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catena-Poly[[μ-5,5′-iminoditetrazolato-$\kappa^3N,N′:N″$-bis[triaquazinc(II)]] bis[[triaquazinc(II)]-μ-5,5′-iminoditetrazolato-$\kappa^3N,N′:N″$] dihydrate]

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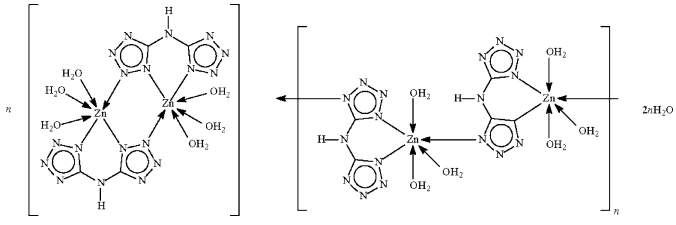
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(N–N) = 0.003 Å; R factor = 0.020; wR factor = 0.054; data-to-parameter ratio = 11.7.

The title compound, $\{[Zn_2(C_2HN_9)_2(H_2O)_6][Zn_2(C_2HN_9)_2(H_2O)_6]\cdot 2H_2O\}_n$, consists of one dinuclear $[Zn(C_2HN_9)(H_2O)_3]_2$ molecule, in which the two $C_2HN_9^-$ monoanions each N,N'-chelate a $[Zn(H_2O)_3]$ unit while using a third N atom to bind to the other triaquazinc unit. In the second $[Zn(C_2HN_9)(H_2O)_3]$ unit, the monoanion similarly N,N'-chelates a triaquazinc unit, but the bridging interaction furnishes a zigzag chain structure. For both Zn centres, a *mer*-ZnN_3O_3 octahedral coordination arises. A network of N—H···N, O—H···N and O—H···O hydrogen bonds helps to establish the structure.

Related literature

For background literature on the ligand, see: Jones *et al.* (2006); Nedel'ko *et al.* (2005); Marecek *et al.* (2004). For related structures, see Klapötke *et al.* (2006); Manfred *et al.* (2005). For related literature, see: Allen (2002).



Experimental

Crystal data

$[Zn_2(C_2HN_9)_2(H_2O)_6]$-$[Zn_2(C_2HN_9)_2(H_2O)_6]\cdot 2H_2O$
M_r = 1118.18
Orthorhombic, $P2_12_12$
a = 10.1201 (1) Å
b = 23.7418 (3) Å
c = 7.3346 (1) Å
V = 1762.28 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 2.81 mm^{-1}
T = 295 (2) K
0.32 × 0.17 × 0.06 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.581, T_{max} = 0.850
25915 measured reflections
4048 independent reflections
3844 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.020
$wR(F^2)$ = 0.054
S = 1.01
4048 reflections
345 parameters
22 restraints
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.43 e Å^{-3}
Absolute structure: Flack (1983), with 1710 Friedel pairs
Flack parameter: 0.026 (8)

Table 1
Selected bond lengths (Å).

Zn1—O2	2.122 (2)	Zn2—O4	2.130 (2)
Zn1—O1	2.148 (2)	Zn2—O5	2.096 (1)
Zn1—O3	2.069 (2)	Zn2—O6	2.132 (2)
Zn1—N1	2.140 (2)	Zn2—N10	2.146 (2)
Zn1—N4^{i}	2.199 (2)	Zn2—N11^{ii}	2.152 (2)
Zn1—N9	2.125 (2)	Zn2—N18	2.113 (2)

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

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

D—H···A	D—H	H···A	D···A	D—H···A
N5—H5···N2^{iii}	0.84 (1)	1.94 (1)	2.773 (2)	171 (3)
N14—H14···N16^{iv}	0.82 (1)	2.23 (1)	3.049 (2)	176 (2)
O1—H11···N13^{iii}	0.85 (1)	1.91 (1)	2.754 (2)	175 (2)
O1—H12···N15^{v}	0.85 (1)	2.14 (2)	2.915 (2)	153 (2)
O2—H21···O6^{iv}	0.84 (1)	2.22 (1)	3.053 (2)	172 (4)
O2—H22···O8^{iii}	0.84 (1)	1.96 (1)	2.796 (2)	173 (3)
O3—H31···N15	0.85 (1)	2.07 (2)	2.835 (3)	148 (3)
O3—H32···N17^{iv}	0.85 (1)	1.96 (1)	2.776 (2)	160 (3)
O4—H41···N3	0.86 (1)	2.00 (1)	2.847 (2)	169 (3)
O4—H42···N6^{i}	0.86 (1)	2.20 (2)	3.000 (3)	155 (3)
O5—H51···O1^{iii}	0.82 (1)	2.19 (1)	3.000 (2)	170 (2)
O5—H52···O7^{vi}	0.83 (1)	1.96 (1)	2.781 (2)	169 (3)
O6—H61···N6^{iv}	0.86 (1)	2.20 (1)	3.042 (3)	167 (3)
O6—H62···N7^{vii}	0.86 (1)	1.84 (1)	2.701 (2)	176 (3)
O7—H7···N8^{viii}	0.84 (1)	2.12 (1)	2.959 (2)	179 (3)
O8—H8···N12^{ix}	0.84 (1)	2.15 (1)	2.974 (2)	166 (4)

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

Data collection: *APEX2* (Bruker, 2006); cell refinement: *SAINT* (Bruker, 2006); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2007).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2619).

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supplementary materials

Acta Cryst. (2007). E**63**, m2943-m2944 [**doi:10.1107/S160053680705578X**]

catena-Poly[[μ-5,5'-iminoditetrazolato-$\kappa^3N,N':N''$-bis[triaquazinc(II)]] bis[[triaquazinc(II)]-μ-5,5'-iminoditetrazolato-$\kappa^3N,N':N''$] dihydrate]

Z.-Q. Liu, W. Dong and S. W. Ng

Comment

Bis(5-tetrazolyl)amine is a high-nitrogen fuel; see Jones *et al.* (2006). Its synthesis in four steps, starting from cyanic chloride, is reported by Nedel'ko *et al.* (2005). The synthesis from sodium azide and sodium dicyanamide in water is reported by Marecek *et al.* (2004). For the crystal structures of the copper complexes, see Klapötke *et al.* (2006); Manfred *et al.* (2005). The structures of several metal derivatives have been deposited with the Cambridge Structural Database (Version 5.28, November 2006; Allen, 2002) as private communications. The title zinc derivative, (I), (Fig. 1) is readily synthesized from sodium azide, sodium dicyanamide and zinc chloride in a hydothermal reaction.

The complex structure of (I) consists of one dinuclear $[Zn(C_2HN_9)_2(H_2O)_3]_2$ moiety in which the two $C_2HN_9^-$ monoanions each *N*,*N*'-chelate to a $Zn(H_2O)_3$ triaquazinc unit while using its third nitrogen atom to bind to the other triaquazinc unit. In the second $Zn(C_2HN_9)_2(H_2O)_3$ unit, the monoanion similarly *N*,*N*'-chelates to a triaquazinc unit, but the bridging interaction furnishes a zigzag chain structure (Fig. 1) For both zinc centres, a *mer*-ZnN_3O_3 octahedral coordination arises (Table 1). Two uncoordinated water molecules complete the structure. A complex network of N—H···N, O—H···N and O—H···O hydrogen bonds helps to establish the structure (Table 2).

Experimental

Zinc chloride (40.9 mg, 0.3 mmol), sodium azide (39.0 mg, 0.6 mmol), sodium dicyanamide (26.7 mg, 0.3 mmol) and water (10 ml) were heated in a 25-ml Teflon-lined, stainless-steel Parr bom at 433 K for 72 h. The bomb was then was cooled to room temperature at 10 K h^{-1}; the colourless blocks of (I) that formed were separated manually.

Refinement

All hydrogen atoms were located in a difference Fourier map, and were refined with distance restraints of O—H = N—H = 0.85 (1) Å; for the water H-atoms, the H···H distances were restrained to 1.39 (1) Å. Their U_{iso} values were refined.

Figures

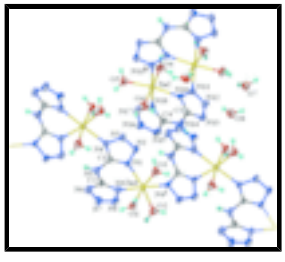


Fig. 1. View of a fragment of (I) depicting the coordination geometries of the two zinc atoms; displacement ellipsoids are drawn at the 70% probability level, and H atoms as spheres of arbitrary radius. Symmetry codes as in Table 1.

catena-poly[μ-5,5'-iminoditetrazolato-κ^3_N_,_N_':_N_''-bis[triaquazinc(II)] bis[[triaquazinc(II)]-μ-5,5'-iminoditetrazolato-κ^3_N_,_N_':_N_'']dihydrate]

Crystal data

$[Zn_2(C_2HN_9)_2(H_2O)_6][Zn_2(C_2HN_9)_2(H_2O)_6]\cdot 2H_2O$	F_{000} = 1128
M_r = 1118.18	D_x = 2.107 Mg m^{-3}
Orthorhombic, $P2_12_12$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2 2ab	Cell parameters from 9121 reflections
a = 10.1201 (1) Å	θ = 1.7–27.5º
b = 23.7418 (3) Å	μ = 2.81 mm^{-1}
c = 7.3346 (1) Å	T = 295 (2) K
V = 1762.28 (4) Å^3	Block, colourless
Z = 2	0.32 × 0.17 × 0.06 mm

Data collection

Bruker APEXII CCD diffractometer	4048 independent reflections
Radiation source: fine-focus sealed tube	3844 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.034
T = 295(2) K	θ_{max} = 27.5º
φ and ω scans	θ_{min} = 1.7º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −13→13
T_{min} = 0.581, T_{max} = 0.850	k = −30→30
25915 measured reflections	l = −9→8

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	All H-atom parameters refined
$R[F^2 > 2\sigma(F^2)]$ = 0.020	$w = 1/[\sigma^2(F_o^2) + (0.0363P)^2P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.054	$(\Delta/\sigma)_{max}$ = 0.001
S = 1.01	$\Delta\rho_{max}$ = 0.29 e Å^{-3}
4048 reflections	$\Delta\rho_{min}$ = −0.43 e Å^{-3}
345 parameters	Extinction correction: none
22 restraints	Absolute structure: Flack (1983), with 1710 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.026 (8)
Secondary atom site location: difference Fourier map	

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.49499 (2)	0.66550 (1)	0.47415 (3)	0.01664 (6)
Zn2	0.36506 (2)	0.93580 (1)	0.01708 (3)	0.01744 (7)
O1	0.4922 (2)	0.6553 (1)	0.7651 (2)	0.0220 (3)
O2	0.6009 (2)	0.5884 (1)	0.4700 (3)	0.0289 (4)
O3	0.5257 (2)	0.6696 (1)	0.1956 (2)	0.0274 (4)
O4	0.3686 (2)	0.9250 (1)	0.3053 (2)	0.0290 (4)
O5	0.1591 (1)	0.9271 (1)	0.0271 (3)	0.0296 (4)
O6	0.3553 (2)	0.9439 (1)	−0.2721 (2)	0.0250 (3)
O7	1.0000	1.0000	−0.1726 (3)	0.0292 (5)
O8	1.0000	1.0000	0.3201 (3)	0.0287 (5)
N1	0.3582 (1)	0.7342 (1)	0.4689 (3)	0.0199 (4)
N2	0.3877 (2)	0.7884 (1)	0.4371 (3)	0.0286 (5)
N3	0.2826 (2)	0.8193 (1)	0.4451 (3)	0.0285 (5)
N4	0.1772 (2)	0.7861 (1)	0.4804 (3)	0.0194 (4)
N5	0.1544 (2)	0.6870 (1)	0.5283 (3)	0.0263 (4)
N6	0.1094 (2)	0.5914 (1)	0.4621 (3)	0.0265 (4)
N7	0.1864 (2)	0.5479 (1)	0.4106 (3)	0.0272 (4)
N8	0.3081 (2)	0.5631 (1)	0.3983 (3)	0.0240 (4)
N9	0.3177 (2)	0.6185 (1)	0.4429 (3)	0.0192 (4)
N10	0.5769 (2)	0.9319 (1)	0.0183 (3)	0.0175 (3)
N11	0.6602 (2)	0.9751 (1)	0.0585 (2)	0.0186 (4)
N12	0.7751 (2)	0.9552 (1)	0.1032 (3)	0.0225 (4)
N13	0.7735 (2)	0.8986 (1)	0.0949 (3)	0.0223 (4)
N14	0.6126 (2)	0.8310 (1)	0.0127 (3)	0.0262 (4)
N15	0.4512 (2)	0.7600 (1)	−0.0351 (3)	0.0270 (4)
N16	0.3182 (2)	0.7617 (1)	−0.0593 (3)	0.0277 (5)
N17	0.2775 (2)	0.8133 (1)	−0.0559 (3)	0.0269 (4)
N18	0.3817 (2)	0.8482 (1)	−0.0277 (3)	0.0215 (4)
C1	0.22764 (2)	0.7341 (1)	0.4936 (3)	0.0168 (4)
C2	0.19376 (2)	0.6338 (1)	0.4795 (3)	0.0191 (4)
C3	0.65014 (2)	0.8860 (1)	0.0409 (3)	0.0178 (4)
C4	0.48487 (2)	0.8141 (1)	−0.0158 (3)	0.0188 (4)
H5	0.073 (1)	0.691 (1)	0.543 (4)	0.03 (1)*
H14	0.671 (2)	0.807 (1)	0.025 (3)	0.02 (1)*
H11	0.423 (2)	0.641 (1)	0.810 (4)	0.04 (1)*
H12	0.505 (3)	0.688 (1)	0.807 (4)	0.05 (1)*
H21	0.667 (2)	0.580 (1)	0.406 (4)	0.08 (1)*
H22	0.571 (2)	0.560 (1)	0.526 (3)	0.04 (1)*
H31	0.496 (3)	0.702 (1)	0.167 (5)	0.08 (1)*
H32	0.608 (1)	0.669 (1)	0.173 (4)	0.05 (1)*
H41	0.333 (3)	0.894 (1)	0.343 (5)	0.09 (2)*
H42	0.448 (2)	0.927 (2)	0.345 (6)	0.11 (2)*
H51	0.119 (2)	0.905 (1)	0.095 (3)	0.04 (1)*
H52	0.112 (2)	0.946 (1)	−0.043 (3)	0.03 (1)*
H61	0.429 (2)	0.931 (1)	−0.310 (5)	0.10 (2)*

H62	0.345 (3)	0.977 (1)	−0.320 (4)	0.04 (1)*
H7	1.055 (2)	1.018 (1)	−0.236 (4)	0.05 (1)*
H8	1.066 (2)	1.007 (2)	0.253 (4)	0.06 (1)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0119 (1)	0.0156 (1)	0.0225 (1)	0.0007 (1)	0.0007 (1)	0.0002 (1)
Zn2	0.0152 (1)	0.0136 (1)	0.0236 (1)	0.0002 (1)	−0.0010 (1)	0.0002 (1)
O1	0.021 (1)	0.021 (1)	0.025 (1)	−0.005 (1)	0.004 (1)	−0.001 (1)
O2	0.022 (1)	0.019 (1)	0.046 (1)	0.004 (1)	0.006 (1)	0.002 (1)
O3	0.023 (1)	0.033 (1)	0.026 (1)	0.005 (1)	0.005 (1)	0.003 (1)
O4	0.034 (1)	0.029 (1)	0.024 (1)	−0.005 (1)	0.000 (1)	0.005 (1)
O5	0.016 (1)	0.024 (1)	0.049 (1)	−0.002 (1)	0.001 (1)	0.007 (1)
O6	0.029 (1)	0.022 (1)	0.023 (1)	0.005 (7)	−0.001 (1)	0.003 (1)
O7	0.024 (1)	0.032 (1)	0.031 (1)	−0.004 (1)	0.000	0.000
O8	0.025 (1)	0.031 (1)	0.030 (1)	−0.003 (1)	0.000	0.000
N1	0.011 (1)	0.015 (1)	0.033 (1)	0.000 (1)	0.001 (1)	0.000 (1)
N2	0.014 (1)	0.016 (1)	0.056 (1)	0.001 (1)	0.003 (1)	0.004 (1)
N3	0.014 (1)	0.018 (1)	0.053 (1)	0.000 (1)	0.004 (1)	0.006 (1)
N4	0.013 (1)	0.015 (1)	0.031 (1)	−0.001 (1)	0.000 (1)	0.001 (1)
N5	0.011 (1)	0.015 (1)	0.053 (1)	0.002 (1)	0.008 (1)	−0.001 (1)
N6	0.016 (1)	0.019 (1)	0.045 (1)	−0.002 (1)	−0.001 (1)	−0.002 (1)
N7	0.019 (1)	0.019 (1)	0.044 (1)	−0.002 (1)	−0.001 (1)	−0.009 (1)
N8	0.020 (1)	0.019 (1)	0.033 (1)	0.000 (1)	0.001 (1)	−0.006 (1)
N9	0.014 (1)	0.015 (1)	0.029 (1)	0.001 (1)	0.000 (1)	−0.004 (1)
N10	0.015 (1)	0.012 (1)	0.026 (1)	−0.001 (1)	−0.002 (1)	0.000 (1)
N11	0.015 (1)	0.015 (1)	0.025 (1)	0.000 (1)	−0.002 (1)	0.001 (1)
N12	0.018 (1)	0.016 (1)	0.034 (1)	0.001 (1)	−0.006 (1)	0.002 (1)
N13	0.016 (1)	0.016 (1)	0.035 (1)	−0.001 (1)	−0.005 (1)	0.001 (1)
N14	0.015 (1)	0.012 (1)	0.052 (1)	0.002 (1)	−0.008 (1)	−0.002 (1)
N15	0.021 (1)	0.014 (1)	0.046 (1)	0.000 (1)	−0.006 (1)	−0.001 (1)
N16	0.019 (1)	0.014 (1)	0.050 (1)	−0.002 (1)	−0.007 (1)	−0.002 (1)
N17	0.019 (1)	0.018 (1)	0.044 (1)	−0.003 (1)	−0.007 (1)	−0.002 (1)
N18	0.018 (1)	0.017 (1)	0.030 (1)	−0.001 (1)	−0.004 (1)	−0.002 (1)
C1	0.011 (1)	0.017 (1)	0.022 (1)	0.002 (1)	0.000 (1)	0.000 (1)
C2	0.014 (1)	0.017 (1)	0.026 (1)	0.001 (1)	0.001 (1)	0.000 (1)
C3	0.016 (1)	0.016 (1)	0.022 (1)	0.000 (1)	−0.002 (1)	0.000 (1)
C4	0.018 (1)	0.014 (1)	0.024 (1)	−0.001 (1)	−0.003 (1)	−0.001 (1)

Geometric parameters (Å, °)

Zn1—O2	2.122 (2)	N10—N11	1.360 (2)
Zn1—O1	2.148 (2)	N11—N12	1.297 (2)
Zn1—O3	2.069 (2)	N12—N13	1.345 (2)
Zn1—N1	2.140 (2)	N13—C3	1.343 (3)
Zn1—N4^{i}	2.199 (2)	N14—C4	1.369 (2)
Zn1—N9	2.125 (2)	N14—C3	1.375 (3)

Zn2—O4	2.130 (2)	N15—C4	1.336 (2)
Zn2—O5	2.096 (1)	N15—N16	1.359 (2)
Zn2—O6	2.132 (2)	N16—N17	1.291 (2)
Zn2—N10	2.146 (2)	N17—N18	1.357 (2)
Zn2—N11^{ii}	2.152 (2)	N18—C4	1.324 (2)
Zn2—N18	2.113 (2)	O1—H11	0.85 (1)
N1—C1	1.334 (2)	O1—H12	0.85 (1)
N1—N2	1.341 (2)	O2—H21	0.84 (1)
N2—N3	1.293 (2)	O2—H22	0.84 (1)
N3—N4	1.351 (2)	O3—H31	0.85 (1)
N4—C1	1.338 (2)	O3—H32	0.85 (1)
N5—C1	1.366 (2)	O4—H41	0.86 (1)
N5—C2	1.371 (2)	O4—H42	0.86 (1)
N6—C2	1.326 (3)	O5—H51	0.82 (1)
N6—N7	1.350 (2)	O5—H52	0.83 (1)
N7—N8	1.287 (3)	O6—H61	0.86 (1)
N8—N9	1.360 (2)	O6—H62	0.86 (1)
N9—C2	1.333 (2)	O7—H7	0.84 (1)
N10—C3	1.329 (2)	O8—H8	0.84 (1)
O3—Zn1—O2	87.17 (7)	N11—N10—Zn2	126.0 (2)
O3—Zn1—N9	92.61 (7)	N12—N11—N10	109.6 (2)
O2—Zn1—N9	88.41 (6)	N12—N11—Zn2^{ii}	120.1 (1)
O3—Zn1—N1	92.48 (7)	N10—N11—Zn2^{ii}	129.6 (1)
O2—Zn1—N1	169.88 (6)	N11—N12—N13	110.0 (2)
N9—Zn1—N1	81.50 (6)	C3—N13—N12	104.3 (2)
O3—Zn1—O1	171.28 (6)	C4—N14—C3	124.2 (2)
O2—Zn1—O1	85.62 (7)	C4—N15—N16	103.7 (2)
N9—Zn1—O1	92.09 (6)	N17—N16—N15	110.1 (2)
N1—Zn1—O1	95.47 (7)	N16—N17—N18	109.5 (2)
O3—Zn1—N4^{i}	89.94 (7)	C4—N18—N17	104.5 (2)
O2—Zn1—N4^{i}	91.70 (6)	C4—N18—Zn2	130.8 (1)
N9—Zn1—N4^{i}	177.45 (7)	N17—N18—Zn2	124.3 (1)
N1—Zn1—N4^{i}	98.42 (6)	N1—C1—N4	111.5 (2)
O1—Zn1—N4^{i}	85.38 (7)	N1—C1—N5	124.3 (2)
O5—Zn2—N18	89.26 (6)	N4—C1—N5	124.2 (2)
O5—Zn2—O4	88.29 (7)	N6—C2—N9	112.3 (2)
N18—Zn2—O4	91.94 (7)	N6—C2—N5	122.5 (2)
O5—Zn2—O6	89.87 (7)	N9—C2—N5	125.2 (2)
N18—Zn2—O6	86.46 (7)	N10—C3—N13	111.9 (2)
O4—Zn2—O6	177.58 (6)	N10—C3—N14	127.3 (2)
O5—Zn2—N10	171.56 (6)	N13—C3—N14	120.8 (2)
N18—Zn2—N10	83.05 (6)	N18—C4—N15	112.3 (2)
O4—Zn2—N10	88.49 (7)	N18—C4—N14	125.1 (2)
O6—Zn2—N10	93.12 (7)	N15—C4—N14	122.6 (2)
O5—Zn2—N11^{ii}	88.51 (6)	Zn1—O1—H11	116 (2)
N18—Zn2—N11^{ii}	177.60 (6)	Zn1—O1—H12	105 (2)

O4—Zn2—N11^{ii}	88.90 (7)	H11—O1—H12	112 (2)
O6—Zn2—N11^{ii}	92.63 (6)	Zn1—O2—H21	128 (2)
N10—Zn2—N11^{ii}	99.22 (6)	Zn1—O2—H22	120 (2)
C1—N1—N2	104.2 (2)	H21—O2—H22	111 (2)
C1—N1—Zn1	129.6 (1)	Zn1—O3—H31	103 (3)
N2—N1—Zn1	126.2 (1)	Zn1—O3—H32	110 (2)
N3—N2—N1	110.6 (2)	H31—O3—H32	108 (2)
N2—N3—N4	109.2 (2)	Zn2—O4—H41	114 (3)
C1—N4—N3	104.5 (2)	Zn2—O4—H42	111 (3)
C1—N4—Zn1^{iii}	142.3 (1)	H41—O4—H42	109 (2)
N3—N4—Zn1^{iii}	112.7 (1)	Zn2—O5—H51	125 (2)
C1—N5—C2	123.2 (2)	Zn2—O5—H52	120 (2)
C2—N6—N7	103.7 (2)	H51—O5—H52	116 (2)
N8—N7—N6	110.9 (2)	Zn2—O6—H61	104 (3)
N7—N8—N9	108.9 (2)	Zn2—O6—H62	120 (2)
C2—N9—N8	104.2 (2)	H61—O6—H62	108 (2)
C2—N9—Zn1	129.0 (1)	C1—N5—H5	118 (2)
N8—N9—Zn1	126.4 (1)	C2—N5—H5	115 (2)
C3—N10—N11	104.3 (2)	C4—N14—H14	119 (2)
C3—N10—Zn2	126.4 (1)	C3—N14—H14	116 (2)
O3—Zn1—N1—C1	109.4 (2)	N16—N17—N18—C4	0.3 (3)
O2—Zn1—N1—C1	21.6 (6)	N16—N17—N18—Zn2	−173.2 (2)
N9—Zn1—N1—C1	17.11 (19)	O5—Zn2—N18—C4	−164.9 (2)
O1—Zn1—N1—C1	−74.2 (2)	O4—Zn2—N18—C4	−76.6 (2)
N4^{i}—Zn1—N1—C1	−160.3 (2)	O6—Zn2—N18—C4	105.2 (2)
O3—Zn1—N1—N2	−69.9 (2)	N10—Zn2—N18—C4	11.6 (2)
O2—Zn1—N1—N2	−157.8 (4)	O5—Zn2—N18—N17	6.7 (2)
N9—Zn1—N1—N2	−162.2 (2)	O4—Zn2—N18—N17	95.0 (2)
O1—Zn1—N1—N2	106.5 (2)	O6—Zn2—N18—N17	−83.2 (2)
N4^{i}—Zn1—N1—N2	20.4 (2)	N10—Zn2—N18—N17	−176.8 (2)
C1—N1—N2—N3	1.1 (3)	N2—N1—C1—N4	−0.8 (3)
Zn1—N1—N2—N3	−179.5 (2)	Zn1—N1—C1—N4	179.8 (2)
N1—N2—N3—N4	−1.0 (3)	N2—N1—C1—N5	179.3 (2)
N2—N3—N4—C1	0.4 (3)	Zn1—N1—C1—N5	−0.2 (3)
N2—N3—N4—Zn1^{iii}	174.0 (2)	N3—N4—C1—N1	0.3 (3)
C2—N6—N7—N8	0.1 (3)	Zn1^{iii}—N4—C1—N1	−170.0 (2)
N6—N7—N8—N9	0.3 (3)	N3—N4—C1—N5	−179.8 (2)
N7—N8—N9—C2	−0.6 (2)	Zn1^{iii}—N4—C1—N5	9.9 (4)
N7—N8—N9—Zn1	173.3 (2)	C2—N5—C1—N1	−24.1 (4)
O3—Zn1—N9—C2	−112.6 (2)	C2—N5—C1—N4	156.0 (2)
O2—Zn1—N9—C2	160.3 (2)	N7—N6—C2—N9	−0.5 (3)
N1—Zn1—N9—C2	−20.5 (2)	N7—N6—C2—N5	179.0 (2)
O1—Zn1—N9—C2	74.7 (2)	N8—N9—C2—N6	0.7 (3)
O3—Zn1—N9—N8	75.0 (2)	Zn1—N9—C2—N6	−173.0 (2)
O2—Zn1—N9—N8	−12.1 (2)	N8—N9—C2—N5	−178.8 (2)
N1—Zn1—N9—N8	167.1 (2)	Zn1—N9—C2—N5	7.5 (3)
O1—Zn1—N9—N8	−97.7 (2)	C1—N5—C2—N6	−159.0 (2)

N18—Zn2—N10—C3	−17.7 (2)	C1—N5—C2—N9	20.4 (4)
O4—Zn2—N10—C3	74.4 (2)	N11—N10—C3—N13	0.8 (2)
O6—Zn2—N10—C3	−103.8 (2)	Zn2—N10—C3—N13	−159.4 (2)
N11^{ii}—Zn2—N10—C3	163.0 (2)	N11—N10—C3—N14	−178.3 (2)
N18—Zn2—N10—N11	−173.7 (2)	Zn2—N10—C3—N14	21.6 (3)
O4—Zn2—N10—N11	−81.6 (2)	N12—N13—C3—N10	−0.7 (3)
O6—Zn2—N10—N11	100.3 (2)	N12—N13—C3—N14	178.4 (2)
N11^{ii}—Zn2—N10—N11	7.1 (2)	C4—N14—C3—N10	−11.1 (4)
C3—N10—N11—N12	−0.5 (2)	C4—N14—C3—N13	169.9 (2)
Zn2—N10—N11—N12	159.7 (2)	N17—N18—C4—N15	0.1 (3)
C3—N10—N11—Zn2^{ii}	169.1 (2)	Zn2—N18—C4—N15	172.9 (2)
Zn2—N10—N11—Zn2^{ii}	−30.7 (2)	N17—N18—C4—N14	180.0 (2)
N10—N11—N12—N13	0.1 (2)	Zn2—N18—C4—N14	−7.1 (4)
Zn2^{ii}—N11—N12—N13	−170.7 (1)	N16—N15—C4—N18	−0.4 (3)
N11—N12—N13—C3	0.4 (2)	N16—N15—C4—N14	179.7 (2)
C4—N15—N16—N17	0.6 (3)	C3—N14—C4—N18	3.0 (4)
N15—N16—N17—N18	−0.5 (3)	C3—N14—C4—N15	−177.1 (2)

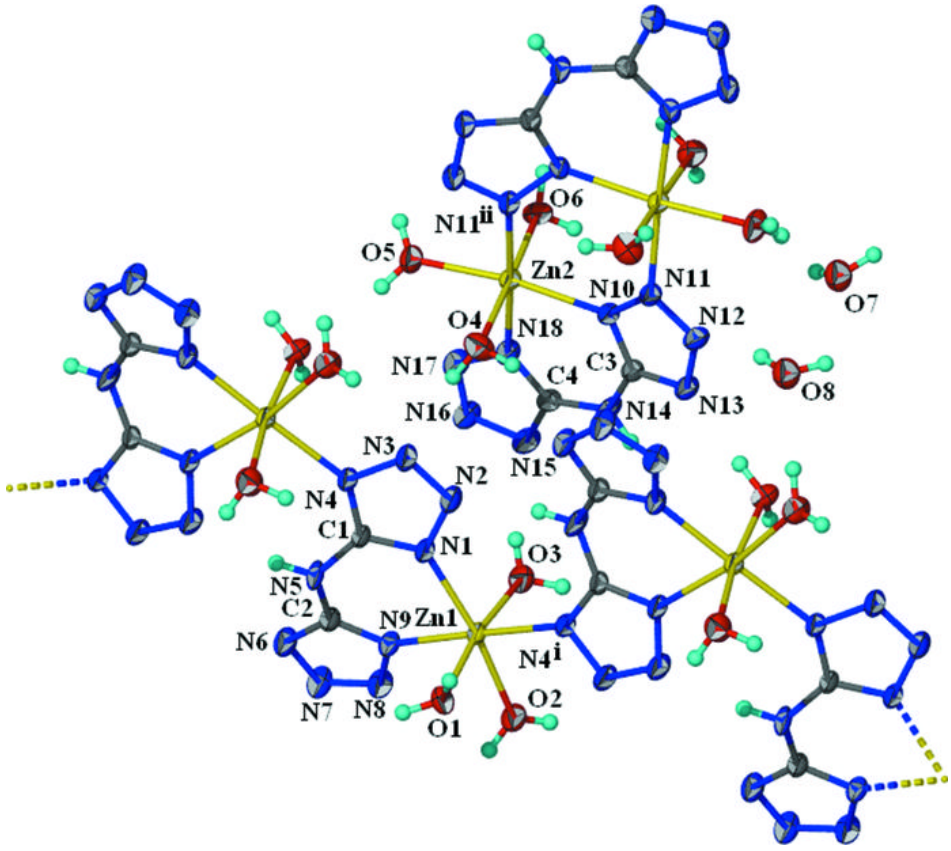
Symmetry codes: (i) *x*+1/2, −*y*+3/2, −*z*+1; (ii) −*x*+1, −*y*+2, *z*; (iii) *x*−1/2, −*y*+3/2, −*z*+1.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N5—H5···N2^{iii}	0.84 (1)	1.94 (1)	2.773 (2)	171 (3)
N14—H14···N16^{iv}	0.82 (1)	2.23 (1)	3.049 (2)	176 (2)
O1—H11···N13^{iii}	0.85 (1)	1.91 (1)	2.754 (2)	175 (2)
O1—H12···N15^{v}	0.85 (1)	2.14 (2)	2.915 (2)	153 (2)
O2—H21···O6^{iv}	0.84 (1)	2.22 (1)	3.053 (2)	172 (4)
O2—H22···O8^{iii}	0.84 (1)	1.96 (1)	2.796 (2)	173 (3)
O3—H31···N15	0.85 (1)	2.07 (2)	2.835 (3)	148 (3)
O3—H32···N17^{iv}	0.85 (1)	1.96 (1)	2.776 (2)	160 (3)
O4—H41···N3	0.86 (1)	2.00 (1)	2.847 (2)	169 (3)
O4—H42···N6^{i}	0.86 (1)	2.20 (2)	3.000 (3)	155 (3)
O5—H51···O1^{iii}	0.82 (1)	2.19 (1)	3.000 (2)	170 (2)
O5—H52···O7^{vi}	0.83 (1)	1.96 (1)	2.781 (2)	169 (3)
O6—H61···N6^{iv}	0.86 (1)	2.20 (1)	3.042 (3)	167 (3)
O6—H62···N7^{vii}	0.86 (1)	1.84 (1)	2.701 (2)	176 (3)
O7—H7···N8^{viii}	0.84 (1)	2.12 (1)	2.959 (2)	179 (3)
O8—H8···N12^{ix}	0.84 (1)	2.15 (1)	2.974 (2)	166 (4)

Symmetry codes: (iii) *x*−1/2, −*y*+3/2, −*z*+1; (iv) *x*+1/2, −*y*+3/2, −*z*; (v) *x*, *y*, *z*+1; (i) *x*+1/2, −*y*+3/2, −*z*+1; (vi) *x*−1, *y*, *z*; (vii) −*x*+1/2, *y*+1/2, −*z*; (viii) −*x*+3/2, *y*+1/2, −*z*; (ix) −*x*+2, −*y*+2, *z*.

Fig. 1


O6
N11ii
O5
Zn2
N10
N11
O7
O4
N18
N12
N17
C4
C3
O8
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N14
N13
N3
N15
N2
N4
C1
N1
O3
N5
C2
N9
Zn1
N6
N4i
N7
N8
O1
O2