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[3-Hydroxy-*N*′-(2-oxidobenzylidene)-2-naphthohydrazidato-κ^3O,N,O']tris(pyridine-κN)nickel(II) pyridine trisolvate

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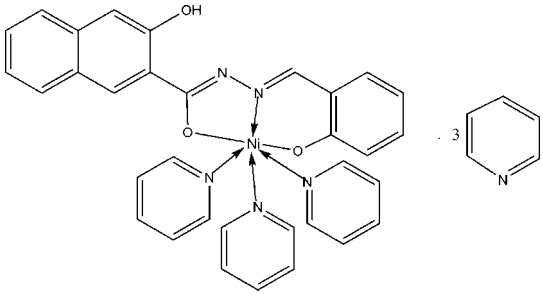
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.019 Å; R factor = 0.081; wR factor = 0.321; data-to-parameter ratio = 13.7.

The asymmetric unit of the crystal structure of the title complex, $[Ni(C_{18}H_{12}N_2O_3)(C_5H_5N)_3]\cdot 3C_5H_5N$, contains two independent Ni^{II} complex molecules and six uncoordinated pyridine molecules. Each Ni^{II} atom is coordinated by two O and four N atoms, from three pyridine and a chelating 3-hydroxy-*N*′-(2-oxidobenzylidene)-2-naphthohydrazide dianionic ligand, with a distorted octahedral geometry. Intramolecular O—H···N hydrogen bonding exists in both complex molecules but no intermolecular hydrogen bonding is observed in the crystal structure.

Related literature

For general background, see Samanta *et al.* (2007). For the specific biological activities of hydrazones, see Bernhardt *et al.* (2006). For the crystal structure of a Ni complex with a related hydrazone derivative, see: Kang *et al.* (2007).



Experimental

Crystal data

$[Ni(C_{18}H_{12}N_2O_3)(C_5H_5N)_3]\cdot 3C_5H_5N$
M_r = 837.59
Monoclinic, $P2_1/c$
a = 18.370 (2) Å
b = 27.720 (3) Å
c = 16.862 (2) Å
β = 90.378 (2)°
V = 8586.3 (18) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.50 mm^{-1}
T = 298 (2) K
0.50 × 0.40 × 0.28 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.787, T_{max} = 0.872
35434 measured reflections
14836 independent reflections
5715 reflections with $I > 2\sigma(I)$
R_{int} = 0.079

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.081
$wR(F^2)$ = 0.321
S = 1.00
14836 reflections
1081 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.77 e Å^{-3}
$\Delta\rho_{min}$ = −0.68 e Å^{-3}

Table 1
Selected bond lengths (Å).

Ni1—O1	2.050 (5)	Ni2—O4	2.061 (5)
Ni1—O3	1.998 (5)	Ni2—O6	1.993 (5)
Ni1—N2	1.989 (7)	Ni2—N7	1.983 (7)
Ni1—N3	2.077 (6)	Ni2—N8	2.067 (7)
Ni1—N4	2.192 (6)	Ni2—N9	2.156 (6)
Ni1—N5	2.173 (7)	Ni2—N10	2.180 (7)

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···N1	0.82	1.82	2.558 (8)	148
O5—H5···N6	0.82	1.80	2.533 (9)	148

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; 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: XU2364).

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supporting information

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Shi-Zhu Sun, Wen-Jun Kang, Da-Cheng Li, Da-Qi Wang and Jian-Min Dou

S1. Comment

Hydrazones and their metal complexes occupy special place due to their chelating capability, structure flexibility, magnetic properties (Samanta *et al.*, 2007) and their biological activities (Bernhardt *et al.*, 2006). As an extension of our work on the structural characterization of hydrazone derivatives (Kang *et al.*, 2007), the title complex, (I), was synthesized and charaterized.

As shown in Fig. 1., the asymmetric unit contains two crystallographically independent Ni^{II} complex molecules, together with six pyridine solvent molecules. structures of the two independent molecules are almost the same, with only few differences in bond lengths and angles (Table 1). In Ni1-complex molecule, the Ni1 atom is coordinated by a L^- ligand [H_2L = 3-hydroxy-*N*′-(2-oxidobenzylidene)-2-naphthohydrazide] and three pyridine molecules with a distorted octahedron geometry. The L^- is coordinated to the Ni atom as a tridentate ligand *via* N atom of the azomethine, O atom of the the hydroxyl and O atom of the phenolate. The tridentate binding leads to one five-numbered chelate ring Ni—N—N—C—O and one six-numbered chelate ring Ni—N—C—C—C—O. The dihedral angle between the two rings is 1.3 (8)°. The atoms N2, O3, N3 and O1 constitute the equatorial plane, with the mean deviation from plane 0.0055 (6) Å. The angles N2—Ni1—N3 and O3—Ni1—O1 are 174.6 (3) and 170.0 (2)°, respectively. The axial positions are occupied by the atoms N5 and N4. The angle of N5—Ni1—N4 is 173.9 (3)°. In the Ni2-complex, the Ni2 atom is also coordinated by two O and four N atoms in a distorted octahedron geometry. There are two intramolecular O2—H2···N1 and O5—H5···N6 hydrogen bonds (Table 2).

S2. Experimental

To a vigorously stirred 20 ml dimethylformamide solution of H_2L (0.077 g, 0.25 mmol) and KOH (0.014 g, 0.25 mmol), 10 ml pyridine solution of $Ni(OAC)_2.4H_2O$ (0.062 g, 0.25 mmol) was added dropwise. And then the mixture was stirred for 4 h and then filtered. Single crystals were obtained from filtrate after two weeks.

S3. Refinement

All H atoms were placed in geometrically idealized positions with O—H = 0.82 and C—H = 0.93 Å, and treated as riding on their parent atoms, with $U_{iso}(H) = 1.5U_{eq}(O)$ and $U_{iso}(H) = 1.2U_{eq}(C)$. Due to the poor quality of the single-crystal, the accuracye of the structure analysis is relatively low.

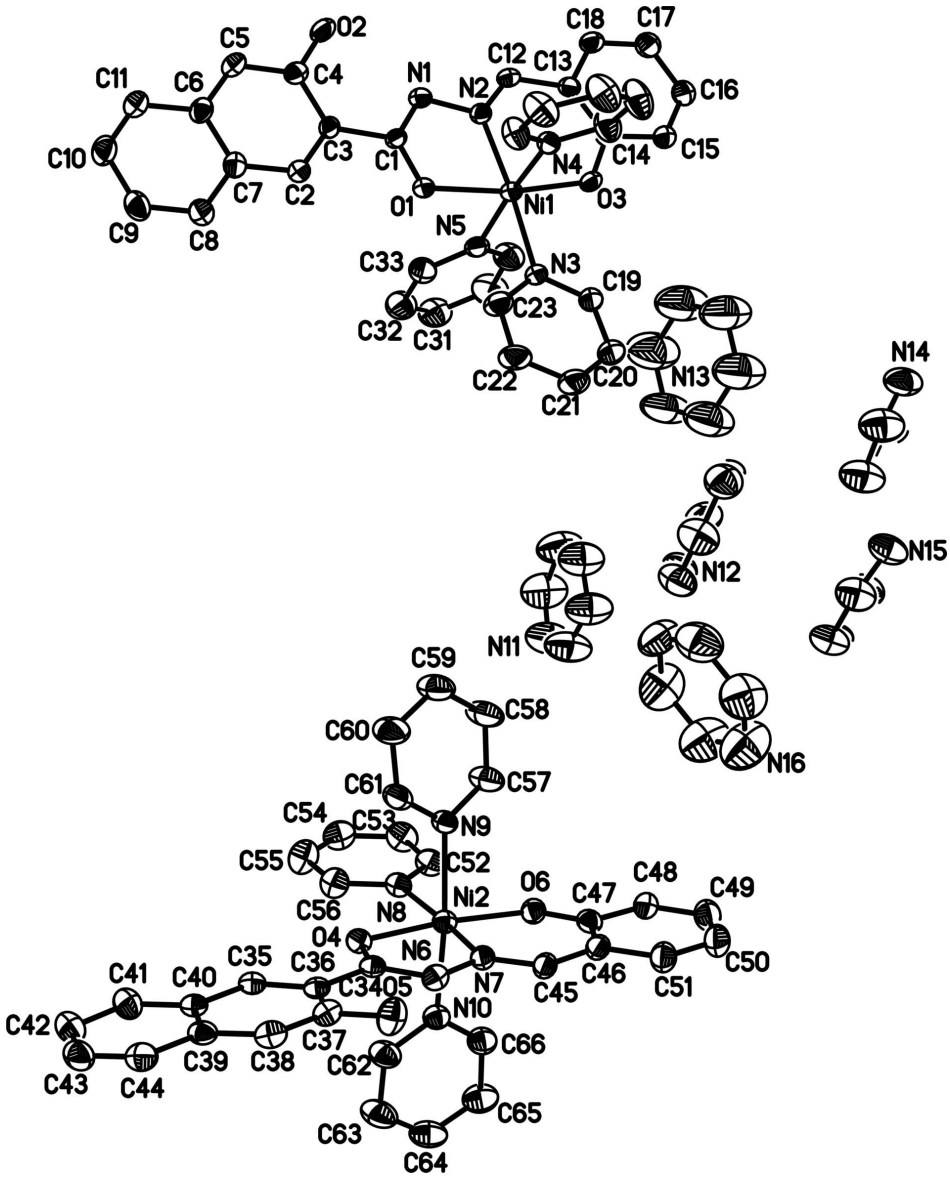

Figure 1

The structure of the title complex, showing 30% probability displacement ellipsoids and the atom-numbering scheme. C-bound H atoms have been omitted for clarity.

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Crystal data

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$c = 16.862$ (2) Å
$\beta = 90.378$ (2)°
$V = 8586.3$ (18) Å^3
$Z = 8$
$F(000) = 3504$
$D_x = 1.296$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4738 reflections
$\theta = 2.2$–20.5°
$\mu = 0.50$ mm^{-1}

T = 298 K
Block, red

0.50 × 0.40 × 0.28 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.787, T_{max} = 0.872

35434 measured reflections
14836 independent reflections
5715 reflections with $I > 2\sigma(I)$
R_{int} = 0.079
θ_{max} = 25.0°, θ_{min} = 1.3°
h = −21→16
k = −29→32
l = −18→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.081
$wR(F^2)$ = 0.321
S = 1.00
14836 reflections
1081 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
$w = 1/[\sigma^2(F_o^2) + (0.1595P)^2 + 3.0585P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.77 e Å^{-3}
$\Delta\rho_{min}$ = −0.68 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	0.03268 (5)	0.27695 (3)	0.16059 (6)	0.0517 (3)
Ni2	0.53241 (5)	0.23392 (4)	0.94731 (6)	0.0552 (3)
O1	0.0273 (3)	0.20424 (18)	0.1821 (3)	0.0562 (14)
O2	−0.0647 (3)	0.1242 (2)	−0.0051 (4)	0.085 (2)
H2	−0.0592	0.1535	−0.0008	0.128*
O3	0.0299 (3)	0.34493 (17)	0.1214 (3)	0.0566 (14)
O4	0.5270 (3)	0.16541 (18)	0.9945 (3)	0.0559 (14)
O5	0.4283 (4)	0.1613 (2)	1.2177 (4)	0.092 (2)
H5	0.4339	0.1841	1.1872	0.137*
O6	0.5316 (3)	0.30395 (19)	0.9206 (3)	0.0639 (15)
N1	−0.0219 (3)	0.2040 (2)	0.0557 (4)	0.0529 (16)
N2	−0.0118 (3)	0.2540 (2)	0.0596 (4)	0.0510 (16)
N3	0.0777 (3)	0.2945 (2)	0.2702 (4)	0.0568 (17)
N4	−0.0738 (3)	0.2859 (2)	0.2166 (4)	0.0572 (17)

N5	0.1433 (4)	0.2687 (3)	0.1177 (4)	0.0649 (19)
N6	0.4775 (3)	0.2078 (3)	1.1004 (4)	0.0607 (18)
N7	0.4885 (3)	0.2480 (2)	1.0519 (4)	0.0585 (18)
N8	0.5757 (3)	0.2122 (3)	0.8402 (4)	0.0600 (18)
N9	0.4274 (3)	0.2233 (2)	0.8922 (4)	0.0599 (18)
N10	0.6439 (4)	0.2400 (3)	0.9913 (4)	0.0653 (19)
N11	0.7971 (10)	0.4330 (9)	0.0620 (15)	0.198 (8)
N12	0.3091 (6)	0.4220 (5)	0.5294 (10)	0.129 (4)
N13	0.2613 (13)	0.4331 (9)	0.1332 (15)	0.290 (12)
N14	0.1890 (7)	0.6197 (7)	0.2569 (12)	0.146 (6)
N15	0.1976 (5)	0.5617 (5)	0.6056 (8)	0.121 (4)
N16	0.2501 (13)	0.4189 (7)	0.9308 (12)	0.222 (8)
C1	−0.0008 (4)	0.1827 (3)	0.1222 (5)	0.051 (2)
C2	0.0190 (4)	0.1045 (3)	0.1887 (5)	0.055 (2)
H2A	0.0389	0.1219	0.2307	0.066*
C3	−0.0072 (4)	0.1289 (3)	0.1241 (5)	0.052 (2)
C4	−0.0395 (4)	0.1023 (3)	0.0607 (6)	0.063 (2)
C5	−0.0434 (4)	0.0526 (3)	0.0651 (6)	0.072 (3)
H5A	−0.0651	0.0355	0.0239	0.087*
C6	−0.0152 (4)	0.0274 (3)	0.1310 (6)	0.064 (2)
C7	0.0169 (4)	0.0542 (3)	0.1936 (5)	0.060 (2)
C8	0.0464 (5)	0.0287 (3)	0.2587 (6)	0.074 (3)
H8	0.0673	0.0457	0.3005	0.089*
C9	0.0449 (5)	−0.0205 (3)	0.2613 (7)	0.083 (3)
H9	0.0643	−0.0368	0.3048	0.099*
C10	0.0138 (5)	−0.0465 (4)	0.1976 (7)	0.086 (3)
H10	0.0134	−0.0800	0.1989	0.103*
C11	−0.0155 (5)	−0.0231 (3)	0.1343 (7)	0.078 (3)
H11	−0.0360	−0.0407	0.0929	0.094*
C12	−0.0321 (4)	0.2787 (3)	0.0004 (5)	0.053 (2)
H12	−0.0525	0.2624	−0.0426	0.063*
C13	−0.0259 (4)	0.3301 (3)	−0.0051 (5)	0.053 (2)
C14	0.0030 (4)	0.3601 (3)	0.0542 (5)	0.056 (2)
C15	0.0044 (4)	0.4102 (3)	0.0385 (6)	0.067 (2)
H15	0.0238	0.4308	0.0766	0.080*
C16	−0.0216 (5)	0.4290 (3)	−0.0302 (6)	0.076 (3)
H16	−0.0196	0.4622	−0.0380	0.091*
C17	−0.0508 (5)	0.4001 (3)	−0.0887 (6)	0.080 (3)
H17	−0.0686	0.4131	−0.1358	0.096*
C18	−0.0528 (4)	0.3512 (3)	−0.0749 (5)	0.066 (2)
H18	−0.0729	0.3313	−0.1137	0.079*
C19	0.0938 (5)	0.3392 (3)	0.2881 (6)	0.085 (3)
H19	0.0871	0.3627	0.2495	0.102*
C20	0.1196 (6)	0.3529 (4)	0.3598 (7)	0.105 (4)
H20	0.1308	0.3850	0.3697	0.126*
C21	0.1289 (6)	0.3191 (5)	0.4171 (7)	0.100 (4)
H21	0.1447	0.3277	0.4677	0.120*
C22	0.1144 (6)	0.2720 (4)	0.3985 (6)	0.095 (3)

H22	0.1224	0.2477	0.4357	0.114*
C23	0.0886 (5)	0.2611 (4)	0.3260 (6)	0.084 (3)
H23	0.0779	0.2291	0.3142	0.100*
C24	−0.1053 (5)	0.2519 (4)	0.2568 (6)	0.087 (3)
H24	−0.0848	0.2212	0.2552	0.104*
C25	−0.1672 (6)	0.2583 (5)	0.3017 (7)	0.106 (4)
H25	−0.1865	0.2326	0.3301	0.128*
C26	−0.1987 (7)	0.3011 (5)	0.3039 (8)	0.119 (4)
H26	−0.2393	0.3066	0.3354	0.143*
C27	−0.1702 (7)	0.3369 (5)	0.2589 (9)	0.127 (5)
H27	−0.1926	0.3669	0.2561	0.152*
C28	−0.1061 (5)	0.3277 (4)	0.2166 (7)	0.095 (3)
H28	−0.0857	0.3526	0.1872	0.114*
C29	0.1770 (6)	0.3032 (4)	0.0792 (7)	0.101 (4)
H29	0.1517	0.3318	0.0702	0.121*
C30	0.2471 (7)	0.3001 (6)	0.0513 (8)	0.129 (5)
H30	0.2688	0.3265	0.0268	0.155*
C31	0.2839 (6)	0.2582 (6)	0.0601 (8)	0.115 (4)
H31	0.3300	0.2540	0.0387	0.138*
C32	0.2509 (6)	0.2223 (5)	0.1016 (9)	0.119 (4)
H32	0.2758	0.1938	0.1127	0.143*
C33	0.1797 (5)	0.2284 (4)	0.1272 (7)	0.092 (3)
H33	0.1568	0.2027	0.1523	0.110*
C34	0.4996 (4)	0.1673 (3)	1.0647 (5)	0.054 (2)
C35	0.5200 (4)	0.0812 (3)	1.0812 (5)	0.055 (2)
H35	0.5399	0.0818	1.0306	0.067*
C36	0.4930 (4)	0.1229 (3)	1.1114 (5)	0.0484 (19)
C37	0.4582 (4)	0.1215 (3)	1.1865 (5)	0.061 (2)
C38	0.4557 (4)	0.0791 (3)	1.2274 (5)	0.070 (2)
H38	0.4326	0.0784	1.2763	0.084*
C39	0.4867 (4)	0.0365 (3)	1.1983 (6)	0.064 (2)
C40	0.5192 (4)	0.0373 (3)	1.1226 (5)	0.058 (2)
C41	0.5496 (5)	−0.0055 (3)	1.0939 (6)	0.082 (3)
H41	0.5707	−0.0055	1.0440	0.098*
C42	0.5493 (6)	−0.0475 (4)	1.1369 (7)	0.092 (3)
H42	0.5699	−0.0755	1.1169	0.111*
C43	0.5171 (5)	−0.0469 (4)	1.2118 (7)	0.090 (3)
H43	0.5174	−0.0749	1.2422	0.108*
C44	0.4865 (5)	−0.0077 (4)	1.2403 (6)	0.078 (3)
H44	0.4640	−0.0091	1.2895	0.094*
C45	0.4684 (4)	0.2890 (3)	1.0809 (6)	0.063 (2)
H45	0.4489	0.2896	1.1317	0.076*
C46	0.4745 (4)	0.3336 (3)	1.0384 (6)	0.067 (2)
C47	0.5048 (4)	0.3392 (3)	0.9619 (6)	0.063 (2)
C48	0.5051 (5)	0.3862 (3)	0.9287 (6)	0.073 (3)
H48	0.5242	0.3908	0.8783	0.088*
C49	0.4779 (5)	0.4253 (4)	0.9690 (8)	0.091 (3)
H49	0.4790	0.4558	0.9460	0.109*

C50	0.4489 (6)	0.4195 (4)	1.0435 (8)	0.097 (3)
H50	0.4299	0.4458	1.0706	0.116*
C51	0.4481 (5)	0.3749 (4)	1.0773 (7)	0.083 (3)
H51	0.4293	0.3716	1.1281	0.100*
C52	0.5885 (5)	0.2427 (4)	0.7825 (6)	0.078 (3)
H52	0.5790	0.2752	0.7915	0.094*
C53	0.6153 (5)	0.2296 (4)	0.7085 (6)	0.088 (3)
H53	0.6233	0.2523	0.6688	0.106*
C54	0.6290 (5)	0.1823 (5)	0.6973 (6)	0.091 (3)
H54	0.6472	0.1722	0.6488	0.110*
C55	0.6170 (6)	0.1492 (4)	0.7547 (7)	0.096 (3)
H55	0.6256	0.1165	0.7462	0.115*
C56	0.5914 (5)	0.1658 (4)	0.8263 (6)	0.082 (3)
H56	0.5846	0.1437	0.8671	0.098*
C57	0.3986 (5)	0.2548 (4)	0.8448 (7)	0.096 (4)
H57	0.4219	0.2844	0.8401	0.115*
C58	0.3372 (6)	0.2479 (5)	0.8014 (8)	0.124 (5)
H58	0.3196	0.2728	0.7696	0.148*
C59	0.3017 (6)	0.2060 (5)	0.8038 (8)	0.117 (4)
H59	0.2605	0.2002	0.7729	0.141*
C60	0.3292 (6)	0.1728 (4)	0.8534 (9)	0.131 (5)
H60	0.3065	0.1430	0.8584	0.158*
C61	0.3906 (5)	0.1828 (4)	0.8968 (7)	0.097 (4)
H61	0.4073	0.1594	0.9319	0.117*
C62	0.6794 (5)	0.2033 (4)	1.0215 (6)	0.089 (3)
H62	0.6558	0.1737	1.0240	0.106*
C63	0.7500 (6)	0.2063 (5)	1.0498 (8)	0.116 (4)
H63	0.7733	0.1793	1.0707	0.140*
C64	0.7839 (6)	0.2490 (5)	1.0464 (7)	0.106 (4)
H64	0.8316	0.2520	1.0646	0.127*
C65	0.7491 (6)	0.2868 (5)	1.0172 (7)	0.105 (4)
H65	0.7714	0.3169	1.0145	0.126*
C66	0.6793 (5)	0.2802 (4)	0.9910 (6)	0.083 (3)
H66	0.6550	0.3071	0.9712	0.100*
C67	0.7641 (17)	0.4404 (9)	0.1201 (17)	0.212 (10)
H67	0.7911	0.4420	0.1669	0.254*
C68	0.6901 (16)	0.4471 (9)	0.1272 (14)	0.195 (9)
H68	0.6691	0.4565	0.1748	0.234*
C69	0.6528 (12)	0.4401 (9)	0.066 (2)	0.206 (9)
H69	0.6022	0.4400	0.0683	0.247*
C70	0.6870 (17)	0.4326 (9)	−0.0024 (16)	0.224 (10)
H70	0.6610	0.4295	−0.0497	0.269*
C71	0.7634 (17)	0.4294 (9)	−0.0012 (18)	0.217 (10)
H71	0.7886	0.4245	−0.0482	0.260*
C72	0.2769 (9)	0.4078 (5)	0.5960 (12)	0.140 (5)
H72	0.3047	0.3953	0.6375	0.168*
C73	0.2048 (9)	0.4113 (6)	0.6034 (11)	0.142 (5)
H73	0.1814	0.4006	0.6488	0.170*

C74	0.1660 (9)	0.4315 (6)	0.5412 (13)	0.145 (5)
H74	0.1156	0.4338	0.5446	0.174*
C75	0.1995 (8)	0.4475 (5)	0.4766 (9)	0.119 (4)
H75	0.1734	0.4625	0.4361	0.143*
C76	0.2728 (9)	0.4416 (6)	0.4712 (10)	0.133 (5)
H76	0.2971	0.4516	0.4258	0.160*
C77	0.3016 (12)	0.4440 (11)	0.2009 (17)	0.247 (13)
H77	0.3503	0.4351	0.2042	0.296*
C78	0.2691 (15)	0.4681 (11)	0.2635 (17)	0.255 (13)
H78	0.2960	0.4754	0.3088	0.307*
C79	0.1962 (16)	0.4814 (10)	0.2585 (17)	0.255 (12)
H79	0.1744	0.4975	0.3005	0.306*
C80	0.1560 (13)	0.4706 (11)	0.191 (2)	0.253 (12)
H80	0.1073	0.4795	0.1874	0.303*
C81	0.1885 (15)	0.4464 (12)	0.1282 (17)	0.273 (14)
H81	0.1616	0.4391	0.0829	0.328*
C82	0.2274 (11)	0.6356 (6)	0.2040 (11)	0.135 (6)
H82	0.2042	0.6494	0.1603	0.162*
C83	0.2988 (12)	0.6346 (6)	0.2042 (11)	0.163 (6)
H83	0.3248	0.6478	0.1623	0.196*
C84	0.3352 (9)	0.6133 (7)	0.2683 (14)	0.168 (7)
H84	0.3857	0.6116	0.2711	0.202*
C85	0.2907 (12)	0.5950 (7)	0.3276 (11)	0.179 (7)
H85	0.3101	0.5806	0.3729	0.215*
C86	0.2179 (12)	0.5990 (8)	0.3164 (13)	0.170 (7)
H86	0.1873	0.5859	0.3545	0.204*
C87	0.2369 (8)	0.5786 (5)	0.5488 (10)	0.134 (5)
H87	0.2135	0.5965	0.5097	0.161*
C88	0.3095 (9)	0.5721 (6)	0.5420 (10)	0.140 (5)
H88	0.3358	0.5849	0.5000	0.169*
C89	0.3403 (7)	0.5468 (5)	0.5982 (10)	0.114 (4)
H89	0.3904	0.5421	0.5971	0.137*
C90	0.3027 (8)	0.5277 (5)	0.6559 (9)	0.129 (5)
H90	0.3261	0.5096	0.6949	0.155*
C91	0.2286 (8)	0.5344 (6)	0.6591 (9)	0.130 (5)
H91	0.2012	0.5197	0.6986	0.156*
C92	0.2952 (11)	0.4024 (9)	0.8709 (16)	0.200 (9)
H92	0.3436	0.4123	0.8693	0.240*
C93	0.2681 (13)	0.3713 (8)	0.8133 (14)	0.183 (8)
H93	0.2984	0.3603	0.7731	0.220*
C94	0.1959 (14)	0.3566 (6)	0.8156 (12)	0.159 (6)
H94	0.1777	0.3358	0.7770	0.191*
C95	0.1507 (11)	0.3731 (9)	0.8756 (17)	0.177 (8)
H95	0.1024	0.3632	0.8772	0.213*
C96	0.1778 (14)	0.4042 (9)	0.9331 (15)	0.189 (8)
H96	0.1476	0.4153	0.9733	0.227*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0510 (6)	0.0552 (6)	0.0488 (7)	−0.0001 (4)	−0.0095 (5)	−0.0051 (5)
Ni2	0.0517 (6)	0.0611 (7)	0.0528 (7)	0.0015 (5)	0.0007 (5)	−0.0008 (5)
O1	0.059 (3)	0.054 (3)	0.055 (4)	0.005 (2)	−0.015 (3)	−0.008 (3)
O2	0.115 (5)	0.064 (4)	0.076 (5)	−0.016 (3)	−0.041 (4)	−0.006 (4)
O3	0.063 (3)	0.056 (3)	0.051 (4)	−0.006 (2)	−0.012 (3)	−0.009 (3)
O4	0.056 (3)	0.066 (4)	0.046 (4)	0.006 (2)	0.007 (3)	−0.001 (3)
O5	0.120 (5)	0.079 (5)	0.076 (5)	−0.003 (4)	0.035 (4)	−0.010 (4)
O6	0.058 (3)	0.059 (4)	0.075 (4)	−0.003 (3)	0.000 (3)	−0.001 (3)
N1	0.051 (4)	0.059 (4)	0.049 (4)	−0.004 (3)	−0.007 (3)	0.001 (4)
N2	0.045 (4)	0.053 (4)	0.056 (5)	−0.001 (3)	−0.001 (3)	−0.005 (3)
N3	0.059 (4)	0.057 (4)	0.054 (5)	0.001 (3)	−0.011 (3)	−0.009 (4)
N4	0.055 (4)	0.059 (4)	0.058 (5)	0.004 (3)	−0.003 (3)	−0.001 (4)
N5	0.052 (4)	0.076 (5)	0.066 (5)	0.000 (4)	−0.010 (4)	−0.015 (4)
N6	0.058 (4)	0.066 (5)	0.058 (5)	−0.002 (3)	0.005 (3)	−0.005 (4)
N7	0.052 (4)	0.055 (4)	0.068 (5)	−0.002 (3)	−0.004 (3)	−0.003 (4)
N8	0.059 (4)	0.066 (5)	0.055 (5)	−0.006 (3)	0.004 (3)	0.014 (4)
N9	0.051 (4)	0.065 (5)	0.064 (5)	−0.001 (3)	−0.007 (3)	0.008 (4)
N10	0.053 (4)	0.078 (5)	0.065 (5)	0.001 (4)	0.002 (4)	−0.004 (4)
N11	0.137 (14)	0.34 (2)	0.117 (15)	0.019 (13)	0.015 (13)	−0.002 (17)
N12	0.076 (8)	0.149 (10)	0.161 (13)	0.016 (7)	0.000 (8)	−0.004 (9)
N13	0.164 (18)	0.45 (3)	0.26 (3)	0.066 (19)	−0.030 (18)	−0.10 (2)
N14	0.085 (9)	0.220 (16)	0.134 (14)	0.020 (9)	−0.010 (9)	−0.029 (12)
N15	0.077 (7)	0.174 (11)	0.113 (10)	0.016 (7)	0.004 (7)	0.023 (8)
N16	0.190 (19)	0.254 (19)	0.22 (2)	−0.047 (15)	0.037 (15)	−0.054 (15)
C1	0.043 (4)	0.052 (5)	0.058 (6)	−0.001 (3)	−0.005 (4)	−0.014 (4)
C2	0.055 (5)	0.054 (5)	0.056 (6)	−0.001 (4)	−0.003 (4)	−0.003 (4)
C3	0.046 (4)	0.050 (5)	0.060 (6)	0.003 (4)	0.003 (4)	−0.010 (4)
C4	0.057 (5)	0.061 (6)	0.070 (7)	−0.008 (4)	−0.006 (5)	0.000 (5)
C5	0.071 (6)	0.061 (6)	0.085 (8)	−0.015 (4)	−0.009 (5)	−0.011 (5)
C6	0.058 (5)	0.056 (5)	0.079 (7)	−0.012 (4)	0.008 (5)	−0.002 (5)
C7	0.053 (5)	0.056 (5)	0.070 (6)	−0.001 (4)	0.014 (4)	0.000 (5)
C8	0.071 (6)	0.069 (6)	0.084 (8)	0.005 (5)	−0.003 (5)	0.001 (6)
C9	0.083 (7)	0.068 (7)	0.097 (9)	0.006 (5)	0.002 (6)	0.024 (6)
C10	0.086 (7)	0.059 (6)	0.114 (10)	−0.013 (5)	0.003 (6)	0.002 (7)
C11	0.078 (7)	0.062 (6)	0.094 (8)	−0.011 (5)	−0.006 (6)	−0.005 (6)
C12	0.049 (5)	0.064 (5)	0.044 (5)	−0.005 (4)	−0.007 (4)	−0.006 (4)
C13	0.048 (5)	0.058 (5)	0.054 (6)	0.000 (4)	−0.007 (4)	0.001 (4)
C14	0.051 (5)	0.063 (6)	0.054 (6)	0.004 (4)	−0.003 (4)	0.000 (5)
C15	0.073 (6)	0.060 (6)	0.068 (7)	0.000 (4)	−0.013 (5)	−0.001 (5)
C16	0.082 (7)	0.062 (6)	0.083 (8)	0.002 (5)	−0.009 (6)	0.009 (6)
C17	0.090 (7)	0.073 (7)	0.076 (8)	0.000 (5)	−0.014 (6)	0.012 (6)
C18	0.071 (6)	0.070 (6)	0.057 (6)	−0.005 (4)	−0.016 (4)	−0.002 (5)
C19	0.107 (8)	0.071 (7)	0.077 (8)	0.018 (5)	−0.038 (6)	−0.015 (6)
C20	0.133 (10)	0.092 (8)	0.088 (9)	0.020 (7)	−0.052 (8)	−0.027 (7)
C21	0.109 (9)	0.119 (10)	0.071 (8)	0.009 (7)	−0.026 (6)	−0.026 (8)

C22	0.111 (9)	0.113 (10)	0.060 (8)	−0.008 (7)	−0.030 (6)	0.012 (7)
C23	0.098 (8)	0.084 (7)	0.069 (8)	−0.019 (5)	−0.023 (6)	0.003 (6)
C24	0.087 (7)	0.080 (7)	0.093 (8)	0.013 (5)	0.019 (6)	0.015 (6)
C25	0.081 (8)	0.126 (10)	0.112 (10)	0.011 (7)	0.031 (7)	0.032 (8)
C26	0.093 (9)	0.138 (12)	0.127 (12)	0.030 (8)	0.039 (8)	0.013 (9)
C27	0.106 (10)	0.118 (10)	0.157 (13)	0.042 (8)	0.043 (9)	0.007 (9)
C28	0.081 (7)	0.085 (8)	0.118 (10)	0.015 (6)	0.023 (6)	0.003 (7)
C29	0.066 (7)	0.116 (9)	0.121 (10)	−0.002 (6)	0.006 (6)	0.006 (8)
C30	0.074 (9)	0.170 (14)	0.144 (12)	−0.006 (8)	0.029 (8)	0.011 (10)
C31	0.065 (8)	0.153 (13)	0.127 (12)	0.001 (8)	0.018 (7)	−0.028 (10)
C32	0.070 (8)	0.135 (11)	0.152 (13)	0.020 (7)	−0.002 (8)	−0.042 (10)
C33	0.064 (7)	0.091 (8)	0.119 (10)	0.002 (5)	−0.007 (6)	−0.008 (6)
C34	0.040 (4)	0.063 (5)	0.057 (6)	−0.004 (4)	−0.005 (4)	0.001 (5)
C35	0.052 (5)	0.068 (6)	0.046 (5)	−0.003 (4)	−0.003 (4)	0.002 (4)
C36	0.039 (4)	0.062 (5)	0.045 (5)	−0.009 (3)	0.000 (3)	0.002 (4)
C37	0.054 (5)	0.072 (6)	0.057 (6)	−0.009 (4)	0.008 (4)	−0.007 (5)
C38	0.066 (6)	0.086 (7)	0.057 (6)	−0.017 (5)	0.005 (4)	0.006 (5)
C39	0.053 (5)	0.072 (6)	0.066 (7)	−0.014 (4)	−0.010 (4)	0.009 (5)
C40	0.049 (5)	0.068 (6)	0.057 (6)	−0.004 (4)	−0.007 (4)	0.000 (5)
C41	0.080 (7)	0.077 (7)	0.088 (8)	0.003 (5)	0.004 (5)	0.014 (6)
C42	0.096 (8)	0.084 (8)	0.097 (9)	0.010 (6)	−0.005 (7)	0.017 (7)
C43	0.088 (8)	0.078 (8)	0.103 (10)	−0.012 (6)	−0.017 (7)	0.026 (7)
C44	0.077 (7)	0.085 (7)	0.073 (7)	−0.018 (5)	−0.005 (5)	0.012 (6)
C45	0.058 (5)	0.057 (5)	0.075 (7)	0.001 (4)	−0.001 (4)	−0.013 (5)
C46	0.057 (5)	0.063 (6)	0.081 (7)	0.003 (4)	−0.005 (5)	−0.017 (5)
C47	0.052 (5)	0.066 (6)	0.072 (7)	0.001 (4)	−0.006 (4)	0.003 (5)
C48	0.082 (6)	0.060 (6)	0.078 (7)	0.000 (5)	−0.008 (5)	−0.002 (5)
C49	0.096 (8)	0.071 (7)	0.106 (10)	0.007 (6)	−0.001 (7)	0.004 (7)
C50	0.096 (8)	0.074 (8)	0.120 (11)	0.017 (6)	−0.003 (7)	−0.018 (7)
C51	0.081 (7)	0.069 (7)	0.101 (9)	0.006 (5)	0.001 (6)	−0.012 (6)
C52	0.073 (6)	0.088 (7)	0.074 (8)	0.002 (5)	0.003 (5)	0.008 (6)
C53	0.096 (8)	0.107 (9)	0.062 (7)	0.000 (6)	0.016 (6)	0.019 (6)
C54	0.097 (8)	0.115 (9)	0.061 (7)	−0.004 (7)	0.015 (6)	−0.007 (7)
C55	0.112 (8)	0.097 (8)	0.079 (8)	−0.009 (6)	0.035 (6)	−0.008 (7)
C56	0.090 (7)	0.081 (7)	0.075 (8)	−0.008 (5)	0.014 (5)	0.007 (6)
C57	0.077 (7)	0.100 (8)	0.111 (9)	−0.029 (6)	−0.033 (6)	0.048 (7)
C58	0.099 (9)	0.116 (10)	0.155 (13)	−0.031 (7)	−0.063 (8)	0.058 (9)
C59	0.098 (9)	0.115 (10)	0.137 (12)	−0.038 (7)	−0.053 (8)	0.047 (8)
C60	0.096 (9)	0.110 (10)	0.187 (14)	−0.039 (7)	−0.066 (9)	0.036 (10)
C61	0.084 (7)	0.075 (7)	0.131 (10)	−0.006 (6)	−0.046 (7)	0.021 (7)
C62	0.056 (6)	0.103 (8)	0.106 (9)	−0.001 (5)	−0.008 (5)	0.010 (7)
C63	0.070 (8)	0.141 (12)	0.137 (12)	0.005 (7)	−0.027 (7)	0.022 (9)
C64	0.051 (7)	0.152 (12)	0.113 (10)	−0.010 (7)	−0.012 (6)	0.003 (9)
C65	0.063 (7)	0.130 (10)	0.123 (11)	−0.026 (7)	−0.006 (6)	−0.003 (8)
C66	0.065 (7)	0.088 (7)	0.097 (8)	−0.004 (5)	−0.004 (5)	0.000 (6)
C67	0.16 (2)	0.34 (3)	0.13 (2)	0.01 (2)	−0.029 (16)	0.01 (2)
C68	0.15 (2)	0.33 (3)	0.107 (16)	−0.019 (19)	0.009 (14)	−0.004 (17)
C69	0.156 (19)	0.30 (3)	0.16 (2)	−0.015 (17)	0.00 (2)	0.00 (2)

C70	0.17 (2)	0.35 (3)	0.15 (2)	−0.02 (2)	−0.016 (17)	−0.05 (2)
C71	0.15 (2)	0.35 (3)	0.15 (2)	0.00 (2)	0.033 (17)	−0.03 (2)
C72	0.101 (12)	0.154 (13)	0.165 (17)	0.011 (9)	−0.021 (11)	0.030 (11)
C73	0.107 (12)	0.175 (15)	0.144 (15)	−0.008 (10)	0.016 (10)	0.034 (11)
C74	0.106 (12)	0.169 (15)	0.160 (17)	0.004 (10)	0.002 (12)	−0.012 (13)
C75	0.097 (11)	0.152 (12)	0.108 (12)	−0.002 (9)	−0.019 (8)	−0.017 (9)
C76	0.098 (12)	0.169 (14)	0.132 (14)	−0.022 (10)	0.010 (10)	−0.032 (11)
C77	0.148 (18)	0.42 (4)	0.17 (2)	0.09 (2)	−0.054 (17)	−0.09 (2)
C78	0.16 (2)	0.38 (4)	0.22 (3)	0.08 (2)	−0.046 (19)	−0.06 (2)
C79	0.17 (2)	0.38 (4)	0.22 (3)	0.02 (2)	−0.03 (2)	−0.05 (2)
C80	0.16 (2)	0.38 (4)	0.22 (3)	0.02 (2)	−0.04 (2)	−0.08 (3)
C81	0.15 (2)	0.44 (4)	0.22 (3)	0.04 (2)	−0.03 (2)	−0.10 (3)
C82	0.105 (13)	0.174 (15)	0.126 (15)	0.027 (11)	−0.051 (11)	0.011 (11)
C83	0.154 (17)	0.212 (18)	0.123 (15)	−0.025 (13)	−0.013 (13)	0.029 (12)
C84	0.109 (13)	0.24 (2)	0.154 (18)	−0.004 (12)	−0.025 (13)	−0.002 (15)
C85	0.139 (17)	0.27 (2)	0.129 (16)	0.013 (15)	−0.014 (13)	0.016 (15)
C86	0.109 (15)	0.26 (2)	0.137 (17)	−0.015 (14)	0.013 (12)	−0.004 (15)
C87	0.097 (11)	0.160 (13)	0.145 (14)	0.025 (9)	−0.014 (10)	0.047 (11)
C88	0.105 (12)	0.175 (14)	0.142 (14)	−0.010 (10)	0.000 (10)	0.033 (11)
C89	0.068 (8)	0.151 (12)	0.124 (12)	−0.002 (8)	−0.016 (8)	0.008 (10)
C90	0.097 (11)	0.174 (14)	0.117 (12)	0.013 (9)	−0.013 (9)	0.020 (10)
C91	0.097 (11)	0.180 (14)	0.113 (12)	0.002 (9)	0.014 (8)	0.016 (11)
C92	0.152 (18)	0.26 (3)	0.19 (2)	−0.039 (17)	0.035 (17)	−0.036 (19)
C93	0.17 (2)	0.21 (2)	0.17 (2)	−0.020 (14)	0.062 (15)	−0.028 (15)
C94	0.164 (18)	0.168 (15)	0.143 (16)	−0.023 (14)	−0.021 (13)	−0.048 (12)
C95	0.130 (16)	0.21 (2)	0.19 (2)	−0.009 (15)	−0.008 (17)	0.034 (18)
C96	0.14 (2)	0.23 (2)	0.19 (2)	0.004 (15)	0.034 (16)	−0.011 (18)

Geometric parameters (Å, º)

Ni1—O1	2.050 (5)	C35—C40	1.404 (10)
Ni1—O3	1.998 (5)	C35—H35	0.9300
Ni1—N2	1.989 (7)	C36—C37	1.424 (11)
Ni1—N3	2.077 (6)	C37—C38	1.364 (11)
Ni1—N4	2.192 (6)	C38—C39	1.403 (12)
Ni1—N5	2.173 (7)	C38—H38	0.9300
Ni2—O4	2.061 (5)	C39—C40	1.412 (11)
Ni2—O6	1.993 (5)	C39—C44	1.416 (12)
Ni2—N7	1.983 (7)	C40—C41	1.399 (11)
Ni2—N8	2.067 (7)	C41—C42	1.371 (12)
Ni2—N9	2.156 (6)	C41—H41	0.9300
Ni2—N10	2.180 (7)	C42—C43	1.397 (14)
O1—C1	1.280 (9)	C42—H42	0.9300
O2—C4	1.346 (10)	C43—C44	1.315 (13)
O2—H2	0.8200	C43—H43	0.9300
O3—C14	1.302 (9)	C44—H44	0.9300
O4—C34	1.291 (9)	C45—C46	1.433 (12)
O5—C37	1.341 (9)	C45—H45	0.9300

O5—H5	0.8200	C46—C51	1.407 (12)
O6—C47	1.300 (10)	C46—C47	1.418 (12)
N1—C1	1.322 (10)	C47—C48	1.418 (11)
N1—N2	1.400 (8)	C48—C49	1.375 (12)
N2—C12	1.266 (9)	C48—H48	0.9300
N3—C19	1.310 (10)	C49—C50	1.377 (14)
N3—C23	1.333 (11)	C49—H49	0.9300
N4—C24	1.298 (10)	C50—C51	1.360 (13)
N4—C28	1.303 (10)	C50—H50	0.9300
N5—C33	1.312 (11)	C51—H51	0.9300
N5—C29	1.313 (12)	C52—C53	1.392 (13)
N6—C34	1.340 (9)	C52—H52	0.9300
N6—N7	1.397 (9)	C53—C54	1.348 (13)
N7—C45	1.293 (9)	C53—H53	0.9300
N8—C52	1.312 (11)	C54—C55	1.354 (13)
N8—C56	1.339 (10)	C54—H54	0.9300
N9—C57	1.293 (10)	C55—C56	1.378 (13)
N9—C61	1.314 (10)	C55—H55	0.9300
N10—C66	1.290 (10)	C56—H56	0.9300
N10—C62	1.309 (11)	C57—C58	1.352 (13)
N11—C67	1.17 (2)	C57—H57	0.9300
N11—C71	1.23 (2)	C58—C59	1.334 (14)
N12—C76	1.302 (17)	C58—H58	0.9300
N12—C72	1.333 (17)	C59—C60	1.340 (14)
N13—C77	1.39 (2)	C59—H59	0.9300
N13—C81	1.39 (2)	C60—C61	1.369 (13)
N14—C82	1.223 (18)	C60—H60	0.9300
N14—C86	1.27 (2)	C61—H61	0.9300
N15—C87	1.290 (15)	C62—C63	1.381 (13)
N15—C91	1.307 (15)	C62—H62	0.9300
N16—C92	1.39 (2)	C63—C64	1.339 (14)
N16—C96	1.39 (2)	C63—H63	0.9300
C1—C3	1.497 (10)	C64—C65	1.322 (14)
C2—C3	1.367 (10)	C64—H64	0.9300
C2—C7	1.398 (10)	C65—C66	1.367 (13)
C2—H2A	0.9300	C65—H65	0.9300
C3—C4	1.425 (11)	C66—H66	0.9300
C4—C5	1.381 (11)	C67—C68	1.38 (2)
C5—C6	1.409 (12)	C67—H67	0.9300
C5—H5A	0.9300	C68—C69	1.25 (2)
C6—C11	1.401 (11)	C68—H68	0.9300
C6—C7	1.414 (12)	C69—C70	1.34 (2)
C7—C8	1.411 (12)	C69—H69	0.9300
C8—C9	1.363 (11)	C70—C71	1.41 (3)
C8—H8	0.9300	C70—H70	0.9300
C9—C10	1.412 (13)	C71—H71	0.9300
C9—H9	0.9300	C72—C73	1.335 (17)
C10—C11	1.357 (13)	C72—H72	0.9300

C10—H10	0.9300	C73—C74	1.381 (19)
C11—H11	0.9300	C73—H73	0.9300
C12—C13	1.432 (10)	C74—C75	1.332 (18)
C12—H12	0.9300	C74—H74	0.9300
C13—C14	1.402 (11)	C75—C76	1.360 (17)
C13—C18	1.403 (11)	C75—H75	0.9300
C14—C15	1.414 (11)	C76—H76	0.9300
C15—C16	1.354 (12)	C77—C78	1.39 (3)
C15—H15	0.9300	C77—H77	0.9300
C16—C17	1.378 (12)	C78—C79	1.39 (2)
C16—H16	0.9300	C78—H78	0.9300
C17—C18	1.373 (11)	C79—C80	1.39 (3)
C17—H17	0.9300	C79—H79	0.9300
C18—H18	0.9300	C80—C81	1.39 (3)
C19—C20	1.349 (13)	C80—H80	0.9300
C19—H19	0.9300	C81—H81	0.9300
C20—C21	1.357 (14)	C82—C83	1.312 (19)
C20—H20	0.9300	C82—H82	0.9300
C21—C22	1.368 (13)	C83—C84	1.40 (2)
C21—H21	0.9300	C83—H83	0.9300
C22—C23	1.343 (13)	C84—C85	1.39 (2)
C22—H22	0.9300	C84—H84	0.9300
C23—H23	0.9300	C85—C86	1.35 (2)
C24—C25	1.382 (13)	C85—H85	0.9300
C24—H24	0.9300	C86—H86	0.9300
C25—C26	1.323 (15)	C87—C88	1.351 (16)
C25—H25	0.9300	C87—H87	0.9300
C26—C27	1.356 (15)	C88—C89	1.305 (17)
C26—H26	0.9300	C88—H88	0.9300
C27—C28	1.404 (14)	C89—C90	1.310 (16)
C27—H27	0.9300	C89—H89	0.9300
C28—H28	0.9300	C90—C91	1.374 (16)
C29—C30	1.377 (14)	C90—H90	0.9300
C29—H29	0.9300	C91—H91	0.9300
C30—C31	1.354 (15)	C92—C93	1.39 (2)
C30—H30	0.9300	C92—H92	0.9300
C31—C32	1.361 (16)	C93—C94	1.39 (2)
C31—H31	0.9300	C93—H93	0.9300
C32—C33	1.391 (14)	C94—C95	1.39 (2)
C32—H32	0.9300	C94—H94	0.9300
C33—H33	0.9300	C95—C96	1.39 (2)
C34—C36	1.465 (10)	C95—H95	0.9300
C35—C36	1.357 (10)	C96—H96	0.9300

N2—Ni1—O3	90.5 (2)	C38—C37—C36	119.3 (8)
N2—Ni1—O1	79.4 (2)	C37—C38—C39	122.3 (8)
O3—Ni1—O1	170.0 (2)	C37—C38—H38	118.8
N2—Ni1—N3	174.6 (3)	C39—C38—H38	118.8

O3—Ni1—N3	94.8 (2)	C38—C39—C40	118.5 (8)
O1—Ni1—N3	95.3 (2)	C38—C39—C44	123.5 (9)
N2—Ni1—N5	93.5 (2)	C40—C39—C44	118.0 (9)
O3—Ni1—N5	90.6 (3)	C41—C40—C35	123.9 (8)
O1—Ni1—N5	90.1 (3)	C41—C40—C39	118.1 (8)
N3—Ni1—N5	87.3 (2)	C35—C40—C39	118.0 (8)
N2—Ni1—N4	92.5 (2)	C42—C41—C40	122.3 (10)
O3—Ni1—N4	90.9 (2)	C42—C41—H41	118.9
O1—Ni1—N4	89.4 (2)	C40—C41—H41	118.9
N3—Ni1—N4	86.7 (2)	C41—C42—C43	118.1 (10)
N5—Ni1—N4	173.9 (3)	C41—C42—H42	120.9
N7—Ni2—O6	90.4 (3)	C43—C42—H42	120.9
N7—Ni2—O4	79.5 (2)	C44—C43—C42	121.6 (10)
O6—Ni2—O4	169.8 (2)	C44—C43—H43	119.2
N7—Ni2—N8	174.4 (3)	C42—C43—H43	119.2
O6—Ni2—N8	95.1 (3)	C43—C44—C39	121.9 (10)
O4—Ni2—N8	95.1 (2)	C43—C44—H44	119.1
N7—Ni2—N9	92.4 (3)	C39—C44—H44	119.1
O6—Ni2—N9	91.7 (2)	N7—C45—C46	123.1 (8)
O4—Ni2—N9	89.7 (2)	N7—C45—H45	118.4
N8—Ni2—N9	86.1 (3)	C46—C45—H45	118.4
N7—Ni2—N10	93.9 (3)	C51—C46—C47	118.3 (9)
O6—Ni2—N10	90.4 (3)	C51—C46—C45	116.1 (9)
O4—Ni2—N10	89.3 (3)	C47—C46—C45	125.6 (8)
N8—Ni2—N10	87.3 (3)	O6—C47—C46	123.9 (8)
N9—Ni2—N10	173.3 (3)	O6—C47—C48	118.5 (9)
C1—O1—Ni1	109.8 (5)	C46—C47—C48	117.6 (9)
C4—O2—H2	109.5	C49—C48—C47	121.8 (10)
C14—O3—Ni1	126.9 (5)	C49—C48—H48	119.1
C34—O4—Ni2	109.7 (5)	C47—C48—H48	119.1
C37—O5—H5	109.5	C48—C49—C50	120.2 (10)
C47—O6—Ni2	127.9 (6)	C48—C49—H49	119.9
C1—N1—N2	111.3 (6)	C50—C49—H49	119.9
C12—N2—N1	117.4 (7)	C51—C50—C49	119.6 (10)
C12—N2—Ni1	128.3 (6)	C51—C50—H50	120.2
N1—N2—Ni1	114.2 (5)	C49—C50—H50	120.2
C19—N3—C23	117.4 (8)	C50—C51—C46	122.6 (10)
C19—N3—Ni1	121.0 (6)	C50—C51—H51	118.7
C23—N3—Ni1	121.6 (6)	C46—C51—H51	118.7
C24—N4—C28	116.3 (8)	N8—C52—C53	124.3 (10)
C24—N4—Ni1	123.0 (6)	N8—C52—H52	117.8
C28—N4—Ni1	120.5 (6)	C53—C52—H52	117.8
C33—N5—C29	116.0 (9)	C54—C53—C52	116.4 (10)
C33—N5—Ni1	121.7 (7)	C54—C53—H53	121.8
C29—N5—Ni1	122.2 (7)	C52—C53—H53	121.8
C34—N6—N7	111.2 (6)	C53—C54—C55	122.0 (10)
C45—N7—N6	115.9 (7)	C53—C54—H54	119.0
C45—N7—Ni2	129.0 (6)	C55—C54—H54	119.0

N6—N7—Ni2	115.1 (5)	C54—C55—C56	117.2 (10)
C52—N8—C56	116.7 (8)	C54—C55—H55	121.4
C52—N8—Ni2	122.2 (7)	C56—C55—H55	121.4
C56—N8—Ni2	121.1 (6)	N8—C56—C55	123.3 (9)
C57—N9—C61	113.8 (8)	N8—C56—H56	118.3
C57—N9—Ni2	122.4 (6)	C55—C56—H56	118.3
C61—N9—Ni2	123.4 (6)	N9—C57—C58	125.2 (10)
C66—N10—C62	115.0 (8)	N9—C57—H57	117.4
C66—N10—Ni2	122.5 (7)	C58—C57—H57	117.4
C62—N10—Ni2	122.5 (7)	C59—C58—C57	120.8 (11)
C67—N11—C71	118 (3)	C59—C58—H58	119.6
C76—N12—C72	122.1 (14)	C57—C58—H58	119.6
C77—N13—C81	120 (2)	C58—C59—C60	115.8 (10)
C82—N14—C86	120.0 (18)	C58—C59—H59	122.1
C87—N15—C91	118.6 (12)	C60—C59—H59	122.1
C92—N16—C96	120 (2)	C59—C60—C61	120.0 (11)
O1—C1—N1	125.2 (7)	C59—C60—H60	120.0
O1—C1—C3	118.6 (8)	C61—C60—H60	120.0
N1—C1—C3	116.1 (7)	N9—C61—C60	124.3 (10)
C3—C2—C7	122.1 (8)	N9—C61—H61	117.8
C3—C2—H2A	119.0	C60—C61—H61	117.8
C7—C2—H2A	119.0	N10—C62—C63	123.5 (10)
C2—C3—C4	119.0 (7)	N10—C62—H62	118.2
C2—C3—C1	118.9 (7)	C63—C62—H62	118.2
C4—C3—C1	122.1 (8)	C64—C63—C62	118.2 (11)
O2—C4—C5	118.5 (8)	C64—C63—H63	120.9
O2—C4—C3	121.6 (7)	C62—C63—H63	120.9
C5—C4—C3	119.9 (9)	C65—C64—C63	119.6 (11)
C4—C5—C6	121.2 (8)	C65—C64—H64	120.2
C4—C5—H5A	119.4	C63—C64—H64	120.2
C6—C5—H5A	119.4	C64—C65—C66	117.6 (11)
C11—C6—C5	121.7 (9)	C64—C65—H65	121.2
C11—C6—C7	119.7 (9)	C66—C65—H65	121.2
C5—C6—C7	118.5 (8)	N10—C66—C65	126.0 (10)
C2—C7—C8	122.3 (9)	N10—C66—H66	117.0
C2—C7—C6	119.4 (8)	C65—C66—H66	117.0
C8—C7—C6	118.3 (8)	N11—C67—C68	128 (2)
C9—C8—C7	121.2 (9)	N11—C67—H67	116.2
C9—C8—H8	119.4	C68—C67—H67	116.2
C7—C8—H8	119.4	C69—C68—C67	116 (2)
C8—C9—C10	119.5 (10)	C69—C68—H68	121.8
C8—C9—H9	120.2	C67—C68—H68	121.8
C10—C9—H9	120.2	C68—C69—C70	119 (3)
C11—C10—C9	120.7 (9)	C68—C69—H69	120.7
C11—C10—H10	119.6	C70—C69—H69	120.7
C9—C10—H10	119.6	C69—C70—C71	118 (2)
C10—C11—C6	120.5 (10)	C69—C70—H70	120.9
C10—C11—H11	119.8	C71—C70—H70	120.9

C6—C11—H11	119.8	N11—C71—C70	120 (2)
N2—C12—C13	124.4 (8)	N11—C71—H71	119.9
N2—C12—H12	117.8	C70—C71—H71	119.9
C13—C12—H12	117.8	N12—C72—C73	120.2 (15)
C14—C13—C18	118.7 (8)	N12—C72—H72	119.9
C14—C13—C12	125.0 (8)	C73—C72—H72	119.9
C18—C13—C12	116.2 (7)	C72—C73—C74	117.8 (16)
O3—C14—C13	124.7 (7)	C72—C73—H73	121.1
O3—C14—C15	118.2 (8)	C74—C73—H73	121.1
C13—C14—C15	117.1 (8)	C75—C74—C73	121.1 (16)
C16—C15—C14	122.2 (9)	C75—C74—H74	119.5
C16—C15—H15	118.9	C73—C74—H74	119.5
C14—C15—H15	118.9	C74—C75—C76	118.5 (15)
C15—C16—C17	121.4 (9)	C74—C75—H75	120.7
C15—C16—H16	119.3	C76—C75—H75	120.7
C17—C16—H16	119.3	N12—C76—C75	120.2 (15)
C18—C17—C16	117.6 (9)	N12—C76—H76	119.9
C18—C17—H17	121.2	C75—C76—H76	119.9
C16—C17—H17	121.2	C78—C77—N13	120 (2)
C17—C18—C13	123.0 (8)	C78—C77—H77	120.0
C17—C18—H18	118.5	N13—C77—H77	120.0
C13—C18—H18	118.5	C77—C78—C79	120 (2)
N3—C19—C20	123.5 (10)	C77—C78—H78	120.0
N3—C19—H19	118.3	C79—C78—H78	120.0
C20—C19—H19	118.3	C80—C79—C78	120 (3)
C19—C20—C21	119.0 (11)	C80—C79—H79	120.0
C19—C20—H20	120.5	C78—C79—H79	120.0
C21—C20—H20	120.5	C81—C80—C79	120 (3)
C20—C21—C22	118.2 (10)	C81—C80—H80	120.0
C20—C21—H21	120.9	C79—C80—H80	120.0
C22—C21—H21	120.9	C80—C81—N13	120 (2)
C23—C22—C21	119.3 (10)	C80—C81—H81	120.0
C23—C22—H22	120.4	N13—C81—H81	120.0
C21—C22—H22	120.4	N14—C82—C83	124.8 (17)
N3—C23—C22	122.6 (10)	N14—C82—H82	117.6
N3—C23—H23	118.7	C83—C82—H82	117.6
C22—C23—H23	118.7	C82—C83—C84	119.0 (17)
N4—C24—C25	124.3 (10)	C82—C83—H83	120.5
N4—C24—H24	117.9	C84—C83—H83	120.5
C25—C24—H24	117.9	C85—C84—C83	115.5 (17)
C26—C25—C24	119.6 (11)	C85—C84—H84	122.3
C26—C25—H25	120.2	C83—C84—H84	122.3
C24—C25—H25	120.2	C86—C85—C84	116.9 (18)
C25—C26—C27	118.0 (11)	C86—C85—H85	121.5
C25—C26—H26	121.0	C84—C85—H85	121.5
C27—C26—H26	121.0	N14—C86—C85	123.7 (19)
C26—C27—C28	118.7 (11)	N14—C86—H86	118.1
C26—C27—H27	120.6	C85—C86—H86	118.1

C28—C27—H27	120.6	N15—C87—C88	124.9 (13)
N4—C28—C27	122.9 (10)	N15—C87—H87	117.5
N4—C28—H28	118.5	C88—C87—H87	117.5
C27—C28—H28	118.5	C89—C88—C87	115.7 (14)
N5—C29—C30	124.7 (11)	C89—C88—H88	122.2
N5—C29—H29	117.6	C87—C88—H88	122.2
C30—C29—H29	117.6	C88—C89—C90	121.9 (14)
C31—C30—C29	118.9 (13)	C88—C89—H89	119.0
C31—C30—H30	120.5	C90—C89—H89	119.0
C29—C30—H30	120.5	C89—C90—C91	120.1 (14)
C30—C31—C32	117.5 (12)	C89—C90—H90	119.9
C30—C31—H31	121.3	C91—C90—H90	119.9
C32—C31—H31	121.3	N15—C91—C90	118.6 (13)
C31—C32—C33	119.5 (12)	N15—C91—H91	120.7
C31—C32—H32	120.2	C90—C91—H91	120.7
C33—C32—H32	120.2	N16—C92—C93	120 (2)
N5—C33—C32	123.2 (11)	N16—C92—H92	120.0
N5—C33—H33	118.4	C93—C92—H92	120.0
C32—C33—H33	118.4	C92—C93—C94	120.0 (18)
O4—C34—N6	124.5 (7)	C92—C93—H93	120.0
O4—C34—C36	119.5 (7)	C94—C93—H93	120.0
N6—C34—C36	116.0 (7)	C95—C94—C93	119.9 (18)
C36—C35—C40	123.1 (8)	C95—C94—H94	120.0
C36—C35—H35	118.4	C93—C94—H94	120.0
C40—C35—H35	118.4	C96—C95—C94	120 (2)
C35—C36—C37	118.6 (7)	C96—C95—H95	120.0
C35—C36—C34	118.8 (7)	C94—C95—H95	120.0
C37—C36—C34	122.6 (7)	C95—C96—N16	120 (2)
O5—C37—C38	119.7 (8)	C95—C96—H96	120.0
O5—C37—C36	121.0 (8)	N16—C96—H96	120.0

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···N1	0.82	1.82	2.558 (8)	148
O5—H5···N6	0.82	1.80	2.533 (9)	148