Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Bis(2-aminobenzothiazol-3-ium) bis(7-oxabicyclo[2.2.1]heptane-2,3-dicarboxylato-κ^3O^2,O^3,O^7)zincate hexahydrate

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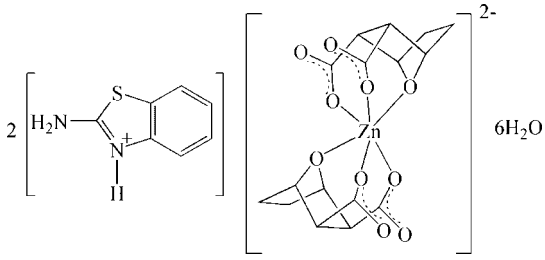
Received 19 April 2012; accepted 21 April 2012

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.005 Å; R factor = 0.047; wR factor = 0.087; data-to-parameter ratio = 12.9.

In the title hydrated molecular salt, $(C_7H_7N_2S)_2[Zn(C_8H_8O_5)_2]\cdot6H_2O$, which is isotypic with its Mn^{II}, Co^{II} and Ni^{II} analogues, the Zn^{2+} ion lies on a crystallographic inversion centre and a distorted ZnO_6 octahedral coordination geometry arises from the two doubly deprotonated O,O',O''-tridentate ligands. In the crystal, the components are linked by $N-H\cdots O_a$, $N-H\cdots O_w$, $O_w-H\cdots O_a$ and $O_w-H\cdots O_w$ hydrogen bonds (w = water and a = anion).

Related literature

For background to the applications of norcantharidin (systematic name: 7-oxabicyclo[2,2,1]heptane-2,3-dicarboxylic anhydride), see: Zeng & Lu (2006). For the isotypic Mn^{II}, Co^{II} and Ni^{II} structures, see: Wang *et al.* (2010*a*,*b*, 2012).



Experimental

Crystal data

$(C_7H_7N_2S)_2[Zn(C_8H_8O_5)_2]\cdot6H_2O$
M_r = 844.21
Triclinic, $P\overline{1}$
a = 6.6983 (7) Å
b = 10.1497 (11) Å
c = 13.2082 (14) Å
α = 90.172 (7)°
β = 91.097 (7)°
γ = 99.251 (7)°
V = 886.11 (16) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 0.89 mm^{-1}
T = 296 K
0.12 × 0.08 × 0.06 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.914, T_{max} = 0.951
11657 measured reflections
3108 independent reflections
1839 reflections with $I > 2\sigma(I)$
R_{int} = 0.228

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.087
S = 0.91
3108 reflections
241 parameters
9 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.48 e Å^{-3}
$\Delta\rho_{min}$ = −0.74 e Å^{-3}

Table 1
Selected bond lengths (Å).

Zn1—O1	2.014 (2)	Zn1—O5	2.176 (3)
Zn1—O3	2.132 (2)		

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1*A*···O4^{i}	0.86	1.82	2.675 (4)	173
N2—H2*A*···O3^{i}	0.86	2.00	2.853 (4)	172
N2—H2*B*···O2*W*^{ii}	0.86	2.02	2.838 (4)	158
O1*W*—H1*WA*···O4	0.85	2.01	2.818 (3)	160
O1*W*—H1*WB*···O2*W*	0.85	1.95	2.793 (4)	170
O2*W*—H2*WA*···O2	0.85	1.85	2.683 (3)	167
O2*W*—H2*WB*···O3*W*	0.85	1.92	2.765 (3)	170
O3*W*—H3*WA*···O1*W*^{ii}	0.85	2.21	3.024 (3)	160
O3*W*—H3*WB*···O1*W*^{iii}	0.85	2.00	2.793 (4)	156

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

Data collection: *APEX2* (Bruker, 2006); cell refinement: *SAINT* (Bruker, 2006); 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: *SHELXL97*.

The authors thank the Natural Science Foundation of Zhejiang Province, China (grant No. Y407301) for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6746).

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supplementary materials

Acta Cryst. (2012). E**68**, m684 [doi:10.1107/S1600536812017886]

Bis(2-aminobenzothiazol-3-ium) bis(7-oxabicyclo[2.2.1]heptane-2,3-dicarboxylato-κ^3O^2,O^3,O^7)zincate hexahydrate

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Comment

7-oxabicyclo[2,2,1]heptane-2,3-dicarboxylic anhydride (norcantharidin), as a traditional Chinese drug, has great anti-cancer activity. (Zeng *et al.*, 2006). A isostructural manganese complex (Wang *et al.*, 2010*a*) and a cobalt complex (Wang *et al.*, 2010*b*) has been reported. The molecular structure of the title complex is shown in Fig.1. The zinc atom is six-coordinated in a distorted octahedral coordination mode, binding to two bridging O atoms of the bicycloheptane unit and four carboxylate O atoms of two symmetry-related and fully deprotonated ligands. 2-aminobenzothiazole don't involved the coordination, and N atom of thiazole ring is protonated.The crystal structure is stabilized by N—H···O hydrogen-bonding interactions between the cations and anions and O—H···O hydrogen bonds including the crystal water molecules.

Experimental

A mixture of 0.5 mmol norcantharidin, 0.5 mmol zinc acetate, 0.5 mmol 2-aminobenzothiazole and 15 mL distilled water was sealed in a 25 mL Teflon-lined stainless vessel and heated at 443 K for 3 d, then cooled slowly to room temperature. The solution was filtered and colourless blocks were recovered.

Refinement

H atoms bonded to C atoms were positioned geometrically and refined using a riding model [aliphatic of tertiary carbon C—H = 0.98 Å, aliphatic of secondary carbon C—H = 0.97 Å, N—H = 0.86 Å, both with U_{iso}(H) = 1.2U_{eq}(C)]. The H atoms bonded to O atoms were located in a difference Fourier maps and refined with O—H distance restraints of 0.85 (4) Å and U_{iso}(H) = 1.5U_{eq}(O).

Computing details

Data collection: *APEX2* (Bruker, 2006); cell refinement: *SAINT* (Bruker, 2006); data reduction: *SAINT* (Bruker, 2006); 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: *SHELXL97* (Sheldrick, 2008).

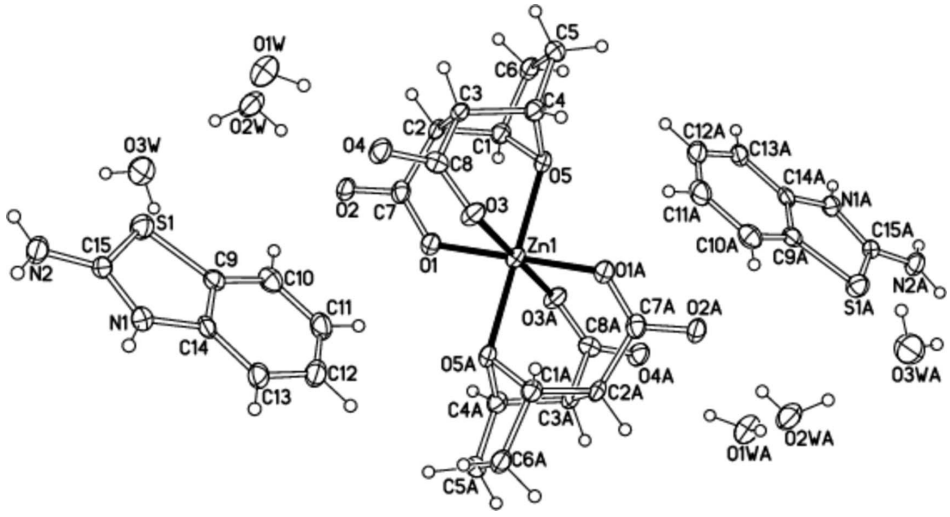

Figure 1

A view of (I) showing displacement ellipsoids drawn at the 30% probability level. Atoms with label suffix A are generatd by (1–x, –y, –z).

Bis(2-aminobenzothiazol-3-ium) bis(7-oxabicyclo[2.2.1]heptane-2,3- dicarboxylato-κ^3O^2,O^3,O^7)zincate hexahydrate

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$(C_7H_7N_2S)_2[Zn(C_8H_8O_5)_2]\cdot 6H_2O$
M_r = 844.21
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 6.6983 (7) Å
b = 10.1497 (11) Å
c = 13.2082 (14) Å
α = 90.172 (7)°
β = 91.097 (7)°
γ = 99.251 (7)°
V = 886.11 (16) Å^3
Z = 1
$F(000)$ = 440
D_x = 1.582 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2505 reflections
θ = 1.5–25.0°
μ = 0.89 mm^{-1}
T = 296 K
Block, colorless
0.12 × 0.08 × 0.06 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.914, T_{max} = 0.951
11657 measured reflections
3108 independent reflections
1839 reflections with $I > 2\sigma(I)$
R_{int} = 0.228
θ_{max} = 25.0°, θ_{min} = 1.5°
h = −7→7
k = −12→12
l = −15→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.087
S = 0.91
3108 reflections
241 parameters
9 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0123P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.48$ e Å^{-3}
$\Delta\rho_{min} = -0.74$ e Å^{-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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.5000	0.0000	0.0000	0.0324 (2)
S1	0.32760 (16)	0.26730 (12)	0.52749 (7)	0.0407 (3)
O1	0.3674 (4)	0.1456 (3)	0.06056 (17)	0.0375 (8)
O1W	0.8090 (4)	0.3956 (3)	0.37387 (17)	0.0545 (9)
H1WA	0.8277	0.3325	0.3345	0.082*
H1WB	0.7307	0.4430	0.3454	0.082*
H2WA	0.4603	0.4745	0.2298	0.082*
H2WB	0.4268	0.5366	0.3202	0.082*
H3WA	0.1928	0.5407	0.4659	0.082*
H3WB	0.0922	0.4941	0.3767	0.082*
O2	0.3636 (4)	0.3401 (3)	0.13832 (18)	0.0398 (8)
O2W	0.5164 (4)	0.5222 (3)	0.27869 (18)	0.0509 (9)
O3	0.6904 (4)	0.0121 (3)	0.13199 (17)	0.0372 (8)
O3W	0.1943 (4)	0.5453 (3)	0.40167 (19)	0.0681 (11)
O4	0.7729 (4)	0.1592 (3)	0.25795 (16)	0.0391 (8)
O5	0.7162 (3)	0.1550 (3)	−0.06915 (16)	0.0318 (8)
N1	0.2772 (4)	0.0314 (3)	0.6011 (2)	0.0314 (9)
H1A	0.2680	−0.0334	0.6434	0.038*
N2	0.3461 (4)	0.1984 (3)	0.7235 (2)	0.0407 (10)
H2A	0.3394	0.1405	0.7712	0.049*
H2B	0.3717	0.2822	0.7379	0.049*
C6	0.8584 (6)	0.3726 (4)	−0.1096 (2)	0.0353 (11)
H6A	0.8806	0.4636	−0.0841	0.042*
H6B	0.8494	0.3736	−0.1829	0.042*
C5	1.0257 (5)	0.2946 (4)	−0.0715 (3)	0.0360 (11)
H5A	1.0917	0.2585	−0.1276	0.043*
H5B	1.1265	0.3507	−0.0300	0.043*
C1	0.6712 (5)	0.2907 (4)	−0.0644 (2)	0.0318 (11)
H1B	0.5458	0.3011	−0.1008	0.038*
C4	0.9066 (5)	0.1842 (4)	−0.0096 (3)	0.0313 (11)
H4A	0.9750	0.1065	−0.0007	0.038*
C2	0.6616 (5)	0.3148 (4)	0.0498 (2)	0.0284 (10)

H2C	0.6979	0.4103	0.0652	0.034*
C3	0.8342 (5)	0.2369 (4)	0.0902 (2)	0.0281 (11)
H3A	0.9440	0.3005	0.1213	0.034*
C7	0.4500 (6)	0.2624 (4)	0.0880 (3)	0.0326 (11)
C8	0.7611 (5)	0.1281 (4)	0.1656 (3)	0.0299 (10)
C9	0.2753 (5)	0.1307 (4)	0.4436 (3)	0.0335 (11)
C10	0.2575 (5)	0.1337 (4)	0.3394 (3)	0.0407 (12)
H10A	0.2714	0.2138	0.3043	0.049*
C11	0.2178 (6)	0.0109 (5)	0.2894 (3)	0.0468 (14)
H11A	0.2094	0.0088	0.2190	0.056*
C12	0.1909 (6)	−0.1066 (5)	0.3418 (3)	0.0467 (14)
H12A	0.1586	−0.1865	0.3061	0.056*
C13	0.2104 (5)	−0.1101 (4)	0.4473 (3)	0.0386 (12)
H13A	0.1969	−0.1901	0.4826	0.046*
C14	0.2511 (5)	0.0122 (4)	0.4961 (3)	0.0293 (11)
C15	0.3173 (5)	0.1590 (4)	0.6289 (3)	0.0304 (11)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0350 (4)	0.0305 (5)	0.0304 (4)	0.0014 (4)	−0.0001 (3)	−0.0092 (3)
S1	0.0497 (7)	0.0374 (9)	0.0338 (6)	0.0033 (6)	0.0004 (5)	−0.0002 (6)
O1	0.0345 (16)	0.038 (2)	0.0393 (16)	0.0037 (15)	0.0032 (12)	−0.0124 (15)
O1W	0.066 (2)	0.045 (2)	0.0543 (19)	0.0145 (18)	−0.0097 (15)	−0.0099 (17)
O2	0.0357 (16)	0.038 (2)	0.0468 (17)	0.0079 (15)	0.0043 (13)	−0.0186 (15)
O2W	0.056 (2)	0.041 (2)	0.0537 (18)	0.0038 (17)	−0.0062 (14)	−0.0156 (17)
O3	0.0510 (19)	0.027 (2)	0.0307 (15)	−0.0005 (16)	−0.0063 (13)	−0.0028 (14)
O3W	0.063 (2)	0.083 (3)	0.053 (2)	−0.002 (2)	0.0003 (16)	−0.014 (2)
O4	0.0530 (19)	0.037 (2)	0.0254 (15)	0.0015 (16)	−0.0020 (13)	−0.0036 (14)
O5	0.0363 (16)	0.032 (2)	0.0266 (14)	0.0046 (15)	0.0020 (12)	−0.0110 (14)
N1	0.0330 (19)	0.033 (3)	0.0284 (18)	0.0064 (18)	0.0029 (14)	0.0008 (17)
N2	0.055 (2)	0.036 (3)	0.0313 (19)	0.007 (2)	0.0034 (16)	−0.0062 (18)
C6	0.051 (3)	0.026 (3)	0.028 (2)	0.004 (2)	0.0034 (19)	−0.003 (2)
C5	0.039 (3)	0.035 (3)	0.032 (2)	0.000 (2)	0.0097 (18)	−0.002 (2)
C1	0.034 (2)	0.031 (3)	0.031 (2)	0.005 (2)	−0.0005 (18)	−0.003 (2)
C4	0.027 (2)	0.030 (3)	0.037 (2)	0.008 (2)	−0.0026 (18)	−0.005 (2)
C2	0.036 (2)	0.021 (3)	0.028 (2)	0.005 (2)	0.0018 (17)	−0.0092 (19)
C3	0.025 (2)	0.028 (3)	0.029 (2)	0.001 (2)	−0.0013 (17)	−0.011 (2)
C7	0.031 (2)	0.043 (3)	0.024 (2)	0.010 (2)	−0.0052 (17)	−0.007 (2)
C8	0.025 (2)	0.031 (3)	0.034 (2)	0.007 (2)	−0.0009 (18)	0.008 (2)
C9	0.024 (2)	0.043 (3)	0.032 (2)	0.001 (2)	0.0043 (18)	−0.004 (2)
C10	0.039 (3)	0.049 (4)	0.034 (2)	0.007 (2)	0.0040 (19)	0.007 (2)
C11	0.042 (3)	0.070 (4)	0.026 (2)	0.002 (3)	0.004 (2)	−0.008 (3)
C12	0.033 (3)	0.061 (4)	0.046 (3)	0.006 (3)	0.000 (2)	−0.024 (3)
C13	0.029 (2)	0.048 (3)	0.039 (2)	0.008 (2)	0.0051 (18)	−0.012 (2)
C14	0.023 (2)	0.042 (3)	0.023 (2)	0.005 (2)	0.0062 (16)	−0.002 (2)
C15	0.028 (2)	0.030 (3)	0.033 (2)	0.003 (2)	0.0066 (18)	−0.006 (2)

Geometric parameters (Å, º)

Zn1—O1	2.014 (2)	C6—C1	1.521 (5)
Zn1—O1^{i}	2.014 (2)	C6—C5	1.550 (5)
Zn1—O3^{i}	2.132 (2)	C6—H6A	0.9700
Zn1—O3	2.132 (2)	C6—H6B	0.9700
Zn1—O5^{i}	2.176 (3)	C5—C4	1.518 (5)
Zn1—O5	2.176 (3)	C5—H5A	0.9700
S1—C15	1.731 (4)	C5—H5B	0.9700
S1—C9	1.759 (4)	C1—C2	1.532 (4)
O1—C7	1.274 (4)	C1—H1B	0.9800
O1W—H1WA	0.8499	C4—C3	1.536 (4)
O1W—H1WB	0.8500	C4—H4A	0.9800
O2—C7	1.248 (3)	C2—C7	1.527 (5)
O2W—H2WA	0.8499	C2—C3	1.587 (5)
O2W—H2WB	0.8501	C2—H2C	0.9800
O3—C8	1.272 (4)	C3—C8	1.517 (5)
O3W—H3WA	0.8504	C3—H3A	0.9800
O3W—H3WB	0.8502	C9—C14	1.379 (5)
O4—C8	1.257 (3)	C9—C10	1.379 (4)
O5—C1	1.458 (4)	C10—C11	1.393 (5)
O5—C4	1.473 (4)	C10—H10A	0.9300
N1—C15	1.329 (4)	C11—C12	1.370 (5)
N1—C14	1.403 (4)	C11—H11A	0.9300
N1—H1A	0.8600	C12—C13	1.398 (5)
N2—C15	1.312 (4)	C12—H12A	0.9300
N2—H2A	0.8600	C13—C14	1.382 (5)
N2—H2B	0.8600	C13—H13A	0.9300
O1—Zn1—O1^{i}	180.0	C2—C1—H1B	113.1
O1—Zn1—O3^{i}	92.14 (9)	O5—C4—C5	101.4 (3)
O1^{i}—Zn1—O3^{i}	87.86 (9)	O5—C4—C3	101.8 (3)
O1—Zn1—O3	87.86 (9)	C5—C4—C3	112.1 (3)
O1^{i}—Zn1—O3	92.14 (9)	O5—C4—H4A	113.4
O3^{i}—Zn1—O3	180.0	C5—C4—H4A	113.4
O1—Zn1—O5^{i}	91.98 (9)	C3—C4—H4A	113.4
O1^{i}—Zn1—O5^{i}	88.02 (9)	C7—C2—C1	110.4 (3)
O3^{i}—Zn1—O5^{i}	89.22 (10)	C7—C2—C3	115.0 (3)
O3—Zn1—O5^{i}	90.78 (10)	C1—C2—C3	100.7 (2)
O1—Zn1—O5	88.02 (9)	C7—C2—H2C	110.1
O1^{i}—Zn1—O5	91.98 (9)	C1—C2—H2C	110.1
O3^{i}—Zn1—O5	90.78 (10)	C3—C2—H2C	110.1
O3—Zn1—O5	89.22 (10)	C8—C3—C4	113.7 (3)
O5^{i}—Zn1—O5	180.0	C8—C3—C2	113.7 (3)
C15—S1—C9	90.10 (19)	C4—C3—C2	101.0 (3)
C7—O1—Zn1	128.1 (2)	C8—C3—H3A	109.4
H1WA—O1W—H1WB	110.0	C4—C3—H3A	109.4
H2WA—O2W—H2WB	109.4	C2—C3—H3A	109.4
C8—O3—Zn1	117.2 (3)	O2—C7—O1	124.0 (4)
H3WA—O3W—H3WB	109.6	O2—C7—C2	117.8 (4)

C1—O5—C4	95.2 (3)	O1—C7—C2	118.0 (3)
C1—O5—Zn1	116.69 (19)	O4—C8—O3	124.0 (4)
C4—O5—Zn1	112.0 (2)	O4—C8—C3	117.5 (3)
C15—N1—C14	113.7 (3)	O3—C8—C3	118.5 (3)
C15—N1—H1A	123.1	C14—C9—C10	121.7 (4)
C14—N1—H1A	123.1	C14—C9—S1	110.6 (3)
C15—N2—H2A	120.0	C10—C9—S1	127.7 (4)
C15—N2—H2B	120.0	C9—C10—C11	116.9 (4)
H2A—N2—H2B	120.0	C9—C10—H10A	121.6
C1—C6—C5	101.2 (3)	C11—C10—H10A	121.6
C1—C6—H6A	111.5	C12—C11—C10	121.3 (4)
C5—C6—H6A	111.5	C12—C11—H11A	119.4
C1—C6—H6B	111.5	C10—C11—H11A	119.4
C5—C6—H6B	111.5	C11—C12—C13	122.0 (4)
H6A—C6—H6B	109.4	C11—C12—H12A	119.0
C4—C5—C6	102.2 (3)	C13—C12—H12A	119.0
C4—C5—H5A	111.3	C14—C13—C12	116.1 (4)
C6—C5—H5A	111.3	C14—C13—H13A	121.9
C4—C5—H5B	111.3	C12—C13—H13A	121.9
C6—C5—H5B	111.3	C9—C14—C13	121.9 (4)
H5A—C5—H5B	109.2	C9—C14—N1	112.6 (3)
O5—C1—C6	102.7 (3)	C13—C14—N1	125.4 (4)
O5—C1—C2	102.4 (3)	N2—C15—N1	123.4 (4)
C6—C1—C2	111.6 (3)	N2—C15—S1	123.7 (3)
O5—C1—H1B	113.1	N1—C15—S1	113.0 (3)
C6—C1—H1B	113.1		

O3^{i}—Zn1—O1—C7	−122.1 (3)	C5—C4—C3—C2	72.1 (4)
O3—Zn1—O1—C7	57.9 (3)	C7—C2—C3—C8	−3.6 (4)
O5^{i}—Zn1—O1—C7	148.6 (3)	C1—C2—C3—C8	−122.3 (3)
O5—Zn1—O1—C7	−31.4 (3)	C7—C2—C3—C4	118.6 (3)
O1—Zn1—O3—C8	−42.4 (3)	C1—C2—C3—C4	−0.1 (3)
O1^{i}—Zn1—O3—C8	137.6 (3)	Zn1—O1—C7—O2	−169.1 (3)
O5^{i}—Zn1—O3—C8	−134.3 (2)	Zn1—O1—C7—C2	16.1 (5)
O5—Zn1—O3—C8	45.7 (2)	C1—C2—C7—O2	−127.5 (4)
O1—Zn1—O5—C1	−10.4 (2)	C3—C2—C7—O2	119.3 (4)
O1^{i}—Zn1—O5—C1	169.6 (2)	C1—C2—C7—O1	47.6 (5)
O3^{i}—Zn1—O5—C1	81.7 (2)	C3—C2—C7—O1	−65.6 (4)
O3—Zn1—O5—C1	−98.3 (2)	Zn1—O3—C8—O4	138.6 (3)
O1—Zn1—O5—C4	97.84 (19)	Zn1—O3—C8—C3	−40.8 (4)
O1^{i}—Zn1—O5—C4	−82.16 (19)	C4—C3—C8—O4	153.4 (3)
O3^{i}—Zn1—O5—C4	−170.05 (19)	C2—C3—C8—O4	−91.7 (4)
O3—Zn1—O5—C4	9.95 (19)	C4—C3—C8—O3	−27.2 (5)
C1—C6—C5—C4	−1.3 (3)	C2—C3—C8—O3	87.7 (4)
C4—O5—C1—C6	57.0 (3)	C15—S1—C9—C14	0.6 (3)
Zn1—O5—C1—C6	174.86 (19)	C15—S1—C9—C10	−179.7 (3)
C4—O5—C1—C2	−58.8 (3)	C14—C9—C10—C11	−1.2 (5)
Zn1—O5—C1—C2	59.0 (3)	S1—C9—C10—C11	179.2 (3)
C5—C6—C1—O5	−34.6 (3)	C9—C10—C11—C12	2.2 (6)

C5—C6—C1—C2	74.5 (3)	C10—C11—C12—C13	−2.9 (6)
C1—O5—C4—C5	−57.3 (3)	C11—C12—C13—C14	2.3 (5)
Zn1—O5—C4—C5	−178.88 (18)	C10—C9—C14—C13	0.9 (6)
C1—O5—C4—C3	58.4 (3)	S1—C9—C14—C13	−179.4 (3)
Zn1—O5—C4—C3	−63.2 (3)	C10—C9—C14—N1	179.5 (3)
C6—C5—C4—O5	36.1 (3)	S1—C9—C14—N1	−0.9 (4)
C6—C5—C4—C3	−71.8 (3)	C12—C13—C14—C9	−1.4 (5)
O5—C1—C2—C7	−85.8 (3)	C12—C13—C14—N1	−179.7 (3)
C6—C1—C2—C7	165.0 (3)	C15—N1—C14—C9	0.8 (4)
O5—C1—C2—C3	36.2 (3)	C15—N1—C14—C13	179.3 (3)
C6—C1—C2—C3	−73.0 (4)	C14—N1—C15—N2	179.8 (3)
O5—C4—C3—C8	86.7 (4)	C14—N1—C15—S1	−0.3 (4)
C5—C4—C3—C8	−165.7 (3)	C9—S1—C15—N2	179.8 (3)
O5—C4—C3—C2	−35.5 (4)	C9—S1—C15—N1	−0.2 (3)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···O4^{ii}	0.86	1.82	2.675 (4)	173
N2—H2*A*···O3^{ii}	0.86	2.00	2.853 (4)	172
N2—H2*B*···O2*W*^{iii}	0.86	2.02	2.838 (4)	158
O1*W*—H1*WA*···O4	0.85	2.01	2.818 (3)	160
O1*W*—H1*WB*···O2*W*	0.85	1.95	2.793 (4)	170
O2*W*—H2*WA*···O2	0.85	1.85	2.683 (3)	167
O2*W*—H2*WB*···O3*W*	0.85	1.92	2.765 (3)	170
O3*W*—H3*WA*···O1*W*^{iii}	0.85	2.21	3.024 (3)	160
O3*W*—H3*WB*···O1*W*^{iv}	0.85	2.00	2.793 (4)	156

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