (9) | 0.0365 (9) | 0.0019 (7) | 0.0006 (6) | −0.0082 (7) |
| C5 | 0.0337 (8) | 0.0372 (9) | 0.0442 (10) | −0.0028 (7) | 0.0040 (7) | −0.0086 (7) |
| C6 | 0.0366 (8) | 0.0377 (9) | 0.0395 (9) | 0.0019 (7) | 0.0082 (7) | −0.0019 (7) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C7 | 0.0382 (9) | 0.0612 (12) | 0.0391 (10) | 0.0070 (8) | −0.0048 (7) | 0.0064 (9) |
| C8 | 0.0358 (10) | 0.0771 (15) | 0.0569 (13) | 0.0145 (10) | −0.0002 (9) | 0.0079 (11) |
| C9 | 0.0406 (10) | 0.0522 (11) | 0.0583 (13) | −0.0106 (8) | −0.0028 (9) | −0.0086 (10) |
| C10 | 0.0540 (12) | 0.0411 (11) | 0.0712 (15) | 0.0064 (9) | 0.0054 (10) | 0.0025 (10) |
| C12 | 0.0338 (8) | 0.0507 (10) | 0.0400 (10) | −0.0015 (7) | 0.0008 (7) | −0.0080 (8) |
| C13 | 0.0310 (8) | 0.0549 (11) | 0.0399 (10) | 0.0011 (7) | 0.0034 (7) | −0.0087 (8) |
| C14 | 0.0317 (8) | 0.0471 (10) | 0.0380 (9) | 0.0013 (7) | 0.0003 (7) | −0.0002 (8) |
| C15 | 0.0391 (9) | 0.0613 (12) | 0.0366 (10) | 0.0061 (8) | −0.0023 (7) | −0.0105 (8) |
| C16 | 0.0363 (9) | 0.0532 (11) | 0.0408 (10) | 0.0074 (7) | 0.0042 (7) | −0.0036 (8) |
| C17 | 0.0316 (8) | 0.0511 (11) | 0.0574 (12) | −0.0015 (8) | 0.0010 (8) | 0.0057 (9) |
| C18 | 0.0505 (13) | 0.0731 (15) | 0.0773 (17) | 0.0136 (11) | −0.0076 (11) | 0.0157 (13) |
| C19 | 0.0414 (11) | 0.0977 (19) | 0.0556 (13) | −0.0049 (11) | −0.0026 (9) | −0.0305 (13) |
| C20 | 0.0456 (12) | 0.106 (2) | 0.0580 (14) | 0.0179 (12) | 0.0083 (10) | −0.0213 (14) |
| Cl1 | 0.0609 (3) | 0.0442 (3) | 0.0936 (5) | −0.0149 (2) | 0.0257 (3) | −0.0035 (3) |
| Cl2 | 0.0553 (3) | 0.0670 (3) | 0.0395 (3) | −0.0098 (2) | 0.0095 (2) | 0.0006 (2) |
| N1 | 0.0302 (7) | 0.0440 (8) | 0.0349 (8) | 0.0032 (6) | 0.0014 (5) | −0.0004 (6) |
| N11 | 0.0280 (7) | 0.0478 (9) | 0.0439 (8) | 0.0019 (6) | −0.0009 (6) | −0.0009 (7) |
| O1 | 0.0375 (7) | 0.0462 (7) | 0.0660 (9) | 0.0066 (6) | −0.0154 (6) | −0.0122 (7) |
| O2 | 0.0296 (6) | 0.0840 (10) | 0.0399 (7) | 0.0028 (6) | −0.0032 (5) | −0.0090 (7) |
| Zn1 | 0.02879 (11) | 0.03822 (13) | 0.03829 (13) | −0.00233 (7) | 0.00007 (8) | −0.00281 (8) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C2—C3 | 1.362 (2) | C12—C19 | 1.498 (3) |
| C2—N1 | 1.371 (2) | C13—C14 | 1.406 (3) |
| C2—C9 | 1.500 (2) | C13—H13 | 0.93 |
| C3—C4 | 1.416 (2) | C14—O2 | 1.286 (2) |
| C3—H3 | 0.93 | C14—C15 | 1.409 (3) |
| C4—O1 | 1.278 (2) | C15—C16 | 1.364 (3) |
| C4—C5 | 1.412 (3) | C15—H15 | 0.93 |
| C5—C6 | 1.363 (2) | C16—N11 | 1.368 (2) |
| C5—H5 | 0.93 | C16—C20 | 1.502 (3) |
| C6—N1 | 1.372 (2) | C17—N11 | 1.490 (2) |
| C6—C10 | 1.496 (3) | C17—C18 | 1.503 (3) |
| C7—N1 | 1.488 (2) | C17—H17A | 0.97 |
| C7—C8 | 1.515 (3) | C17—H17B | 0.97 |
| C7—H7A | 0.97 | C18—H18A | 0.96 |
| C7—H7B | 0.97 | C18—H18B | 0.96 |
| C8—H8A | 0.96 | C18—H18C | 0.96 |
| C8—H8B | 0.96 | C19—H19A | 0.96 |
| C8—H8C | 0.96 | C19—H19B | 0.96 |
| C9—H9A | 0.96 | C19—H19C | 0.96 |
| C9—H9B | 0.96 | C20—H20A | 0.96 |
| C9—H9C | 0.96 | C20—H20B | 0.96 |
| C10—H10A | 0.96 | C20—H20C | 0.96 |
| C10—H10B | 0.96 | Cl1—Zn1 | 2.2292 (5) |
| C10—H10C | 0.96 | Cl2—Zn1 | 2.2349 (6) |
| C12—C13 | 1.361 (2) | O1—Zn1 | 1.9649 (13) |

| | | | |
|---|---|---|---|
| C12—N11 | 1.367 (2) | O2—Zn1 | 1.9472 (13) |
| | | | |
| C3—C2—N1 | 120.57 (15) | O2—C14—C15 | 124.24 (17) |
| C3—C2—C9 | 120.36 (17) | C13—C14—C15 | 115.41 (16) |
| N1—C2—C9 | 119.07 (16) | C16—C15—C14 | 121.93 (18) |
| C2—C3—C4 | 121.94 (16) | C16—C15—H15 | 119.0 |
| C2—C3—H3 | 119.0 | C14—C15—H15 | 119.0 |
| C4—C3—H3 | 119.0 | C15—C16—N11 | 120.19 (17) |
| O1—C4—C5 | 120.54 (16) | C15—C16—C20 | 120.50 (19) |
| O1—C4—C3 | 124.33 (17) | N11—C16—C20 | 119.30 (17) |
| C5—C4—C3 | 115.12 (15) | N11—C17—C18 | 112.90 (17) |
| C6—C5—C4 | 122.31 (16) | N11—C17—H17A | 109.0 |
| C6—C5—H5 | 118.8 | C18—C17—H17A | 109.0 |
| C4—C5—H5 | 118.8 | N11—C17—H17B | 109.0 |
| C5—C6—N1 | 120.23 (16) | C18—C17—H17B | 109.0 |
| C5—C6—C10 | 120.08 (17) | H17A—C17—H17B | 107.8 |
| N1—C6—C10 | 119.67 (16) | C17—C18—H18A | 109.5 |
| N1—C7—C8 | 112.78 (16) | C17—C18—H18B | 109.5 |
| N1—C7—H7A | 109.0 | H18A—C18—H18B | 109.5 |
| C8—C7—H7A | 109.0 | C17—C18—H18C | 109.5 |
| N1—C7—H7B | 109.0 | H18A—C18—H18C | 109.5 |
| C8—C7—H7B | 109.0 | H18B—C18—H18C | 109.5 |
| H7A—C7—H7B | 107.8 | C12—C19—H19A | 109.5 |
| C7—C8—H8A | 109.5 | C12—C19—H19B | 109.5 |
| C7—C8—H8B | 109.5 | H19A—C19—H19B | 109.5 |
| H8A—C8—H8B | 109.5 | C12—C19—H19C | 109.5 |
| C7—C8—H8C | 109.5 | H19A—C19—H19C | 109.5 |
| H8A—C8—H8C | 109.5 | H19B—C19—H19C | 109.5 |
| H8B—C8—H8C | 109.5 | C16—C20—H20A | 109.5 |
| C2—C9—H9A | 109.5 | C16—C20—H20B | 109.5 |
| C2—C9—H9B | 109.5 | H20A—C20—H20B | 109.5 |
| H9A—C9—H9B | 109.5 | C16—C20—H20C | 109.5 |
| C2—C9—H9C | 109.5 | H20A—C20—H20C | 109.5 |
| H9A—C9—H9C | 109.5 | H20B—C20—H20C | 109.5 |
| H9B—C9—H9C | 109.5 | C2—N1—C6 | 119.74 (14) |
| C6—C10—H10A | 109.5 | C2—N1—C7 | 120.04 (15) |
| C6—C10—H10B | 109.5 | C6—N1—C7 | 120.21 (15) |
| H10A—C10—H10B | 109.5 | C12—N11—C16 | 119.99 (15) |
| C6—C10—H10C | 109.5 | C12—N11—C17 | 119.84 (15) |
| H10A—C10—H10C | 109.5 | C16—N11—C17 | 120.15 (16) |
| H10B—C10—H10C | 109.5 | C4—O1—Zn1 | 134.31 (12) |
| C13—C12—N11 | 120.20 (16) | C14—O2—Zn1 | 133.29 (12) |
| C13—C12—C19 | 120.27 (17) | O2—Zn1—O1 | 98.22 (6) |
| N11—C12—C19 | 119.51 (16) | O2—Zn1—Cl1 | 107.99 (5) |
| C12—C13—C14 | 122.15 (17) | O1—Zn1—Cl1 | 114.29 (5) |
| C12—C13—H13 | 118.9 | O2—Zn1—Cl2 | 115.09 (4) |
| C14—C13—H13 | 118.9 | O1—Zn1—Cl2 | 105.10 (5) |
| O2—C14—C13 | 120.34 (16) | Cl1—Zn1—Cl2 | 115.06 (2) |

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|---|---|---|---|
| N1—C2—C3—C4 | 0.7 (3) | C10—C6—N1—C7 | 4.0 (2) |
| C9—C2—C3—C4 | −179.34 (17) | C8—C7—N1—C2 | 93.7 (2) |
| C2—C3—C4—O1 | −179.80 (18) | C8—C7—N1—C6 | −85.9 (2) |
| C2—C3—C4—C5 | 1.7 (3) | C13—C12—N11—C16 | −3.0 (3) |
| O1—C4—C5—C6 | 179.59 (18) | C19—C12—N11—C16 | 178.4 (2) |
| C3—C4—C5—C6 | −1.8 (3) | C13—C12—N11—C17 | 175.60 (18) |
| C4—C5—C6—N1 | −0.4 (3) | C19—C12—N11—C17 | −3.0 (3) |
| C4—C5—C6—C10 | 178.01 (17) | C15—C16—N11—C12 | 2.7 (3) |
| N11—C12—C13—C14 | 0.2 (3) | C20—C16—N11—C12 | −178.4 (2) |
| C19—C12—C13—C14 | 178.8 (2) | C15—C16—N11—C17 | −175.92 (18) |
| C12—C13—C14—O2 | −178.01 (19) | C20—C16—N11—C17 | 3.0 (3) |
| C12—C13—C14—C15 | 2.7 (3) | C18—C17—N11—C12 | 90.0 (2) |
| O2—C14—C15—C16 | 177.7 (2) | C18—C17—N11—C16 | −91.4 (2) |
| C13—C14—C15—C16 | −3.0 (3) | C5—C4—O1—Zn1 | −160.08 (14) |
| C14—C15—C16—N11 | 0.4 (3) | C3—C4—O1—Zn1 | 21.5 (3) |
| C14—C15—C16—C20 | −178.5 (2) | C13—C14—O2—Zn1 | 169.24 (15) |
| C3—C2—N1—C6 | −3.1 (3) | C15—C14—O2—Zn1 | −11.6 (3) |
| C9—C2—N1—C6 | 176.98 (17) | C14—O2—Zn1—O1 | −127.09 (19) |
| C3—C2—N1—C7 | 177.37 (16) | C14—O2—Zn1—Cl1 | 113.97 (19) |
| C9—C2—N1—C7 | −2.6 (2) | C14—O2—Zn1—Cl2 | −16.1 (2) |
| C5—C6—N1—C2 | 2.9 (3) | C4—O1—Zn1—O2 | −159.12 (19) |
| C10—C6—N1—C2 | −175.51 (17) | C4—O1—Zn1—Cl1 | −45.1 (2) |
| C5—C6—N1—C7 | −177.53 (17) | C4—O1—Zn1—Cl2 | 82.02 (19) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C8—H8*A*···O1$^{i}$ | 0.96 | 2.53 | 3.344 (3) | 143 |
| C10—H10*A*···Cl1$^{ii}$ | 0.96 | 2.82 | 3.740 (2) | 162 |
| C10—H10*C*···Cl1$^{iii}$ | 0.96 | 2.82 | 3.745 (2) | 162 |
| C13—H13···Cl2$^{iv}$ | 0.93 | 2.82 | 3.709 (2) | 161 |

Symmetry codes: (i) −*x*, *y*, −*z*+1/2; (ii) −*x*, *y*+1, −*z*+1/2; (iii) *x*, *y*+1, *z*; (iv) *x*, −*y*+2, *z*+1/2.