Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

{6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethanylylidene)]diphenolato}nickel(II) dimethylformamide monosolvate

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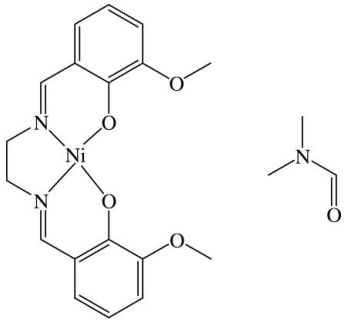
Received 31 January 2011; accepted 8 February 2011

Key indicators: single-crystal X-ray study; T = 110 K; mean σ(C–C) = 0.003 Å; R factor = 0.041; wR factor = 0.114; data-to-parameter ratio = 14.2.

In the title compound, $[Ni(C_{18}H_{18}N_2O_4)]\cdot C_3H_7NO$, the central Ni^{II} atom is in a square-planar O_2N_2 coordination environment. The planar Ni–salen moieties (r.m.s. deviation for the plane through the conjugated part of the Ni–salen group = 0.07 Å) form parallel stacks in the a-axis direction, with alternating Ni···Ni separations of 3.5339 (7) and 3.6165 (7) Å. In the crystal, there are weak intermolecular C—H···O interactions involving the dimethylformamide O and phenolate O atoms.

Related literature

For stacking of Ni–salen units, see: Abe *et al.* (2006); Assey *et al.* (2010); Feng *et al.* (2007); Miyamura *et al.* (1995); Vasil'eva *et al.* (2003). For a description of the Cambridge Structural Database, see: Allen (2002).



Experimental

Crystal data

$[Ni(C_{18}H_{18}N_2O_4)]\cdot C_3H_7NO$
M_r = 458.15
Monoclinic, $P2_1/c$
a = 6.8601 (1) Å
b = 15.3432 (3) Å
c = 18.9065 (4) Å
β = 91.676 (2)°
V = 1989.17 (6) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 1.75 mm^{-1}
T = 110 K
0.53 × 0.35 × 0.28 mm

Data collection

Oxford Diffraction Xcalibur diffractometer with a Ruby detector
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2009)
T_{min} = 0.750, T_{max} = 1.000
7909 measured reflections
3911 independent reflections
3513 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.114
S = 1.10
3911 reflections
275 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

Table 1
Selected bond lengths (Å).

Ni—N1	1.8503 (17)	Ni—O1	1.8609 (13)
Ni—N2	1.8502 (17)	Ni—O2	1.8594 (13)

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

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4A···O1S	0.95	2.62	3.310 (3)	130
C9—H9A···O2^{i}	0.99	2.45	3.334 (3)	148
C10—H10A···O1^{ii}	0.99	2.45	3.348 (3)	151

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $-x+2, -y+1, -z+1$.

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2009); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; 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*.

RJB wishes to acknowledge the NSF–MRI program (grant No. CHE-0619278) for funds to purchase the diffractometer. KA wishes to thank the National Science Foundation's AGEP Fellowship for support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2717).

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supporting information

Acta Cryst. (2011). E**67**, m328 [doi:10.1107/S1600536811004818]

{6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethanylylidene)]diphenolato}nickel(II) dimethylformamide monosolvate

Kouassi Ayikoé, Ray J. Butcher and Yilma Gultneh

S1. Comment

The title compound is a composed of one mononuclear nickel salen-type complex and one molecule of dimethylformamide as solvate. The central Ni is in a square planar O_2N_2 coordination environment (Fig. 1). The Ni—N and Ni—O bond distances, Table 1, are in the normal range for Ni-salen type complexes (Allen, 2002). The planar Ni salen moieties form parallel stacks in the *a* direction with alternating Ni—Ni separations of 3.5339 (7) and 3.6165 (7) Å as is common for this type of complex (Abe *et al.*, 2006; Assey *et al.*, 2010; Feng *et al.*, 2007; Miyamura *et al.*, 1995; Vasil'eva *et al.*, 2003). There are weak intermolecular C—H···O interactions involving the DMF O and phenolic O atoms (Table 2 and Fig. 2).

S2. Experimental

The ligand, *N*,*N*′-bis(3-methoxysalicylaldehyde)ethylenediimine (H_2L_1), was synthesized in a conventional way by mixing *o*-vanillin with ethylenediamine. To 10 g (0.066 mole) of *o*-vanillin weighed into a 100 ml round-bottom flask, 30 ml of methanol and 3 mL (0.035 mole) of ethylenediamine were added drop-wise while stirring. The resulting mixture was refluxed at a regulated temperature of 313 K overnight. The yellow precipitate was filtered under vacuum, dissolved in methanol and filtered a second time.

To a stirred bright yellow solution of 20 ml methanol containing 0.9 g (2.74 mmol) of H_2L_1, a 20 ml green methanol solution of 0.65 g $NiCl_2.6H_2O$ (2.73 mmol) was added drop-wise with continuous stirring. About 2 to 3 drops of triethylamine was added to activate deprotonation of the 2-hydroxyl group on the aldehyde moiety and promote oxygen binding to the metal. The resulting dark brown complex solution was stirred and refluxed overnight at 313 K, rotary-evaporated and washed with ethanol to obtain a brown solid in over 90% yield. The complex (7 mg) was dissolved in 5 ml of *N*,*N*′-dimethyl formamide and filtered into a crystallization tube. Sufficient amount of diethyl ether was slowly layered over the dissolved complex yielding red brown crystals after several days.

S3. Refinement

H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms with C—H distances of 0.95 to 0.99 Å and U_{iso}(H) = 1.2U_{eq}(C) [U_{iso}(H) = 1.5U_{eq}(C) for CH_3].

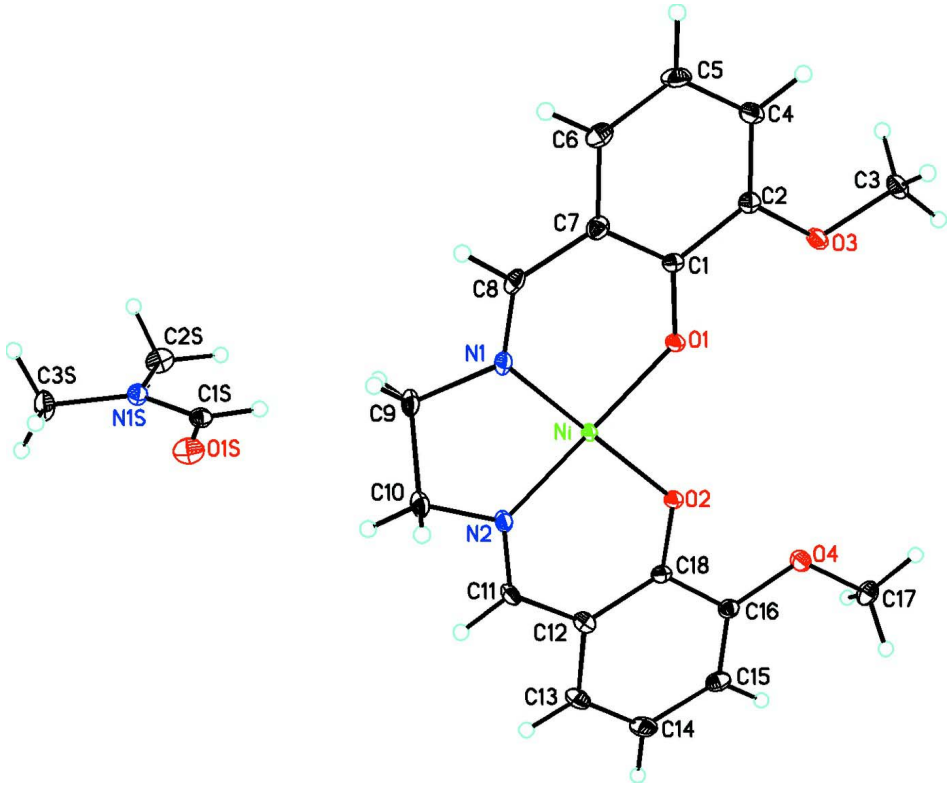

Figure 1

The molecular structures of the complex, $C_{18}H_{18}N_3NiO_5$, and solvent, C_3H_7NO, showing the atom numbering scheme and 50% probability displacement ellipsoids.

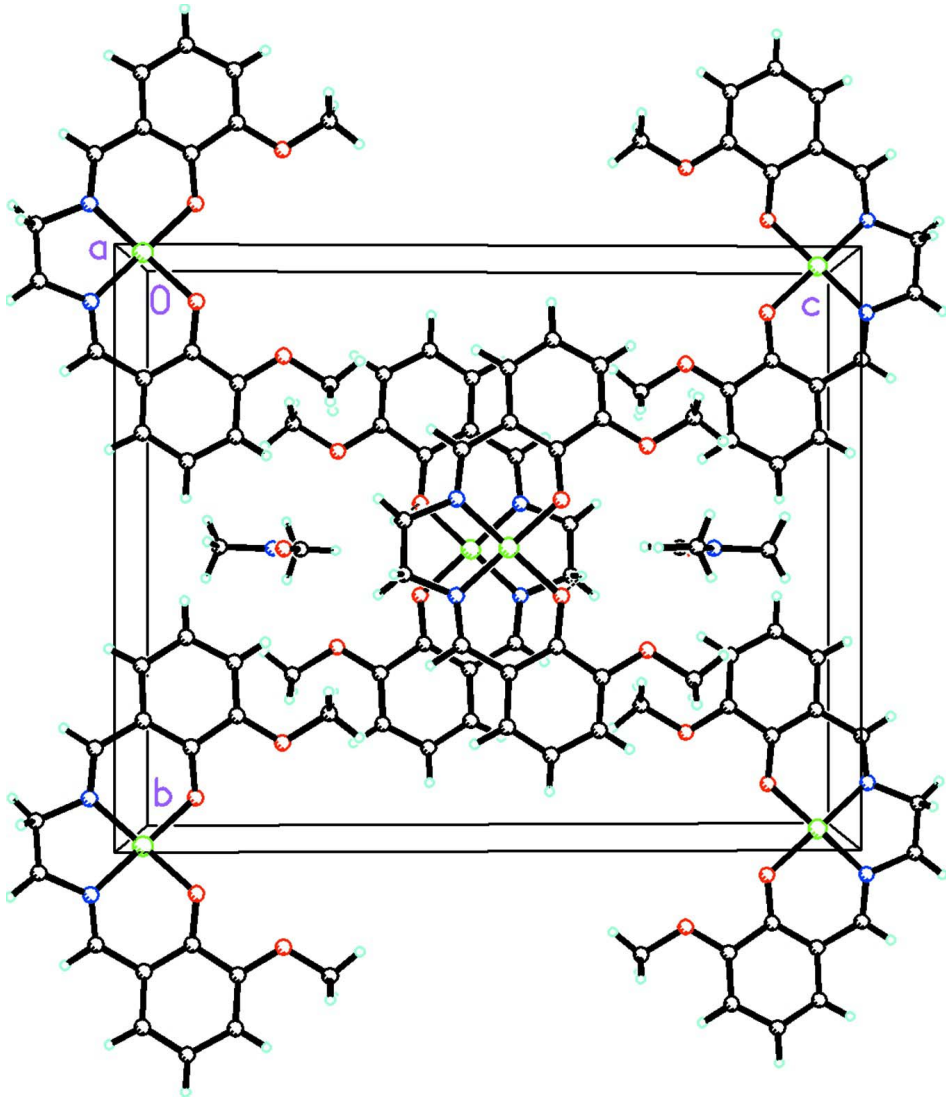

Figure 2

The molecular packing for $C_{18}H_{18}N_3NiO_5.C_3H_7NO$, viewed down the *a* axis showing overlapping Nisalen units.

{6,6′-Dimethoxy-2,2′-[ethane-1,2- diylbis(nitrilomethanylylidene)]diphenolato}nickel(II) dimethylformamide monosolvate

Crystal data

$[Ni(C_{18}H_{18}N_2O_4)]\cdot C_3H_7NO$
$M_r = 458.15$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 6.8601\ (1)$ Å
$b = 15.3432\ (3)$ Å
$c = 18.9065\ (4)$ Å
$\beta = 91.676\ (2)°$
$V = 1989.17\ (6)$ Å^3
$Z = 4$

$F(000) = 960$
$D_x = 1.530$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å
Cell parameters from 5823 reflections
$\theta = 5.5–73.9°$
$\mu = 1.75$ mm^{-1}
$T = 110$ K
Prism, red brown
0.53 × 0.35 × 0.28 mm

Data collection

Oxford Diffraction Xcalibur diffractometer with a Ruby (Gemini Mo) detector
Radiation source: Enhance (Cu) X-ray Source
Graphite monochromator
Detector resolution: 10.5081 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2009)
T_{min} = 0.750, T_{max} = 1.000
7909 measured reflections
3911 independent reflections
3513 reflections with $I > 2\sigma(I)$
R_{int} = 0.020
θ_{max} = 74.1°, θ_{min} = 5.5°
h = −8→6
k = −18→18
l = −22→23

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.114
S = 1.10
3911 reflections
275 parameters
0 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
$w = 1/[\sigma^2(F_o^2) + (0.0443P)^2 + 2.5615P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 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}
Ni	0.74901 (5)	0.498467 (19)	0.526650 (16)	0.01230 (13)
O1	0.7304 (2)	0.41708 (9)	0.59911 (7)	0.0156 (3)
O2	0.7642 (2)	0.58041 (9)	0.59906 (7)	0.0153 (3)
O3	0.7206 (2)	0.32568 (9)	0.71759 (7)	0.0202 (3)
O4	0.7569 (2)	0.67226 (9)	0.71712 (7)	0.0219 (3)
O1S	0.5907 (2)	−0.00040 (9)	0.71449 (9)	0.0270 (4)
N1	0.7406 (2)	0.41614 (11)	0.45511 (9)	0.0159 (3)
N2	0.7631 (2)	0.57987 (11)	0.45478 (9)	0.0160 (3)
N1S	0.2629 (3)	−0.00026 (10)	0.69058 (10)	0.0191 (4)
C1	0.7385 (3)	0.33191 (13)	0.59320 (10)	0.0143 (4)
C2	0.7330 (3)	0.27939 (13)	0.65578 (10)	0.0159 (4)
C3	0.7344 (3)	0.27729 (14)	0.78197 (11)	0.0214 (4)
H3A	0.7272	0.3173	0.8222	0.032*
H3B	0.8588	0.2459	0.7845	0.032*
H3C	0.6266	0.2355	0.7834	0.032*
C4	0.7376 (3)	0.18962 (13)	0.65251 (11)	0.0198 (4)

H4A	0.7304	0.1564	0.6948	0.024*
C5	0.7531 (3)	0.14675 (13)	0.58720 (12)	0.0257 (5)
H5A	0.7577	0.0849	0.5853	0.031*
C6	0.7613 (3)	0.19459 (15)	0.52644 (12)	0.0251 (5)
H6A	0.7735	0.1657	0.4823	0.030*
C7	0.7518 (3)	0.28656 (14)	0.52840 (11)	0.0191 (4)
C8	0.7480 (3)	0.33263 (14)	0.46263 (11)	0.0194 (4)
H8A	0.7513	0.2987	0.4207	0.023*
C9	0.7123 (3)	0.45208 (15)	0.38295 (10)	0.0219 (4)
H9A	0.5720	0.4523	0.3692	0.026*
H9B	0.7824	0.4159	0.3486	0.026*
C10	0.7908 (3)	0.54324 (14)	0.38323 (10)	0.0215 (4)
H10A	0.9310	0.5429	0.3722	0.026*
H10B	0.7202	0.5789	0.3472	0.026*
C11	0.7590 (3)	0.66365 (14)	0.46181 (11)	0.0195 (4)
H11A	0.7622	0.6974	0.4197	0.023*
C12	0.7500 (3)	0.71005 (14)	0.52714 (11)	0.0192 (4)
C13	0.7388 (3)	0.80217 (15)	0.52450 (12)	0.0252 (5)
H13A	0.7355	0.8308	0.4799	0.030*
C14	0.7328 (3)	0.85024 (14)	0.58504 (13)	0.0268 (5)
H14A	0.7254	0.9120	0.5827	0.032*
C15	0.7376 (3)	0.80773 (13)	0.65102 (12)	0.0203 (4)
H15A	0.7318	0.8411	0.6933	0.024*
C16	0.7506 (3)	0.71821 (13)	0.65496 (10)	0.0164 (4)
C17	0.7597 (3)	0.72153 (15)	0.78123 (11)	0.0220 (4)
H17A	0.7687	0.6818	0.8218	0.033*
H17B	0.6397	0.7559	0.7836	0.033*
H17C	0.8726	0.7607	0.7823	0.033*
C18	0.7554 (3)	0.66541 (13)	0.59253 (10)	0.0146 (4)
C1S	0.4214 (3)	−0.00156 (11)	0.73382 (12)	0.0181 (4)
H1SA	0.4011	−0.0035	0.7833	0.022*
C2S	0.0692 (3)	−0.00288 (14)	0.71929 (14)	0.0270 (5)
H2SA	0.0795	−0.0017	0.7711	0.040*
H2SB	0.0029	−0.0564	0.7038	0.040*
H2SC	−0.0057	0.0478	0.7024	0.040*
C3S	0.2806 (5)	0.00255 (16)	0.61430 (13)	0.0347 (6)
H3SA	0.4173	0.0120	0.6028	0.052*
H3SB	0.2009	0.0503	0.5948	0.052*
H3SC	0.2355	−0.0528	0.5938	0.052*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni	0.0174 (2)	0.0113 (2)	0.00815 (19)	−0.00089 (12)	0.00040 (13)	0.00026 (11)
O1	0.0232 (7)	0.0109 (6)	0.0127 (6)	−0.0014 (5)	0.0010 (5)	0.0000 (5)
O2	0.0216 (7)	0.0113 (6)	0.0131 (6)	−0.0013 (5)	0.0005 (5)	−0.0001 (5)
O3	0.0333 (8)	0.0145 (7)	0.0130 (7)	0.0003 (6)	0.0024 (6)	0.0026 (5)
O4	0.0373 (9)	0.0150 (7)	0.0135 (7)	−0.0009 (6)	0.0018 (6)	−0.0027 (5)

O1S	0.0217 (8)	0.0249 (9)	0.0347 (9)	0.0000 (6)	0.0039 (7)	0.0014 (6)
N1	0.0175 (8)	0.0195 (9)	0.0105 (8)	−0.0004 (7)	−0.0001 (6)	−0.0017 (6)
N2	0.0169 (8)	0.0201 (9)	0.0110 (8)	−0.0018 (6)	−0.0002 (6)	0.0023 (6)
N1S	0.0239 (9)	0.0172 (9)	0.0162 (9)	−0.0004 (7)	−0.0001 (7)	0.0003 (6)
C1	0.0135 (9)	0.0121 (9)	0.0173 (9)	−0.0003 (7)	0.0005 (7)	−0.0002 (7)
C2	0.0140 (9)	0.0163 (10)	0.0176 (9)	−0.0002 (7)	0.0012 (7)	0.0000 (7)
C3	0.0244 (11)	0.0227 (10)	0.0171 (10)	−0.0001 (8)	0.0008 (8)	0.0067 (8)
C4	0.0203 (10)	0.0152 (10)	0.0238 (11)	−0.0002 (8)	−0.0001 (8)	0.0035 (8)
C5	0.0328 (12)	0.0108 (9)	0.0334 (13)	−0.0007 (8)	−0.0017 (10)	−0.0022 (8)
C6	0.0339 (12)	0.0177 (11)	0.0237 (11)	−0.0002 (9)	0.0001 (9)	−0.0073 (8)
C7	0.0207 (10)	0.0175 (10)	0.0190 (10)	0.0012 (8)	−0.0008 (8)	−0.0036 (8)
C8	0.0233 (10)	0.0202 (10)	0.0146 (9)	−0.0008 (8)	0.0001 (8)	−0.0074 (8)
C9	0.0272 (11)	0.0281 (11)	0.0104 (9)	−0.0022 (9)	−0.0006 (8)	−0.0006 (8)
C10	0.0259 (11)	0.0274 (11)	0.0114 (9)	−0.0025 (9)	0.0018 (8)	0.0014 (8)
C11	0.0235 (10)	0.0194 (10)	0.0155 (9)	−0.0012 (8)	−0.0005 (8)	0.0079 (8)
C12	0.0205 (10)	0.0175 (10)	0.0195 (10)	0.0008 (8)	0.0020 (8)	0.0034 (8)
C13	0.0320 (12)	0.0164 (10)	0.0272 (12)	−0.0003 (9)	−0.0001 (9)	0.0087 (8)
C14	0.0347 (13)	0.0111 (10)	0.0344 (13)	−0.0007 (9)	0.0005 (10)	0.0022 (9)
C15	0.0192 (10)	0.0146 (10)	0.0270 (11)	−0.0005 (8)	0.0018 (8)	−0.0043 (8)
C16	0.0137 (9)	0.0161 (9)	0.0192 (10)	−0.0008 (7)	−0.0002 (7)	0.0000 (8)
C17	0.0250 (11)	0.0232 (11)	0.0178 (10)	0.0007 (8)	0.0010 (8)	−0.0079 (8)
C18	0.0135 (9)	0.0124 (9)	0.0179 (10)	−0.0008 (7)	−0.0002 (7)	0.0002 (7)
C1S	0.0229 (10)	0.0114 (9)	0.0200 (10)	−0.0017 (7)	0.0006 (8)	−0.0005 (7)
C2S	0.0208 (11)	0.0254 (12)	0.0347 (13)	−0.0012 (8)	0.0004 (9)	0.0028 (9)
C3S	0.0537 (17)	0.0342 (14)	0.0161 (11)	0.0016 (11)	−0.0033 (11)	−0.0005 (9)

Geometric parameters (Å, º)

Ni—N1	1.8503 (17)	C6—H6A	0.9500
Ni—N2	1.8502 (17)	C7—C8	1.430 (3)
Ni—O1	1.8609 (13)	C8—H8A	0.9500
Ni—O2	1.8594 (13)	C9—C10	1.499 (3)
O1—C1	1.313 (2)	C9—H9A	0.9900
O2—C18	1.311 (2)	C9—H9B	0.9900
O3—C2	1.372 (2)	C10—H10A	0.9900
O3—C3	1.427 (2)	C10—H10B	0.9900
O4—C16	1.370 (2)	C11—C12	1.429 (3)
O4—C17	1.428 (2)	C11—H11A	0.9500
O1S—C1S	1.228 (3)	C12—C18	1.413 (3)
N1—C8	1.290 (3)	C12—C13	1.416 (3)
N1—C9	1.479 (2)	C13—C14	1.363 (3)
N2—C11	1.293 (3)	C13—H13A	0.9500
N2—C10	1.482 (2)	C14—C15	1.407 (3)
N1S—C1S	1.341 (3)	C14—H14A	0.9500
N1S—C2S	1.451 (3)	C15—C16	1.378 (3)
N1S—C3S	1.451 (3)	C15—H15A	0.9500
C1—C7	1.414 (3)	C16—C18	1.433 (3)
C1—C2	1.433 (3)	C17—H17A	0.9800

C2—C4	1.379 (3)	C17—H17B	0.9800
C3—H3A	0.9800	C17—H17C	0.9800
C3—H3B	0.9800	C1S—H1SA	0.9500
C3—H3C	0.9800	C2S—H2SA	0.9800
C4—C5	1.406 (3)	C2S—H2SB	0.9800
C4—H4A	0.9500	C2S—H2SC	0.9800
C5—C6	1.366 (3)	C3S—H3SA	0.9800
C5—H5A	0.9500	C3S—H3SB	0.9800
C6—C7	1.413 (3)	C3S—H3SC	0.9800

N2—Ni—N1	85.71 (8)	C10—C9—H9B	110.1
N2—Ni—O2	94.66 (7)	H9A—C9—H9B	108.4
N1—Ni—O2	178.51 (7)	N2—C10—C9	107.53 (16)
N2—Ni—O1	179.01 (7)	N2—C10—H10A	110.2
N1—Ni—O1	94.51 (7)	C9—C10—H10A	110.2
O2—Ni—O1	85.14 (6)	N2—C10—H10B	110.2
C1—O1—Ni	126.96 (12)	C9—C10—H10B	110.2
C18—O2—Ni	127.00 (12)	H10A—C10—H10B	108.5
C2—O3—C3	116.94 (16)	N2—C11—C12	125.87 (19)
C16—O4—C17	117.06 (16)	N2—C11—H11A	117.1
C8—N1—C9	118.40 (17)	C12—C11—H11A	117.1
C8—N1—Ni	126.67 (15)	C18—C12—C13	120.97 (19)
C9—N1—Ni	114.85 (13)	C18—C12—C11	120.96 (19)
C11—N2—C10	118.33 (17)	C13—C12—C11	118.07 (19)
C11—N2—Ni	126.45 (14)	C14—C13—C12	120.9 (2)
C10—N2—Ni	115.16 (13)	C14—C13—H13A	119.6
C1S—N1S—C2S	120.44 (19)	C12—C13—H13A	119.6
C1S—N1S—C3S	121.1 (2)	C13—C14—C15	119.53 (19)
C2S—N1S—C3S	118.5 (2)	C13—C14—H14A	120.2
O1—C1—C7	124.57 (18)	C15—C14—H14A	120.2
O1—C1—C2	119.16 (17)	C16—C15—C14	120.6 (2)
C7—C1—C2	116.27 (18)	C16—C15—H15A	119.7
O3—C2—C4	123.86 (18)	C14—C15—H15A	119.7
O3—C2—C1	114.57 (17)	O4—C16—C15	124.02 (19)
C4—C2—C1	121.56 (18)	O4—C16—C18	114.50 (17)
O3—C3—H3A	109.5	C15—C16—C18	121.47 (19)
O3—C3—H3B	109.5	O4—C17—H17A	109.5
H3A—C3—H3B	109.5	O4—C17—H17B	109.5
O3—C3—H3C	109.5	H17A—C17—H17B	109.5
H3A—C3—H3C	109.5	O4—C17—H17C	109.5
H3B—C3—H3C	109.5	H17A—C17—H17C	109.5
C2—C4—C5	120.60 (19)	H17B—C17—H17C	109.5
C2—C4—H4A	119.7	O2—C18—C12	124.36 (18)
C5—C4—H4A	119.7	O2—C18—C16	119.15 (17)
C6—C5—C4	119.57 (19)	C12—C18—C16	116.49 (18)
C6—C5—H5A	120.2	O1S—C1S—N1S	125.1 (2)
C4—C5—H5A	120.2	O1S—C1S—H1SA	117.4
C5—C6—C7	120.8 (2)	N1S—C1S—H1SA	117.4

C5—C6—H6A	119.6	N1S—C2S—H2SA	109.5
C7—C6—H6A	119.6	N1S—C2S—H2SB	109.5
C6—C7—C1	121.21 (19)	H2SA—C2S—H2SB	109.5
C6—C7—C8	118.07 (19)	N1S—C2S—H2SC	109.5
C1—C7—C8	120.68 (19)	H2SA—C2S—H2SC	109.5
N1—C8—C7	125.91 (19)	H2SB—C2S—H2SC	109.5
N1—C8—H8A	117.0	N1S—C3S—H3SA	109.5
C7—C8—H8A	117.0	N1S—C3S—H3SB	109.5
N1—C9—C10	107.90 (16)	H3SA—C3S—H3SB	109.5
N1—C9—H9A	110.1	N1S—C3S—H3SC	109.5
C10—C9—H9A	110.1	H3SA—C3S—H3SC	109.5
N1—C9—H9B	110.1	H3SB—C3S—H3SC	109.5

N2—Ni—O1—C1	111 (4)	C2—C1—C7—C8	176.74 (18)
N1—Ni—O1—C1	8.14 (16)	C9—N1—C8—C7	−172.29 (19)
O2—Ni—O1—C1	−170.41 (16)	Ni—N1—C8—C7	4.3 (3)
N2—Ni—O2—C18	8.98 (16)	C6—C7—C8—N1	−179.6 (2)
N1—Ni—O2—C18	113 (3)	C1—C7—C8—N1	2.8 (3)
O1—Ni—O2—C18	−170.05 (16)	C8—N1—C9—C10	−156.46 (19)
N2—Ni—N1—C8	172.71 (18)	Ni—N1—C9—C10	26.6 (2)
O2—Ni—N1—C8	68 (3)	C11—N2—C10—C9	−157.70 (19)
O1—Ni—N1—C8	−8.25 (18)	Ni—N2—C10—C9	25.0 (2)
N2—Ni—N1—C9	−10.60 (14)	N1—C9—C10—N2	−31.2 (2)
O2—Ni—N1—C9	−115 (3)	C10—N2—C11—C12	−174.43 (19)
O1—Ni—N1—C9	168.43 (14)	Ni—N2—C11—C12	2.5 (3)
N1—Ni—N2—C11	174.22 (18)	N2—C11—C12—C18	3.5 (3)
O2—Ni—N2—C11	−7.22 (18)	N2—C11—C12—C13	−177.6 (2)
O1—Ni—N2—C11	71 (4)	C18—C12—C13—C14	−0.1 (3)
N1—Ni—N2—C10	−8.76 (14)	C11—C12—C13—C14	−179.0 (2)
O2—Ni—N2—C10	169.79 (14)	C12—C13—C14—C15	0.0 (3)
O1—Ni—N2—C10	−112 (4)	C13—C14—C15—C16	0.8 (3)
Ni—O1—C1—C7	−4.0 (3)	C17—O4—C16—C15	−3.2 (3)
Ni—O1—C1—C2	176.32 (13)	C17—O4—C16—C18	177.79 (16)
C3—O3—C2—C4	6.9 (3)	C14—C15—C16—O4	179.68 (19)
C3—O3—C2—C1	−173.86 (17)	C14—C15—C16—C18	−1.4 (3)
O1—C1—C2—O3	−0.4 (3)	Ni—O2—C18—C12	−6.0 (3)
C7—C1—C2—O3	179.85 (17)	Ni—O2—C18—C16	173.96 (13)
O1—C1—C2—C4	178.85 (18)	C13—C12—C18—O2	179.44 (19)
C7—C1—C2—C4	−0.9 (3)	C11—C12—C18—O2	−1.6 (3)
O3—C2—C4—C5	−179.16 (18)	C13—C12—C18—C16	−0.5 (3)
C1—C2—C4—C5	1.6 (3)	C11—C12—C18—C16	178.44 (18)
C2—C4—C5—C6	−0.7 (3)	O4—C16—C18—O2	0.3 (3)
C4—C5—C6—C7	−0.9 (3)	C15—C16—C18—O2	−178.73 (18)
C5—C6—C7—C1	1.6 (3)	O4—C16—C18—C12	−179.74 (17)
C5—C6—C7—C8	−175.9 (2)	C15—C16—C18—C12	1.2 (3)
O1—C1—C7—C6	179.6 (2)	C2S—N1S—C1S—O1S	179.27 (18)
C2—C1—C7—C6	−0.7 (3)	C3S—N1S—C1S—O1S	0.1 (3)
O1—C1—C7—C8	−3.0 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4*A*···O1*S*	0.95	2.62	3.310 (3)	130
C9—H9*A*···O2^{i}	0.99	2.45	3.334 (3)	148
C10—H10*A*···O1^{ii}	0.99	2.45	3.348 (3)	151

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