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

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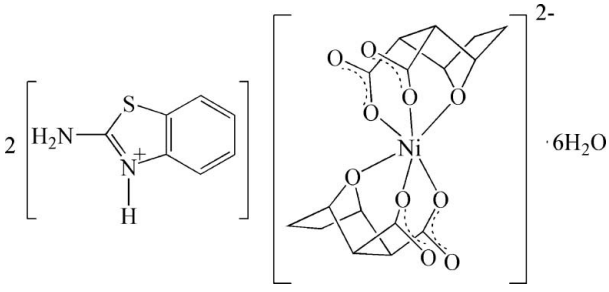
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.032; wR factor = 0.089; data-to-parameter ratio = 12.8.

In the title compound, $(C_7H_7N_2S)_2[Ni(C_8H_8O_5)_2]\cdot 6H_2O$, the Ni^{II} cation is located on an inversion center and is O,O',O''-chelated by two symmetry-related 7-oxabicyclo[2.2.1]heptane-2,3-dicarboxylate anions in a distorted octahedral geometry. The 2-aminobenzothiazol-3-ium cation links with the Ni complex anion *via* N—H···O hydrogen bonding. Extensive O—H···O and N—H···O hydrogen bonds involving the lattice water molecules also occur in the crystal structure.

Related literature

For background to the applications of norcantharidin (systematic name: 7-oxabicyclo[2,2,1]heptane-2,3-dicarboxylic anhydride), see: Hill *et al.* (2007). The isotypic Mn^{II}, Co^{II} and Ni^{II} analogues were reported by Wang *et al.* (2010*a*,*b*) and Zhang *et al.* (2012), respectively.



Experimental

Crystal data

$(C_7H_7N_2S)_2[Ni(C_8H_8O_5)_2]\cdot 6H_2O$
M_r = 837.51
Triclinic, $P\overline{1}$
a = 6.6907 (1) Å
b = 10.0963 (2) Å
c = 13.2283 (3) Å
α = 90.284 (1)°
β = 91.192 (1)°
γ = 99.709 (1)°
V = 880.57 (3) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 0.75 mm^{-1}
T = 296 K
0.27 × 0.21 × 0.07 mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.828, T_{max} = 0.951
11942 measured reflections
3083 independent reflections
2654 reflections with $I > 2\sigma(I)$
R_{int} = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.089
S = 1.06
3083 reflections
241 parameters
3 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.44 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1W—H1WA···O4^{i}	0.85	1.97	2.815 (2)	179
O1W—H1WB···O3W	0.85	2.28	3.029 (3)	147
O2W—H2WA···O2^{ii}	0.85	1.83	2.682 (2)	179
O2W—H2WB···O1W^{iii}	0.85	1.95	2.798 (3)	178
O3W—H3WA···O1W^{iv}	0.85	1.92	2.769 (3)	179
O3W—H3WB···O2W	0.85	1.95	2.772 (3)	161
N1—H1A···O4^{i}	0.86	1.82	2.673 (2)	173
N2—H2A···O3^{i}	0.86	2.01	2.863 (2)	173
N2—H2B···O2W^{i}	0.86	2.00	2.818 (3)	158

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

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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5517).

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supplementary materials

Acta Cryst. (2012). E**68**, m683 [doi:10.1107/S1600536812017722]

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

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Comment

7-oxabicyclo[2,2,1]heptane-2,3-dicarboxylic anhydride (norcantharidin), which has been considered as potent inhibitor of the serine/threonine protein, has great anti-cancer activity (Hill *et al.*, 2007). 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 nickel 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 nickel 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 block green crystals were obtained.

Refinement

The H atoms bonded to O atoms were located in a difference Fourier maps and refined with O—H distance restraints of 0.85 (3) Å and U_{iso}(H) = 1.5U_{eq}(O). Other H atoms were positioned geometrically and refined using a riding model with C—H = 0.97–0.98 and N—H = 0.86 Å, U_{iso}(H) = 1.2U_{eq}(C,N).

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).

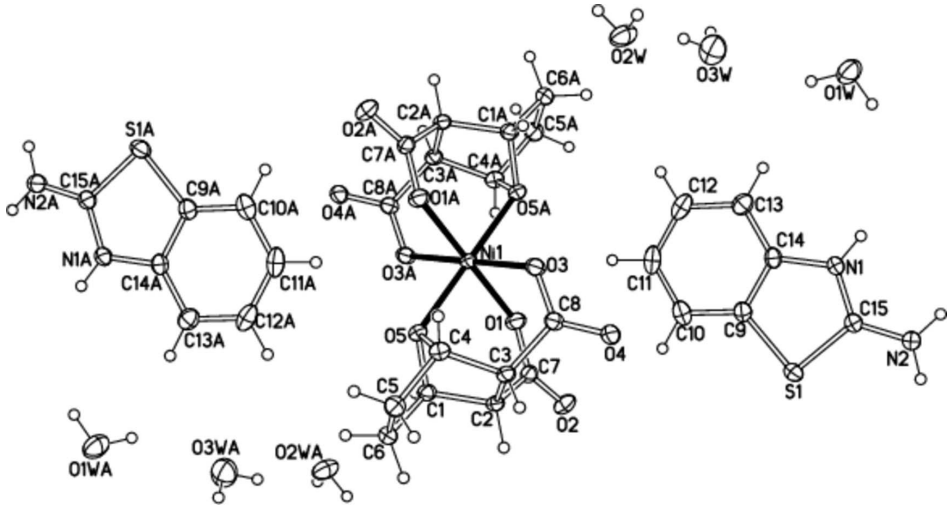

Figure 1

A view of the molecule of (I) showing the atom-labelling scheme with displacement ellipsoids drawn at the 30% probability.

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

Crystal data

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Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 6.6907$ (1) Å
$b = 10.0963$ (2) Å
$c = 13.2283$ (3) Å
$\alpha = 90.284$ (1)°
$\beta = 91.192$ (1)°
$\gamma = 99.709$ (1)°
$V = 880.57$ (3) Å^3
$Z = 1$
$F(000) = 438$
$D_x = 1.579$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3486 reflections
$\theta = 1.5$–$25.0°$
$\mu = 0.75$ mm^{-1}
$T = 296$ K
Block, green
0.27 × 0.21 × 0.07 mm

Data collection

Bruker APEXII area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.828$, $T_{max} = 0.951$
11942 measured reflections
3083 independent reflections
2654 reflections with $I > 2\sigma(I)$
$R_{int} = 0.032$
$\theta_{max} = 25.0°$, $\theta_{min} = 1.5°$
$h = -7\rightarrow7$
$k = -11\rightarrow11$
$l = -15\rightarrow15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.032$
$wR(F^2) = 0.089$
$S = 1.06$
3083 reflections
241 parameters
3 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

$w = 1/[\sigma^2(F_o^2) + (0.0485P)^2 + 0.2846P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.38$ e Å^{-3}
$\Delta\rho_{min} = -0.44$ 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}
Ni1	0.5000	0.5000	0.0000	0.02482 (13)
S1	0.32763 (10)	0.76888 (6)	0.52853 (4)	0.03601 (17)
O1	0.3599 (2)	0.64286 (15)	0.06025 (12)	0.0324 (4)
O1W	0.1930 (3)	0.1034 (2)	0.62809 (15)	0.0559 (5)
H1WA	0.2029	0.1747	0.6636	0.084*
H1WB	0.2102	0.1218	0.5659	0.084*
H2WA	0.4613	−0.0379	0.2341	0.084*
H2WB	0.6001	−0.0155	0.3078	0.084*
H3WA	0.0734	−0.0017	0.3946	0.084*
H3WB	0.2721	0.0206	0.3603	0.084*
O2	0.3555 (2)	0.83685 (16)	0.13816 (12)	0.0374 (4)
O2W	0.5108 (3)	0.02150 (17)	0.27766 (14)	0.0495 (5)
O3	0.6790 (2)	0.51244 (15)	0.13147 (11)	0.0330 (4)
O3W	0.1917 (3)	0.0438 (2)	0.40342 (16)	0.0651 (6)
O4	0.7719 (3)	0.65778 (16)	0.25730 (11)	0.0358 (4)
O5	0.7091 (2)	0.65098 (14)	−0.06734 (11)	0.0284 (3)
N1	0.2773 (3)	0.53206 (18)	0.60097 (13)	0.0275 (4)
H1A	0.2670	0.4669	0.6432	0.033*
N2	0.3472 (3)	0.6994 (2)	0.72380 (14)	0.0369 (5)
H2A	0.3401	0.6413	0.7715	0.044*
H2B	0.3734	0.7838	0.7380	0.044*
C6	0.8514 (4)	0.8692 (2)	−0.10948 (17)	0.0347 (5)
H6A	0.8737	0.9613	−0.0848	0.042*
H6B	0.8424	0.8689	−0.1828	0.042*
C5	1.0189 (4)	0.7933 (2)	−0.07100 (18)	0.0356 (5)
H5A	1.0851	0.7565	−0.1266	0.043*
H5B	1.1199	0.8510	−0.0299	0.043*
C1	0.6635 (3)	0.7873 (2)	−0.06430 (16)	0.0277 (5)
H1B	0.5377	0.7965	−0.1009	0.033*
C4	0.8995 (3)	0.6828 (2)	−0.00850 (16)	0.0286 (5)
H4A	0.9683	0.6053	0.0013	0.034*
C2	0.6554 (3)	0.8135 (2)	0.04989 (15)	0.0253 (5)

H2C	0.6916	0.9099	0.0643	0.030*
C3	0.8288 (3)	0.7379 (2)	0.08999 (16)	0.0259 (5)
H3A	0.9391	0.8026	0.1208	0.031*
C7	0.4422 (3)	0.7606 (2)	0.08724 (16)	0.0271 (5)
C8	0.7543 (3)	0.6281 (2)	0.16535 (16)	0.0261 (5)
C9	0.2752 (3)	0.6322 (2)	0.44420 (17)	0.0305 (5)
C10	0.2573 (4)	0.6336 (3)	0.34006 (18)	0.0417 (6)
H10A	0.2723	0.7142	0.3050	0.050*
C11	0.2165 (4)	0.5119 (3)	0.28954 (19)	0.0466 (7)
H11A	0.2056	0.5102	0.2193	0.056*
C12	0.1917 (4)	0.3922 (3)	0.34191 (19)	0.0433 (6)
H12A	0.1622	0.3114	0.3062	0.052*
C13	0.2098 (3)	0.3900 (3)	0.44640 (18)	0.0356 (5)
H13A	0.1941	0.3093	0.4813	0.043*
C14	0.2521 (3)	0.5118 (2)	0.49681 (16)	0.0278 (5)
C15	0.3181 (3)	0.6592 (2)	0.62951 (16)	0.0284 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0312 (2)	0.0187 (2)	0.0230 (2)	0.00043 (16)	−0.00167 (16)	−0.00208 (15)
S1	0.0480 (4)	0.0277 (3)	0.0308 (3)	0.0020 (3)	−0.0013 (3)	0.0062 (2)
O1	0.0328 (8)	0.0246 (8)	0.0385 (9)	0.0009 (7)	0.0025 (7)	−0.0048 (7)
O1W	0.0682 (13)	0.0494 (12)	0.0491 (11)	0.0083 (10)	−0.0104 (10)	−0.0136 (9)
O2	0.0374 (9)	0.0340 (9)	0.0420 (9)	0.0097 (7)	0.0030 (8)	−0.0128 (7)
O2W	0.0574 (12)	0.0350 (10)	0.0550 (11)	0.0068 (9)	−0.0154 (9)	−0.0122 (8)
O3	0.0443 (9)	0.0234 (8)	0.0281 (8)	−0.0023 (7)	−0.0070 (7)	0.0032 (6)
O3W	0.0550 (12)	0.0735 (15)	0.0625 (13)	−0.0023 (11)	0.0085 (10)	−0.0073 (11)
O4	0.0520 (10)	0.0285 (9)	0.0250 (8)	0.0017 (7)	−0.0048 (7)	0.0019 (6)
O5	0.0357 (8)	0.0213 (8)	0.0266 (8)	0.0006 (6)	−0.0005 (7)	−0.0037 (6)
N1	0.0330 (10)	0.0266 (10)	0.0230 (9)	0.0049 (8)	−0.0001 (8)	0.0033 (7)
N2	0.0556 (13)	0.0273 (10)	0.0265 (10)	0.0036 (9)	−0.0016 (9)	0.0004 (8)
C6	0.0505 (15)	0.0250 (12)	0.0266 (11)	0.0000 (10)	0.0037 (11)	0.0014 (9)
C5	0.0372 (13)	0.0330 (13)	0.0352 (13)	0.0012 (10)	0.0068 (11)	−0.0012 (10)
C1	0.0339 (12)	0.0226 (11)	0.0264 (11)	0.0051 (9)	−0.0043 (9)	0.0014 (9)
C4	0.0284 (11)	0.0247 (11)	0.0328 (12)	0.0051 (9)	−0.0005 (10)	−0.0011 (9)
C2	0.0317 (12)	0.0176 (10)	0.0256 (11)	0.0021 (9)	−0.0015 (9)	−0.0012 (8)
C3	0.0284 (11)	0.0209 (11)	0.0263 (11)	−0.0014 (9)	−0.0034 (9)	−0.0013 (9)
C7	0.0331 (12)	0.0251 (12)	0.0235 (10)	0.0062 (9)	−0.0029 (9)	−0.0015 (9)
C8	0.0260 (11)	0.0251 (11)	0.0261 (11)	0.0019 (9)	−0.0059 (9)	0.0025 (9)
C9	0.0291 (12)	0.0351 (13)	0.0267 (11)	0.0039 (10)	0.0005 (9)	0.0016 (9)
C10	0.0430 (14)	0.0522 (16)	0.0298 (12)	0.0069 (12)	0.0026 (11)	0.0089 (12)
C11	0.0444 (15)	0.071 (2)	0.0244 (12)	0.0112 (14)	0.0016 (11)	−0.0049 (13)
C12	0.0362 (14)	0.0556 (17)	0.0378 (14)	0.0075 (12)	−0.0013 (11)	−0.0194 (12)
C13	0.0319 (12)	0.0374 (14)	0.0379 (13)	0.0067 (10)	0.0014 (10)	−0.0053 (11)
C14	0.0230 (11)	0.0353 (13)	0.0253 (11)	0.0051 (9)	0.0023 (9)	0.0016 (9)
C15	0.0298 (12)	0.0292 (12)	0.0262 (11)	0.0049 (9)	0.0006 (9)	0.0024 (9)

Geometric parameters (Å, º)

Ni1—O1^{i}	2.0174 (15)	C6—C1	1.520 (3)
Ni1—O1	2.0174 (15)	C6—C5	1.541 (3)
Ni1—O3^{i}	2.0823 (15)	C6—H6A	0.9700
Ni1—O3	2.0823 (15)	C6—H6B	0.9700
Ni1—O5	2.1024 (14)	C5—C4	1.517 (3)
Ni1—O5^{i}	2.1024 (14)	C5—H5A	0.9700
S1—C15	1.735 (2)	C5—H5B	0.9700
S1—C9	1.754 (2)	C1—C2	1.536 (3)
O1—C7	1.269 (3)	C1—H1B	0.9800
O1W—H1WA	0.8500	C4—C3	1.529 (3)
O1W—H1WB	0.8500	C4—H4A	0.9800
O2—C7	1.243 (3)	C2—C7	1.529 (3)
O2W—H2WA	0.8502	C2—C3	1.577 (3)
O2W—H2WB	0.8503	C2—H2C	0.9800
O3—C8	1.267 (3)	C3—C8	1.522 (3)
O3W—H3WA	0.8503	C3—H3A	0.9800
O3W—H3WB	0.8503	C9—C10	1.381 (3)
O4—C8	1.250 (3)	C9—C14	1.391 (3)
O5—C1	1.459 (3)	C10—C11	1.379 (4)
O5—C4	1.467 (3)	C10—H10A	0.9300
N1—C15	1.318 (3)	C11—C12	1.383 (4)
N1—C14	1.394 (3)	C11—H11A	0.9300
N1—H1A	0.8600	C12—C13	1.386 (3)
N2—C15	1.310 (3)	C12—H12A	0.9300
N2—H2A	0.8600	C13—C14	1.380 (3)
N2—H2B	0.8600	C13—H13A	0.9300
O1^{i}—Ni1—O1	180.0	C2—C1—H1B	113.3
O1^{i}—Ni1—O3^{i}	87.63 (6)	O5—C4—C5	101.81 (17)
O1—Ni1—O3^{i}	92.37 (6)	O5—C4—C3	101.95 (16)
O1^{i}—Ni1—O3	92.37 (6)	C5—C4—C3	111.62 (18)
O1—Ni1—O3	87.63 (6)	O5—C4—H4A	113.4
O3^{i}—Ni1—O3	180.00 (9)	C5—C4—H4A	113.4
O1^{i}—Ni1—O5	90.51 (6)	C3—C4—H4A	113.4
O1—Ni1—O5	89.49 (6)	C7—C2—C1	109.66 (17)
O3^{i}—Ni1—O5	89.20 (6)	C7—C2—C3	116.01 (17)
O3—Ni1—O5	90.80 (6)	C1—C2—C3	100.63 (16)
O1^{i}—Ni1—O5^{i}	89.49 (6)	C7—C2—H2C	110.0
O1—Ni1—O5^{i}	90.51 (6)	C1—C2—H2C	110.0
O3^{i}—Ni1—O5^{i}	90.80 (6)	C3—C2—H2C	110.0
O3—Ni1—O5^{i}	89.20 (6)	C8—C3—C4	112.85 (17)
O5—Ni1—O5^{i}	180.0	C8—C3—C2	112.99 (17)
C15—S1—C9	90.16 (11)	C4—C3—C2	101.37 (16)
C7—O1—Ni1	126.63 (14)	C8—C3—H3A	109.8
H1WA—O1W—H1WB	111.0	C4—C3—H3A	109.8
H2WA—O2W—H2WB	102.3	C2—C3—H3A	109.8
C8—O3—Ni1	118.10 (13)	O2—C7—O1	123.6 (2)
H3WA—O3W—H3WB	110.3	O2—C7—C2	118.55 (19)

C1—O5—C4	95.27 (15)	O1—C7—C2	117.79 (18)
C1—O5—Ni1	116.89 (12)	O4—C8—O3	123.94 (19)
C4—O5—Ni1	112.33 (12)	O4—C8—C3	117.72 (19)
C15—N1—C14	114.58 (18)	O3—C8—C3	118.34 (18)
C15—N1—H1A	122.7	C10—C9—C14	121.1 (2)
C14—N1—H1A	122.7	C10—C9—S1	128.6 (2)
C15—N2—H2A	120.0	C14—C9—S1	110.31 (16)
C15—N2—H2B	120.0	C11—C10—C9	118.0 (2)
H2A—N2—H2B	120.0	C11—C10—H10A	121.0
C1—C6—C5	101.64 (17)	C9—C10—H10A	121.0
C1—C6—H6A	111.4	C10—C11—C12	120.9 (2)
C5—C6—H6A	111.4	C10—C11—H11A	119.6
C1—C6—H6B	111.4	C12—C11—H11A	119.6
C5—C6—H6B	111.4	C11—C12—C13	121.4 (2)
H6A—C6—H6B	109.3	C11—C12—H12A	119.3
C4—C5—C6	101.95 (19)	C13—C12—H12A	119.3
C4—C5—H5A	111.4	C14—C13—C12	117.6 (2)
C6—C5—H5A	111.4	C14—C13—H13A	121.2
C4—C5—H5B	111.4	C12—C13—H13A	121.2
C6—C5—H5B	111.4	C13—C14—C9	120.9 (2)
H5A—C5—H5B	109.2	C13—C14—N1	126.8 (2)
O5—C1—C6	102.53 (17)	C9—C14—N1	112.23 (19)
O5—C1—C2	102.03 (16)	N2—C15—N1	124.1 (2)
C6—C1—C2	111.26 (18)	N2—C15—S1	123.20 (17)
O5—C1—H1B	113.3	N1—C15—S1	112.73 (16)
C6—C1—H1B	113.3		

O3^{i}—Ni1—O1—C7	−120.43 (17)	C5—C4—C3—C2	72.7 (2)
O3—Ni1—O1—C7	59.57 (17)	C7—C2—C3—C8	−3.4 (2)
O5—Ni1—O1—C7	−31.25 (17)	C1—C2—C3—C8	−121.57 (18)
O5^{i}—Ni1—O1—C7	148.75 (17)	C7—C2—C3—C4	117.67 (19)
O1^{i}—Ni1—O3—C8	134.35 (16)	C1—C2—C3—C4	−0.53 (19)
O1—Ni1—O3—C8	−45.65 (16)	Ni1—O1—C7—O2	−168.26 (16)
O5—Ni1—O3—C8	43.80 (16)	Ni1—O1—C7—C2	15.2 (3)
O5^{i}—Ni1—O3—C8	−136.20 (16)	C1—C2—C7—O2	−128.9 (2)
O1^{i}—Ni1—O5—C1	169.62 (13)	C3—C2—C7—O2	118.0 (2)
O1—Ni1—O5—C1	−10.38 (13)	C1—C2—C7—O1	47.8 (2)
O3^{i}—Ni1—O5—C1	82.01 (13)	C3—C2—C7—O1	−65.2 (2)
O3—Ni1—O5—C1	−97.99 (13)	Ni1—O3—C8—O4	142.42 (18)
O1^{i}—Ni1—O5—C4	−81.74 (13)	Ni1—O3—C8—C3	−37.8 (2)
O1—Ni1—O5—C4	98.26 (13)	C4—C3—C8—O4	151.24 (19)
O3^{i}—Ni1—O5—C4	−169.35 (13)	C2—C3—C8—O4	−94.5 (2)
O3—Ni1—O5—C4	10.65 (13)	C4—C3—C8—O3	−28.5 (3)
C1—C6—C5—C4	−1.2 (2)	C2—C3—C8—O3	85.8 (2)
C4—O5—C1—C6	56.54 (18)	C15—S1—C9—C10	−179.3 (2)
Ni1—O5—C1—C6	174.86 (12)	C15—S1—C9—C14	0.40 (17)
C4—O5—C1—C2	−58.75 (18)	C14—C9—C10—C11	−0.2 (4)
Ni1—O5—C1—C2	59.58 (17)	S1—C9—C10—C11	179.49 (19)
C5—C6—C1—O5	−34.3 (2)	C9—C10—C11—C12	0.8 (4)

C5—C6—C1—C2	74.1 (2)	C10—C11—C12—C13	−1.0 (4)
C1—O5—C4—C5	−57.14 (18)	C11—C12—C13—C14	0.5 (4)
Ni1—O5—C4—C5	−179.07 (13)	C12—C13—C14—C9	0.1 (3)
C1—O5—C4—C3	58.27 (18)	C12—C13—C14—N1	−179.7 (2)
Ni1—O5—C4—C3	−63.67 (16)	C10—C9—C14—C13	−0.2 (3)
C6—C5—C4—O5	36.1 (2)	S1—C9—C14—C13	180.00 (18)
C6—C5—C4—C3	−72.0 (2)	C10—C9—C14—N1	179.5 (2)
O5—C1—C2—C7	−86.34 (19)	S1—C9—C14—N1	−0.2 (2)
C6—C1—C2—C7	164.94 (18)	C15—N1—C14—C13	179.6 (2)
O5—C1—C2—C3	36.40 (19)	C15—N1—C14—C9	−0.2 (3)
C6—C1—C2—C3	−72.3 (2)	C14—N1—C15—N2	−179.9 (2)
O5—C4—C3—C8	85.9 (2)	C14—N1—C15—S1	0.5 (2)
C5—C4—C3—C8	−166.13 (18)	C9—S1—C15—N2	179.9 (2)
O5—C4—C3—C2	−35.25 (19)	C9—S1—C15—N1	−0.52 (18)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*WA*···O4^{ii}	0.85	1.97	2.815 (2)	179
O1*W*—H1*WB*···O3*W*	0.85	2.28	3.029 (3)	147
O2*W*—H2*WA*···O2^{iii}	0.85	1.83	2.682 (2)	179
O2*W*—H2*WB*···O1*W*^{iv}	0.85	1.95	2.798 (3)	178
O3*W*—H3*WA*···O1*W*^{v}	0.85	1.92	2.769 (3)	179
O3*W*—H3*WB*···O2*W*	0.85	1.95	2.772 (3)	161
N1—H1*A*···O4^{ii}	0.86	1.82	2.673 (2)	173
N2—H2*A*···O3^{ii}	0.86	2.01	2.863 (2)	173
N2—H2*B*···O2*W*^{vi}	0.86	2.00	2.818 (3)	158

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