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# Bis(1,10-phenanthrolin-1-ium) tetrachloridozincate monohydrate

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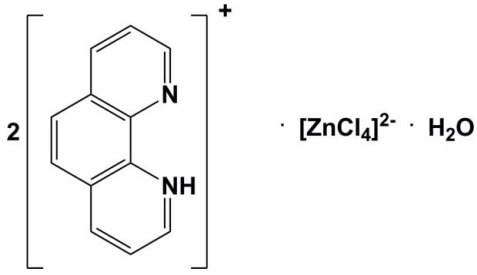
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.031; $wR$ factor = 0.068; data-to-parameter ratio = 13.2.

In the crystal structure of the title compound, $(C_{12}H_9N_2)_2[ZnCl_4]\cdot H_2O$, the two independent 1,10-phenanthrolinium cations are bridged by the water molecule and the tetrahedral tetrachloridozincate anion *via* N—H···O, O—H···Cl and N—H···Cl hydrogen bonds, forming chains along [100]. The chains are linked *via* C—H···Cl hydrogen bonds and a number of $\pi$–$\pi$ interactions [centroid–centroid distances vary from 3.5594 (14) to 3.7057 (13) Å], forming a three-dimensional network. In each 1,10-phenanthrolinium cation, there is a short N—H···N interaction.

## Related literature

For an example of the crystal structure of a hybrid compound combining an organic cation and the tetrachloridozincate anion, see: Dong & Liu (2012). For details of the Cambridge Structural Database, see: Allen (2002).




## Experimental

### Crystal data

$(C_{12}H_9N_2)_2[ZnCl_4]\cdot H_2O$
$M_r$ = 587.61
Monoclinic, $P2_1/a$
$a$ = 14.6046 (5) Å
$b$ = 10.8008 (3) Å
$c$ = 16.3151 (6) Å
$\beta$ = 107.390 (4)°
$V$ = 2455.93 (14) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 1.46 mm$^{-1}$
$T$ = 293 K
0.21 × 0.18 × 0.15 mm

### Data collection

Oxford Diffraction Xcalibur diffractometer with Eos detector
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2009)
$T_{min}$ = 0.743, $T_{max}$ = 0.803
10373 measured reflections
4293 independent reflections
3414 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.028

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.068
$S$ = 1.05
4293 reflections
324 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.38 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.29 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1···O1$^{i}$ | 0.74 (3) | 2.01 (3) | 2.711 (4) | 158 (2) |
| O1—H1$A$···Cl1 | 0.80 (4) | 2.44 (4) | 3.231 (3) | 172 (3) |
| O1—H1$B$···Cl2$^{ii}$ | 0.73 (3) | 2.82 (4) | 3.317 (3) | 128 (4) |
| N15—H15···Cl3 | 0.83 (3) | 2.50 (2) | 3.225 (2) | 146 (2) |
| C3—H3···Cl2$^{iii}$ | 0.93 | 2.80 | 3.728 (3) | 172 |
| C24—H24···Cl2$^{iv}$ | 0.93 | 2.74 | 3.629 (3) | 160 |
| N1—H1···N12 | 0.74 (3) | 2.42 (2) | 2.737 (3) | 107 (2) |
| N15—H15···N26 | 0.83 (3) | 2.41 (2) | 2.731 (3) | 104 (2) |

Symmetry codes: (i) $x+\frac{1}{2}, -y+\frac{3}{2}, z$; (ii) $x-\frac{1}{2}, -y+\frac{1}{2}, z$; (iii) $-x, -y+2, -z+1$; (iv) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+2$.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2009); cell refinement: *CrysAlis CCD*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2009); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008) and *PLATON* (Spek, 2009).

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Supporting information for this paper is available from the IUCr electronic archives (Reference: SU2681).

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# supporting information

*Acta Cryst.* (2014). E**70**, m53 [doi:10.1107/S1600536814000208]

## Bis(1,10-phenanthrolin-1-ium) tetrachloridozincate monohydrate

**E. Govindan, Subramani Thirumurugan, Ayyakannu Sundaram Ganeshraja, Krishnamoorthy Anbalagan and A. SubbiahPandi**

### S1. Comment

As part of an ongoing investigation of the structures of and non-covalent interactions present in self-assembling organic and inorganic hybrid materials prepared by the combination of an organic cation and the tetrachloridozincate anion we synthesized the title compound. There are only a small number of structures of materials containing bis(1,10-phenanthrolinium) cations and perhalometallate anions in the Cambridge Structural Database (CSD; V5.35, last update Nov. 2013; Allen, 2002), and none of them involve the tetrachloridozincate anion.

The molecule structure of the title compound is shown in Fig. 1. The asymmetric unit contains one inorganic tetrachloridozincate anion and two 1,10-phenanthrolinium organic cations. The compound crystallized as a monohydrate. The tetrachlorozincate anion has a perfect tetrahedral coordination environment. The bond lengths Zn—Cl [2.556 (7) - 2.3085 (7) Å] and C—N [1.320 (3) - 1.362 (3) Å] are comparable with the values reported for Bis(10-methoxy-benzo[*h*]quinolinium) tetrachloridozinc [Dong & Liu, 2012]. The sum of the bond angles around atoms N1 and N15 (360°) in the 1,10-phenanthrolinium cations indicates $sp^2$ hybridization states. The two 1,10-phenanthrolinium ring systems (N1/N12/C2-C11/C13/C14) and (N15/N26/C16-C25/C27/C28) are planar with r.m.s values of 0.029 (3) and 0.022 (2) Å, respectively. In each 1,10-phenanthrolinium cation there is a short N-H···N interaction (Table 1).

In the crystal, the two independent 1,10-phenanthrolinium cations are bridged by the water molecule and the tetrachloridozinc anion via N-H···O, O-H···Cl and N-H···Cl hydrogen bonds (Table 1 and Fig. 2) forming chains along [100]. The chains are linked via C-H···Cl hydrogen bonds (Table 1) and a number of $\pi$-$\pi$ interactions forming a three-dimensional network.

The centroid-centroid distances are 3.5594 (14) Å for Cg1···Cg2$^{i}$ [Cg1 and Cg2 and the centroids of rings N1/C2-C5/C14 and N12/C8-C11/C13, respectively; symmetry code: (i) = -x, -y+2, -z+1 ], 3.6501 (15) Å for Cg1···Cg3$^{i}$ [Cg3 is the centroid of ring C5-C8/C13/C14] and 3.7057 (13) Å for Cg8···Cg9$^{ii}$ [Cg8 and Cg9 are the centroids of rings N26/C22-C25/C27 and C19-C22/C27/C28, respectively; symmetry code: (ii) -x, -y, -z+2].

### S2. Experimental

Zinc chloride (136 mg, 1 mmol) was dissolved in 10 mL of water. To this 1,10-phenanthroline (396 mg, 2 mmol) in 20 ml of an EtOH/HCl mixture (1:9 *v*/*v*) was added drop wise. The mixture was heated to 323 K for 2–3 hrs and then allowed to stand. On slow evaporation colourless crystals separated out. They were filtered off and recrystallized using acidified water.

### S3. Refinement

The NH and water H atoms were located in a difference Fourier map and freely refined. The C bound H atoms were positioned geometrically and allowed to ride on their parent atoms: C–H = 0.93 Å with $U_{iso}$(H) = 1.2$U_{eq}$(C).

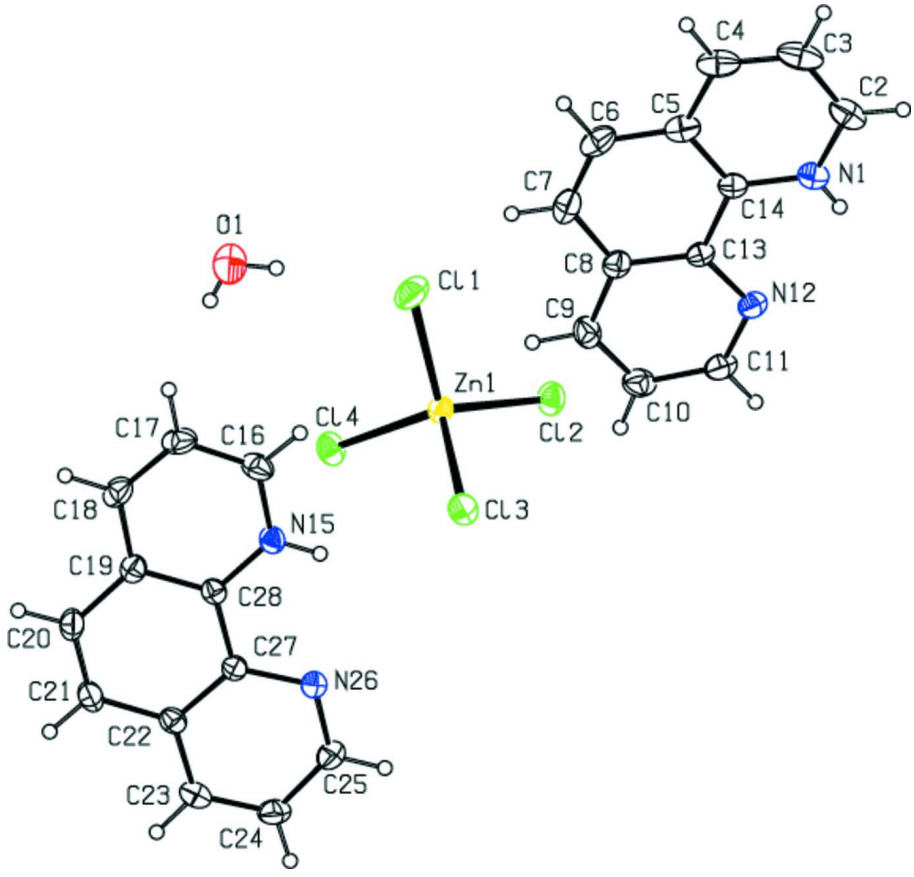


**Figure 1**

The molecular structure of the title compound, with the atom labelling. Displacement ellipsoids are drawn at 30% probability level.

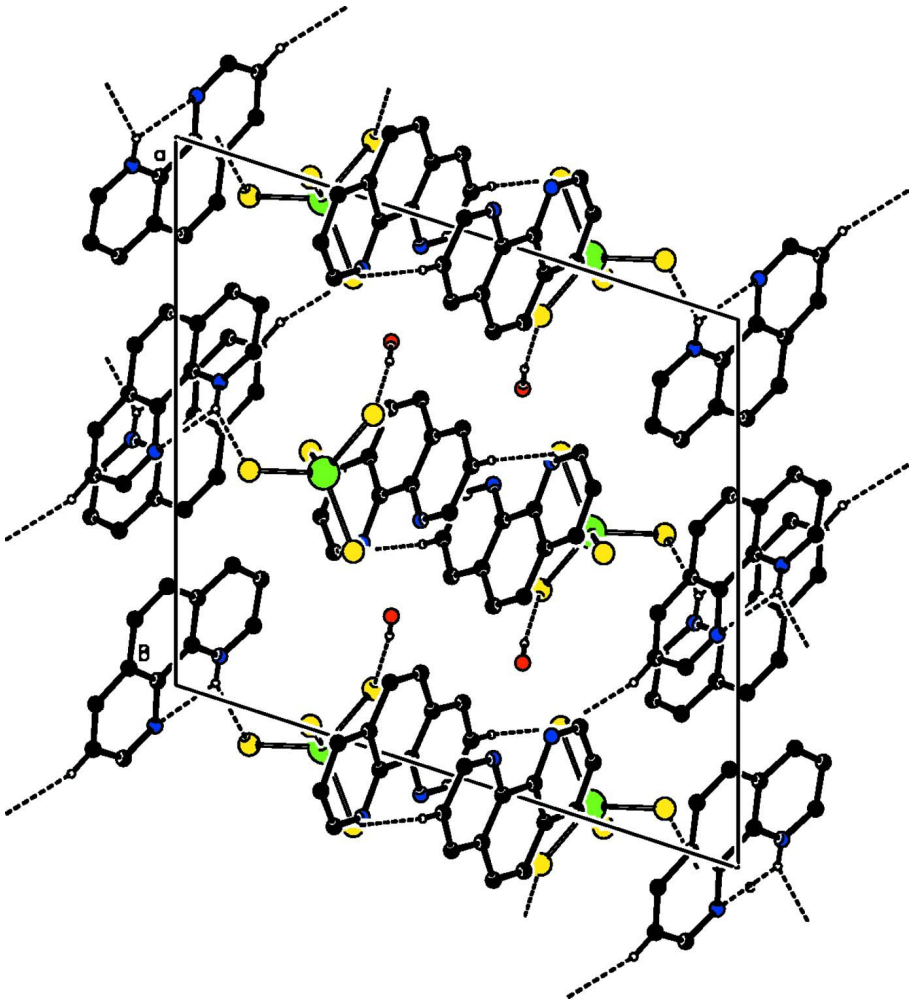


**Figure 2**

A view along the *b*-axis of the crystal packing of the title compound. Hydrogen bonds are shown as dashed lines (see Table 1 for details).

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*Crystal data*

$(C_{12}H_9N_2)_2[ZnCl_4]\cdot H_2O$
$M_r = 587.61$
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Hall symbol: -P 2yab
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$c = 16.3151\ (6)$ Å
$\beta = 107.390\ (4)°$
$V = 2455.93\ (14)$ Å$^3$
$Z = 4$
$F(000) = 1192$
$D_x = 1.589$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3414 reflections
$\theta = 3.8–25.0°$
$\mu = 1.46$ mm$^{-1}$
$T = 293$ K
Block, colourless
0.21 × 0.18 × 0.15 mm

*Data collection*

Oxford Diffraction Xcalibur diffractometer with Eos detector
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$ and $\varphi$ scans
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2009)
$T_{min}$ = 0.743, $T_{max}$ = 0.803
10373 measured reflections
4293 independent reflections
3414 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.028
$\theta_{max}$ = 25.0°, $\theta_{min}$ = 3.8°
$h$ = −17→17
$k$ = −11→12
$l$ = −19→19

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.068
$S$ = 1.05
4293 reflections
324 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0278P)^2 + 0.2557P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.38 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.29 e Å$^{-3}$
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0165 (5)

*Special details*

**Geometry**. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

**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 (Å²)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| N1 | 0.05391 (18) | 1.17583 (19) | 0.56437 (14) | 0.0382 (8) |
| N12 | 0.13002 (14) | 0.97933 (17) | 0.66837 (13) | 0.0364 (7) |
| C2 | 0.0227 (2) | 1.2729 (2) | 0.51338 (17) | 0.0498 (10) |
| C3 | −0.0746 (2) | 1.2890 (3) | 0.47489 (18) | 0.0574 (10) |
| C4 | −0.1379 (2) | 1.2056 (3) | 0.49016 (18) | 0.0533 (11) |
| C5 | −0.10528 (18) | 1.1038 (2) | 0.54406 (16) | 0.0401 (9) |
| C6 | −0.16693 (19) | 1.0148 (3) | 0.56456 (18) | 0.0497 (10) |
| C7 | −0.13202 (18) | 0.9219 (3) | 0.61895 (18) | 0.0475 (10) |
| C8 | −0.03095 (17) | 0.9048 (2) | 0.65657 (15) | 0.0354 (8) |
| C9 | 0.0097 (2) | 0.8067 (2) | 0.71173 (17) | 0.0437 (9) |
| C10 | 0.1068 (2) | 0.7959 (2) | 0.74208 (18) | 0.0469 (10) |
| C11 | 0.16361 (19) | 0.8837 (2) | 0.71874 (16) | 0.0427 (9) |
| C13 | 0.03328 (16) | 0.9889 (2) | 0.63748 (14) | 0.0293 (7) |
| C14 | −0.00593 (17) | 1.0909 (2) | 0.58142 (14) | 0.0306 (8) |
| N15 | −0.07856 (15) | 0.34171 (18) | 0.92218 (13) | 0.0339 (7) |

| | | | | |
|---|---|---|---|---|
| N26 | 0.08664 (14) | 0.25794 (18) | 1.03725 (13) | 0.0378 (7) |
| C16 | −0.15449 (18) | 0.3854 (2) | 0.86201 (17) | 0.0424 (9) |
| C17 | −0.24346 (18) | 0.3314 (3) | 0.84870 (17) | 0.0460 (9) |
| C18 | −0.25201 (17) | 0.2333 (2) | 0.89907 (17) | 0.0428 (9) |
| C19 | −0.17174 (16) | 0.1862 (2) | 0.96188 (15) | 0.0339 (8) |
| C20 | −0.17495 (18) | 0.0817 (2) | 1.01531 (17) | 0.0411 (9) |
| C21 | −0.09527 (18) | 0.0398 (2) | 1.07310 (16) | 0.0407 (9) |
| C22 | −0.00318 (17) | 0.0967 (2) | 1.08369 (15) | 0.0327 (8) |
| C23 | 0.08261 (19) | 0.0549 (2) | 1.14257 (16) | 0.0417 (9) |
| C24 | 0.16602 (19) | 0.1130 (2) | 1.14723 (17) | 0.0473 (9) |
| C25 | 0.16456 (18) | 0.2136 (3) | 1.09347 (18) | 0.0470 (9) |
| C27 | 0.00304 (16) | 0.1986 (2) | 1.03291 (15) | 0.0291 (7) |
| C28 | −0.08273 (16) | 0.2437 (2) | 0.97183 (15) | 0.0287 (7) |
| Zn1 | 0.02573 (2) | 0.43561 (2) | 0.73719 (2) | 0.0324 (1) |
| Cl1 | −0.11018 (5) | 0.52315 (6) | 0.64898 (5) | 0.0584 (3) |
| Cl2 | 0.15128 (4) | 0.45542 (6) | 0.68453 (4) | 0.0445 (2) |
| Cl3 | 0.06504 (5) | 0.53130 (5) | 0.86969 (4) | 0.0429 (2) |
| Cl4 | −0.00552 (5) | 0.23479 (5) | 0.76075 (4) | 0.0433 (2) |
| O1 | −0.25358 (17) | 0.2883 (3) | 0.61679 (19) | 0.0609 (9) |
| H1 | 0.1064 (18) | 1.169 (2) | 0.5852 (17) | 0.033 (8)* |
| H2 | 0.06620 | 1.32970 | 0.50370 | 0.0600* |
| H3 | −0.09690 | 1.35620 | 0.43880 | 0.0690* |
| H4 | −0.20340 | 1.21660 | 0.46450 | 0.0640* |
| H6 | −0.23290 | 1.02140 | 0.53950 | 0.0600* |
| H7 | −0.17430 | 0.86710 | 0.63270 | 0.0570* |
| H9 | −0.02950 | 0.74930 | 0.72740 | 0.0530* |
| H10 | 0.13470 | 0.73060 | 0.77800 | 0.0560* |
| H11 | 0.22980 | 0.87460 | 0.74000 | 0.0510* |
| H15 | −0.0270 (18) | 0.379 (2) | 0.9296 (16) | 0.040 (8)* |
| H16 | −0.14770 | 0.45270 | 0.82870 | 0.0510* |
| H17 | −0.29670 | 0.36120 | 0.80630 | 0.0550* |
| H18 | −0.31190 | 0.19750 | 0.89150 | 0.0510* |
| H20 | −0.23320 | 0.04250 | 1.00970 | 0.0490* |
| H21 | −0.09940 | −0.02770 | 1.10720 | 0.0490* |
| H23 | 0.08200 | −0.01220 | 1.17810 | 0.0500* |
| H24 | 0.22340 | 0.08620 | 1.18570 | 0.0570* |
| H25 | 0.22260 | 0.25230 | 1.09750 | 0.0560* |
| H1A | −0.217 (3) | 0.344 (3) | 0.620 (2) | 0.083 (15)* |
| H1B | −0.239 (3) | 0.241 (3) | 0.650 (2) | 0.079 (16)* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| N1 | 0.0427 (15) | 0.0374 (13) | 0.0337 (13) | 0.0058 (11) | 0.0103 (11) | 0.0005 (10) |
| N12 | 0.0342 (11) | 0.0336 (11) | 0.0368 (12) | 0.0014 (9) | 0.0034 (9) | −0.0013 (9) |
| C2 | 0.081 (2) | 0.0349 (15) | 0.0369 (17) | 0.0056 (14) | 0.0228 (15) | 0.0018 (12) |
| C3 | 0.087 (2) | 0.0461 (17) | 0.0368 (17) | 0.0339 (17) | 0.0149 (16) | 0.0047 (13) |
| C4 | 0.0546 (18) | 0.066 (2) | 0.0358 (17) | 0.0293 (16) | 0.0081 (14) | −0.0022 (14) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C5 | 0.0395 (15) | 0.0489 (15) | 0.0312 (15) | 0.0145 (12) | 0.0096 (12) | −0.0083 (12) |
| C6 | 0.0301 (14) | 0.0680 (19) | 0.0472 (18) | 0.0052 (14) | 0.0058 (13) | −0.0136 (15) |
| C7 | 0.0374 (15) | 0.0549 (17) | 0.0524 (18) | −0.0112 (13) | 0.0168 (13) | −0.0128 (14) |
| C8 | 0.0396 (14) | 0.0367 (13) | 0.0299 (14) | −0.0049 (11) | 0.0105 (11) | −0.0108 (11) |
| C9 | 0.0582 (18) | 0.0342 (14) | 0.0405 (16) | −0.0133 (13) | 0.0173 (14) | −0.0057 (12) |
| C10 | 0.0600 (19) | 0.0330 (14) | 0.0402 (16) | 0.0000 (13) | 0.0036 (14) | 0.0023 (12) |
| C11 | 0.0407 (15) | 0.0394 (14) | 0.0388 (16) | 0.0024 (12) | −0.0019 (12) | −0.0012 (12) |
| C13 | 0.0325 (13) | 0.0291 (12) | 0.0248 (13) | 0.0011 (10) | 0.0062 (10) | −0.0079 (10) |
| C14 | 0.0365 (13) | 0.0317 (13) | 0.0241 (13) | 0.0034 (11) | 0.0099 (11) | −0.0065 (10) |
| N15 | 0.0305 (12) | 0.0374 (12) | 0.0362 (13) | 0.0010 (10) | 0.0138 (10) | 0.0036 (10) |
| N26 | 0.0319 (11) | 0.0453 (12) | 0.0355 (13) | −0.0040 (9) | 0.0090 (9) | 0.0053 (10) |
| C16 | 0.0423 (15) | 0.0481 (15) | 0.0396 (16) | 0.0136 (13) | 0.0164 (12) | 0.0134 (12) |
| C17 | 0.0326 (15) | 0.0642 (18) | 0.0382 (16) | 0.0129 (13) | 0.0059 (12) | 0.0039 (14) |
| C18 | 0.0282 (13) | 0.0558 (17) | 0.0437 (17) | −0.0009 (12) | 0.0098 (12) | −0.0058 (13) |
| C19 | 0.0320 (13) | 0.0379 (13) | 0.0340 (15) | −0.0021 (11) | 0.0131 (11) | −0.0053 (11) |
| C20 | 0.0382 (15) | 0.0454 (15) | 0.0435 (16) | −0.0125 (12) | 0.0180 (13) | −0.0040 (13) |
| C21 | 0.0482 (16) | 0.0377 (14) | 0.0404 (16) | −0.0082 (12) | 0.0195 (13) | 0.0033 (12) |
| C22 | 0.0389 (14) | 0.0338 (13) | 0.0277 (13) | 0.0002 (11) | 0.0137 (11) | −0.0008 (11) |
| C23 | 0.0520 (17) | 0.0420 (15) | 0.0316 (15) | 0.0045 (13) | 0.0133 (12) | 0.0067 (12) |
| C24 | 0.0388 (15) | 0.0594 (17) | 0.0373 (16) | 0.0056 (13) | 0.0015 (12) | 0.0101 (14) |
| C25 | 0.0305 (14) | 0.0625 (18) | 0.0444 (17) | −0.0057 (13) | 0.0057 (12) | 0.0052 (14) |
| C27 | 0.0302 (12) | 0.0321 (13) | 0.0264 (13) | −0.0010 (10) | 0.0106 (10) | −0.0030 (10) |
| C28 | 0.0336 (13) | 0.0285 (12) | 0.0267 (13) | −0.0002 (10) | 0.0132 (10) | −0.0025 (10) |
| Zn1 | 0.0315 (2) | 0.0318 (2) | 0.0336 (2) | −0.0033 (1) | 0.0091 (1) | −0.0023 (1) |
| Cl1 | 0.0373 (4) | 0.0486 (4) | 0.0735 (5) | −0.0010 (3) | −0.0074 (3) | 0.0052 (4) |
| Cl2 | 0.0409 (4) | 0.0505 (4) | 0.0470 (4) | −0.0073 (3) | 0.0208 (3) | −0.0059 (3) |
| Cl3 | 0.0575 (4) | 0.0369 (3) | 0.0369 (4) | −0.0085 (3) | 0.0182 (3) | −0.0086 (3) |
| Cl4 | 0.0575 (4) | 0.0299 (3) | 0.0460 (4) | −0.0072 (3) | 0.0210 (3) | −0.0050 (3) |
| O1 | 0.0530 (14) | 0.0493 (14) | 0.083 (2) | 0.0033 (13) | 0.0242 (13) | 0.0021 (14) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Zn1—Cl4 | 2.2728 (6) | C2—H2 | 0.9300 |
| Zn1—Cl1 | 2.2798 (8) | C3—H3 | 0.9300 |
| Zn1—Cl2 | 2.2556 (7) | C4—H4 | 0.9300 |
| Zn1—Cl3 | 2.3085 (7) | C6—H6 | 0.9300 |
| O1—H1A | 0.80 (4) | C7—H7 | 0.9300 |
| O1—H1B | 0.73 (3) | C9—H9 | 0.9300 |
| N1—C2 | 1.331 (3) | C10—H10 | 0.9300 |
| N1—C14 | 1.352 (3) | C11—H11 | 0.9300 |
| N12—C13 | 1.355 (3) | C16—C17 | 1.381 (4) |
| N12—C11 | 1.320 (3) | C17—C18 | 1.369 (4) |
| N1—H1 | 0.74 (3) | C18—C19 | 1.402 (3) |
| N15—C28 | 1.345 (3) | C19—C20 | 1.435 (3) |
| N15—C16 | 1.329 (3) | C19—C28 | 1.406 (3) |
| N26—C25 | 1.320 (4) | C20—C21 | 1.339 (4) |
| N26—C27 | 1.362 (3) | C21—C22 | 1.441 (4) |
| N15—H15 | 0.83 (3) | C22—C27 | 1.397 (3) |

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| C2—C3 | 1.382 (4) | C22—C23 | 1.406 (4) |
| C3—C4 | 1.366 (4) | C23—C24 | 1.352 (4) |
| C4—C5 | 1.400 (4) | C24—C25 | 1.393 (4) |
| C5—C6 | 1.424 (4) | C27—C28 | 1.433 (3) |
| C5—C14 | 1.403 (4) | C16—H16 | 0.9300 |
| C6—C7 | 1.336 (4) | C17—H17 | 0.9300 |
| C7—C8 | 1.431 (4) | C18—H18 | 0.9300 |
| C8—C13 | 1.406 (3) | C20—H20 | 0.9300 |
| C8—C9 | 1.402 (3) | C21—H21 | 0.9300 |
| C9—C10 | 1.360 (4) | C23—H23 | 0.9300 |
| C10—C11 | 1.386 (4) | C24—H24 | 0.9300 |
| C13—C14 | 1.437 (3) | C25—H25 | 0.9300 |

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| Cl3—Zn1—Cl4 | 105.98 (2) | C8—C7—H7 | 119.00 |
| Cl1—Zn1—Cl4 | 108.76 (3) | C8—C9—H9 | 120.00 |
| Cl1—Zn1—Cl2 | 111.95 (3) | C10—C9—H9 | 120.00 |
| Cl1—Zn1—Cl3 | 109.35 (3) | C9—C10—H10 | 120.00 |
| Cl2—Zn1—Cl3 | 108.14 (3) | C11—C10—H10 | 120.00 |
| Cl2—Zn1—Cl4 | 112.47 (3) | N12—C11—H11 | 118.00 |
| H1A—O1—H1B | 116 (4) | C10—C11—H11 | 118.00 |
| C2—N1—C14 | 122.8 (3) | N15—C16—C17 | 120.3 (2) |
| C11—N12—C13 | 116.3 (2) | C16—C17—C18 | 118.9 (2) |
| C14—N1—H1 | 118.7 (18) | C17—C18—C19 | 120.9 (2) |
| C2—N1—H1 | 118.5 (18) | C18—C19—C28 | 117.8 (2) |
| C16—N15—C28 | 123.1 (2) | C18—C19—C20 | 123.9 (2) |
| C25—N26—C27 | 116.0 (2) | C20—C19—C28 | 118.3 (2) |
| C28—N15—H15 | 119.8 (16) | C19—C20—C21 | 121.0 (2) |
| C16—N15—H15 | 117.1 (16) | C20—C21—C22 | 121.6 (2) |
| N1—C2—C3 | 119.8 (3) | C21—C22—C27 | 119.3 (2) |
| C2—C3—C4 | 119.6 (3) | C23—C22—C27 | 117.1 (2) |
| C3—C4—C5 | 120.7 (3) | C21—C22—C23 | 123.6 (2) |
| C4—C5—C14 | 117.7 (2) | C22—C23—C24 | 119.6 (2) |
| C4—C5—C6 | 123.9 (3) | C23—C24—C25 | 118.9 (2) |
| C6—C5—C14 | 118.4 (2) | N26—C25—C24 | 124.7 (3) |
| C5—C6—C7 | 121.4 (3) | C22—C27—C28 | 118.8 (2) |
| C6—C7—C8 | 121.5 (3) | N26—C27—C28 | 117.4 (2) |
| C9—C8—C13 | 116.6 (2) | N26—C27—C22 | 123.8 (2) |
| C7—C8—C13 | 119.5 (2) | C19—C28—C27 | 121.1 (2) |
| C7—C8—C9 | 123.9 (2) | N15—C28—C19 | 119.0 (2) |
| C8—C9—C10 | 119.6 (2) | N15—C28—C27 | 119.9 (2) |
| C9—C10—C11 | 119.1 (2) | N15—C16—H16 | 120.00 |
| N12—C11—C10 | 124.4 (3) | C17—C16—H16 | 120.00 |
| C8—C13—C14 | 118.1 (2) | C18—C17—H17 | 121.00 |
| N12—C13—C14 | 117.9 (2) | C16—C17—H17 | 121.00 |
| N12—C13—C8 | 124.0 (2) | C17—C18—H18 | 120.00 |
| N1—C14—C5 | 119.4 (2) | C19—C18—H18 | 120.00 |
| N1—C14—C13 | 119.5 (2) | C21—C20—H20 | 120.00 |
| C5—C14—C13 | 121.1 (2) | C19—C20—H20 | 120.00 |

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|---|---|---|---|
| N1—C2—H2 | 120.00 | C20—C21—H21 | 119.00 |
| C3—C2—H2 | 120.00 | C22—C21—H21 | 119.00 |
| C4—C3—H3 | 120.00 | C22—C23—H23 | 120.00 |
| C2—C3—H3 | 120.00 | C24—C23—H23 | 120.00 |
| C3—C4—H4 | 120.00 | C23—C24—H24 | 121.00 |
| C5—C4—H4 | 120.00 | C25—C24—H24 | 121.00 |
| C5—C6—H6 | 119.00 | N26—C25—H25 | 118.00 |
| C7—C6—H6 | 119.00 | C24—C25—H25 | 118.00 |
| C6—C7—H7 | 119.00 | | |

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| C14—N1—C2—C3 | −0.6 (4) | C8—C9—C10—C11 | 1.0 (4) |
| C2—N1—C14—C13 | −179.7 (2) | C9—C10—C11—N12 | 0.2 (4) |
| C2—N1—C14—C5 | 0.3 (4) | C8—C13—C14—C5 | −2.4 (3) |
| C11—N12—C13—C14 | −179.1 (2) | N12—C13—C14—C5 | 177.2 (2) |
| C11—N12—C13—C8 | 0.5 (3) | C8—C13—C14—N1 | 177.6 (2) |
| C13—N12—C11—C10 | −0.9 (4) | N12—C13—C14—N1 | −2.7 (3) |
| C16—N15—C28—C27 | 177.3 (2) | N15—C16—C17—C18 | 0.7 (4) |
| C28—N15—C16—C17 | 1.0 (4) | C16—C17—C18—C19 | −1.4 (4) |
| C16—N15—C28—C19 | −1.9 (3) | C17—C18—C19—C28 | 0.6 (4) |
| C25—N26—C27—C28 | −179.4 (2) | C17—C18—C19—C20 | −178.3 (2) |
| C25—N26—C27—C22 | 0.0 (3) | C20—C19—C28—C27 | 0.8 (3) |
| C27—N26—C25—C24 | −0.3 (4) | C18—C19—C20—C21 | 178.7 (2) |
| N1—C2—C3—C4 | 0.6 (4) | C28—C19—C20—C21 | −0.1 (4) |
| C2—C3—C4—C5 | −0.3 (4) | C18—C19—C28—C27 | −178.2 (2) |
| C3—C4—C5—C14 | 0.0 (4) | C20—C19—C28—N15 | 180.0 (2) |
| C3—C4—C5—C6 | 178.5 (3) | C18—C19—C28—N15 | 1.1 (3) |
| C4—C5—C14—N1 | 0.0 (4) | C19—C20—C21—C22 | −0.5 (4) |
| C4—C5—C6—C7 | −177.5 (3) | C20—C21—C22—C23 | −179.0 (2) |
| C14—C5—C6—C7 | 1.0 (4) | C20—C21—C22—C27 | 0.5 (4) |
| C4—C5—C14—C13 | −180.0 (2) | C23—C22—C27—N26 | 0.3 (3) |
| C6—C5—C14—C13 | 1.5 (3) | C21—C22—C27—N26 | −179.2 (2) |
| C6—C5—C14—N1 | −178.6 (2) | C21—C22—C27—C28 | 0.2 (3) |
| C5—C6—C7—C8 | −2.4 (4) | C23—C22—C27—C28 | 179.7 (2) |
| C6—C7—C8—C9 | −177.8 (3) | C21—C22—C23—C24 | 179.1 (2) |
| C6—C7—C8—C13 | 1.4 (4) | C27—C22—C23—C24 | −0.5 (3) |
| C7—C8—C9—C10 | 177.8 (3) | C22—C23—C24—C25 | 0.3 (4) |
| C9—C8—C13—N12 | 0.6 (3) | C23—C24—C25—N26 | 0.2 (4) |
| C7—C8—C13—N12 | −178.6 (2) | N26—C27—C28—N15 | −0.6 (3) |
| C9—C8—C13—C14 | −179.7 (2) | C22—C27—C28—C19 | −0.8 (3) |
| C7—C8—C13—C14 | 1.0 (3) | N26—C27—C28—C19 | 178.6 (2) |
| C13—C8—C9—C10 | −1.4 (4) | C22—C27—C28—N15 | −180.0 (2) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1···O1$^{i}$ | 0.74 (3) | 2.01 (3) | 2.711 (4) | 158 (2) |
| O1—H1*A*···Cl1 | 0.80 (4) | 2.44 (4) | 3.231 (3) | 172 (3) |
| O1—H1*B*···Cl2$^{ii}$ | 0.73 (3) | 2.82 (4) | 3.317 (3) | 128 (4) |

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| N15—H15···Cl3 | 0.83 (3) | 2.50 (2) | 3.225 (2) | 146 (2) |
| C3—H3···Cl2$^{iii}$ | 0.93 | 2.80 | 3.728 (3) | 172 |
| C24—H24···Cl2$^{iv}$ | 0.93 | 2.74 | 3.629 (3) | 160 |
| N1—H1···N12 | 0.74 (3) | 2.42 (2) | 2.737 (3) | 107 (2) |
| N15—H15···N26 | 0.83 (3) | 2.41 (2) | 2.731 (3) | 104 (2) |

Symmetry codes: (i) $x+1/2, -y+3/2, z$; (ii) $x-1/2, -y+1/2, z$; (iii) $-x, -y+2, -z+1$; (iv) $-x+1/2, y-1/2, -z+2$.