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# *catena*-Poly[[(dichloridozinc)-$\mu$-4,4′-bis(1*H*-imidazol-1-yl)biphenyl-$\kappa^2N^3:N^{3'}$] 0.25-hydrate]

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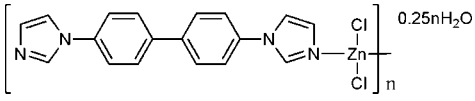
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.005 Å; disorder in solvent or counterion; $R$ factor = 0.052; $wR$ factor = 0.092; data-to-parameter ratio = 14.2.

In the title one-dimensional coordination polymer, $\{[ZnCl_2(C_{18}H_{14}N_4)]\cdot 0.25H_2O\}_n$, the $Zn^{II}$ atom is coordinated by two chloride ions and two 4,4′-bis(1*H*-imidazol-1-yl)biphenyl ligands, generating a distorted tetrahedral $ZnCl_2N_2$ geometry. The dihedral angle between the benzene rings of the ligand is 51.0 (1)° and the dihedral angles between the benzene rings and their attached imidazole rings are 18.7 (2) and 45.9 (1)°. The bridging ligand leads to [10$\bar{1}$] polymeric chains in the crystal and the disordered water molecule (occupancy 0.25) forms O—H···Cl hydrogen bonds.

## Related literature

For background to coordination polymers containing imidazole-derived ligands, see: Li *et al.* (2010, 2011).




## Experimental

### Crystal data

$[ZnCl_2(C_{18}H_{14}N_4)]\cdot 0.25H_2O$
$M_r$ = 427.11
Monoclinic, $P2_1/n$
$a$ = 8.1565 (16) Å
$b$ = 12.554 (3) Å
$c$ = 18.411 (4) Å
$\beta$ = 101.08 (3)°
$V$ = 1850.0 (6) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 1.63 mm$^{-1}$
$T$ = 293 K
0.25 × 0.22 × 0.20 mm

### Data collection

Rigaku Mercury CCD diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
$T_{min}$ = 0.687, $T_{max}$ = 0.737
15655 measured reflections
3256 independent reflections
2622 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.058

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.092
$S$ = 1.16
3256 reflections
230 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.35 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.31 e Å$^{-3}$

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

| | | | |
|---|---|---|---|
| Zn1—N1 | 2.021 (3) | Zn1—Cl2 | 2.2368 (13) |
| Zn1—N3$^{i}$ | 2.024 (3) | Zn1—Cl1 | 2.2370 (12) |

Symmetry code: (i) $x+\frac{1}{2}, -y+\frac{3}{2}, z-\frac{1}{2}$.

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1$W$—H1$A$···Cl2$^{ii}$ | 0.85 | 2.55 | 3.270 (14) | 143 |
| O1$W$—H1$B$···Cl1$^{iii}$ | 0.85 | 2.19 | 3.038 (14) | 179 |

Symmetry codes: (ii) $-x+1, -y+2, -z+1$; (iii) $x-\frac{1}{2}, -y+\frac{5}{2}, z+\frac{1}{2}$.

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); 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: HB6628).

## References

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# supporting information

*Acta Cryst.* (2012). E**68**, m406 [https://doi.org/10.1107/S1600536812009543]

## *catena*-Poly[[(dichloridozinc)-$\mu$-4,4′-bis(1*H*-imidazol-1-yl)biphenyl-$\kappa^2N^3$:$N^{3'}$] 0.25-hydrate]

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### S1. Comment

In recent years, imidazole has been well used in crystal engineering, and a large number of imidazole-containing flexible ligands have been extensively studied. However, to our knowledge, the research on imidazole ligands bearing rigid spacers is less developed (Li *et al.*, 2010; Li *et al.*, 2011).

Single-crystal X-ray diffraction analysis reveals that the title compound (I) crystallizes in the monoclinic space group P21/n. For the title compound, the geometry of the $Zn^{II}$ ion is bound by two imidazole rings of individual **L** ligands, and two chlorine anions, which illustrates a slightly distorted tetrahedral coordination environment (Fig 1). Notably, as shown in Fig. 2, the four-coordinate $Zn^{II}$ center is bridged by the ligand **L** to form an infinite one-dimensional architecture.

### S2. Experimental

A mixture of $CH_3OH$ and $H_2O$ (1:1, 8 ml), as a buffer layer, was carefully layered over a solution of $ZnCl_2$ (0.02 mmol) in $H_2O$ (6 ml). Then a solution of 4,4′-bis(1*H*-imidazol-1-yl)phenyl (**L**, 0.06 mmol) in $CH_3OH$ (6 ml) was layered over the buffer layer, and the resultant reaction was left to stand at room temperature. After *ca* three weeks, colorless block single crystals appeared at the boundary. Yield: ~25% (based on **L**).

### S3. Refinement

The dispalcement parameters for the water O atom were very large at full occupancy. When refined, its fractional occupancy converged to close to 0.25 and was then set at this value. C-bound H atoms were positioned geometrically and refined in the riding-model approximation, with C—H = 0.93Å and $U_{iso}$(H) = 1.2$U_{eq}$ (C).

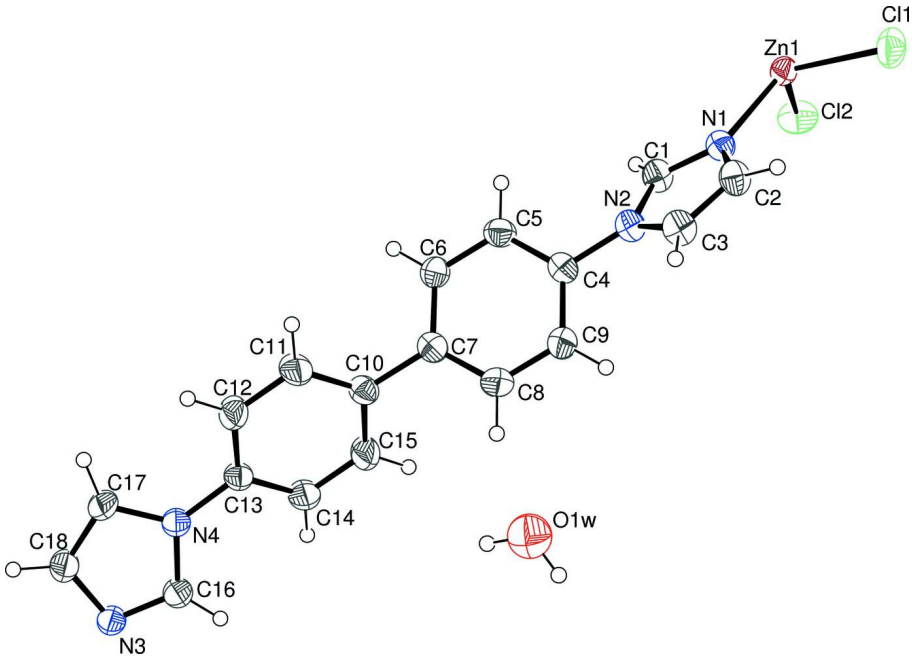


**Figure 1**

The molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level.

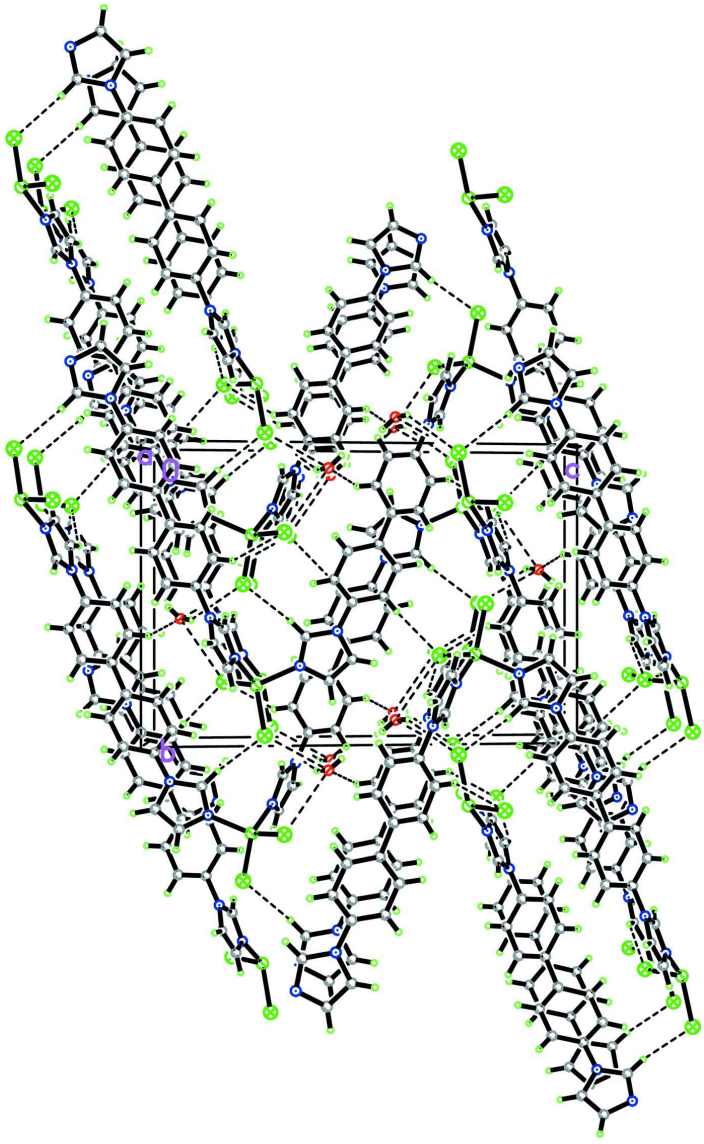

**Figure 2**

The crystal packing for (**I**).

***catena*-Poly[[(dichloridozinc)-$\mu$-4,4′-bis(1*H*- imidazol-1-yl)biphenyl-$\kappa^2N^3$:$N^{3'}$] 0.25-hydrate]**

*Crystal data*

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$b = 12.554$ (3) Å
$c = 18.411$ (4) Å
$\beta = 101.08$ (3)°
$V = 1850.0$ (6) Å$^3$
$Z = 4$
$F(000) = 866$
$D_x = 1.533$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 15648 reflections
$\theta = 3.0$–$27.6$°
$\mu = 1.63$ mm$^{-1}$
$T = 293$ K
Block, colorless
0.25 × 0.22 × 0.20 mm

*Data collection*

Rigaku Mercury CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 9 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
$T_{min}$ = 0.687, $T_{max}$ = 0.737
15655 measured reflections
3256 independent reflections
2622 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.058
$\theta_{max}$ = 25.0°, $\theta_{min}$ = 3.1°
$h$ = −9→9
$k$ = −14→14
$l$ = −21→21

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.092
$S$ = 1.16
3256 reflections
230 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
$w = 1/[\sigma^2(F_o^2) + (0.0291P)^2 + 1.2964P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.35 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.31 e Å$^{-3}$

*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$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| N3 | 0.1785 (4) | 0.2607 (2) | 0.64336 (16) | 0.0383 (8) | |
| C16 | 0.2231 (5) | 0.3586 (3) | 0.6299 (2) | 0.0405 (10) | |
| H16 | 0.2570 | 0.4097 | 0.6663 | 0.049* | |
| N4 | 0.2135 (4) | 0.3755 (2) | 0.55687 (16) | 0.0380 (8) | |
| C13 | 0.2497 (5) | 0.4730 (3) | 0.5231 (2) | 0.0370 (9) | |
| C14 | 0.3472 (6) | 0.5486 (3) | 0.5650 (2) | 0.0570 (12) | |
| H14 | 0.3939 | 0.5347 | 0.6143 | 0.068* | |
| C15 | 0.3752 (6) | 0.6452 (3) | 0.5337 (2) | 0.0566 (12) | |
| H15 | 0.4387 | 0.6964 | 0.5630 | 0.068* | |
| C10 | 0.3122 (5) | 0.6681 (3) | 0.4604 (2) | 0.0385 (9) | |
| Zn1 | 0.67056 (5) | 1.30302 (3) | 0.24360 (2) | 0.03635 (15) | |
| N1 | 0.5135 (4) | 1.2116 (2) | 0.28937 (16) | 0.0371 (8) | |
| N2 | 0.4081 (4) | 1.0778 (2) | 0.34273 (17) | 0.0385 (8) | |
| C1 | 0.5385 (5) | 1.1127 (3) | 0.3145 (2) | 0.0411 (10) | |
| H1 | 0.6337 | 1.0728 | 0.3128 | 0.049* | |
| C2 | 0.3587 (5) | 1.2400 (3) | 0.3021 (2) | 0.0430 (10) | |

| | | | | | |
|---|---|---|---|---|---|
| H2 | 0.3073 | 1.3055 | 0.2900 | 0.052* | |
| C3 | 0.2931 (5) | 1.1594 (3) | 0.3345 (2) | 0.0448 (10) | |
| H3 | 0.1897 | 1.1585 | 0.3488 | 0.054* | |
| C4 | 0.3885 (4) | 0.9745 (3) | 0.3733 (2) | 0.0361 (9) | |
| C5 | 0.4253 (5) | 0.8852 (3) | 0.3368 (2) | 0.0429 (10) | |
| H5 | 0.4660 | 0.8918 | 0.2931 | 0.051* | |
| C6 | 0.4018 (5) | 0.7850 (3) | 0.3650 (2) | 0.0413 (10) | |
| H6 | 0.4273 | 0.7245 | 0.3402 | 0.050* | |
| C7 | 0.3404 (5) | 0.7745 (3) | 0.4297 (2) | 0.0384 (9) | |
| C8 | 0.3060 (5) | 0.8666 (3) | 0.4660 (2) | 0.0481 (11) | |
| H8 | 0.2670 | 0.8609 | 0.5101 | 0.058* | |
| C9 | 0.3285 (5) | 0.9661 (3) | 0.4380 (2) | 0.0471 (10) | |
| H9 | 0.3033 | 1.0269 | 0.4625 | 0.056* | |
| C18 | 0.1364 (6) | 0.2126 (3) | 0.5758 (2) | 0.0503 (11) | |
| H18 | 0.0996 | 0.1427 | 0.5680 | 0.060* | |
| C17 | 0.1562 (6) | 0.2820 (3) | 0.5223 (2) | 0.0520 (12) | |
| H17 | 0.1352 | 0.2690 | 0.4716 | 0.062* | |
| C12 | 0.1883 (5) | 0.4928 (3) | 0.4495 (2) | 0.0505 (11) | |
| H12 | 0.1239 | 0.4417 | 0.4205 | 0.061* | |
| C11 | 0.2221 (5) | 0.5887 (3) | 0.4187 (2) | 0.0503 (11) | |
| H11 | 0.1832 | 0.6001 | 0.3684 | 0.060* | |
| Cl1 | 0.56577 (14) | 1.46719 (8) | 0.22217 (6) | 0.0567 (3) | |
| Cl2 | 0.91696 (13) | 1.29605 (10) | 0.32170 (6) | 0.0563 (3) | |
| O1W | 0.0484 (16) | 0.9183 (11) | 0.5755 (7) | 0.080 (4)* | 0.25 |
| H1B | 0.0526 | 0.9507 | 0.6164 | 0.120* | 0.25 |
| H1A | 0.0731 | 0.8530 | 0.5831 | 0.120* | 0.25 |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| N3 | 0.045 (2) | 0.0354 (18) | 0.0334 (19) | 0.0009 (15) | 0.0035 (15) | 0.0016 (15) |
| C16 | 0.043 (2) | 0.042 (2) | 0.035 (2) | −0.004 (2) | 0.0025 (19) | 0.0000 (19) |
| N4 | 0.044 (2) | 0.0363 (18) | 0.0319 (19) | −0.0018 (15) | 0.0035 (15) | 0.0015 (15) |
| C13 | 0.040 (2) | 0.037 (2) | 0.032 (2) | 0.0002 (18) | 0.0032 (18) | 0.0035 (18) |
| C14 | 0.085 (3) | 0.054 (3) | 0.028 (2) | −0.017 (3) | −0.001 (2) | 0.003 (2) |
| C15 | 0.078 (3) | 0.046 (3) | 0.041 (3) | −0.020 (2) | −0.001 (2) | −0.001 (2) |
| C10 | 0.039 (2) | 0.039 (2) | 0.037 (2) | −0.0005 (18) | 0.0054 (18) | 0.0047 (18) |
| Zn1 | 0.0407 (3) | 0.0323 (2) | 0.0346 (3) | −0.0028 (2) | 0.00384 (19) | −0.0020 (2) |
| N1 | 0.0362 (19) | 0.036 (2) | 0.0378 (19) | −0.0013 (15) | 0.0044 (15) | 0.0014 (15) |
| N2 | 0.0329 (18) | 0.0384 (18) | 0.044 (2) | −0.0008 (15) | 0.0069 (15) | 0.0023 (15) |
| C1 | 0.035 (2) | 0.039 (2) | 0.051 (3) | 0.0049 (19) | 0.011 (2) | 0.002 (2) |
| C2 | 0.039 (2) | 0.038 (2) | 0.050 (3) | 0.0075 (19) | 0.003 (2) | 0.005 (2) |
| C3 | 0.034 (2) | 0.047 (2) | 0.054 (3) | 0.003 (2) | 0.009 (2) | 0.003 (2) |
| C4 | 0.028 (2) | 0.039 (2) | 0.040 (2) | −0.0021 (17) | 0.0032 (17) | 0.0047 (19) |
| C5 | 0.046 (2) | 0.046 (3) | 0.039 (2) | 0.001 (2) | 0.014 (2) | 0.002 (2) |
| C6 | 0.045 (2) | 0.036 (2) | 0.044 (2) | 0.0053 (19) | 0.011 (2) | −0.0004 (18) |
| C7 | 0.033 (2) | 0.042 (2) | 0.037 (2) | −0.0034 (18) | −0.0002 (18) | 0.0035 (18) |
| C8 | 0.055 (3) | 0.050 (3) | 0.043 (2) | −0.005 (2) | 0.019 (2) | −0.001 (2) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C9 | 0.057 (3) | 0.038 (2) | 0.049 (3) | −0.001 (2) | 0.018 (2) | −0.003 (2) |
| C18 | 0.070 (3) | 0.039 (2) | 0.039 (3) | −0.008 (2) | 0.003 (2) | 0.000 (2) |
| C17 | 0.077 (3) | 0.046 (3) | 0.029 (2) | −0.013 (2) | 0.002 (2) | −0.005 (2) |
| C12 | 0.065 (3) | 0.042 (2) | 0.040 (3) | −0.012 (2) | −0.004 (2) | −0.001 (2) |
| C11 | 0.062 (3) | 0.049 (3) | 0.034 (2) | −0.006 (2) | −0.005 (2) | 0.010 (2) |
| Cl1 | 0.0701 (8) | 0.0351 (6) | 0.0578 (7) | 0.0074 (5) | −0.0061 (6) | −0.0028 (5) |
| Cl2 | 0.0412 (6) | 0.0771 (8) | 0.0463 (6) | 0.0007 (6) | −0.0021 (5) | 0.0011 (6) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| N3—C16 | 1.319 (5) | N2—C4 | 1.435 (5) |
| N3—C18 | 1.365 (5) | C1—H1 | 0.9300 |
| N3—Zn1$^{i}$ | 2.024 (3) | C2—C3 | 1.338 (5) |
| C16—N4 | 1.349 (5) | C2—H2 | 0.9300 |
| C16—H16 | 0.9300 | C3—H3 | 0.9300 |
| N4—C17 | 1.374 (5) | C4—C5 | 1.370 (5) |
| N4—C13 | 1.429 (5) | C4—C9 | 1.375 (5) |
| C13—C12 | 1.373 (5) | C5—C6 | 1.388 (5) |
| C13—C14 | 1.376 (5) | C5—H5 | 0.9300 |
| C14—C15 | 1.380 (6) | C6—C7 | 1.385 (5) |
| C14—H14 | 0.9300 | C6—H6 | 0.9300 |
| C15—C10 | 1.379 (5) | C7—C8 | 1.391 (5) |
| C15—H15 | 0.9300 | C8—C9 | 1.377 (5) |
| C10—C11 | 1.381 (5) | C8—H8 | 0.9300 |
| C10—C7 | 1.486 (5) | C9—H9 | 0.9300 |
| Zn1—N1 | 2.021 (3) | C18—C17 | 1.349 (5) |
| Zn1—N3$^{ii}$ | 2.024 (3) | C18—H18 | 0.9300 |
| Zn1—Cl2 | 2.2368 (13) | C17—H17 | 0.9300 |
| Zn1—Cl1 | 2.2370 (12) | C12—C11 | 1.381 (5) |
| N1—C1 | 1.326 (4) | C12—H12 | 0.9300 |
| N1—C2 | 1.375 (5) | C11—H11 | 0.9300 |
| N2—C1 | 1.344 (5) | O1W—H1B | 0.8500 |
| N2—C3 | 1.377 (5) | O1W—H1A | 0.8499 |
| | | | |
| C16—N3—C18 | 105.7 (3) | C3—C2—H2 | 125.1 |
| C16—N3—Zn1$^{i}$ | 126.7 (3) | N1—C2—H2 | 125.1 |
| C18—N3—Zn1$^{i}$ | 127.5 (3) | C2—C3—N2 | 106.8 (3) |
| N3—C16—N4 | 111.6 (3) | C2—C3—H3 | 126.6 |
| N3—C16—H16 | 124.2 | N2—C3—H3 | 126.6 |
| N4—C16—H16 | 124.2 | C5—C4—C9 | 120.7 (4) |
| C16—N4—C17 | 106.1 (3) | C5—C4—N2 | 119.7 (3) |
| C16—N4—C13 | 126.3 (3) | C9—C4—N2 | 119.6 (4) |
| C17—N4—C13 | 127.6 (3) | C4—C5—C6 | 119.9 (4) |
| C12—C13—C14 | 119.4 (4) | C4—C5—H5 | 120.1 |
| C12—C13—N4 | 121.1 (3) | C6—C5—H5 | 120.1 |
| C14—C13—N4 | 119.4 (3) | C7—C6—C5 | 120.5 (4) |
| C13—C14—C15 | 119.7 (4) | C7—C6—H6 | 119.8 |
| C13—C14—H14 | 120.1 | C5—C6—H6 | 119.8 |

| | | | |
|---|---|---|---|
| C15—C14—H14 | 120.1 | C6—C7—C8 | 118.3 (4) |
| C10—C15—C14 | 122.1 (4) | C6—C7—C10 | 121.4 (4) |
| C10—C15—H15 | 118.9 | C8—C7—C10 | 120.2 (4) |
| C14—C15—H15 | 118.9 | C9—C8—C7 | 121.3 (4) |
| C15—C10—C11 | 116.9 (4) | C9—C8—H8 | 119.4 |
| C15—C10—C7 | 120.3 (4) | C7—C8—H8 | 119.4 |
| C11—C10—C7 | 122.8 (3) | C4—C9—C8 | 119.4 (4) |
| N1—Zn1—N3$^{ii}$ | 106.86 (12) | C4—C9—H9 | 120.3 |
| N1—Zn1—Cl2 | 105.84 (9) | C8—C9—H9 | 120.3 |
| N3$^{ii}$—Zn1—Cl2 | 112.85 (10) | C17—C18—N3 | 109.7 (4) |
| N1—Zn1—Cl1 | 110.21 (9) | C17—C18—H18 | 125.2 |
| N3$^{ii}$—Zn1—Cl1 | 106.34 (10) | N3—C18—H18 | 125.2 |
| Cl2—Zn1—Cl1 | 114.52 (5) | C18—C17—N4 | 106.9 (3) |
| C1—N1—C2 | 105.6 (3) | C18—C17—H17 | 126.6 |
| C1—N1—Zn1 | 127.6 (3) | N4—C17—H17 | 126.6 |
| C2—N1—Zn1 | 126.9 (3) | C13—C12—C11 | 119.9 (4) |
| C1—N2—C3 | 106.8 (3) | C13—C12—H12 | 120.0 |
| C1—N2—C4 | 127.0 (3) | C11—C12—H12 | 120.0 |
| C3—N2—C4 | 126.2 (3) | C12—C11—C10 | 121.8 (4) |
| N1—C1—N2 | 111.1 (3) | C12—C11—H11 | 119.1 |
| N1—C1—H1 | 124.5 | C10—C11—H11 | 119.1 |
| N2—C1—H1 | 124.5 | H1B—O1W—H1A | 110.4 |
| C3—C2—N1 | 109.8 (4) | | |

| | | | |
|---|---|---|---|
| C18—N3—C16—N4 | −0.7 (4) | C1—N2—C4—C5 | −45.5 (5) |
| Zn1$^{i}$—N3—C16—N4 | −179.6 (2) | C3—N2—C4—C5 | 132.2 (4) |
| N3—C16—N4—C17 | 1.0 (4) | C1—N2—C4—C9 | 136.4 (4) |
| N3—C16—N4—C13 | 178.8 (3) | C3—N2—C4—C9 | −46.0 (5) |
| C16—N4—C13—C12 | −159.4 (4) | C9—C4—C5—C6 | 0.1 (6) |
| C17—N4—C13—C12 | 17.9 (6) | N2—C4—C5—C6 | −178.0 (3) |
| C16—N4—C13—C14 | 20.2 (6) | C4—C5—C6—C7 | 0.3 (6) |
| C17—N4—C13—C14 | −162.4 (4) | C5—C6—C7—C8 | −1.0 (6) |
| C12—C13—C14—C15 | 3.1 (7) | C5—C6—C7—C10 | 179.2 (4) |
| N4—C13—C14—C15 | −176.6 (4) | C15—C10—C7—C6 | 129.7 (4) |
| C13—C14—C15—C10 | −1.8 (7) | C11—C10—C7—C6 | −51.0 (6) |
| C14—C15—C10—C11 | −1.5 (7) | C15—C10—C7—C8 | −50.1 (6) |
| C14—C15—C10—C7 | 177.8 (4) | C11—C10—C7—C8 | 129.3 (4) |
| N3$^{ii}$—Zn1—N1—C1 | 70.1 (3) | C6—C7—C8—C9 | 1.3 (6) |
| Cl2—Zn1—N1—C1 | −50.4 (3) | C10—C7—C8—C9 | −178.9 (4) |
| Cl1—Zn1—N1—C1 | −174.8 (3) | C5—C4—C9—C8 | 0.2 (6) |
| N3$^{ii}$—Zn1—N1—C2 | −111.1 (3) | N2—C4—C9—C8 | 178.4 (4) |
| Cl2—Zn1—N1—C2 | 128.4 (3) | C7—C8—C9—C4 | −1.0 (6) |
| Cl1—Zn1—N1—C2 | 4.0 (3) | C16—N3—C18—C17 | 0.1 (5) |
| C2—N1—C1—N2 | −0.4 (4) | Zn1$^{i}$—N3—C18—C17 | 179.0 (3) |
| Zn1—N1—C1—N2 | 178.6 (2) | N3—C18—C17—N4 | 0.5 (5) |
| C3—N2—C1—N1 | 0.4 (4) | C16—N4—C17—C18 | −0.9 (5) |
| C4—N2—C1—N1 | 178.5 (3) | C13—N4—C17—C18 | −178.6 (4) |
| C1—N1—C2—C3 | 0.2 (4) | C14—C13—C12—C11 | −1.2 (6) |

| | | | |
|---|---|---|---|
| Zn1—N1—C2—C3 | −178.8 (3) | N4—C13—C12—C11 | 178.5 (4) |
| N1—C2—C3—N2 | 0.1 (5) | C13—C12—C11—C10 | −2.3 (7) |
| C1—N2—C3—C2 | −0.3 (4) | C15—C10—C11—C12 | 3.6 (6) |
| C4—N2—C3—C2 | −178.4 (3) | C7—C10—C11—C12 | −175.8 (4) |

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

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1*W*—H1*A*···Cl2$^{iii}$ | 0.85 | 2.55 | 3.270 (14) | 143 |
| O1*W*—H1*B*···Cl1$^{iv}$ | 0.85 | 2.19 | 3.038 (14) | 179 |

Symmetry codes: (iii) $-x+1, -y+2, -z+1$; (iv) $x-1/2, -y+5/2, z+1/2$.