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Bis[1,3-dihydroxy-2-hydroxymethyl-2-(5-nitro-2-oxidobenzylideneamino)propane-κ^3N,O,O']zinc(II) trihydrate

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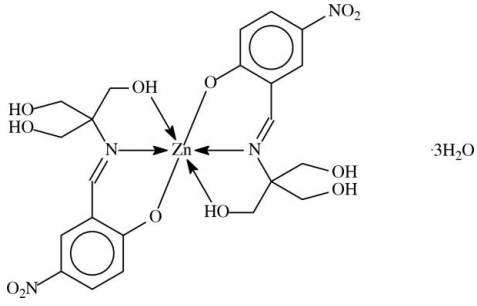
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.002 Å; R factor = 0.023; wR factor = 0.069; data-to-parameter ratio = 14.5.

The Zn atom in the title compound, $[Zn(C_{11}H_{13}N_2O_6)_2]\cdot 3H_2O$, is chelated by the two terdentate Schiff base anions, resulting in a *trans*-ZnN_2O_4 octahedral geometry. The crystal packing is stabilized by O—H···O hydrogen bonds, leading to a three-dimensional network structure.

Related literature

For the same metal complex as a pyridine solvate, see: Ali *et al.* (2006).



Experimental

Crystal data

$[Zn(C_{11}H_{13}N_2O_6)_2]\cdot 3H_2O$
M_r = 657.89
Monoclinic, $P2_1/n$
a = 10.7231 (2) Å
b = 11.7429 (2) Å
c = 21.7538 (3) Å
β = 100.227 (1)°
V = 2695.72 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.99 mm^{-1}
T = 173 (2) K
0.52 × 0.35 × 0.35 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.590, T_{max} = 0.722
55575 measured reflections
6185 independent reflections
5696 reflections with $I > 2\sigma(I)$
R_{int} = 0.029

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.023
$wR(F^2)$ = 0.069
S = 1.02
6185 reflections
427 parameters
12 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.46 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

Table 1
Selected bond lengths (Å).

Zn1—O1	2.062 (1)	Zn1—O8	2.162 (1)
Zn1—O2	2.196 (1)	Zn1—N2	2.079 (1)
Zn1—O7	2.030 (1)	Zn1—N4	2.087 (1)

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2*o*···O10^{i}	0.84 (1)	1.85 (1)	2.686 (1)	173 (2)
O3—H3*o*···O7^{ii}	0.83 (1)	1.90 (1)	2.687 (1)	158 (2)
O4—H4*o*···O3*w*^{iii}	0.83 (1)	1.94 (1)	2.774 (2)	175 (2)
O8—H8*o*···O1*w*	0.83 (1)	1.80 (1)	2.625 (1)	171 (2)
O9—H9*o*···O4^{iv}	0.82 (1)	1.83 (1)	2.640 (1)	168 (2)
O10—H10*o*···O9^{v}	0.83 (1)	1.87 (1)	2.685 (1)	171 (2)
O1*w*—H1*w*1···O2*w*	0.85 (1)	1.85 (1)	2.702 (2)	173 (2)
O1*w*—H1*w*2···O3	0.84 (1)	1.94 (1)	2.780 (2)	174 (2)
O2*w*—H2*w*1···O3*w*	0.86 (1)	2.03 (1)	2.863 (2)	162 (3)
O2*w*—H2*w*2···O6^{vi}	0.86 (1)	2.25 (1)	3.085 (2)	166 (4)
O3*w*—H3*w*1···O1^{vii}	0.85 (1)	2.00 (1)	2.817 (1)	163 (2)
O3*w*—H3*w*2···O11^{viii}	0.85 (1)	2.02 (1)	2.825 (2)	159 (2)

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

Data collection: *APEXII* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); 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: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2383).

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Ali, H. M., Puvaneswary, S. & Ng, S. W. (2006). *Acta Cryst.* E**62**, m2737–m2738.
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supplementary materials

Acta Cryst. (2007). E**63**, m1532 [**doi:10.1107/S1600536807020521**]

Bis[1,3-dihydroxy-2-hydroxymethyl-2-(5-nitro-2-oxidobenzylideneamino)propane-κ^3N,O,O']zinc(II) trihydrate

H. M. Ali, S. Puvaneswary, B. Wan Jefrey and S. W. Ng

Comment

A previous study (Ali *et al.*, 2006) reported the structure of the complex ion found in the title compound as a bis-pyridine solvate. The use of DMSO as solvent yielded the title trihdrate (I) (Fig. 1). Two deprotonated Schiff-base ligands chelate through their phenoxy oxygen atoms, imino nitrogen and hydroxyl oxygen atoms (Table 1). The hydroxy groups of the ligands are engaged in extensive hydrogen bonding with the the uncoordinated water molecules to lead to a three-dimensional network (Table 2).

Experimental

The Schiff base used to make the title compound was synthesized from tris(hydroxymethyl)aminomethane and 5-nitrosalicylaldehyde. The ligand (0.23 g, 0.85 mmol) was dissolved in ethanol (25 ml) and several drops of aqueous sodium hydroxide were added to raise the pH of the solution to about 8.5. Zinc acetate (0.09 g, 0.43 mmol) was then added and the mixture heated for 5 h. The solvent was removed and the product recrystallized from DMSO to yield faint yellow blocks of (I). The water in (I) was presumably incorporated from the atmosphere.

Refinement

The carbon-bound H atoms were placed at calculated positions (C–H = 0.95–0.99 Å), and they were included in the refinement in the riding model approximation with U_{iso}(H) = 1.2U_{eq}(C). The hydroxy and water H atoms were located in a difference Fourier map, and were refined with a distance restraint (O–H = 0.84±0.01 Å); their U_{iso} values were freely refined.

Figures

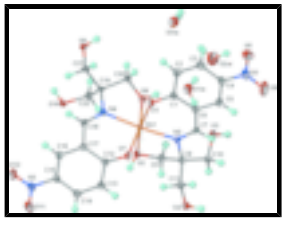


Fig. 1. View of the molecular structure of (I). Displacement ellipsoids are drawn at the 70% probability level (H atoms are shown as spheres of arbitrary radius).

Bis[1,3-dihydroxy-2-hydroxymethyl-2-(5-nitro-2-oxidobenzylideneamino)propane- κ^3N,O,O']zinc(II) trihydrate

Crystal data

$[Zn(C_{11}H_{13}N_2O_6)_2]\cdot 3H_2O$ F_{000} = 1368

M_r = 657.89	D_x = 1.621 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 8727 reflections
a = 10.7231 (2) Å	θ = 2.5–34.6º
b = 11.7429 (2) Å	μ = 0.99 mm^{-1}
c = 21.7538 (3) Å	T = 173 (2) K
β = 100.227 (1)º	Irregular block, faint yellow
V = 2695.72 (8) Å^3	0.52 × 0.35 × 0.35 mm
Z = 4	

Data collection

Bruker APEXII CCD diffractometer	6185 independent reflections
Radiation source: fine-focus sealed tube	5696 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.029
T = 173(2) K	θ_{max} = 27.5º
φ and ω scans	θ_{min} = 1.9º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −13→13
T_{min} = 0.590, T_{max} = 0.722	k = −15→15
55575 measured reflections	l = −28→28

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.023	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.069	$w = 1/[\sigma^2(F_o^2) + (0.04P)^2 + 1.457P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.02	$(\Delta/\sigma)_{max}$ = 0.001
6185 reflections	$\Delta\rho_{max}$ = 0.46 e Å^{-3}
427 parameters	$\Delta\rho_{min}$ = −0.27 e Å^{-3}
12 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.484037 (13)	0.450449 (12)	0.344186 (6)	0.01048 (5)
O1	0.56842 (9)	0.36478 (8)	0.27965 (4)	0.01451 (18)
O2	0.37281 (9)	0.56145 (8)	0.39519 (4)	0.01370 (18)
O3	0.28019 (9)	0.73088 (8)	0.22313 (5)	0.0176 (2)
O4	0.02639 (9)	0.55207 (9)	0.31518 (5)	0.0186 (2)
O5	0.55010 (11)	0.32881 (12)	−0.00644 (5)	0.0315 (3)
O6	0.36276 (12)	0.39495 (12)	−0.00592 (5)	0.0374 (3)
O7	0.38730 (9)	0.31709 (8)	0.37207 (4)	0.01398 (18)
O8	0.60464 (9)	0.59756 (8)	0.34246 (4)	0.01519 (19)
O9	0.97710 (9)	0.50096 (9)	0.42660 (5)	0.0196 (2)
O10	0.77487 (9)	0.53162 (9)	0.53065 (4)	0.01668 (19)
O11	0.39461 (11)	−0.00756 (10)	0.59767 (5)	0.0300 (3)
O12	0.57778 (11)	0.07193 (10)	0.62595 (5)	0.0273 (2)
O1W	0.54356 (11)	0.73526 (11)	0.24683 (6)	0.0280 (2)
O2W	0.61738 (14)	0.65040 (14)	0.14354 (6)	0.0417 (3)
O3W	0.87436 (10)	0.63095 (9)	0.20693 (5)	0.0229 (2)
N1	0.46896 (12)	0.36639 (11)	0.02166 (5)	0.0201 (2)
N2	0.34315 (10)	0.50587 (9)	0.27214 (5)	0.0106 (2)
N3	0.47816 (12)	0.05985 (10)	0.58859 (6)	0.0180 (2)
N4	0.63672 (10)	0.41467 (9)	0.41535 (5)	0.0112 (2)
C1	0.54691 (12)	0.37682 (10)	0.21976 (6)	0.0125 (2)
C2	0.63983 (13)	0.33967 (12)	0.18453 (6)	0.0166 (3)
H2	0.7201	0.3149	0.2061	0.020*
C3	0.61644 (13)	0.33876 (12)	0.12065 (6)	0.0173 (3)
H3	0.6798	0.3139	0.0982	0.021*
C4	0.49776 (13)	0.37499 (11)	0.08866 (6)	0.0159 (3)
C5	0.40829 (13)	0.41975 (11)	0.12047 (6)	0.0147 (2)
H5	0.3301	0.4473	0.0979	0.018*
C6	0.43230 (12)	0.42464 (11)	0.18558 (6)	0.0120 (2)
C7	0.33752 (12)	0.48409 (11)	0.21393 (6)	0.0122 (2)
H7	0.2639	0.5094	0.1864	0.015*
C8	0.23991 (12)	0.57477 (11)	0.29063 (6)	0.0116 (2)
C9	0.29593 (12)	0.63565 (11)	0.35181 (6)	0.0143 (2)
H9A	0.3479	0.7009	0.3424	0.017*
H9B	0.2260	0.6660	0.3712	0.017*
C10	0.18367 (12)	0.66386 (11)	0.24237 (6)	0.0136 (2)
H10A	0.1339	0.6252	0.2056	0.016*
H10B	0.1255	0.7140	0.2606	0.016*
C11	0.13271 (12)	0.49241 (11)	0.29965 (6)	0.0145 (2)
H11A	0.1055	0.4486	0.2607	0.017*
H11B	0.1650	0.4378	0.3334	0.017*
C12	0.41320 (12)	0.25775 (10)	0.42287 (6)	0.0117 (2)
C13	0.31940 (12)	0.18237 (11)	0.43848 (6)	0.0153 (3)
H13	0.2401	0.1770	0.4111	0.018*
C14	0.33969 (13)	0.11756 (11)	0.49157 (6)	0.0157 (3)

H14	0.2756	0.0680	0.5009	0.019*
C15	0.45667 (13)	0.12566 (11)	0.53189 (6)	0.0147 (2)
C16	0.55135 (12)	0.19657 (11)	0.51877 (6)	0.0141 (2)
H16	0.6302	0.1997	0.5467	0.017*
C17	0.53229 (12)	0.26373 (11)	0.46495 (6)	0.0122 (2)
C18	0.63767 (12)	0.33792 (11)	0.45755 (6)	0.0129 (2)
H18	0.7142	0.3287	0.4867	0.015*
C19	0.74779 (11)	0.49089 (11)	0.41778 (6)	0.0118 (2)
C20	0.73077 (12)	0.55311 (11)	0.35481 (6)	0.0137 (2)
H20A	0.7931	0.6158	0.3566	0.016*
H20B	0.7438	0.4997	0.3213	0.016*
C21	0.87318 (12)	0.42490 (12)	0.42665 (6)	0.0155 (3)
H21A	0.8850	0.3829	0.4667	0.019*
H21B	0.8705	0.3687	0.3925	0.019*
C22	0.74665 (13)	0.57977 (11)	0.46974 (6)	0.0145 (2)
H22A	0.8096	0.6398	0.4659	0.017*
H22B	0.6621	0.6161	0.4640	0.017*
H2O	0.3294 (17)	0.5271 (16)	0.4177 (8)	0.031 (5)*
H3O	0.2450 (18)	0.7667 (16)	0.1918 (7)	0.036 (5)*
H4O	−0.0227 (18)	0.5733 (19)	0.2831 (7)	0.042 (6)*
H8O	0.5937 (19)	0.6421 (15)	0.3125 (7)	0.033 (5)*
H9O	0.9814 (19)	0.5166 (18)	0.3901 (5)	0.032 (5)*
H10O	0.8525 (9)	0.5287 (18)	0.5423 (10)	0.034 (5)*
H1W1	0.5666 (18)	0.7032 (15)	0.2156 (7)	0.028 (5)*
H1W2	0.4639 (9)	0.735 (2)	0.2426 (11)	0.049 (7)*
H2W1	0.6926 (14)	0.629 (3)	0.1600 (13)	0.079 (10)*
H2W2	0.609 (4)	0.643 (4)	0.1038 (5)	0.131 (15)*
H3W1	0.887 (2)	0.7015 (9)	0.2026 (11)	0.052 (7)*
H3W2	0.900 (2)	0.601 (2)	0.1756 (8)	0.056 (7)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.00938 (8)	0.01265 (8)	0.00889 (8)	−0.00022 (5)	0.00021 (5)	0.00146 (5)
O1	0.0148 (4)	0.0169 (4)	0.0114 (4)	0.0034 (3)	0.0012 (3)	0.0012 (3)
O2	0.0138 (4)	0.0172 (4)	0.0101 (4)	0.0009 (3)	0.0021 (3)	0.0016 (3)
O3	0.0148 (5)	0.0183 (5)	0.0184 (5)	−0.0012 (4)	−0.0008 (4)	0.0084 (4)
O4	0.0137 (5)	0.0263 (5)	0.0170 (5)	0.0051 (4)	0.0059 (4)	0.0039 (4)
O5	0.0277 (6)	0.0523 (7)	0.0172 (5)	0.0038 (5)	0.0114 (4)	−0.0083 (5)
O6	0.0385 (7)	0.0569 (8)	0.0141 (5)	0.0253 (6)	−0.0026 (5)	−0.0056 (5)
O7	0.0144 (4)	0.0158 (4)	0.0105 (4)	−0.0031 (3)	−0.0013 (3)	0.0025 (3)
O8	0.0119 (4)	0.0175 (5)	0.0154 (5)	0.0004 (4)	0.0003 (3)	0.0065 (4)
O9	0.0102 (4)	0.0335 (6)	0.0152 (5)	−0.0036 (4)	0.0026 (4)	0.0056 (4)
O10	0.0116 (5)	0.0272 (5)	0.0110 (4)	−0.0020 (4)	0.0012 (4)	0.0021 (4)
O11	0.0308 (6)	0.0332 (6)	0.0245 (6)	−0.0131 (5)	0.0012 (5)	0.0149 (5)
O12	0.0233 (5)	0.0340 (6)	0.0215 (5)	−0.0036 (5)	−0.0049 (4)	0.0126 (5)
O1W	0.0201 (5)	0.0355 (6)	0.0271 (6)	0.0006 (5)	0.0006 (5)	0.0118 (5)
O2W	0.0358 (7)	0.0589 (9)	0.0284 (7)	0.0008 (6)	0.0000 (6)	−0.0022 (6)

O3W	0.0245 (5)	0.0215 (5)	0.0221 (5)	0.0005 (4)	0.0024 (4)	−0.0056 (4)
N1	0.0262 (6)	0.0213 (6)	0.0132 (5)	0.0032 (5)	0.0050 (5)	−0.0015 (4)
N2	0.0094 (5)	0.0112 (5)	0.0114 (5)	0.0005 (4)	0.0020 (4)	0.0005 (4)
N3	0.0196 (6)	0.0183 (6)	0.0158 (6)	−0.0007 (4)	0.0025 (5)	0.0047 (4)
N4	0.0096 (5)	0.0129 (5)	0.0110 (5)	−0.0014 (4)	0.0021 (4)	0.0000 (4)
C1	0.0133 (6)	0.0114 (5)	0.0128 (6)	−0.0008 (4)	0.0022 (5)	−0.0002 (4)
C2	0.0134 (6)	0.0191 (6)	0.0174 (6)	0.0039 (5)	0.0032 (5)	0.0004 (5)
C3	0.0180 (6)	0.0181 (6)	0.0176 (6)	0.0030 (5)	0.0076 (5)	−0.0002 (5)
C4	0.0211 (7)	0.0166 (6)	0.0107 (6)	0.0015 (5)	0.0046 (5)	−0.0004 (5)
C5	0.0160 (6)	0.0147 (6)	0.0127 (6)	0.0020 (5)	0.0009 (5)	−0.0001 (5)
C6	0.0120 (6)	0.0120 (5)	0.0124 (6)	0.0004 (4)	0.0030 (5)	−0.0004 (4)
C7	0.0101 (6)	0.0132 (5)	0.0126 (6)	0.0005 (4)	0.0001 (4)	−0.0001 (5)
C8	0.0111 (6)	0.0123 (5)	0.0117 (6)	0.0014 (4)	0.0027 (4)	−0.0001 (5)
C9	0.0168 (6)	0.0139 (6)	0.0118 (6)	0.0024 (5)	0.0013 (5)	−0.0007 (5)
C10	0.0125 (6)	0.0141 (6)	0.0140 (6)	0.0023 (5)	0.0019 (5)	0.0016 (5)
C11	0.0124 (6)	0.0153 (6)	0.0163 (6)	0.0009 (5)	0.0042 (5)	0.0005 (5)
C12	0.0131 (6)	0.0113 (5)	0.0104 (5)	−0.0001 (4)	0.0014 (4)	−0.0013 (4)
C13	0.0130 (6)	0.0178 (6)	0.0143 (6)	−0.0033 (5)	0.0002 (5)	0.0005 (5)
C14	0.0155 (6)	0.0158 (6)	0.0163 (6)	−0.0039 (5)	0.0041 (5)	0.0007 (5)
C15	0.0183 (6)	0.0135 (6)	0.0121 (6)	−0.0004 (5)	0.0026 (5)	0.0032 (5)
C16	0.0140 (6)	0.0147 (6)	0.0128 (6)	−0.0003 (5)	−0.0001 (5)	0.0009 (5)
C17	0.0129 (6)	0.0120 (5)	0.0118 (6)	−0.0008 (4)	0.0020 (5)	0.0007 (4)
C18	0.0107 (6)	0.0155 (6)	0.0115 (6)	−0.0004 (5)	−0.0004 (4)	0.0005 (5)
C19	0.0090 (5)	0.0145 (6)	0.0117 (6)	−0.0021 (4)	0.0012 (4)	0.0014 (5)
C20	0.0101 (6)	0.0175 (6)	0.0132 (6)	−0.0020 (5)	0.0012 (5)	0.0028 (5)
C21	0.0102 (6)	0.0197 (6)	0.0168 (6)	−0.0004 (5)	0.0025 (5)	0.0020 (5)
C22	0.0153 (6)	0.0161 (6)	0.0117 (6)	−0.0021 (5)	0.0016 (5)	0.0006 (5)

Geometric parameters (Å, °)

Zn1—O1	2.062 (1)	C2—C3	1.3676 (19)
Zn1—O2	2.196 (1)	C2—H2	0.9500
Zn1—O7	2.030 (1)	C3—C4	1.4038 (19)
Zn1—O8	2.162 (1)	C3—H3	0.9500
Zn1—N2	2.079 (1)	C4—C5	1.3825 (18)
Zn1—N4	2.087 (1)	C5—C6	1.3952 (18)
O1—C1	1.2898 (15)	C5—H5	0.9500
O2—C9	1.4329 (15)	C6—C7	1.4570 (17)
O2—H2O	0.837 (9)	C7—H7	0.9500
O3—C10	1.4211 (16)	C8—C10	1.5282 (17)
O3—H3O	0.832 (9)	C8—C9	1.5360 (17)
O4—C11	1.4288 (15)	C8—C11	1.5412 (17)
O4—H4O	0.834 (10)	C9—H9A	0.9900
O5—N1	1.2305 (16)	C9—H9B	0.9900
O6—N1	1.2355 (17)	C10—H10A	0.9900
O7—C12	1.2941 (15)	C10—H10B	0.9900
O8—C20	1.4300 (15)	C11—H11A	0.9900
O8—H8O	0.828 (9)	C11—H11B	0.9900
O9—C21	1.4283 (16)	C12—C13	1.4254 (18)

O9—H9O	0.824 (9)	C12—C17	1.4348 (17)
O10—C22	1.4229 (15)	C13—C14	1.3679 (18)
O10—H10O	0.826 (9)	C13—H13	0.9500
O11—N3	1.2375 (16)	C14—C15	1.4004 (18)
O12—N3	1.2301 (16)	C14—H14	0.9500
O1W—H1W1	0.852 (9)	C15—C16	1.3814 (18)
O1W—H1W2	0.843 (10)	C16—C17	1.3964 (17)
O2W—H2W1	0.860 (10)	C16—H16	0.9500
O2W—H2W2	0.857 (10)	C17—C18	1.4581 (17)
O3W—H3W1	0.848 (10)	C18—H18	0.9500
O3W—H3W2	0.851 (10)	C19—C21	1.5341 (17)
N1—C4	1.4387 (17)	C19—C20	1.5345 (17)
N2—C7	1.2828 (16)	C19—C22	1.5402 (18)
N2—C8	1.4833 (16)	C20—H20A	0.9900
N3—C15	1.4391 (17)	C20—H20B	0.9900
N4—C18	1.2853 (17)	C21—H21A	0.9900
N4—C19	1.4833 (15)	C21—H21B	0.9900
C1—C2	1.4289 (18)	C22—H22A	0.9900
C1—C6	1.4332 (17)	C22—H22B	0.9900
O7—Zn1—O1	97.84 (4)	N2—C8—C11	107.55 (10)
O7—Zn1—N2	97.20 (4)	C10—C8—C11	107.75 (10)
O1—Zn1—N2	89.28 (4)	C9—C8—C11	111.57 (10)
O7—Zn1—N4	89.90 (4)	O2—C9—C8	112.23 (10)
O1—Zn1—N4	91.46 (4)	O2—C9—H9A	109.2
N2—Zn1—N4	172.70 (4)	C8—C9—H9A	109.2
O7—Zn1—O8	163.85 (4)	O2—C9—H9B	109.2
O1—Zn1—O8	92.40 (4)	C8—C9—H9B	109.2
N2—Zn1—O8	95.37 (4)	H9A—C9—H9B	107.9
N4—Zn1—O8	77.34 (4)	O3—C10—C8	111.24 (10)
O7—Zn1—O2	87.40 (4)	O3—C10—H10A	109.4
O1—Zn1—O2	167.64 (4)	C8—C10—H10A	109.4
N2—Zn1—O2	78.92 (4)	O3—C10—H10B	109.4
N4—Zn1—O2	99.77 (4)	C8—C10—H10B	109.4
O8—Zn1—O2	85.11 (4)	H10A—C10—H10B	108.0
C1—O1—Zn1	127.78 (8)	O4—C11—C8	111.52 (11)
C9—O2—Zn1	109.20 (7)	O4—C11—H11A	109.3
C9—O2—H2O	111.3 (14)	C8—C11—H11A	109.3
Zn1—O2—H2O	114.8 (14)	O4—C11—H11B	109.3
C10—O3—H3O	105.8 (14)	C8—C11—H11B	109.3
C11—O4—H4O	111.2 (16)	H11A—C11—H11B	108.0
C12—O7—Zn1	128.83 (8)	O7—C12—C13	118.97 (11)
C20—O8—Zn1	104.71 (7)	O7—C12—C17	123.38 (11)
C20—O8—H8O	112.1 (14)	C13—C12—C17	117.66 (11)
Zn1—O8—H8O	121.1 (14)	C14—C13—C12	122.24 (12)
C21—O9—H9O	108.4 (15)	C14—C13—H13	118.9
C22—O10—H10O	109.7 (15)	C12—C13—H13	118.9
H1W1—O1W—H1W2	110 (2)	C13—C14—C15	118.78 (12)
H2W1—O2W—H2W2	108 (3)	C13—C14—H14	120.6
H3W1—O3W—H3W2	103 (2)	C15—C14—H14	120.6

O5—N1—O6	121.88 (12)	C16—C15—C14	121.40 (12)
O5—N1—C4	119.00 (12)	C16—C15—N3	119.27 (12)
O6—N1—C4	119.11 (12)	C14—C15—N3	119.32 (12)
C7—N2—C8	118.03 (10)	C15—C16—C17	120.67 (12)
C7—N2—Zn1	125.62 (9)	C15—C16—H16	119.7
C8—N2—Zn1	116.35 (8)	C17—C16—H16	119.7
O12—N3—O11	122.46 (12)	C16—C17—C12	119.24 (11)
O12—N3—C15	119.50 (12)	C16—C17—C18	115.41 (11)
O11—N3—C15	118.03 (12)	C12—C17—C18	125.33 (11)
C18—N4—C19	119.55 (11)	N4—C18—C17	126.14 (12)
C18—N4—Zn1	125.23 (9)	N4—C18—H18	116.9
C19—N4—Zn1	115.10 (8)	C17—C18—H18	116.9
O1—C1—C2	119.44 (11)	N4—C19—C21	112.33 (10)
O1—C1—C6	123.37 (11)	N4—C19—C20	106.74 (10)
C2—C1—C6	117.18 (12)	C21—C19—C20	108.39 (10)
C3—C2—C1	121.86 (12)	N4—C19—C22	108.91 (10)
C3—C2—H2	119.1	C21—C19—C22	111.78 (10)
C1—C2—H2	119.1	C20—C19—C22	108.50 (10)
C2—C3—C4	119.21 (12)	O8—C20—C19	107.46 (10)
C2—C3—H3	120.4	O8—C20—H20A	110.2
C4—C3—H3	120.4	C19—C20—H20A	110.2
C5—C4—C3	121.04 (12)	O8—C20—H20B	110.2
C5—C4—N1	119.38 (12)	C19—C20—H20B	110.2
C3—C4—N1	119.58 (12)	H20A—C20—H20B	108.5
C4—C5—C6	120.30 (12)	O9—C21—C19	110.52 (11)
C4—C5—H5	119.8	O9—C21—H21A	109.5
C6—C5—H5	119.9	C19—C21—H21A	109.5
C5—C6—C1	119.82 (12)	O9—C21—H21B	109.5
C5—C6—C7	115.63 (11)	C19—C21—H21B	109.5
C1—C6—C7	124.51 (12)	H21A—C21—H21B	108.1
N2—C7—C6	126.81 (12)	O10—C22—C19	112.71 (11)
N2—C7—H7	116.6	O10—C22—H22A	109.0
C6—C7—H7	116.6	C19—C22—H22A	109.0
N2—C8—C10	114.18 (10)	O10—C22—H22B	109.0
N2—C8—C9	107.04 (10)	C19—C22—H22B	109.0
C10—C8—C9	108.81 (10)	H22A—C22—H22B	107.8
O7—Zn1—O1—C1	112.03 (10)	C5—C6—C7—N2	−175.06 (13)
N2—Zn1—O1—C1	14.87 (11)	C1—C6—C7—N2	2.4 (2)
N4—Zn1—O1—C1	−157.87 (11)	C7—N2—C8—C10	−32.67 (16)
O8—Zn1—O1—C1	−80.48 (10)	Zn1—N2—C8—C10	148.33 (9)
O2—Zn1—O1—C1	−2.5 (2)	C7—N2—C8—C9	−153.16 (11)
O7—Zn1—O2—C9	−116.17 (8)	Zn1—N2—C8—C9	27.84 (12)
O1—Zn1—O2—C9	−0.6 (2)	C7—N2—C8—C11	86.83 (13)
N2—Zn1—O2—C9	−18.31 (8)	Zn1—N2—C8—C11	−92.17 (10)
N4—Zn1—O2—C9	154.38 (8)	Zn1—O2—C9—C8	39.50 (12)
O8—Zn1—O2—C9	78.15 (8)	N2—C8—C9—O2	−44.26 (13)
O1—Zn1—O7—C12	103.45 (11)	C10—C8—C9—O2	−168.11 (10)
N2—Zn1—O7—C12	−166.29 (10)	C11—C8—C9—O2	73.15 (13)
N4—Zn1—O7—C12	11.98 (11)	N2—C8—C10—O3	−50.24 (14)

O8—Zn1—O7—C12	−25.4 (2)	C9—C8—C10—O3	69.25 (13)
O2—Zn1—O7—C12	−87.80 (11)	C11—C8—C10—O3	−169.64 (10)
O7—Zn1—O8—C20	76.02 (16)	N2—C8—C11—O4	−177.65 (10)
O1—Zn1—O8—C20	−53.45 (8)	C10—C8—C11—O4	−54.13 (13)
N2—Zn1—O8—C20	−142.95 (8)	C9—C8—C11—O4	65.25 (13)
N4—Zn1—O8—C20	37.51 (8)	Zn1—O7—C12—C13	167.87 (9)
O2—Zn1—O8—C20	138.68 (8)	Zn1—O7—C12—C17	−12.00 (18)
O7—Zn1—N2—C7	−99.37 (11)	O7—C12—C13—C14	−179.56 (12)
O1—Zn1—N2—C7	−1.56 (11)	C17—C12—C13—C14	0.32 (19)
O8—Zn1—N2—C7	90.78 (11)	C12—C13—C14—C15	0.0 (2)
O2—Zn1—N2—C7	174.71 (11)	C13—C14—C15—C16	−0.6 (2)
O7—Zn1—N2—C8	79.54 (9)	C13—C14—C15—N3	178.61 (12)
O1—Zn1—N2—C8	177.35 (9)	O12—N3—C15—C16	3.6 (2)
O8—Zn1—N2—C8	−90.31 (9)	O11—N3—C15—C16	−176.19 (13)
O2—Zn1—N2—C8	−6.38 (8)	O12—N3—C15—C14	−175.59 (13)
O7—Zn1—N4—C18	−4.94 (11)	O11—N3—C15—C14	4.6 (2)
O1—Zn1—N4—C18	−102.78 (11)	C14—C15—C16—C17	0.8 (2)
O8—Zn1—N4—C18	165.09 (11)	N3—C15—C16—C17	−178.35 (12)
O2—Zn1—N4—C18	82.41 (11)	C15—C16—C17—C12	−0.51 (19)
O7—Zn1—N4—C19	179.02 (8)	C15—C16—C17—C18	177.86 (12)
O1—Zn1—N4—C19	81.18 (8)	O7—C12—C17—C16	179.82 (12)
O8—Zn1—N4—C19	−10.95 (8)	C13—C12—C17—C16	−0.06 (18)
O2—Zn1—N4—C19	−93.63 (8)	O7—C12—C17—C18	1.6 (2)
Zn1—O1—C1—C2	159.57 (9)	C13—C12—C17—C18	−178.24 (12)
Zn1—O1—C1—C6	−21.42 (18)	C19—N4—C18—C17	174.09 (12)
O1—C1—C2—C3	172.67 (13)	Zn1—N4—C18—C17	−1.78 (19)
C6—C1—C2—C3	−6.40 (19)	C16—C17—C18—N4	−172.61 (12)
C1—C2—C3—C4	−0.2 (2)	C12—C17—C18—N4	5.6 (2)
C2—C3—C4—C5	5.1 (2)	C18—N4—C19—C21	49.08 (15)
C2—C3—C4—N1	−175.41 (13)	Zn1—N4—C19—C21	−134.64 (9)
O5—N1—C4—C5	178.41 (13)	C18—N4—C19—C20	167.74 (11)
O6—N1—C4—C5	−2.9 (2)	Zn1—N4—C19—C20	−15.98 (12)
O5—N1—C4—C3	−1.1 (2)	C18—N4—C19—C22	−75.30 (14)
O6—N1—C4—C3	177.61 (14)	Zn1—N4—C19—C22	100.98 (10)
C3—C4—C5—C6	−3.1 (2)	Zn1—O8—C20—C19	−57.53 (10)
N1—C4—C5—C6	177.42 (12)	N4—C19—C20—O8	48.97 (13)
C4—C5—C6—C1	−3.77 (19)	C21—C19—C20—O8	170.18 (10)
C4—C5—C6—C7	173.81 (12)	C22—C19—C20—O8	−68.25 (12)
O1—C1—C6—C5	−170.72 (12)	N4—C19—C21—O9	178.03 (10)
C2—C1—C6—C5	8.31 (18)	C20—C19—C21—O9	60.34 (13)
O1—C1—C6—C7	11.9 (2)	C22—C19—C21—O9	−59.19 (14)
C2—C1—C6—C7	−169.05 (12)	N4—C19—C22—O10	70.23 (13)
C8—N2—C7—C6	175.80 (12)	C21—C19—C22—O10	−54.47 (14)
Zn1—N2—C7—C6	−5.30 (19)	C20—C19—C22—O10	−173.93 (10)

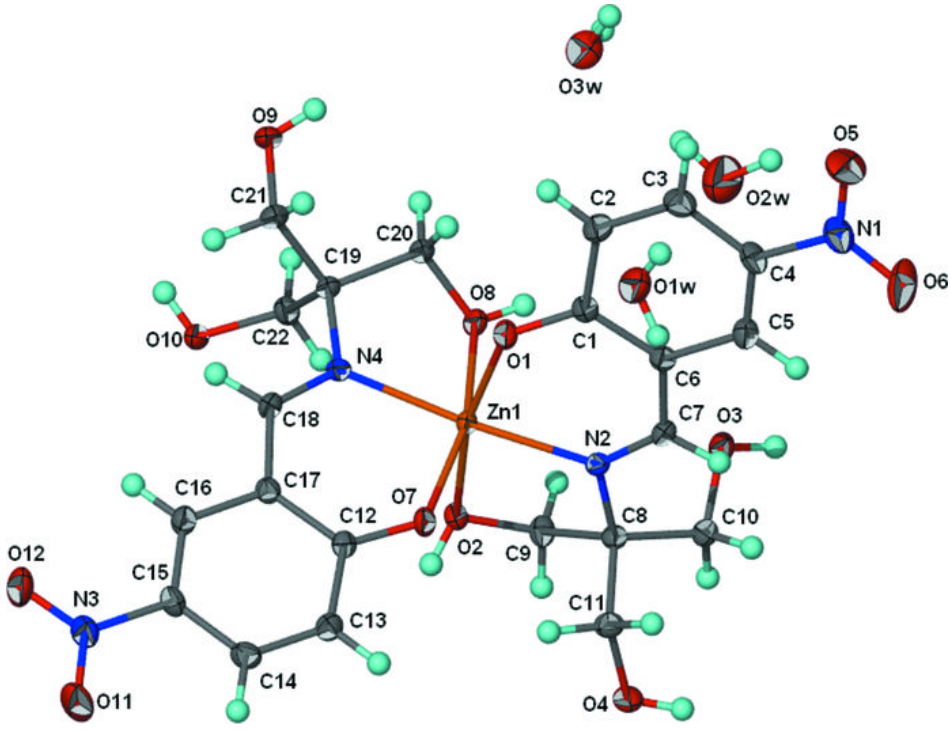
Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2o···O10^{i}	0.84 (1)	1.85 (1)	2.686 (1)	173 (2)

O3—H3o···O7^{ii}	0.83 (1)	1.90 (1)	2.687 (1)	158 (2)
O4—H4o···O3w^{iii}	0.83 (1)	1.94 (1)	2.774 (2)	175 (2)
O8—H8o···O1w	0.83 (1)	1.80 (1)	2.625 (1)	171 (2)
O9—H9o···O4^{iv}	0.82 (1)	1.83 (1)	2.640 (1)	168 (2)
O10—H10o···O9^{v}	0.83 (1)	1.87 (1)	2.685 (1)	171 (2)
O1w—H1w1···O2W	0.85 (1)	1.85 (1)	2.702 (2)	173 (2)
O1w—H1w2···O3	0.84 (1)	1.94 (1)	2.780 (2)	174 (2)
O2w—H2w1···O3W	0.86 (1)	2.03 (1)	2.863 (2)	162 (3)
O2w—H2w2···O6^{vi}	0.86 (1)	2.25 (1)	3.085 (2)	166 (4)
O3w—H3w1···O1^{vii}	0.85 (1)	2.00 (1)	2.817 (1)	163 (2)
O3w—H3w2···O11^{viii}	0.85 (1)	2.02 (1)	2.825 (2)	159 (2)

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

Fig. 1


O3w
O9
C21
C20
C19
O8
O10
C22
N4
O1
C1
C2
C3
O2w
O5
N1
C4
O1w
O6
C5
C6
C7
O3
Zn1
N2
C18
C17
C16
O7
C12
O2
C9
C8
C10
O12
C15
N3
C13
C11
C14
O11
O4