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Hexaaquazinc(II) dichloride bis(hexamethylenetetramine) tetrahydrate

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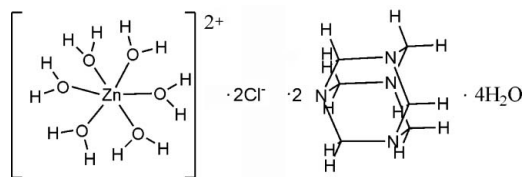
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Key indicators: single-crystal X-ray study; $T = 291$ K; mean $\sigma(\text{N}-\text{C}) = 0.004$ Å; R factor = 0.038; wR factor = 0.113; data-to-parameter ratio = 17.1.

The title compound, $[\text{Zn}(\text{H}_2\text{O})_6]\text{Cl}_2 \cdot 2\text{C}_6\text{H}_{12}\text{N}_4 \cdot 4\text{H}_2\text{O}$, has been prepared under mild hydrothermal conditions. The Zn^{II} atom, located on a centre of symmetry, is coordinated by six water molecules in a distorted octahedral coordination geometry. The hexamethylenetetramine molecule is not coordinated to Zn^{II} but links the Zn complexes *via* three $\text{O}-\text{H} \cdots \text{N}$ hydrogen bonds. The remaining N atom of the hexamethylenetetramine molecule is hydrogen-bonded to a solvent water molecule. In the crystal structure, intermolecular $\text{O}-\text{H} \cdots \text{O}$, $\text{O}-\text{H} \cdots \text{N}$ and $\text{O}-\text{H} \cdots \text{Cl}$ hydrogen bonds link the components into a three-dimensional network.

Related literature

For related compounds, see: Zhang *et al.* (2000).

Experimental

Crystal data

 $[\text{Zn}(\text{H}_2\text{O})_6]\text{Cl}_2 \cdot 2\text{C}_6\text{H}_{12}\text{N}_4 \cdot 4\text{H}_2\text{O}$ $M_r = 596.84$ Triclinic, $P\bar{1}$ $a = 9.345$ (3) Å $b = 9.4176$ (15) Å $c = 9.4535$ (15) Å $\alpha = 119.521$ (1)° $\beta = 94.218$ (2)° $\gamma = 100.969$ (2)° $V = 697.0$ (3) Å³ $Z = 1$ Mo $K\alpha$ radiation $\mu = 1.13$ mm⁻¹ $T = 291$ (2) K $0.36 \times 0.29 \times 0.15$ mm

Data collection

Bruker SMART CCD area-detector diffractometer

Absorption correction: multi-scan

(SADABS; Sheldrick, 1996)

 $T_{\text{min}} = 0.690$, $T_{\text{max}} = 0.849$

5184 measured reflections

2576 independent reflections

2466 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.018$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.038$ $wR(F^2) = 0.113$ $S = 1.05$

2576 reflections

151 parameters

H-atom parameters constrained

 $\Delta\rho_{\text{max}} = 0.51$ e Å⁻³ $\Delta\rho_{\text{min}} = -0.68$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

| $D-\text{H} \cdots A$ | $D-\text{H}$ | $\text{H} \cdots A$ | $D \cdots A$ | $D-\text{H} \cdots A$ |
|--|--------------|---------------------|--------------|-----------------------|
| $\text{O1}-\text{H1W} \cdots \text{N3}$ | 0.82 | 2.05 | 2.827 (3) | 158 |
| $\text{O1}-\text{H2W} \cdots \text{O5}^{\text{i}}$ | 0.83 | 1.94 | 2.743 (3) | 162 |
| $\text{O2}-\text{H3W} \cdots \text{N2}^{\text{ii}}$ | 0.83 | 1.99 | 2.804 (3) | 167 |
| $\text{O2}-\text{H4W} \cdots \text{O4}^{\text{ii}}$ | 0.84 | 1.90 | 2.711 (3) | 165 |
| $\text{O3}-\text{H5W} \cdots \text{Cl1}$ | 0.82 | 2.55 | 3.197 (2) | 137 |
| $\text{O3}-\text{H6W} \cdots \text{N1}^{\text{iii}}$ | 0.83 | 2.01 | 2.813 (3) | 165 |
| $\text{O4}-\text{H7W} \cdots \text{Cl1}$ | 0.83 | 2.36 | 3.175 (2) | 168 |
| $\text{O4}-\text{H8W} \cdots \text{N4}^{\text{iv}}$ | 0.84 | 2.00 | 2.835 (3) | 174 |
| $\text{O5}-\text{H9W} \cdots \text{Cl1}$ | 0.83 | 2.43 | 3.255 (3) | 168 |
| $\text{O5}-\text{H10W} \cdots \text{Cl1}^{\text{v}}$ | 0.83 | 2.38 | 3.213 (3) | 175 |

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

Data collection: SMART (Bruker, 2002); cell refinement: SAINT (Bruker, 2002); data reduction: SAINT; 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: KP2186).

References

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- Sheldrick, G. M. (2008). Acta Cryst. A64, 112–122.
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supporting information

Acta Cryst. (2008). E64, m1132 [doi:10.1107/S1600536808024793]

Hexaaquazinc(II) dichloride bis(hexamethylenetetramine) tetrahydrate

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S1. Comment

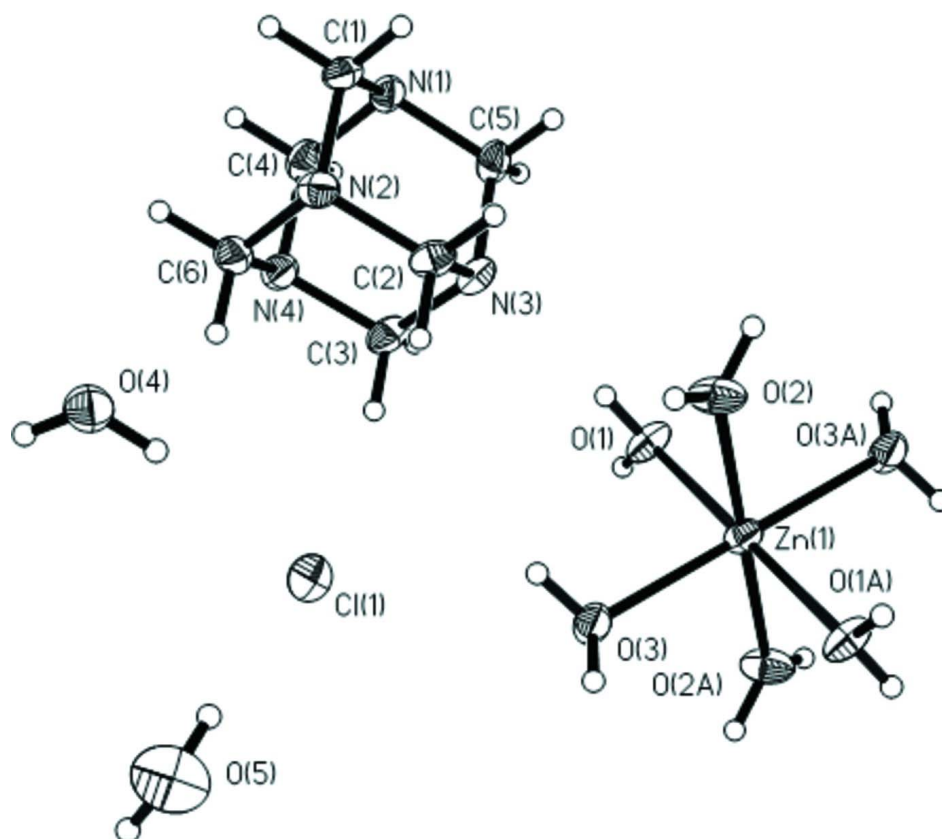
The asymmetric unit (Fig.1) consists of one half of hexaaqua Zn^{II} octahedron, one chloride ion, one uncoordinated neutral hexamethylenetetramine and two molecules of water of crystallization. The hexamethylenetetramine molecule is linked to the $[Zn(H_2O)_6]^{2+}$ via three $O-H\cdots N$ hydrogen bonds, while atom N3 of hexamethylenetetramine is hydrogen-bonded to O5 of the solvent water molecule. The Cl^- anions link to the $[Zn(H_2O)_6]^{2+}$ and water of crystallization via $O-H\cdots Cl$ hydrogen bonding. Hydrogen bonding of these anionic and cationic frameworks results in the formation of a three-dimensional network (Table 1, Fig. 2).

S2. Experimental

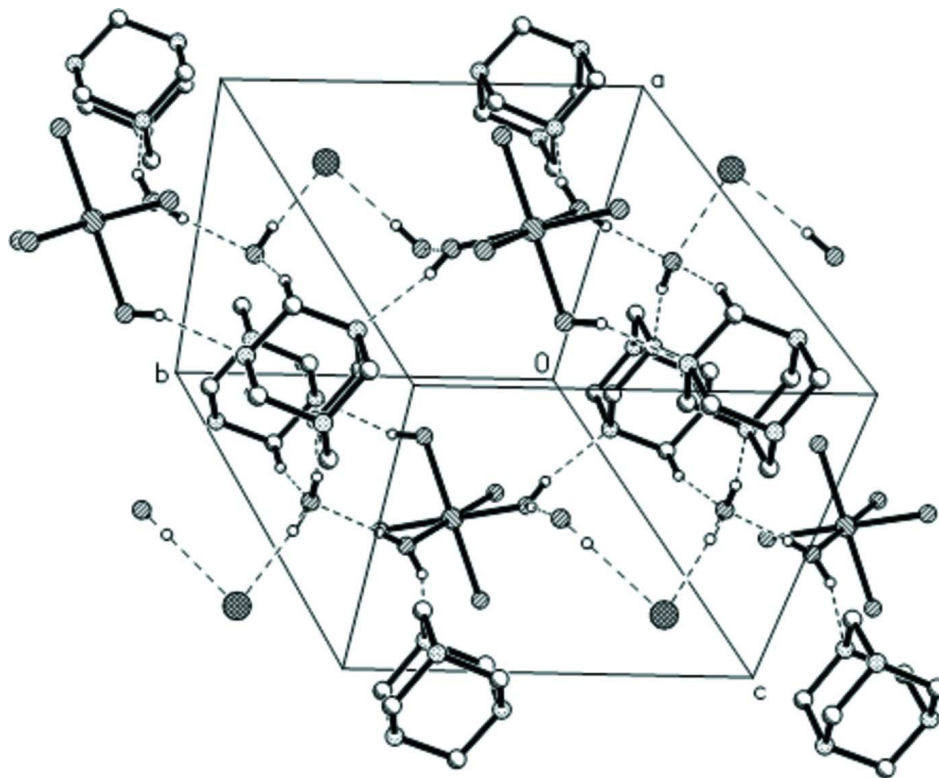
All the reagents were of AR grade and used without further purification. $C_6H_{12}N_4$ (1.401 g, 10 mmol) were dissolved in 50 mL H_2O solution, then the resultant solution was added in 10 mL double-distilled water containing $ZnCl_2$ (0.273 g, 2 mmol). The resulting solution was heated at 423 K for 96 h. After cooling to room temperature, block crystals were obtained in a yield up to 21.1%.

S3. Refinement

H atoms bonded to O atoms were located in a difference map and included in their 'as found' positions with $U_{iso}(H) = 1.5U_{eq}(O)$. Other H atoms were positioned geometrically with $C-H = 0.97 \text{ \AA}$ and with $U_{iso}(H) = 1.2U_{eq}(C)$. All H atoms were treated as riding.

**Figure 1**

Plot of an asymmetric unit with the 30% probability ellipsoids.

**Figure 2**

Three-dimensional network of hydrogen-bonding pattern with the motif $R_4^4(16)$ linking the cationic moieties with hexamine which are in turn interwoven with anionic moieties via water molecules.

Hexaaquazinc(II) dichloride bis(hexamethylenetetramine) tetrahydrate

Crystal data

$[\text{Zn}(\text{H}_2\text{O})_6]\text{Cl}_2 \cdot 2\text{C}_6\text{H}_{12}\text{N}_4 \cdot 4\text{H}_2\text{O}$

$M_r = 596.84$

Triclinic, $P\bar{1}$

Hall symbol: $-\text{P } 1$

$a = 9.345(3) \text{ \AA}$

$b = 9.4176(15) \text{ \AA}$

$c = 9.4535(15) \text{ \AA}$

$\alpha = 119.521(1)^\circ$

$\beta = 94.218(2)^\circ$

$\gamma = 100.969(2)^\circ$

$V = 697.0(3) \text{ \AA}^3$

$Z = 1$

$F(000) = 316$

$D_x = 1.422 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 2143 reflections

$\theta = 2.5\text{--}25.5^\circ$

$\mu = 1.13 \text{ mm}^{-1}$

$T = 291 \text{ K}$

Block, colorless

$0.36 \times 0.29 \times 0.15 \text{ mm}$

Data collection

Bruker SMART CCD area-detector
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Detector resolution: 0 pixels mm^{-1}

φ and ω scans

Absorption correction: multi-scan

(*SADABS*; Sheldrick, 1996)

$T_{\min} = 0.690$, $T_{\max} = 0.849$

5184 measured reflections

2576 independent reflections

2466 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.018$

$\theta_{\max} = 25.5^\circ$, $\theta_{\min} = 2.5^\circ$

$h = -11 \rightarrow 11$

$k = -11 \rightarrow 11$

$l = -11 \rightarrow 11$

*Refinement*Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.038$ $wR(F^2) = 0.113$ $S = 1.05$

2576 reflections

151 parameters

0 restraints

Primary atom site location: structure-invariant
direct methodsSecondary atom site location: difference Fourier
mapHydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.0645P)^2 + 0.6988P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\max} < 0.001$ $\Delta\rho_{\max} = 0.51 \text{ e } \text{\AA}^{-3}$ $\Delta\rho_{\min} = -0.68 \text{ e } \text{\AA}^{-3}$ *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 (\AA^2)

| | x | y | z | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|------|--------------|--------------|--------------|----------------------------------|
| Zn1 | 0.5000 | 0.0000 | 0.0000 | 0.02942 (16) |
| Cl1 | 0.18939 (10) | 0.17479 (10) | 0.43496 (10) | 0.0530 (2) |
| O1 | 0.3835 (2) | 0.1347 (2) | -0.0573 (2) | 0.0385 (5) |
| H1W | 0.3888 | 0.2257 | 0.0269 | 0.058* |
| H2W | 0.3035 | 0.0961 | -0.1235 | 0.058* |
| O2 | 0.6192 (2) | 0.2238 (2) | 0.1987 (2) | 0.0445 (5) |
| H3W | 0.6176 | 0.2521 | 0.2964 | 0.067* |
| H4W | 0.6833 | 0.2949 | 0.1930 | 0.067* |
| O3 | 0.3580 (2) | -0.0281 (3) | 0.1463 (3) | 0.0449 (5) |
| H5W | 0.3405 | 0.0629 | 0.2078 | 0.067* |
| H6W | 0.3658 | -0.0839 | 0.1907 | 0.067* |
| O4 | 0.1961 (2) | 0.5028 (3) | 0.7778 (3) | 0.0453 (5) |
| H7W | 0.2082 | 0.4201 | 0.6931 | 0.068* |
| H8W | 0.1053 | 0.4939 | 0.7784 | 0.068* |
| O5 | 0.1487 (3) | 0.0521 (4) | 0.7002 (4) | 0.0734 (8) |
| H9W | 0.1699 | 0.0950 | 0.6431 | 0.110* |
| H10W | 0.0600 | -0.0024 | 0.6715 | 0.110* |
| N1 | 0.3345 (3) | 0.7407 (3) | 0.2554 (3) | 0.0330 (5) |
| N2 | 0.3362 (3) | 0.6543 (3) | 0.4602 (3) | 0.0333 (5) |
| N3 | 0.3418 (3) | 0.4524 (3) | 0.1728 (3) | 0.0321 (5) |
| N4 | 0.1152 (2) | 0.5427 (3) | 0.2441 (3) | 0.0340 (5) |
| C1 | 0.3865 (3) | 0.7935 (3) | 0.4289 (3) | 0.0356 (6) |
| H1A | 0.3492 | 0.8886 | 0.5010 | 0.043* |
| H1B | 0.4942 | 0.8302 | 0.4552 | 0.043* |
| C2 | 0.3944 (3) | 0.5116 (3) | 0.3488 (3) | 0.0342 (6) |

| | | | | |
|-----|------------|------------|------------|------------|
| H2A | 0.3628 | 0.4191 | 0.3677 | 0.041* |
| H2B | 0.5022 | 0.5466 | 0.3743 | 0.041* |
| C3 | 0.1782 (3) | 0.4021 (3) | 0.1376 (3) | 0.0381 (6) |
| H3A | 0.1440 | 0.3088 | 0.1546 | 0.046* |
| H3B | 0.1422 | 0.3632 | 0.0223 | 0.046* |
| C4 | 0.1706 (3) | 0.6838 (4) | 0.2176 (4) | 0.0375 (6) |
| H4A | 0.1348 | 0.6480 | 0.1032 | 0.045* |
| H4B | 0.1311 | 0.7778 | 0.2876 | 0.045* |
| C5 | 0.3925 (3) | 0.5955 (4) | 0.1482 (3) | 0.0353 (6) |
| H5A | 0.3595 | 0.5592 | 0.0331 | 0.042* |
| H5B | 0.5003 | 0.6306 | 0.1729 | 0.042* |
| C6 | 0.1728 (3) | 0.5995 (4) | 0.4186 (3) | 0.0369 (6) |
| H6A | 0.1333 | 0.6925 | 0.4910 | 0.044* |
| H6B | 0.1386 | 0.5076 | 0.4377 | 0.044* |

Atomic displacement parameters (Å²)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|-------------|-------------|--------------|--------------|--------------|
| Zn1 | 0.0395 (3) | 0.0233 (2) | 0.0250 (2) | 0.00991 (17) | 0.00711 (17) | 0.01148 (18) |
| Cl1 | 0.0591 (5) | 0.0399 (4) | 0.0534 (5) | 0.0135 (3) | 0.0246 (4) | 0.0173 (4) |
| O1 | 0.0604 (11) | 0.0278 (9) | 0.0329 (10) | 0.0192 (8) | -0.0009 (8) | 0.0105 (8) |
| O2 | 0.0710 (13) | 0.0280 (10) | 0.0220 (9) | -0.0076 (9) | 0.0009 (9) | 0.0081 (8) |
| O3 | 0.0675 (14) | 0.0422 (11) | 0.0548 (12) | 0.0327 (10) | 0.0401 (11) | 0.0367 (10) |
| O4 | 0.0398 (11) | 0.0386 (11) | 0.0417 (11) | 0.0003 (9) | 0.0055 (9) | 0.0130 (9) |
| O5 | 0.0604 (16) | 0.086 (2) | 0.0720 (18) | 0.0027 (14) | -0.0156 (13) | 0.0485 (16) |
| N1 | 0.0423 (12) | 0.0298 (11) | 0.0371 (12) | 0.0160 (10) | 0.0161 (10) | 0.0214 (10) |
| N2 | 0.0426 (12) | 0.0285 (11) | 0.0242 (10) | 0.0036 (9) | 0.0050 (9) | 0.0125 (9) |
| N3 | 0.0407 (12) | 0.0255 (11) | 0.0275 (11) | 0.0144 (9) | 0.0046 (9) | 0.0102 (9) |
| N4 | 0.0345 (11) | 0.0289 (11) | 0.0335 (11) | 0.0088 (9) | 0.0063 (9) | 0.0124 (9) |
| C1 | 0.0433 (15) | 0.0221 (12) | 0.0348 (14) | 0.0048 (10) | 0.0100 (11) | 0.0110 (11) |
| C2 | 0.0432 (15) | 0.0284 (13) | 0.0326 (13) | 0.0090 (11) | 0.0007 (11) | 0.0178 (11) |
| C3 | 0.0417 (15) | 0.0264 (13) | 0.0327 (14) | 0.0086 (11) | -0.0005 (11) | 0.0066 (11) |
| C4 | 0.0443 (15) | 0.0376 (15) | 0.0404 (15) | 0.0219 (12) | 0.0136 (12) | 0.0226 (12) |
| C5 | 0.0452 (15) | 0.0399 (15) | 0.0314 (13) | 0.0217 (12) | 0.0167 (11) | 0.0214 (12) |
| C6 | 0.0427 (15) | 0.0337 (14) | 0.0326 (14) | 0.0055 (11) | 0.0128 (11) | 0.0167 (11) |

Geometric parameters (Å, °)

| | | | |
|---------------------|-------------|--------|-----------|
| Zn1—O2 ⁱ | 2.0269 (18) | N2—C2 | 1.476 (3) |
| Zn1—O2 | 2.0269 (18) | N2—C1 | 1.481 (3) |
| Zn1—O1 | 2.0507 (17) | N3—C3 | 1.472 (4) |
| Zn1—O1 ⁱ | 2.0507 (17) | N3—C5 | 1.476 (3) |
| Zn1—O3 ⁱ | 2.0595 (18) | N3—C2 | 1.477 (3) |
| Zn1—O3 | 2.0595 (18) | N4—C4 | 1.477 (4) |
| O1—H1W | 0.8223 | N4—C3 | 1.478 (3) |
| O1—H2W | 0.8281 | N4—C6 | 1.479 (4) |
| O2—H3W | 0.8279 | C1—H1A | 0.9700 |
| O2—H4W | 0.8360 | C1—H1B | 0.9700 |

| | | | |
|--------------------------------------|-------------|------------|-----------|
| O3—H5W | 0.8221 | C2—H2A | 0.9700 |
| O3—H6W | 0.8267 | C2—H2B | 0.9700 |
| O4—H7W | 0.8326 | C3—H3A | 0.9700 |
| O4—H8W | 0.8374 | C3—H3B | 0.9700 |
| O5—H9W | 0.8338 | C4—H4A | 0.9700 |
| O5—H10W | 0.8316 | C4—H4B | 0.9700 |
| N1—C1 | 1.470 (4) | C5—H5A | 0.9700 |
| N1—C4 | 1.476 (4) | C5—H5B | 0.9700 |
| N1—C5 | 1.479 (3) | C6—H6A | 0.9700 |
| N2—C6 | 1.471 (4) | C6—H6B | 0.9700 |
| O2 ⁱ —Zn1—O2 | 180.00 (11) | C3—N4—C6 | 107.8 (2) |
| O2 ⁱ —Zn1—O1 | 92.66 (8) | N1—C1—N2 | 111.7 (2) |
| O2—Zn1—O1 | 87.34 (8) | N1—C1—H1A | 109.3 |
| O2 ⁱ —Zn1—O1 ⁱ | 87.34 (8) | N2—C1—H1A | 109.3 |
| O2—Zn1—O1 ⁱ | 92.66 (8) | N1—C1—H1B | 109.3 |
| O1—Zn1—O1 ⁱ | 180.00 (12) | N2—C1—H1B | 109.3 |
| O2 ⁱ —Zn1—O3 ⁱ | 89.59 (9) | H1A—C1—H1B | 107.9 |
| O2—Zn1—O3 ⁱ | 90.41 (9) | N2—C2—N3 | 111.6 (2) |
| O1—Zn1—O3 ⁱ | 86.57 (8) | N2—C2—H2A | 109.3 |
| O1 ⁱ —Zn1—O3 ⁱ | 93.43 (8) | N3—C2—H2A | 109.3 |
| O2 ⁱ —Zn1—O3 | 90.41 (9) | N2—C2—H2B | 109.3 |
| O2—Zn1—O3 | 89.59 (9) | N3—C2—H2B | 109.3 |
| O1—Zn1—O3 | 93.43 (8) | H2A—C2—H2B | 108.0 |
| O1 ⁱ —Zn1—O3 | 86.57 (8) | N3—C3—N4 | 112.2 (2) |
| O3 ⁱ —Zn1—O3 | 180.00 (19) | N3—C3—H3A | 109.2 |
| Zn1—O1—H1W | 109.5 | N4—C3—H3A | 109.2 |
| Zn1—O1—H2W | 126.6 | N3—C3—H3B | 109.2 |
| H1W—O1—H2W | 113.2 | N4—C3—H3B | 109.2 |
| Zn1—O2—H3W | 124.5 | H3A—C3—H3B | 107.9 |
| Zn1—O2—H4W | 124.2 | N1—C4—N4 | 112.2 (2) |
| H3W—O2—H4W | 111.0 | N1—C4—H4A | 109.2 |
| Zn1—O3—H5W | 109.6 | N4—C4—H4A | 109.2 |
| Zn1—O3—H6W | 123.5 | N1—C4—H4B | 109.2 |
| H5W—O3—H6W | 113.5 | N4—C4—H4B | 109.2 |
| H7W—O4—H8W | 110.1 | H4A—C4—H4B | 107.9 |
| H9W—O5—H10W | 111.5 | N3—C5—N1 | 111.7 (2) |
| C1—N1—C4 | 108.4 (2) | N3—C5—H5A | 109.3 |
| C1—N1—C5 | 108.2 (2) | N1—C5—H5A | 109.3 |
| C4—N1—C5 | 108.3 (2) | N3—C5—H5B | 109.3 |
| C6—N2—C2 | 108.5 (2) | N1—C5—H5B | 109.3 |
| C6—N2—C1 | 108.5 (2) | H5A—C5—H5B | 108.0 |
| C2—N2—C1 | 108.0 (2) | N2—C6—N4 | 112.0 (2) |
| C3—N3—C5 | 108.7 (2) | N2—C6—H6A | 109.2 |
| C3—N3—C2 | 108.4 (2) | N4—C6—H6A | 109.2 |
| C5—N3—C2 | 107.9 (2) | N2—C6—H6B | 109.2 |
| C4—N4—C3 | 108.0 (2) | N4—C6—H6B | 109.2 |
| C4—N4—C6 | 108.1 (2) | H6A—C6—H6B | 107.9 |

| | | | |
|-------------|-----------|-------------|-----------|
| C4—N1—C1—N2 | 58.4 (3) | C1—N1—C4—N4 | -58.6 (3) |
| C5—N1—C1—N2 | -58.8 (3) | C5—N1—C4—N4 | 58.6 (3) |
| C6—N2—C1—N1 | -58.6 (3) | C3—N4—C4—N1 | -58.3 (3) |
| C2—N2—C1—N1 | 58.9 (3) | C6—N4—C4—N1 | 58.1 (3) |
| C6—N2—C2—N3 | 58.3 (3) | C3—N3—C5—N1 | 58.1 (3) |
| C1—N2—C2—N3 | -59.1 (3) | C2—N3—C5—N1 | -59.2 (3) |
| C3—N3—C2—N2 | -58.2 (3) | C1—N1—C5—N3 | 59.2 (3) |
| C5—N3—C2—N2 | 59.4 (3) | C4—N1—C5—N3 | -58.1 (3) |
| C5—N3—C3—N4 | -58.3 (3) | C2—N2—C6—N4 | -58.8 (3) |
| C2—N3—C3—N4 | 58.7 (3) | C1—N2—C6—N4 | 58.4 (3) |
| C4—N4—C3—N3 | 58.0 (3) | C4—N4—C6—N2 | -58.0 (3) |
| C6—N4—C3—N3 | -58.6 (3) | C3—N4—C6—N2 | 58.5 (3) |

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

Hydrogen-bond geometry (\AA , $^\circ$)

| <i>D</i> —H \cdots <i>A</i> | <i>D</i> —H | H \cdots <i>A</i> | <i>D</i> \cdots <i>A</i> | <i>D</i> —H \cdots <i>A</i> |
|--|-------------|---------------------|----------------------------|-------------------------------|
| O1—H1 <i>W</i> \cdots N3 | 0.82 | 2.05 | 2.827 (3) | 158 |
| O1—H2 <i>W</i> \cdots O5 ⁱⁱ | 0.83 | 1.94 | 2.743 (3) | 162 |
| O2—H3 <i>W</i> \cdots N2 ⁱⁱⁱ | 0.83 | 1.99 | 2.804 (3) | 167 |
| O2—H4 <i>W</i> \cdots O4 ⁱⁱⁱ | 0.84 | 1.90 | 2.711 (3) | 165 |
| O3—H5 <i>W</i> \cdots C11 | 0.82 | 2.55 | 3.197 (2) | 137 |
| O3—H6 <i>W</i> \cdots N1 ^{iv} | 0.83 | 2.01 | 2.813 (3) | 165 |
| O4—H7 <i>W</i> \cdots C11 | 0.83 | 2.36 | 3.175 (2) | 168 |
| O4—H8 <i>W</i> \cdots N4 ^v | 0.84 | 2.00 | 2.835 (3) | 174 |
| O5—H9 <i>W</i> \cdots C11 | 0.83 | 2.43 | 3.255 (3) | 168 |
| O5—H10 <i>W</i> \cdots C11 ^{vi} | 0.83 | 2.38 | 3.213 (3) | 175 |

Symmetry codes: (ii) $x, y, z-1$; (iii) $-x+1, -y+1, -z+1$; (iv) $x, y-1, z$; (v) $-x, -y+1, -z+1$; (vi) $-x, -y, -z+1$.