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Bis{4-bromo-2-[(2-hydroxyethyl)iminomethyl]phenolato}nickel(II) monohydrate

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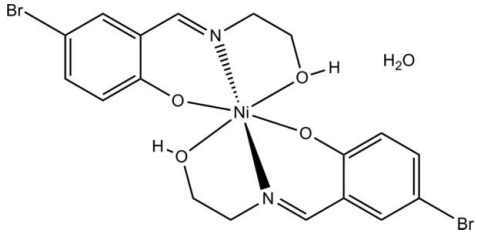
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.012 Å; R factor = 0.048; wR factor = 0.128; data-to-parameter ratio = 17.3.

The title mononuclear nickel complex, $[Ni(C_9H_9BrNO_2)_2]\cdot H_2O$, was obtained by the reaction of 5-bromosalicylaldehyde, 2-aminoethanol and nickel nitrate in methanol. The Ni^{II} atom is six-coordinated by two phenolate O, two imine N and two hydroxy O atoms from two crystallographically different Schiff base ligands, forming an octahedral geometry. In the crystal, molecules are linked by intermolecular O—H···O and O—H···Br hydrogen bonds, forming a three-dimensional network.

Related literature

For urease inhibitors, see: Wang (2009); Wang & Ye (2011). For related nickel(II) complexes, see: Arıcı *et al.* (2005); Liu *et al.* (2006); Li & Wang (2007); Ali *et al.* (2006).



Experimental

Crystal data

$[Ni(C_9H_9BrNO_2)_2]\cdot H_2O$
M_r = 562.89
Orthorhombic, $P2_12_12_1$
a = 9.835 (3) Å
b = 12.851 (2) Å
c = 16.226 (3) Å
V = 2050.8 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 4.87 mm^{-1}
T = 298 K
0.21 × 0.20 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.428, T_{max} = 0.442
13318 measured reflections
4474 independent reflections
2310 reflections with $I > 2\sigma(I)$
R_{int} = 0.099

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.128
S = 1.02
4474 reflections
259 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.60 e Å^{-3}
$\Delta\rho_{min}$ = −0.95 e Å^{-3}
Absolute structure: Flack (1983), 1930 Friedel pairs
Flack parameter: 0.013 (19)

Table 1
Selected bond lengths (Å).

Ni1—N1	1.976 (7)	Ni1—O3	2.014 (6)
Ni1—N2	1.981 (7)	Ni1—O2	2.132 (5)
Ni1—O1	2.008 (6)	Ni1—O4	2.160 (6)

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

D—H···A	D—H	H···A	D···A	D—H···A
O5—H5B···O1	0.85 (1)	2.22 (7)	2.898 (8)	136 (8)
O5—H5A···Br2^{i}	0.85 (1)	2.92 (5)	3.666 (9)	146 (8)
O4—H4A···Br1^{ii}	0.93	2.90	3.532 (6)	126
O4—H4A···O5^{i}	0.93	2.16	2.841 (9)	130
O2—H2A···O3^{iii}	0.93	1.97	2.694 (7)	133

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); 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: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI5196).

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supporting information

Acta Cryst. (2011). E**67**, m1227–m1228 [doi:10.1107/S1600536811031771]

Bis{4-bromo-2-[(2-hydroxyethyl)iminomethyl]phenolato}nickel(II) monohydrate

Chen-Yi Wang, Jing-Fen Li, Ping Wang and Cai-Jun Yuan

S1. Comment

As part of our investigations into novel urease inhibitors (Wang & Ye, 2011; Wang, 2009), we have synthesized the title compound, a new mononuclear nickel(II) complex, Fig. 1. The compound contains a mononuclear nickel(II) complex molecule and a water molecule of crystallization. The Ni atom in the complex is six-coordinated by two phenolate O, two imine N, and two hydroxy O atoms from two Schiff base ligands, forming an octahedral geometry. The *trans* angles at the Ni atom are in the range 173.1 (3)–174.0 (2)°; the other angles are close to 90°, ranging from 80.4 (3) to 94.8 (2)°, indicating a slightly distorted octahedral coordination. The Ni—O and Ni—N bond lengths (Table 1) are typical and are comparable to those observed in other similar nickel(II) complexes (Arıcı *et al.*, 2005; Liu *et al.*, 2006; Li & Wang, 2007; Ali *et al.*, 2006).

In the crystal structure of the compound, molecules are linked through intermolecular O—H···O and O—H···Br hydrogen bonds (Table 2), to form a three-dimensional network (Fig. 2).

S2. Experimental

5-Bromosalicylaldehyde (1.0 mmol, 0.201 g), 2-aminoethanol (1.0 mmol, 0.061 g), and nickel nitrate hexahydrate (0.5 mmol, 0.146 g) were dissolved in MeOH (30 ml). The mixture was stirred at room temperature for 10 min to give a clear green solution. After keeping the solution in air for a week, green block-shaped crystals were formed at the bottom of the vessel.

S3. Refinement

The water H atoms were located in a difference Fourier map and refined isotropically, with O–H and H···H distances restrained to 0.85 (1) and 1.37 (2) Å, respectively. The remaining H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C–H distances in the range 0.93–0.97 Å, O—H distance of 0.93 Å, and with U_{iso}(H) set at 1.2U_{eq}(C and O).

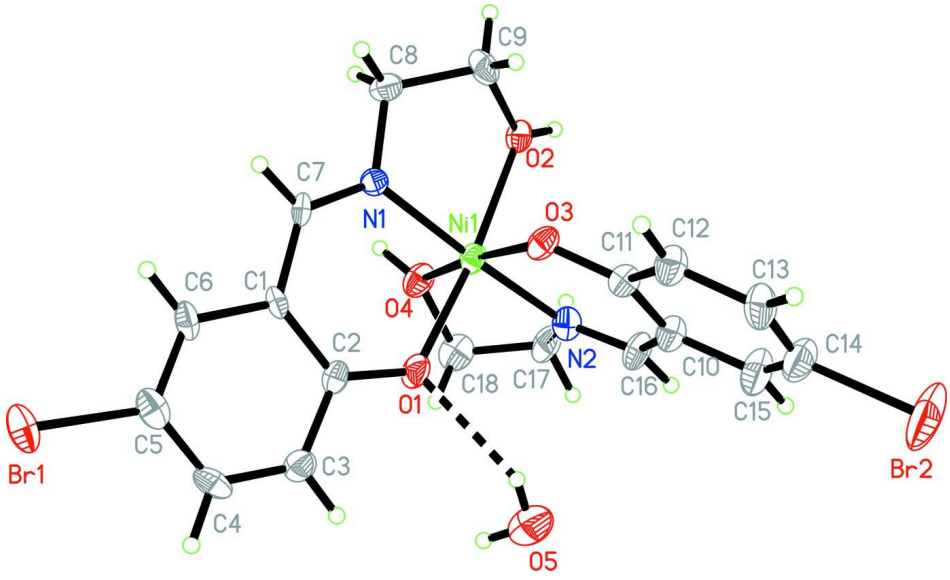

Figure 1

The molecular structure of the title compound, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. The dashed line indicates a hydrogen bond.

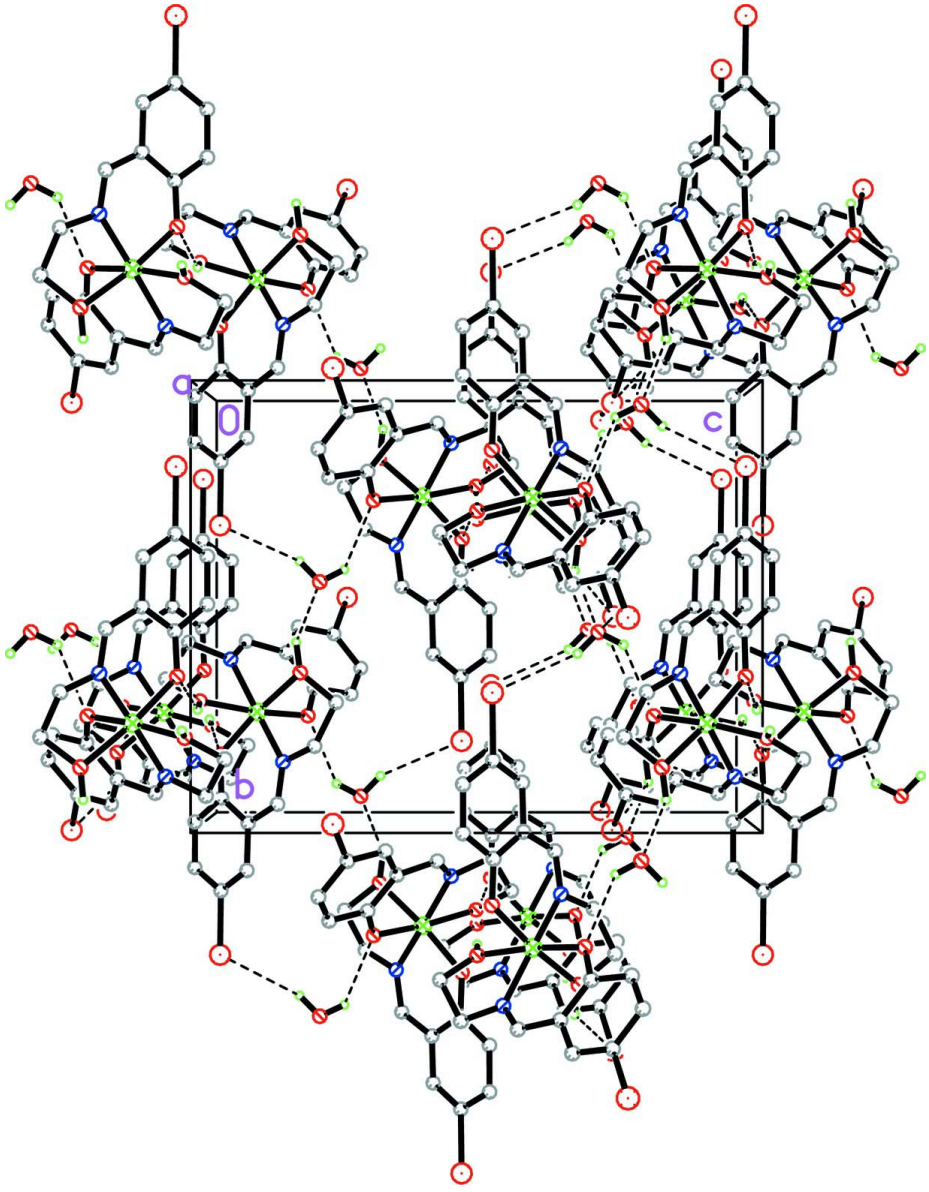

Figure 2

The crystal packing of the title compound. Hydrogen bonds are shown as dashed lines.

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Crystal data

$[Ni(C_9H_9BrNO_2)_2]\cdot H_2O$
$M_r = 562.89$
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a = 9.835$ (3) Å
$b = 12.851$ (2) Å
$c = 16.226$ (3) Å
$V = 2050.8$ (8) Å^3
$Z = 4$
$F(000) = 1120$
$D_x = 1.823$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2063 reflections
$\theta = 2.5$–25.3°
$\mu = 4.87$ mm^{-1}
$T = 298$ K
BlocK, green
0.21 × 0.20 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.428, T_{max} = 0.442
13318 measured reflections
4474 independent reflections
2310 reflections with $I > 2\sigma(I)$
R_{int} = 0.099
θ_{max} = 27.0°, θ_{min} = 2.4°
h = −12→12
k = −16→16
l = −20→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.128
S = 1.02
4474 reflections
259 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0374P)^2 + 1.9512P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.60 e Å^{-3}
$\Delta\rho_{min}$ = −0.95 e Å^{-3}
Absolute structure: Flack (1983), 1930 Friedel pairs
Absolute structure parameter: 0.013 (19)

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}
Br1	1.08191 (9)	−0.02277 (7)	0.25079 (7)	0.0550 (3)
Br2	0.5363 (2)	0.81053 (8)	0.47258 (10)	0.1150 (7)
Ni1	0.45998 (10)	0.24321 (8)	0.40117 (7)	0.0323 (3)
O1	0.6019 (5)	0.2555 (4)	0.3127 (4)	0.0425 (15)
O2	0.3198 (5)	0.2157 (4)	0.4990 (3)	0.0364 (16)
H2A	0.2280	0.2329	0.4989	0.044*
O3	0.5614 (6)	0.3443 (4)	0.4733 (4)	0.0366 (15)
O4	0.3367 (6)	0.1508 (4)	0.3188 (4)	0.0451 (17)
H4A	0.3131	0.0812	0.3251	0.054*
O5	0.5810 (10)	0.4431 (5)	0.2144 (5)	0.074 (2)
N1	0.5494 (7)	0.1225 (5)	0.4536 (4)	0.0307 (17)
N2	0.3496 (7)	0.3550 (5)	0.3502 (5)	0.0371 (19)
C1	0.7389 (8)	0.1086 (6)	0.3572 (5)	0.029 (2)
C2	0.7047 (8)	0.1925 (6)	0.3039 (5)	0.032 (2)
C3	0.7945 (8)	0.2085 (6)	0.2369 (6)	0.040 (2)

H3	0.7772	0.2640	0.2016	0.048*
C4	0.9041 (9)	0.1480 (7)	0.2209 (6)	0.042 (2)
H4	0.9582	0.1617	0.1752	0.051*
C5	0.9358 (9)	0.0658 (7)	0.2726 (6)	0.042 (2)
C6	0.8539 (8)	0.0483 (6)	0.3384 (6)	0.038 (2)
H6	0.8751	−0.0070	0.3732	0.046*
C7	0.6629 (8)	0.0814 (6)	0.4292 (5)	0.028 (2)
H7	0.6986	0.0286	0.4620	0.033*
C8	0.4827 (8)	0.0827 (6)	0.5276 (5)	0.040 (2)
H8A	0.5507	0.0620	0.5676	0.047*
H8B	0.4287	0.0220	0.5138	0.047*
C9	0.3914 (9)	0.1664 (7)	0.5646 (6)	0.045 (3)
H9A	0.3276	0.1353	0.6030	0.054*
H9B	0.4458	0.2171	0.5941	0.054*
C10	0.4558 (9)	0.5003 (6)	0.4176 (5)	0.041 (2)
C11	0.5478 (8)	0.4458 (6)	0.4704 (5)	0.033 (2)
C12	0.6275 (8)	0.5055 (6)	0.5233 (6)	0.045 (2)
H12	0.6845	0.4714	0.5602	0.055*
C13	0.6258 (10)	0.6126 (7)	0.5234 (6)	0.051 (3)
H13	0.6819	0.6502	0.5586	0.061*
C14	0.5408 (13)	0.6614 (7)	0.4712 (7)	0.060 (3)
C15	0.4569 (12)	0.6097 (7)	0.4200 (7)	0.062 (3)
H15	0.3987	0.6469	0.3857	0.075*
C16	0.3650 (8)	0.4525 (6)	0.3608 (6)	0.041 (2)
H16	0.3121	0.4964	0.3285	0.049*
C17	0.2488 (9)	0.3159 (7)	0.2904 (6)	0.051 (3)
H17A	0.2340	0.3675	0.2477	0.061*
H17B	0.1628	0.3033	0.3180	0.061*
C18	0.2992 (9)	0.2178 (6)	0.2530 (7)	0.051 (3)
H18A	0.2286	0.1858	0.2198	0.062*
H18B	0.3771	0.2316	0.2180	0.062*
H5A	0.584 (12)	0.395 (5)	0.178 (4)	0.080*
H5B	0.605 (11)	0.415 (6)	0.260 (3)	0.080*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0343 (4)	0.0641 (6)	0.0666 (7)	0.0118 (5)	0.0052 (6)	−0.0190 (6)
Br2	0.2030 (18)	0.0286 (5)	0.1133 (12)	0.0049 (9)	−0.0640 (13)	−0.0095 (7)
Ni1	0.0245 (5)	0.0278 (5)	0.0446 (7)	0.0024 (5)	0.0003 (5)	0.0031 (5)
O1	0.032 (3)	0.036 (3)	0.059 (4)	0.013 (3)	0.003 (3)	0.011 (3)
O2	0.026 (3)	0.038 (4)	0.045 (4)	0.015 (3)	−0.003 (3)	0.004 (3)
O3	0.030 (4)	0.032 (3)	0.048 (4)	0.001 (3)	−0.006 (3)	0.009 (3)
O4	0.051 (4)	0.035 (3)	0.050 (5)	−0.003 (3)	−0.012 (4)	0.001 (3)
O5	0.076 (5)	0.062 (4)	0.083 (6)	−0.010 (5)	0.002 (5)	0.017 (4)
N1	0.031 (4)	0.025 (3)	0.036 (5)	−0.005 (3)	0.008 (4)	0.000 (3)
N2	0.027 (4)	0.034 (4)	0.050 (5)	−0.005 (3)	−0.002 (4)	−0.005 (4)
C1	0.026 (5)	0.031 (5)	0.029 (6)	0.008 (4)	0.001 (4)	−0.012 (4)

C2	0.030 (5)	0.024 (4)	0.041 (6)	0.000 (4)	−0.006 (5)	−0.002 (4)
C3	0.043 (5)	0.034 (5)	0.044 (7)	−0.002 (4)	0.000 (5)	0.004 (5)
C4	0.029 (5)	0.060 (6)	0.037 (6)	−0.011 (5)	0.013 (4)	−0.006 (5)
C5	0.034 (5)	0.045 (5)	0.046 (7)	−0.007 (4)	0.001 (5)	−0.022 (5)
C6	0.027 (5)	0.033 (5)	0.055 (7)	0.006 (4)	0.007 (5)	−0.012 (5)
C7	0.026 (5)	0.019 (4)	0.038 (6)	0.007 (3)	−0.005 (4)	−0.006 (4)
C8	0.036 (5)	0.043 (5)	0.039 (6)	0.001 (4)	0.002 (5)	0.012 (5)
C9	0.031 (5)	0.058 (6)	0.045 (7)	0.013 (4)	0.007 (5)	−0.008 (5)
C10	0.043 (5)	0.034 (4)	0.048 (6)	0.004 (4)	−0.008 (5)	0.000 (4)
C11	0.027 (5)	0.035 (5)	0.036 (6)	−0.001 (4)	−0.008 (5)	0.001 (4)
C12	0.046 (6)	0.038 (5)	0.052 (7)	0.007 (4)	−0.009 (5)	−0.001 (5)
C13	0.057 (7)	0.037 (5)	0.059 (8)	−0.001 (5)	−0.009 (6)	−0.016 (5)
C14	0.080 (8)	0.031 (5)	0.067 (8)	−0.001 (6)	−0.008 (8)	0.001 (5)
C15	0.077 (7)	0.037 (5)	0.073 (8)	0.013 (6)	−0.018 (7)	−0.004 (5)
C16	0.036 (5)	0.029 (5)	0.057 (7)	0.004 (4)	−0.018 (5)	0.002 (5)
C17	0.040 (6)	0.040 (5)	0.072 (8)	0.012 (5)	−0.008 (5)	0.011 (5)
C18	0.048 (5)	0.053 (6)	0.053 (7)	−0.002 (4)	−0.020 (6)	0.000 (6)

Geometric parameters (Å, º)

Ni1—N1	1.976 (7)	C4—C5	1.385 (12)
Ni1—N2	1.981 (7)	C4—H4	0.93
Ni1—O1	2.008 (6)	C5—C6	1.356 (11)
Ni1—O3	2.014 (6)	C6—H6	0.93
Ni1—O2	2.132 (5)	C7—H7	0.93
Ni1—O4	2.160 (6)	C8—C9	1.523 (11)
Br1—C5	1.867 (9)	C8—H8A	0.97
Br2—C14	1.917 (8)	C8—H8B	0.97
O1—C2	1.303 (9)	C9—H9A	0.97
O2—C9	1.424 (10)	C9—H9B	0.97
O2—H2A	0.9298	C10—C15	1.407 (12)
O3—C11	1.312 (8)	C10—C16	1.423 (11)
O4—C18	1.420 (10)	C10—C11	1.430 (11)
O4—H4A	0.9298	C11—C12	1.392 (11)
O5—H5A	0.853 (10)	C12—C13	1.377 (11)
O5—H5B	0.854 (10)	C12—H12	0.93
N1—C7	1.297 (10)	C13—C14	1.346 (13)
N1—C8	1.461 (10)	C13—H13	0.93
N2—C16	1.274 (10)	C14—C15	1.346 (14)
N2—C17	1.476 (11)	C15—H15	0.93
C1—C6	1.405 (10)	C16—H16	0.93
C1—C2	1.422 (11)	C17—C18	1.485 (12)
C1—C7	1.431 (11)	C17—H17A	0.97
C2—C3	1.416 (12)	C17—H17B	0.97
C3—C4	1.354 (11)	C18—H18A	0.97
C3—H3	0.93	C18—H18B	0.97
N1—Ni1—N2	173.1 (3)	N1—C7—C1	126.8 (8)

N1—Ni1—O1	93.4 (2)	N1—C7—H7	116.6
N2—Ni1—O1	91.5 (3)	C1—C7—H7	116.6
N1—Ni1—O3	92.1 (2)	N1—C8—C9	110.0 (7)
N2—Ni1—O3	92.6 (2)	N1—C8—H8A	109.7
O1—Ni1—O3	91.2 (2)	C9—C8—H8A	109.7
N1—Ni1—O2	80.6 (2)	N1—C8—H8B	109.7
N2—Ni1—O2	94.4 (3)	C9—C8—H8B	109.7
O1—Ni1—O2	174.0 (2)	H8A—C8—H8B	108.2
O3—Ni1—O2	89.7 (2)	O2—C9—C8	108.1 (7)
N1—Ni1—O4	94.8 (2)	O2—C9—H9A	110.1
N2—Ni1—O4	80.4 (3)	C8—C9—H9A	110.1
O1—Ni1—O4	89.5 (2)	O2—C9—H9B	110.1
O3—Ni1—O4	173.0 (2)	C8—C9—H9B	110.1
O2—Ni1—O4	90.4 (2)	H9A—C9—H9B	108.4
C2—O1—Ni1	124.7 (5)	C15—C10—C16	117.0 (8)
C9—O2—Ni1	108.1 (5)	C15—C10—C11	117.9 (8)
C9—O2—H2A	126.0	C16—C10—C11	125.0 (7)
Ni1—O2—H2A	125.9	O3—C11—C12	117.9 (7)
C11—O3—Ni1	124.8 (5)	O3—C11—C10	125.0 (7)
C18—O4—Ni1	106.1 (5)	C12—C11—C10	117.1 (7)
C18—O4—H4A	126.9	C13—C12—C11	123.0 (8)
Ni1—O4—H4A	126.9	C13—C12—H12	118.5
H5A—O5—H5B	106 (3)	C11—C12—H12	118.5
C7—N1—C8	119.7 (7)	C14—C13—C12	118.2 (9)
C7—N1—Ni1	124.9 (6)	C14—C13—H13	120.9
C8—N1—Ni1	115.4 (5)	C12—C13—H13	120.9
C16—N2—C17	120.2 (8)	C13—C14—C15	122.6 (9)
C16—N2—Ni1	126.3 (6)	C13—C14—Br2	118.3 (8)
C17—N2—Ni1	113.3 (5)	C15—C14—Br2	119.1 (8)
C6—C1—C2	118.5 (8)	C14—C15—C10	121.0 (9)
C6—C1—C7	117.5 (8)	C14—C15—H15	119.5
C2—C1—C7	123.9 (7)	C10—C15—H15	119.5
O1—C2—C3	118.5 (7)	N2—C16—C10	125.9 (8)
O1—C2—C1	126.0 (8)	N2—C16—H16	117.0
C3—C2—C1	115.4 (7)	C10—C16—H16	117.0
C4—C3—C2	124.0 (8)	N2—C17—C18	109.5 (7)
C4—C3—H3	118.0	N2—C17—H17A	109.8
C2—C3—H3	118.0	C18—C17—H17A	109.8
C3—C4—C5	120.1 (9)	N2—C17—H17B	109.8
C3—C4—H4	119.9	C18—C17—H17B	109.8
C5—C4—H4	119.9	H17A—C17—H17B	108.2
C6—C5—C4	118.0 (8)	O4—C18—C17	107.1 (8)
C6—C5—Br1	120.3 (7)	O4—C18—H18A	110.3
C4—C5—Br1	121.6 (7)	C17—C18—H18A	110.3
C5—C6—C1	123.8 (9)	O4—C18—H18B	110.3
C5—C6—H6	118.1	C17—C18—H18B	110.3
C1—C6—H6	118.1	H18A—C18—H18B	108.6

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H5*B*···O1	0.85 (1)	2.22 (7)	2.898 (8)	136 (8)
O5—H5*A*···Br2^{i}	0.85 (1)	2.92 (5)	3.666 (9)	146 (8)
O4—H4*A*···Br1^{ii}	0.93	2.90	3.532 (6)	126
O4—H4*A*···O5^{i}	0.93	2.16	2.841 (9)	130
O2—H2*A*···O3^{iii}	0.93	1.97	2.694 (7)	133

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