Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Diaquadimethanolbis[4-(1*H*-tetrazol-1-yl)benzoato]zinc(II) dihydrate

Shu-Ming Zhang

Department of Chemistry, Nankai University, Tianjin 300071, People's Republic of China, and School of Chemical Engineering and Technology, Hebei University of Technology, Tianjin 300130, People's Republic of China
Correspondence e-mail: zsmchange@sina.com

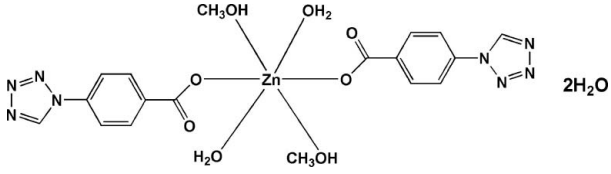
Received 15 March 2008; accepted 29 March 2008

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.032; wR factor = 0.076; data-to-parameter ratio = 14.6.

In the title compound, $[Zn(C_8H_5N_4O_2)_2(CH_3OH)_2(H_2O)_2]\cdot 2H_2O$, the Zn^{II} ion lies on an inversion centre and is coordinated by two O atoms from two 4-(tetrazol-1-yl)benzoate ligands, two O atoms from two methanol molecules and two O atoms from two water molecules in a slightly distorted octahedral geometry. In addition, there are two uncoordinated water molecules in the crystal structure. The crystal structure is stabilized by intermolecular O—H···O hydrogen bonds.

Related literature

For related literature, see: Zou *et al.* (2005); Dinca *et al.* (2006); Li *et al.* (2007); Zhang & Du (2007).



Experimental

Crystal data

$[Zn(C_8H_5N_4O_2)_2(CH_4O)_2(H_2O)_2]\cdot 2H_2O$
M_r = 579.84
Monoclinic, $P2_1/c$
a = 13.220 (3) Å
b = 7.1551 (14) Å
c = 12.636 (3) Å
β = 90.24 (3)°
V = 1195.3 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.10 mm^{-1}
T = 293 (2) K
0.20 × 0.18 × 0.16 mm

Data collection

Bruker P4 diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
T_{min} = 0.810, T_{max} = 0.844
12254 measured reflections
2746 independent reflections
2359 reflections with $I > 2\sigma(I)$
R_{int} = 0.045

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.076
S = 1.04
2746 reflections
188 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—O1	2.0483 (14)	Zn1—O1*W*	2.1342 (14)
Zn1—O3	2.1078 (15)		
O1—Zn1—O3	93.56 (6)	O3—Zn1—O1*W*	92.25 (6)
O1—Zn1—O1*W*	91.02 (6)		

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*WA*···O2*W*^{i}	0.82	1.97	2.759 (2)	160
O2*W*—H2*WB*···O1*W*^{ii}	0.77 (3)	2.07 (3)	2.831 (2)	175 (3)
O3—H3*M*···O2*W*^{iii}	0.75 (3)	1.99 (3)	2.726 (2)	167 (3)

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); 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*.

The authors thank the Natural Science Foundation of Tianjin, China (No. 07JCZDJC00500) for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2552).

References

Bruker (1998). *SMART*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Dinca, M., Dailly, A., Liu, Y., Brown, C. M., Neumann, D. A. & Long, J. R. (2006). *J. Am. Chem. Soc.* **128**, 16876–16883.
Li, J. R., Tao, Y., Yu, Q. & Bu, X. H. (2007). *Chem. Commun.* pp. 1527–1529.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Zhang, S.-M. & Du, J.-L. (2007). *Acta Cryst.* E**63**, m3139.
Zou, R.-Q., Cai, L.-Z. & Guo, G.-C. (2005). *J. Mol. Struct.* **737**, 125–129.

supporting information

Acta Cryst. (2008). E**64**, m624 [doi:10.1107/S1600536808008490]

Diaquadimethanolbis[4-(1*H*-tetrazol-1-yl)benzoato]zinc(II) dihydrate

Shu-Ming Zhang

S1. Comment

Coordination architectures formed from 1*H*-tetrazol and its derivatives have attracted wide attentions in recent years, due to not only their fascinating structures and topologies, but also their potential applications in luminescence, magnetism and gas storage (Dinca, *et al.*, 2006; Li, *et al.*, 2007). However, there are rare reports (Zou, *et al.*, 2005) of the coordination systems using the benzoic acids with N-heterocycle as ligands. So we synthesized several coordination compounds by such ligands. And here we report the structure of title compound (I).

The structure of (I) consists of discrete neutral unit $[Zn(C_8H_5N_4O_2)_2(CH_3OH)_2(H_2O)_2]$, and two lattice water molecules (Fig. 1), atom Zn1 lies on an inversion centre and is coordinated by two O atoms from two 4-(tetrazol-1-yl) benzoate ligands, two O atoms from two methanol molecules and two O atoms from two water molecules in a distorted octahedral geometry.The metal ion of (I) is bonded to the carboxyl group of 4-(tetrazol-1-yl) benzoate, which is remarkably different from our previous reported compound that using the same ligand with N donor coordinating to metal ion (Zhang *et al.*, 2007). The crystal stacking of (I) (Fig. 2) is stabilized by the intermolecular O—H···O hydrogen bonds (Table 2).

S2. Experimental

A solution of $Zn(NO_3)_2.6H_2O$ (0.1 mmol) in water (5 ml) was added to a solution of 4-(tetrazol-1-yl) benzoic acid (38 mg, 0.2 mmol) and sodium hydroxide (8 mg, 0.2 mmol) in methanol (5 mL). The reaction mixture was stirred for 30 min and then filtered. Colourless crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation after two weeks [yield: 46%].

S3. Refinement

H atoms of C were included in calculated positions and treated in the subsequent refinement as riding atoms, with C—H = 0.93 and 0.96 Å and U_{iso}(H) = 1.2 and 1.5 U_{eq}(C,*N*). The H atoms of water was located in Fourier difference map and refined without restraint.

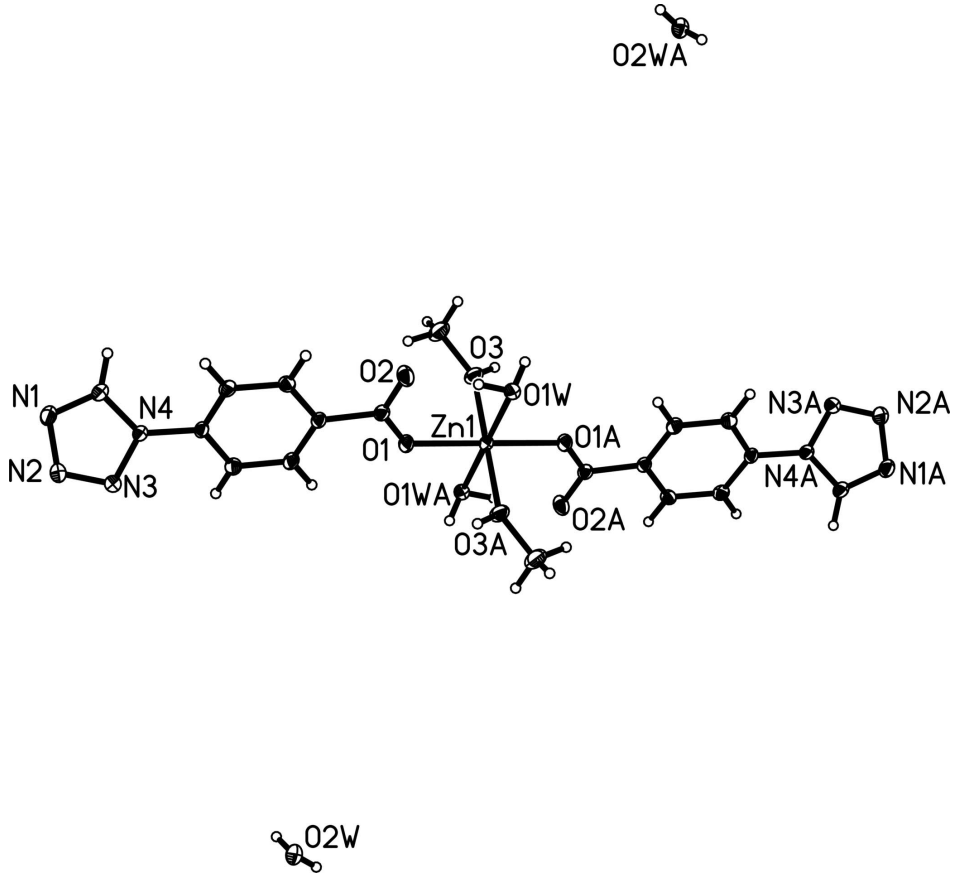


Figure 1

The molecular structure of (I), with 30% probability displacement ellipsoids. [Symmetry code: (A) -x+1, -y, -z+2.]

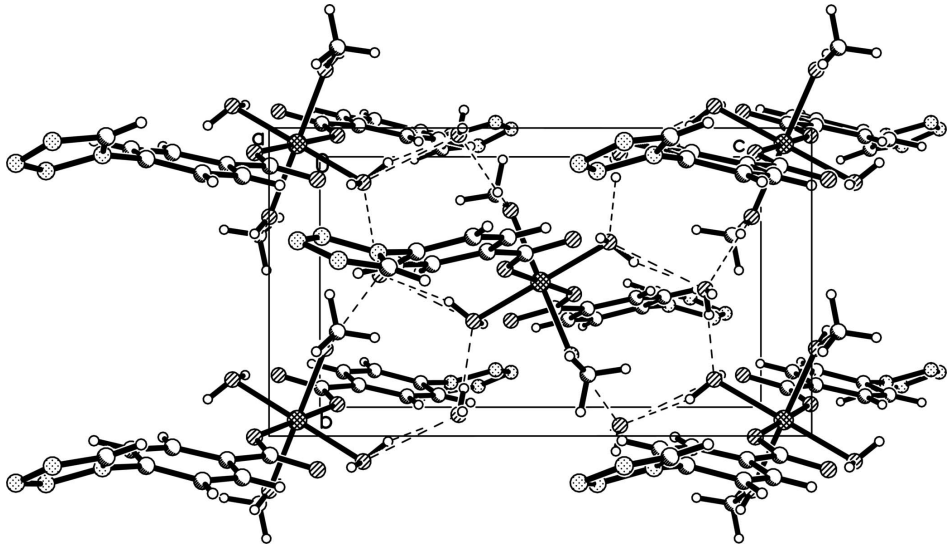


Figure 2

A portion of the crystal stacking structure, showing the intermolecular O—H···O, hydrogen bonds as dashed lines.

Diaquadimethanolbis[4-(1H-tetrazol-1-yl)benzoato]zinc(II) dihydrate

Crystal data

$[Zn(C_8H_5N_4O_2)_2(CH_4O)_2(H_2O)_2]\cdot 2H_2O$
$M_r = 579.84$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 13.220$ (3) Å
$b = 7.1551$ (14) Å
$c = 12.636$ (3) Å
$\beta = 90.24$ (3)°
$V = 1195.3$ (4) Å^3
$Z = 2$
$F(000) = 600$
$D_x = 1.611$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 11248 reflections
$\theta = 3.1$–$27.6°$
$\mu = 1.10$ mm^{-1}
$T = 293$ K
Block, colourless
0.20 × 0.18 × 0.16 mm

Data collection

Bruker P4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
$T_{min} = 0.810$, $T_{max} = 0.844$
12254 measured reflections
2746 independent reflections
2359 reflections with $I > 2\sigma(I)$
$R_{int} = 0.045$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.1°$
$h = -17\rightarrow17$
$k = -9\rightarrow9$
$l = -16\rightarrow16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.032$
$wR(F^2) = 0.076$
$S = 1.04$
2746 reflections
188 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
$w = 1/[\sigma^2(F_o^2) + (0.0297P)^2 + 0.5826P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.29$ e Å^{-3}
$\Delta\rho_{min} = -0.23$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0228 (12)

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}
Zn1	0.5000	0.0000	1.0000	0.02298 (11)
O1	0.63696 (9)	0.0452 (2)	0.92928 (10)	0.0313 (3)
O2	0.73211 (10)	0.1468 (2)	1.06367 (10)	0.0399 (4)

C2	0.97854 (12)	0.0991 (2)	0.77039 (14)	0.0231 (4)
N4	1.06694 (11)	0.0940 (2)	0.70586 (12)	0.0243 (3)
C5	0.80990 (13)	0.1028 (2)	0.89760 (14)	0.0228 (4)
N3	1.06465 (12)	0.1453 (3)	0.60316 (13)	0.0339 (4)
C4	0.90418 (13)	0.1480 (3)	0.93867 (14)	0.0259 (4)
H4	0.9104	0.1793	1.0098	0.031*
N1	1.21854 (12)	0.0669 (3)	0.64661 (14)	0.0342 (4)
C7	0.88492 (14)	0.0580 (3)	0.72624 (15)	0.0282 (4)
H7	0.8786	0.0294	0.6547	0.034*
C3	0.98863 (14)	0.1470 (3)	0.87560 (15)	0.0274 (4)
H3	1.0516	0.1782	0.9035	0.033*
C8	0.71954 (13)	0.0989 (3)	0.96960 (14)	0.0256 (4)
C1	1.16184 (14)	0.0462 (3)	0.72993 (16)	0.0291 (4)
H1	1.1840	0.0047	0.7958	0.035*
C6	0.80137 (14)	0.0608 (3)	0.79125 (15)	0.0279 (4)
H6	0.7380	0.0339	0.7629	0.033*
N2	1.15560 (13)	0.1290 (3)	0.56869 (14)	0.0375 (4)
O3	0.54347 (11)	−0.2616 (2)	1.06193 (13)	0.0380 (4)
C9	0.63908 (16)	−0.3252 (3)	1.0949 (2)	0.0470 (6)
H9A	0.6907	−0.2579	1.0578	0.071*
H9B	0.6451	−0.4563	1.0799	0.071*
H9C	0.6467	−0.3050	1.1696	0.071*
O2W	0.43377 (14)	0.4734 (2)	0.16558 (13)	0.0340 (3)
O1W	0.54904 (11)	0.14327 (19)	1.13919 (10)	0.0289 (3)
H1WA	0.5471	0.0718	1.1898	0.043*
H2WA	0.378 (2)	0.457 (4)	0.156 (2)	0.053 (9)*
H2WB	0.463 (2)	0.382 (4)	0.156 (2)	0.061 (10)*
H1WB	0.612 (2)	0.155 (4)	1.121 (2)	0.058 (8)*
H3M	0.5060 (19)	−0.325 (4)	1.088 (2)	0.047 (8)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.01705 (16)	0.02848 (18)	0.02340 (17)	0.00002 (12)	−0.00056 (11)	0.00133 (13)
O1	0.0173 (6)	0.0487 (9)	0.0279 (7)	−0.0049 (6)	0.0003 (5)	0.0000 (6)
O2	0.0265 (7)	0.0670 (11)	0.0261 (7)	−0.0095 (7)	0.0019 (6)	−0.0061 (7)
C2	0.0174 (9)	0.0241 (9)	0.0279 (9)	−0.0001 (7)	0.0021 (7)	0.0030 (7)
N4	0.0191 (7)	0.0275 (8)	0.0261 (8)	0.0008 (6)	−0.0003 (6)	0.0027 (7)
C5	0.0184 (8)	0.0231 (9)	0.0270 (9)	−0.0014 (7)	0.0000 (7)	0.0016 (7)
N3	0.0277 (9)	0.0455 (10)	0.0284 (9)	0.0043 (7)	0.0021 (7)	0.0072 (8)
C4	0.0240 (9)	0.0310 (10)	0.0227 (9)	−0.0040 (7)	−0.0023 (7)	0.0004 (8)
N1	0.0239 (9)	0.0384 (9)	0.0403 (10)	0.0029 (7)	0.0040 (7)	0.0031 (8)
C7	0.0244 (9)	0.0352 (10)	0.0249 (9)	−0.0018 (8)	−0.0025 (8)	−0.0039 (8)
C3	0.0190 (9)	0.0330 (10)	0.0301 (10)	−0.0040 (7)	−0.0053 (7)	0.0009 (8)
C8	0.0199 (9)	0.0283 (10)	0.0287 (10)	−0.0013 (7)	−0.0004 (7)	0.0038 (8)
C1	0.0214 (9)	0.0331 (11)	0.0328 (10)	0.0023 (7)	−0.0020 (8)	0.0010 (8)
C6	0.0179 (9)	0.0362 (10)	0.0294 (10)	−0.0033 (7)	−0.0039 (7)	−0.0030 (8)
N2	0.0290 (9)	0.0478 (11)	0.0358 (10)	0.0035 (8)	0.0080 (7)	0.0093 (8)

O3	0.0261 (7)	0.0373 (9)	0.0505 (9)	0.0028 (7)	−0.0007 (7)	0.0194 (7)
C9	0.0323 (12)	0.0468 (14)	0.0620 (15)	0.0093 (10)	−0.0041 (11)	0.0120 (12)
O2W	0.0277 (8)	0.0361 (9)	0.0382 (8)	−0.0020 (7)	0.0031 (7)	−0.0057 (7)
O1W	0.0251 (7)	0.0359 (8)	0.0257 (7)	0.0002 (6)	0.0004 (6)	0.0029 (6)

Geometric parameters (Å, º)

Zn1—O1	2.0483 (14)	C4—H4	0.9300
Zn1—O1^{i}	2.0483 (14)	N1—C1	1.304 (3)
Zn1—O3	2.1078 (15)	N1—N2	1.361 (2)
Zn1—O3^{i}	2.1078 (15)	C7—C6	1.379 (3)
Zn1—O1W^{i}	2.1342 (14)	C7—H7	0.9300
Zn1—O1W	2.1342 (14)	C3—H3	0.9300
O1—C8	1.263 (2)	C1—H1	0.9300
O2—C8	1.247 (2)	C6—H6	0.9300
C2—C3	1.379 (3)	O3—C9	1.405 (2)
C2—C7	1.387 (2)	O3—H3M	0.75 (3)
C2—N4	1.428 (2)	C9—H9A	0.9600
N4—C1	1.334 (2)	C9—H9B	0.9600
N4—N3	1.349 (2)	C9—H9C	0.9600
C5—C6	1.381 (3)	O2W—H2WA	0.75 (3)
C5—C4	1.386 (2)	O2W—H2WB	0.77 (3)
C5—C8	1.505 (2)	O1W—H1WA	0.8200
N3—N2	1.286 (2)	O1W—H1WB	0.87 (3)
C4—C3	1.375 (3)		

O1—Zn1—O1^{i}	180.00 (3)	C6—C7—C2	118.22 (17)
O1—Zn1—O3	93.56 (6)	C6—C7—H7	120.9
O1^{i}—Zn1—O3	86.44 (6)	C2—C7—H7	120.9
O1—Zn1—O3^{i}	86.44 (6)	C4—C3—C2	119.00 (17)
O1^{i}—Zn1—O3^{i}	93.56 (6)	C4—C3—H3	120.5
O3—Zn1—O3^{i}	180.0	C2—C3—H3	120.5
O1—Zn1—O1W^{i}	88.98 (6)	O2—C8—O1	125.41 (17)
O1^{i}—Zn1—O1W^{i}	91.02 (6)	O2—C8—C5	117.92 (16)
O3—Zn1—O1W^{i}	87.75 (6)	O1—C8—C5	116.66 (16)
O3^{i}—Zn1—O1W^{i}	92.25 (6)	N1—C1—N4	109.28 (17)
O1—Zn1—O1W	91.02 (6)	N1—C1—H1	125.4
O1^{i}—Zn1—O1W	88.98 (6)	N4—C1—H1	125.4
O3—Zn1—O1W	92.25 (6)	C7—C6—C5	121.35 (17)
O3^{i}—Zn1—O1W	87.75 (6)	C7—C6—H6	119.3
O1W^{i}—Zn1—O1W	180.0	C5—C6—H6	119.3
C8—O1—Zn1	129.52 (12)	N3—N2—N1	110.75 (16)
C3—C2—C7	121.54 (17)	C9—O3—Zn1	129.90 (14)
C3—C2—N4	118.74 (16)	C9—O3—H3M	105 (2)
C7—C2—N4	119.72 (16)	Zn1—O3—H3M	122 (2)
C1—N4—N3	107.84 (15)	O3—C9—H9A	109.5
C1—N4—C2	130.34 (16)	O3—C9—H9B	109.5
N3—N4—C2	121.81 (15)	H9A—C9—H9B	109.5

C6—C5—C4	118.98 (17)	O3—C9—H9C	109.5
C6—C5—C8	121.50 (16)	H9A—C9—H9C	109.5
C4—C5—C8	119.52 (16)	H9B—C9—H9C	109.5
N2—N3—N4	106.50 (15)	H2WA—O2W—H2WB	109 (3)
C3—C4—C5	120.86 (17)	Zn1—O1W—H1WA	109.5
C3—C4—H4	119.6	Zn1—O1W—H1WB	96.5 (17)
C5—C4—H4	119.6	H1WA—O1W—H1WB	107.7
C1—N1—N2	105.63 (15)		

O1^{i}—Zn1—O1—C8	73 (100)	Zn1—O1—C8—C5	174.81 (12)
O3—Zn1—O1—C8	−78.56 (17)	C6—C5—C8—O2	−176.77 (19)
O3^{i}—Zn1—O1—C8	101.44 (17)	C4—C5—C8—O2	3.7 (3)
O1W^{i}—Zn1—O1—C8	−166.24 (17)	C6—C5—C8—O1	3.9 (3)
O1W—Zn1—O1—C8	13.76 (17)	C4—C5—C8—O1	−175.56 (17)
C3—C2—N4—C1	33.9 (3)	N2—N1—C1—N4	−0.2 (2)
C7—C2—N4—C1	−146.7 (2)	N3—N4—C1—N1	0.4 (2)
C3—C2—N4—N3	−144.73 (19)	C2—N4—C1—N1	−178.39 (18)
C7—C2—N4—N3	34.7 (3)	C2—C7—C6—C5	−0.2 (3)
C1—N4—N3—N2	−0.4 (2)	C4—C5—C6—C7	1.8 (3)
C2—N4—N3—N2	178.53 (17)	C8—C5—C6—C7	−177.68 (18)
C6—C5—C4—C3	−1.5 (3)	N4—N3—N2—N1	0.2 (2)
C8—C5—C4—C3	177.97 (17)	C1—N1—N2—N3	0.0 (2)
C3—C2—C7—C6	−1.8 (3)	O1—Zn1—O3—C9	31.19 (19)
N4—C2—C7—C6	178.77 (17)	O1^{i}—Zn1—O3—C9	−148.81 (19)
C5—C4—C3—C2	−0.4 (3)	O3^{i}—Zn1—O3—C9	−165 (73)
C7—C2—C3—C4	2.1 (3)	O1W^{i}—Zn1—O3—C9	120.04 (19)
N4—C2—C3—C4	−178.49 (17)	O1W—Zn1—O3—C9	−59.96 (19)
Zn1—O1—C8—O2	−4.4 (3)		

Symmetry code: (i) −*x*+1, −*y*, −*z*+2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*WA*···O2*W*^{ii}	0.82	1.97	2.759 (2)	160
O2*W*—H2*WB*···O1*W*^{iii}	0.77 (3)	2.07 (3)	2.831 (2)	175 (3)
O3—H3*M*···O2*W*^{iv}	0.75 (3)	1.99 (3)	2.726 (2)	167 (3)

Symmetry codes: (ii) −*x*+1, *y*−1/2, −*z*+3/2; (iii) *x*, *y*, *z*−1; (iv) *x*, *y*−1, *z*+1.