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Dihydroxidobis(melamine-κN)zinc(II) monohydrate

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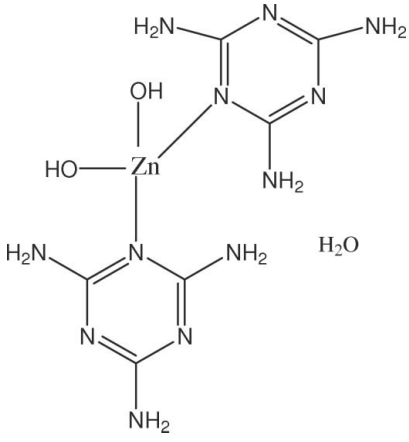
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(N–C) = 0.010 Å; R factor = 0.053; wR factor = 0.143; data-to-parameter ratio = 9.3.

In the title compound, dihydroxidobis(2,4,6-triamino-1,3,5-triazine-κN)zinc(II) monohydrate, $[Zn(OH)_2(C_3N_6H_6)_2]\cdot H_2O$, Zn^{II} is tetrahedrally coordinated by two melamine and two hydroxy groups; there is also a solvent water molecule. The dihedral angle between the two melamine rings is 86.3 (9)°. Intramolecular N—H···O and N—H···N hydrogen bonds help to stabilize the molecular conformation. Numerous intermolecular hydrogen bonds between water, hydroxy and melamine groups link the molecules into a three-dimensional supramolecular network.

Related literature

For general background, see: Ford *et al.* (1999); Tandon *et al.* (1994); Zhu *et al.* (1999). For a related structure, see: Yu *et al.* (2004). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$[Zn(OH)_2(C_3N_6H_6)_2]\cdot H_2O$
M_r = 369.70
Orthorhombic, $Pna2_1$
a = 17.531 (4) Å
b = 6.6251 (13) Å
c = 11.335 (2) Å
V = 1316.5 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.91 mm^{-1}
T = 293 (2) K
0.40 × 0.40 × 0.22 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.508, T_{max} = 0.657
3467 measured reflections
1843 independent reflections
1682 reflections with $I > 2\sigma(I)$
R_{int} = 0.037
3 standard reflections
every 200 reflections
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.143
S = 1.09
1843 reflections
199 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}
Absolute structure: Flack (1983), 636 Friedel pairs
Flack parameter: 0.06 (3)

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O2	0.86	2.44	3.221 (11)	151
N2—H2B···N9^{i}	0.86	2.01	2.865 (9)	174
N4—H4A···O1^{ii}	0.86	2.37	3.120 (8)	146
N4—H4B···O2^{iii}	0.86	2.29	3.089 (11)	156
N6—H6A···O1	0.86	2.14	2.921 (10)	151
N6—H6B···O3^{iv}	0.86	1.91	2.670 (9)	146
N8—H8A···N1	0.86	2.30	3.070 (12)	150
N8—H8B···O3^{v}	0.86	2.03	2.674 (9)	131
N10—H10A···O2^{vi}	0.86	2.34	3.057 (11)	141
N10—H10B···N3^{v}	0.86	1.97	2.826 (9)	176
N12—H12A···O1	0.86	2.31	3.111 (10)	155
N12—H12B···N5^{vii}	0.86	2.29	2.849 (9)	123
O1—H1···O3^{viii}	0.84	2.46	3.209 (14)	150
O2—H2···N8^{ix}	0.84	2.60	3.288 (10)	139
O3—H3A···N11^{x}	0.84	2.43	2.770 (9)	105
O3—H3B···N11^{x}	0.84	2.23	2.770 (9)	122

Symmetry codes: (i) $-x+2, -y+1, z+\frac{1}{2}$; (ii) $x+\frac{1}{2}, -y+\frac{5}{2}, z$; (iii) $x+\frac{1}{2}, -y+\frac{3}{2}, z$; (iv) $-x+2, -y+2, z-\frac{1}{2}$; (v) $-x+2, -y+1, z-\frac{1}{2}$; (vi) $-x+\frac{3}{2}, y-\frac{1}{2}, z-\frac{1}{2}$; (vii) $x-\frac{1}{2}, -y+\frac{5}{2}, z$; (viii) $x, y+1, z$; (ix) $-x+2, -y+2, z+\frac{1}{2}$; (x) $-x+\frac{3}{2}, y-\frac{1}{2}, z+\frac{1}{2}$.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); 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: DN2228).

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supplementary materials

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Dihydroxidobis(melamine-*κN*)zinc(II) monohydrate

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Comment

The transition metal complexes are potential photo-luminescent, paramagnetic and radioactive materials due to their attractive photochemical and photophysical properties(Ford *et al.*, 1999). Low dimensional metal organic complexes have received great attention in recent years for their potential applications in optics, electronics, magnetics, biology, catalyst and medicine (Tandon *et al.*, 1994). The ligand, melamine, has both acceptor and donnor atoms suitable for hydrogen bonding and is analogous to nucleobases that may lead to some interesting new chemotherapeutic possibilities (Zhu *et al.*, 1999).

In the complex I, the zinc cation is coordinated by two melamine and two hydroxyl ligands, forming a distorted tetrahedral geometry, while intramolecular N—H···O and N—H···H hydrogen bonds help to stabilize the molecular conformation (Fig. 1). The two melamine rings make a dihedral angle of 86.3 (9) °. All of the bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The Zn—N bond lengths (2.021 Å and 2.024 Å) in the title compound are slightly shorter than that (2.039 Å) in the compound $[Zn(C_3N_6H_6)(H_2O)_{0.5}Cl_2](C_3N_6H_6)(H_2O)$ (Yu *et al.*, 2004). The Zn—O bond lengths (2.018 Å and 2.041 Å) are slightly longer than that (1.984 Å) in the compound $[Zn(C_3N_6H_6)(H_2O)_{0.5}Cl_2](C_3N_6H_6)(H_2O)$ (Yu *et al.*, 2004).

As can be seen from the packing diagram (Fig. 2), intermolecular N—H···O, N—H···N, O—H.·O and O—H···N hydrogen bonds(Table 1) link the molecules into a three-dimensional network, which may be effective in the stabilization of the crystal structure.

Experimental

A mixture of zinc chloride (0.136 g, 1 mmol), melamine (0.252 g, 2 mmol), and distilled water(8 ml) was heated at 180°C for 4 days in hydrothermal tube. After being cooled to room temperature, colourless block crystals were obtained. Elemental analysis calcd for compound(I): C 19.58%, H 4.40%, N 45.60%; Found: C 19.51%, H 4.35%, N 45.53%.

Refinement

H atoms attached to NH_2 and hydroxyl groups were positioned geometrically (O—H = 0.84 and N—H = 0.86 Å) and constrained to ride on their parent atoms, with $U_{iso}(H) = 1.2U_{eq}(N,O)$. H atoms from water were located in a difference map and refined with distance restraints of O—H = 0.84 \%A and Uĩso~(H) = 1.5U~eq~(O).

Figures

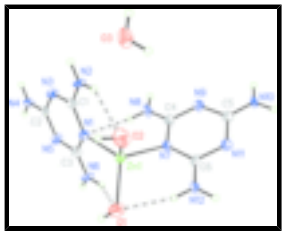

Fig. 1. A view of the molecular structure of (I) showing the atom-numbering scheme and 30% displacement ellipsoids (arbitrary spheres for the H atoms). Intramolecular hydrogen bonds are shown as double dashed lines.

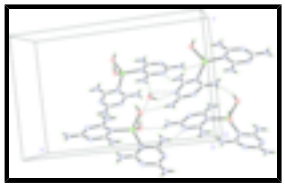

Fig. 2. A packing diagram of complex(I). Hydrogen bonds are shown as dashed lines.

Dihydroxidobis(melamine-κ*N*)zinc(II) monohydrate

Crystal data

$[Zn(OH)_2(C_3N_6H_6)_2]\cdot H_2O$	$F_{000} = 760$
$M_r = 369.70$	$D_x = 1.865$ Mg m^{-3}
Orthorhombic, *Pna*2$_1$	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: P 2c -2n	Cell parameters from 25 reflections
a = 17.531 (4) Å	θ = 9–13º
b = 6.6251 (13) Å	μ = 1.91 mm^{-1}
c = 11.335 (2) Å	*T* = 293 (2) K
V = 1316.5 (5) Å^3	Block, colourless
Z = 4	0.40 × 0.40 × 0.22 mm

Data collection

Enraf–Nonius CAD-4 diffractometer	$R_{int} = 0.037$
Radiation source: fine-focus sealed tube	$\theta_{max} = 25.1$º
Monochromator: graphite	$\theta_{min} = 2.3$º
T = 293(2) K	*h* = −11→20
ω/2θ scans	*k* = −7→7
Absorption correction: ψ scan (North *et al.*, 1968)	*l* = −13→11
$T_{min} = 0.508$, $T_{max} = 0.657$	3 standard reflections
3467 measured reflections	every 200 reflections
1843 independent reflections	intensity decay: none
1682 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.053$	$w = 1/[\sigma^2(F_o^2) + (0.0759P)^2 + 5.1018P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.143$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.09$	$\Delta\rho_{max} = 0.23$ e Å^{-3}
1843 reflections	$\Delta\rho_{min} = -0.38$ e Å^{-3}
199 parameters	Extinction correction: none
1 restraint	Absolute structure: Flack (1983), 636 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.06 (3)
Secondary atom site location: difference Fourier map	

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}
C1	1.0926 (4)	0.8133 (12)	0.2026 (8)	0.0288 (18)
C2	1.2208 (4)	0.9046 (10)	0.1426 (11)	0.0301 (16)
C3	1.1128 (4)	1.1158 (13)	0.0982 (8)	0.032 (2)
C4	0.9359 (4)	0.7899 (13)	−0.0664 (9)	0.0327 (19)
C5	0.8131 (5)	0.6933 (14)	−0.1435 (9)	0.035 (2)
C6	0.8286 (4)	0.9887 (13)	−0.0226 (9)	0.0306 (18)
N1	1.0653 (3)	0.9865 (9)	0.1520 (9)	0.0303 (18)
N2	1.0510 (3)	0.6883 (9)	0.2514 (6)	0.0264 (16)
H2A	1.0026	0.7081	0.2547	0.032*
H2B	1.0705	0.5814	0.2821	0.032*
N3	1.1697 (3)	0.7769 (10)	0.1947 (7)	0.0313 (16)
N4	1.2893 (2)	0.8706 (8)	0.1433 (8)	0.0246 (13)
H4A	1.3205	0.9558	0.1124	0.030*
H4B	1.3064	0.7614	0.1747	0.030*
N5	1.1901 (4)	1.0702 (10)	0.0957 (7)	0.0319 (17)
N6	1.0884 (4)	1.2648 (11)	0.0488 (7)	0.039 (2)

H6A	1.0402	1.2885	0.0479	0.046*
H6B	1.1193	1.3467	0.0145	0.046*
N7	0.9038 (4)	0.9458 (10)	−0.0072 (7)	0.0242 (17)
N8	1.0043 (3)	0.7584 (11)	−0.0641 (8)	0.041 (2)
H8A	1.0338	0.8362	−0.0240	0.050*
H8B	1.0232	0.6582	−0.1025	0.050*
N9	0.8892 (4)	0.6602 (11)	−0.1310 (7)	0.0329 (17)
N10	0.7718 (4)	0.5743 (10)	−0.1966 (7)	0.0318 (17)
H10A	0.7239	0.5988	−0.2035	0.038*
H10B	0.7909	0.4665	−0.2269	0.038*
N11	0.7853 (4)	0.8644 (11)	−0.0947 (7)	0.0338 (16)
N12	0.7985 (3)	1.1327 (10)	0.0259 (7)	0.0333 (18)
H12A	0.8250	1.2100	0.0711	0.040*
H12B	0.7509	1.1568	0.0149	0.040*
O1	0.9360 (3)	1.3630 (9)	0.1356 (11)	0.0580 (17)
H1	0.9357	1.4061	0.2053	0.087*
O2	0.8931 (5)	0.9344 (13)	0.2726 (9)	0.051 (3)
H2	0.9153	0.9581	0.3368	0.077*
O3	0.8689 (4)	0.4538 (10)	0.3936 (8)	0.053 (2)
H3A	0.8521	0.3534	0.4307	0.080*
H3B	0.8286	0.4959	0.3620	0.080*
Zn1	0.95397 (4)	1.06209 (11)	0.13850 (11)	0.0287 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.026 (4)	0.027 (4)	0.033 (5)	0.005 (3)	−0.001 (3)	−0.006 (4)
C2	0.029 (3)	0.030 (4)	0.031 (4)	−0.006 (3)	−0.012 (5)	0.002 (5)
C3	0.026 (4)	0.037 (4)	0.032 (5)	−0.001 (3)	0.005 (3)	−0.003 (4)
C4	0.028 (4)	0.033 (4)	0.037 (5)	0.003 (3)	0.001 (4)	−0.005 (4)
C5	0.036 (4)	0.032 (5)	0.038 (5)	0.004 (4)	0.001 (4)	−0.0041 (4)
C6	0.025 (4)	0.035 (4)	0.033 (5)	0.005 (3)	−0.008 (3)	0.000 (4)
N1	0.020 (2)	0.029 (3)	0.042 (5)	−0.004 (2)	−0.002 (4)	0.009 (4)
N2	0.015 (3)	0.021 (3)	0.043 (4)	0.002 (3)	0.007 (3)	0.018 (3)
N3	0.022 (3)	0.027 (3)	0.045 (4)	−0.002 (3)	0.003 (3)	0.009 (3)
N4	0.009 (2)	0.019 (3)	0.047 (4)	0.0011 (18)	0.008 (4)	0.004 (4)
N5	0.026 (3)	0.034 (4)	0.036 (4)	−0.001 (3)	0.002 (3)	0.010 (3)
N6	0.018 (3)	0.025 (4)	0.043 (5)	0.004 (3)	0.011 (3)	0.018 (4)
N7	0.020 (3)	0.028 (4)	0.025 (5)	0.002 (3)	−0.003 (3)	−0.008 (3)
N8	0.020 (3)	0.040 (4)	0.064 (6)	0.008 (3)	−0.004 (3)	−0.036 (4)
N9	0.028 (3)	0.035 (4)	0.035 (4)	0.003 (3)	−0.001 (3)	−0.012 (4)
N10	0.021 (3)	0.029 (3)	0.045 (5)	0.000 (3)	−0.008 (3)	−0.022 (3)
N11	0.028 (3)	0.033 (4)	0.040 (4)	0.004 (3)	0.002 (3)	−0.010 (4)
N12	0.021 (3)	0.034 (4)	0.054 (5)	0.010 (3)	−0.009 (3)	−0.031 (4)
O1	0.057 (3)	0.046 (3)	0.071 (5)	0.007 (3)	0.000 (6)	0.009 (6)
O2	0.055 (5)	0.047 (6)	0.062 (7)	−0.011 (4)	0.005 (4)	0.002 (5)
O3	0.032 (3)	0.058 (4)	0.069 (5)	0.005 (3)	−0.008 (3)	−0.021 (4)
Zn1	0.0224 (4)	0.0304 (5)	0.0334 (5)	0.0006 (3)	−0.0005 (5)	−0.0012 (6)

Geometric parameters (Å, °)

C1—N2	1.234 (10)	N2—H2A	0.8600
C1—N1	1.369 (11)	N2—H2B	0.8600
C1—N3	1.377 (10)	N4—H4A	0.8600
C2—N4	1.222 (8)	N4—H4B	0.8600
C2—N5	1.334 (10)	N6—H6A	0.8600
C2—N3	1.366 (10)	N6—H6B	0.8600
C3—N6	1.213 (11)	N7—Zn1	2.024 (8)
C3—N1	1.341 (11)	N8—H8A	0.8600
C3—N5	1.389 (10)	N8—H8B	0.8600
C4—N8	1.217 (10)	N10—H10A	0.8600
C4—N7	1.354 (11)	N10—H10B	0.8600
C4—N9	1.395 (11)	N12—H12A	0.8600
C5—N10	1.227 (11)	N12—H12B	0.8600
C5—N11	1.353 (12)	O1—Zn1	2.018 (6)
C5—N9	1.359 (11)	O1—H1	0.8396
C6—N12	1.221 (11)	O2—Zn1	2.041 (10)
C6—N7	1.360 (11)	O2—H2	0.8400
C6—N11	1.387 (11)	O3—H3A	0.8396
N1—Zn1	2.021 (6)	O3—H3B	0.8399
N2—C1—N1	122.9 (7)	C2—N5—C3	124.4 (7)
N2—C1—N3	119.5 (7)	C3—N6—H6A	120.0
N1—C1—N3	117.6 (7)	C3—N6—H6B	120.0
N4—C2—N5	123.5 (8)	H6A—N6—H6B	120.0
N4—C2—N3	121.9 (7)	C4—N7—C6	119.9 (8)
N5—C2—N3	114.6 (6)	C4—N7—Zn1	121.0 (6)
N6—C3—N1	120.8 (7)	C6—N7—Zn1	116.5 (6)
N6—C3—N5	120.7 (8)	C4—N8—H8A	120.0
N1—C3—N5	118.4 (8)	C4—N8—H8B	120.0
N8—C4—N7	122.0 (8)	H8A—N8—H8B	120.0
N8—C4—N9	119.0 (8)	C5—N9—C4	122.2 (7)
N7—C4—N9	119.0 (7)	C5—N10—H10A	120.0
N10—C5—N11	121.8 (8)	C5—N10—H10B	120.0
N10—C5—N9	121.8 (8)	H10A—N10—H10B	120.0
N11—C5—N9	116.5 (9)	C5—N11—C6	122.8 (7)
N12—C6—N7	121.7 (8)	C6—N12—H12A	120.0
N12—C6—N11	119.5 (7)	C6—N12—H12B	120.0
N7—C6—N11	118.9 (8)	H12A—N12—H12B	120.0
C3—N1—C1	120.6 (6)	Zn1—O1—H1	108.8
C3—N1—Zn1	114.0 (5)	Zn1—O2—H2	109.0
C1—N1—Zn1	125.2 (5)	H3A—O3—H3B	100.5
C1—N2—H2A	120.0	O1—Zn1—N1	113.4 (3)
C1—N2—H2B	120.0	O1—Zn1—N7	107.2 (4)
H2A—N2—H2B	120.0	N1—Zn1—N7	112.8 (3)
C2—N3—C1	124.3 (7)	O1—Zn1—O2	109.8 (4)
C2—N4—H4A	120.0	N1—Zn1—O2	110.2 (4)
C2—N4—H4B	120.0	N7—Zn1—O2	102.9 (3)

H4A—N4—H4B	120.0		
N6—C3—N1—C1	176.7 (9)	N12—C6—N7—Zn1	21.0 (12)
N5—C3—N1—C1	−0.4 (14)	N11—C6—N7—Zn1	−158.6 (7)
N6—C3—N1—Zn1	1.3 (12)	N10—C5—N9—C4	−177.1 (9)
N5—C3—N1—Zn1	−175.8 (6)	N11—C5—N9—C4	3.0 (13)
N2—C1—N1—C3	−178.8 (9)	N8—C4—N9—C5	−175.8 (9)
N3—C1—N1—C3	−0.8 (14)	N7—C4—N9—C5	4.9 (13)
N2—C1—N1—Zn1	−3.9 (13)	N10—C5—N11—C6	172.1 (9)
N3—C1—N1—Zn1	174.1 (6)	N9—C5—N11—C6	−8.0 (13)
N4—C2—N3—C1	176.1 (10)	N12—C6—N11—C5	−174.5 (9)
N5—C2—N3—C1	−1.6 (15)	N7—C6—N11—C5	5.1 (14)
N2—C1—N3—C2	180.0 (9)	C3—N1—Zn1—O1	−33.1 (9)
N1—C1—N3—C2	1.8 (14)	C1—N1—Zn1—O1	151.7 (8)
N4—C2—N5—C3	−177.3 (10)	C3—N1—Zn1—N7	88.9 (7)
N3—C2—N5—C3	0.4 (15)	C1—N1—Zn1—N7	−86.3 (9)
N6—C3—N5—C2	−176.5 (10)	C3—N1—Zn1—O2	−156.7 (7)
N1—C3—N5—C2	0.5 (14)	C1—N1—Zn1—O2	28.1 (9)
N8—C4—N7—C6	172.8 (10)	C4—N7—Zn1—O1	143.5 (7)
N9—C4—N7—C6	−8.0 (13)	C6—N7—Zn1—O1	−54.9 (7)
N8—C4—N7—Zn1	−26.2 (13)	C4—N7—Zn1—N1	18.0 (8)
N9—C4—N7—Zn1	153.0 (7)	C6—N7—Zn1—N1	179.6 (6)
N12—C6—N7—C4	−177.2 (9)	C4—N7—Zn1—O2	−100.7 (7)
N11—C6—N7—C4	3.2 (13)	C6—N7—Zn1—O2	60.9 (7)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2A···O2	0.86	2.44	3.221 (11)	151
N2—H2B···N9^{i}	0.86	2.01	2.865 (9)	174
N4—H4A···O1^{ii}	0.86	2.37	3.120 (8)	146
N4—H4B···O2^{iii}	0.86	2.29	3.089 (11)	156
N6—H6A···O1	0.86	2.14	2.921 (10)	151
N6—H6B···O3^{iv}	0.86	1.91	2.670 (9)	146
N8—H8A···N1	0.86	2.30	3.070 (12)	150
N8—H8B···O3^{v}	0.86	2.03	2.674 (9)	131
N10—H10A···O2^{vi}	0.86	2.34	3.057 (11)	141
N10—H10B···N3^{v}	0.86	1.97	2.826 (9)	176
N12—H12A···O1	0.86	2.31	3.111 (10)	155
N12—H12B···N5^{vii}	0.86	2.29	2.849 (9)	123
O1—H1···O3^{viii}	0.84	2.46	3.209 (14)	150
O2—H2···N8^{ix}	0.84	2.60	3.288 (10)	139
O3—H3A···N11^{x}	0.84	2.43	2.770 (9)	105
O3—H3B···N11^{x}	0.84	2.23	2.770 (9)	122

Symmetry codes: (i) −*x*+2, −*y*+1, *z*+1/2; (ii) *x*+1/2, −*y*+5/2, *z*; (iii) *x*+1/2, −*y*+3/2, *z*; (iv) −*x*+2, −*y*+2, *z*−1/2; (v) −*x*+2, −*y*+1, *z*−1/2; (vi) −*x*+3/2, *y*−1/2, *z*−1/2; (vii) *x*−1/2, −*y*+5/2, *z*; (viii) *x*, *y*+1, *z*; (ix) −*x*+2, −*y*+2, *z*+1/2; (x) −*x*+3/2, *y*−1/2, *z*+1/2.

Fig. 1

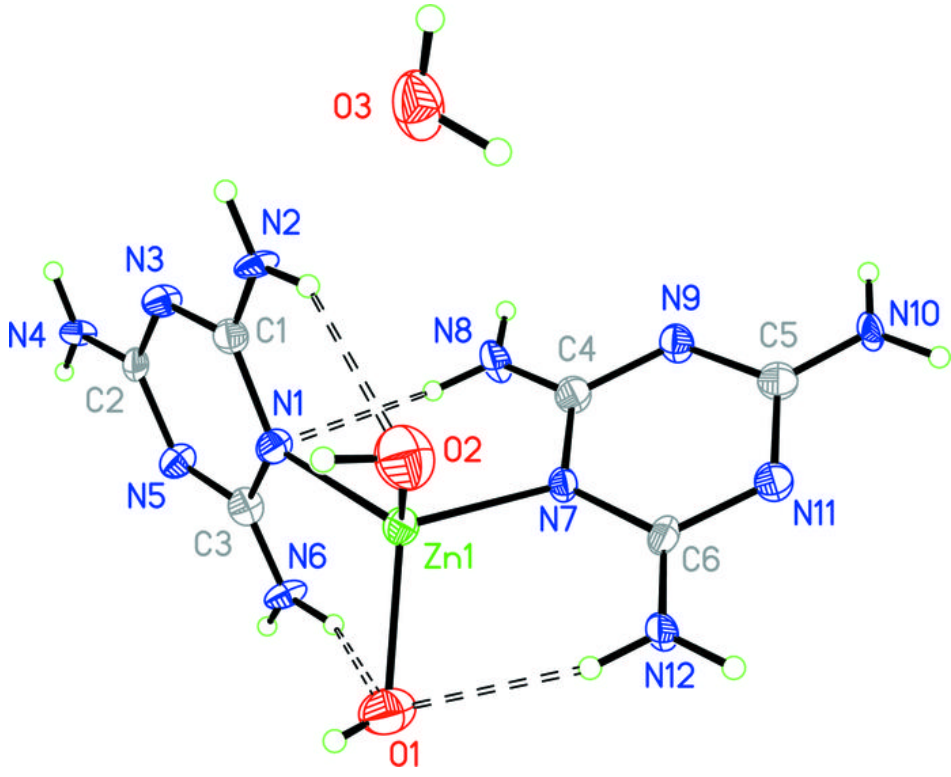

Fig. 2