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[*N*-(8-Quinolylmethyl)iminodiethanol-κ^4N,N',O,O']bis(thiocyanato-κN)-nickel(II) monohydrate

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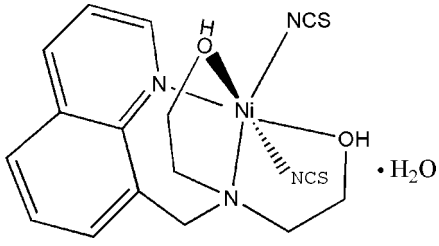
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.006 Å; R factor = 0.043; wR factor = 0.097; data-to-parameter ratio = 16.1.

In the neutral title complex, $[Ni(NCS)_2(C_{14}H_{18}N_2O_2)]\cdot H_2O$, the Ni^{II} ion has a distorted octahedral geometry with *cis*-isothiocyanate ligands.

Related literature

For diethanolamine and N-substituted diethanolamine transition metal coordination compounds, see: Saalfrank *et al.* (2001); Yilmaz *et al.* (2000).



Experimental

Crystal data

$[Ni(NCS)_2(C_{14}H_{18}N_2O_2)]\cdot H_2O$
M_r = 439.19
Monoclinic, $P2_1/c$
a = 14.693 (6) Å
b = 10.142 (4) Å
c = 13.965 (6) Å
β = 115.460 (6)°
V = 1878.9 (13) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.28 mm^{-1}
T = 293 (2) K
0.15 × 0.10 × 0.08 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1998)
T_{min} = 0.800, T_{max} = 1.000
(expected range = 0.722–0.903)
8517 measured reflections
3783 independent reflections
2673 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.097
S = 1.08
3783 reflections
235 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.50 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ni1—N3	2.011 (3)	Ni1—O2	2.067 (2)
Ni1—N4	2.018 (3)	Ni1—O1	2.089 (2)
Ni1—N2	2.061 (3)	Ni1—N1	2.093 (3)
N3—Ni1—N4	96.64 (12)	N2—Ni1—O1	80.54 (10)
N3—Ni1—N2	97.00 (11)	O2—Ni1—O1	89.84 (10)
N3—Ni1—O2	89.15 (12)	N3—Ni1—N1	90.10 (12)
N4—Ni1—O2	91.29 (11)	N4—Ni1—N1	96.35 (11)
N2—Ni1—O2	79.51 (10)	N2—Ni1—N1	93.04 (10)
N4—Ni1—O1	85.70 (10)	O1—Ni1—N1	90.59 (10)

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1999); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); 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: SG2198).

References

Bruker (1998). *SHELXTL* and *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (1999). *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Saalfrank, R. F., Bertnt, I. & Hampel, F. (2001). *Chem. Eur. J.* **7**, 2770–2774.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (1998). *SADABS*. University of Göttingen, Germany.
Yilmaz, V. T., Karadag, A., Thöne, C. & Herbst-Irmer, R. (2000). *Acta Cryst.* C**56**, 948–949.

supporting information

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[*N*-(8-Quinolylmethyl)iminodiethanol-κ^4N,N',O,O']bis(thiocyanato-κN)nickel(II) monohydrate

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S1. Comment

As shown in Fig. 1, (I) is a neutral mononuclear complex, consisting of one nickel(II) ion, one *N*-(8-quinolylmethyl)-iminodiethanol ligand, two SCN^- and one uncoordinated H_2O molecule. Each Ni^{II} center has a distorted octahedral geometry (Table 1) comprised of two isothiocyanate N atoms, the quinoline N donor, the tertiary N donor and two O donor of the ligand. The NSC groups are almost linear [178.9 (3)° and 178.2 (4)°], though he Ni—N—C linkage [158.8 (3)° and 171.5 (3)°] is bent. No intermolecular hydrogen bonds interactions were observed in the complex.

S2. Experimental

Synthesis of the *N*-(8-quinolylmethyl)iminodiethanol ligand. 8-bromomethylquinoline (0.01 mol) was added to the solution of diethanolamine (0.03 mol) in ethanol (50 ml) with stirring. The mixture was refluxed for 15 h, and the solvent was evaporated. The residual oil was dissolved in 10 ml H_2O, and the mixture was extracted with benzene and dried over $MgSO_4$. The solvent was evaporated to give a pale yellow liquid, 1.92 g (78% yield). IR (cm^{-1}): 3357vs, 2926 s, 2869 s, 1454 s, 1425*m*, 1321*m*, 1130*m*, 1071 s, 1438 s, 834*m*. ^{1}H NMR ($CDCl_3$): 4.21 (2*H*,*S*,-CH_2Ar), 8.88 (1*H*, d, Ar—H2), 7.41 (1*H*, t, Ar—H3), 8.16 (1*H*, d, Ar—H4), 7.75 (1*H*, d, Ar—H5), 7.47(1*H*, t, Ar—H6), 7.57 (1*H*, d, Ar—H7), 2.74 (4*H*, t, NCH2C), 3.62 (4*H*, t, CH_2O), 1.25 (2*H*, s, OH). Anal. Found: C, 68.51; H, 7.62; N, 11.39%; calculated for $C_{14}H_{18}N_2O_2$: C, 68.27; H, 7.37; N, 11.37.

Synthesis of the title complex (I). Solid KSCN (0.2 mmol) was added slowly with continuous stirring to a solution of $NiSO_4.6H_2O$ (0.1 mmol) in distilled water (15 ml), the ligand (0.1 mmol) was dissolved in methanol (15 ml) and two solutions were mixed. The mixture was filtered, and green crystals suitable for X-ray diffraction analysis were obtained by slow evaporation from the resulting solution at room temperature. Anal. Found: C, 43.28; H, 4.63; N, 12.78%; calculated for $C_{16}H_{20}N_4NiO_3S_2$: C, 43.76; H, 4.59; N, 12.76%.

S3. Refinement

H atoms were included in calculated positions refined as part of a riding with C—H distances of 0.93 Å (aromatic H) and 0.97 Å (ethyl H), and with U_{iso}(aromatic H, ethyl H) = 1.2U_{eq}(C). H atoms bonded to O atoms were located in a difference map and refined with distance restraints of O—H = 0.93 Å (hydroxy H) and 0.852Å (H_2O molecular H), and with U_{iso} (hydroxy H)= 1.2U_{eq}(O) and U_{iso} (H_2O molecular H) = 1.5U_{eq}(O).

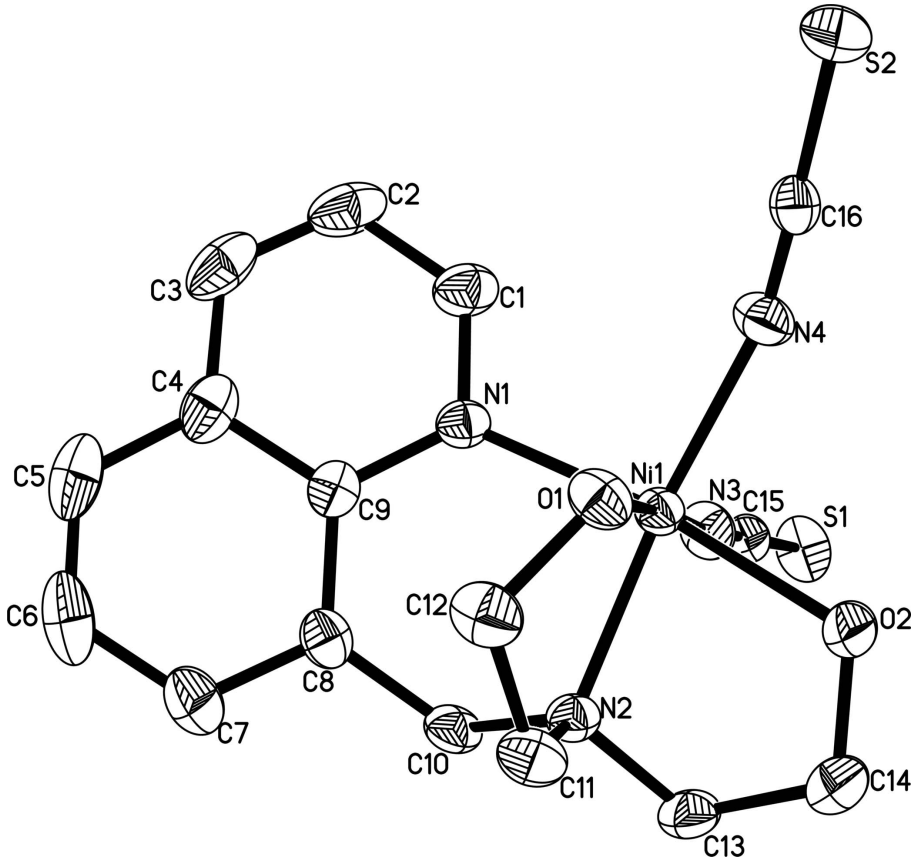

Figure 1

The molecular structure of (I), with atom labels and 30% probability displacement ellipsoids for non-H atoms and uncoordinated H_2O molecular.

[*N*-(8-Quinolylmethyl)iminodiethanol-κ^4N,N',O,O']bis(thiocyanato- κN)nickel(II) monohydrate

Crystal data

$[Ni(NCS)_2(C_{14}H_{18}N_2O_2)]\cdot H_2O$
$M_r = 439.19$
Monoclinic, $P2_1/c$
$a = 14.693$ (6) Å
$b = 10.142$ (4) Å
$c = 13.965$ (6) Å
$\beta = 115.460$ (6)°
$V = 1878.9$ (13) Å^3
$Z = 4$
$F(000) = 912$
$D_x = 1.553$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 783 reflections
$\theta = 2.6$–25.0°
$\mu = 1.28$ mm^{-1}
$T = 293$ K
Block, green
0.15 × 0.10 × 0.08 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1998)
$T_{min} = 0.800$, $T_{max} = 1.000$
8517 measured reflections
3783 independent reflections
2673 reflections with $I > 2\sigma(I)$
$R_{int} = 0.033$
$\theta_{max} = 26.3°$, $\theta_{min} = 2.5°$
$h = -18\rightarrow13$
$k = -11\rightarrow12$
$l = -6\rightarrow17$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.097$
$S = 1.08$
3783 reflections
235 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
$w = 1/[\sigma^2(F_o^2) + (0.0367P)^2 + 0.8315P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.50$ e Å^{-3}
$\Delta\rho_{min} = -0.40$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ni1	0.20147 (3)	0.81623 (4)	0.28870 (3)	0.03578 (13)
O1	0.15578 (17)	0.7221 (2)	0.39381 (17)	0.0461 (6)
H1A	0.1344	0.6349	0.3868	0.055*
O2	0.05232 (18)	0.8491 (2)	0.1858 (2)	0.0596 (7)
H2A	0.0136	0.7863	0.1366	0.072*
O3	0.9140 (3)	0.7780 (4)	1.0013 (3)	0.1413 (18)
H31	0.9448	0.8434	0.9906	0.212*
H32	0.8905	0.7275	0.9473	0.212*
N1	0.35206 (19)	0.8079 (3)	0.4011 (2)	0.0399 (6)
N2	0.1710 (2)	0.9792 (2)	0.3581 (2)	0.0391 (6)
N3	0.2430 (2)	0.9143 (3)	0.1887 (2)	0.0513 (8)
N4	0.1975 (2)	0.6352 (3)	0.2271 (2)	0.0500 (7)
S1	0.27361 (8)	1.03083 (10)	0.02603 (8)	0.0606 (3)
S2	0.20208 (9)	0.36476 (10)	0.22047 (9)	0.0679 (3)
C1	0.4045 (3)	0.7104 (4)	0.3897 (3)	0.0561 (10)
H1	0.3790	0.6661	0.3251	0.067*
C2	0.4961 (3)	0.6688 (4)	0.4681 (4)	0.0707 (12)
H2	0.5323	0.6018	0.4549	0.085*
C3	0.5309 (3)	0.7265 (4)	0.5624 (4)	0.0699 (13)
H3	0.5896	0.6954	0.6175	0.084*
C4	0.4804 (3)	0.8329 (4)	0.5791 (3)	0.0558 (10)
C5	0.5166 (3)	0.9007 (5)	0.6756 (3)	0.0753 (13)
H5	0.5740	0.8707	0.7330	0.090*
C6	0.4696 (4)	1.0072 (6)	0.6857 (3)	0.0832 (15)
H6	0.4936	1.0506	0.7507	0.100*

C7	0.3841 (3)	1.0554 (4)	0.6000 (3)	0.0627 (11)
H7	0.3535	1.1319	0.6086	0.075*
C8	0.3448 (3)	0.9931 (3)	0.5044 (3)	0.0453 (8)
C9	0.3920 (2)	0.8769 (3)	0.4943 (3)	0.0418 (8)
C10	0.2622 (3)	1.0574 (3)	0.4120 (3)	0.0457 (8)
H10A	0.2442	1.1388	0.4361	0.055*
H10B	0.2879	1.0807	0.3609	0.055*
C11	0.1257 (3)	0.9385 (3)	0.4299 (3)	0.0528 (9)
H11A	0.0529	0.9372	0.3907	0.063*
H11B	0.1429	1.0026	0.4866	0.063*
C12	0.1611 (3)	0.8060 (4)	0.4765 (3)	0.0543 (9)
H12A	0.2299	0.8110	0.5309	0.065*
H12B	0.1187	0.7724	0.5085	0.065*
C13	0.0982 (3)	1.0567 (3)	0.2689 (3)	0.0522 (9)
H13A	0.1325	1.0963	0.2302	0.063*
H13B	0.0715	1.1272	0.2962	0.063*
C14	0.0131 (3)	0.9727 (4)	0.1949 (3)	0.0636 (11)
H14A	−0.0369	0.9617	0.2224	0.076*
H14B	−0.0191	1.0145	0.1259	0.076*
C15	0.2565 (2)	0.9625 (3)	0.1223 (3)	0.0412 (8)
C16	0.1984 (2)	0.5241 (4)	0.2227 (2)	0.0410 (8)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0407 (2)	0.0316 (2)	0.0351 (2)	0.00054 (19)	0.01630 (17)	0.00133 (19)
O1	0.0596 (15)	0.0355 (12)	0.0487 (13)	−0.0080 (11)	0.0285 (12)	−0.0020 (11)
O2	0.0500 (15)	0.0436 (15)	0.0632 (16)	0.0030 (12)	0.0033 (13)	−0.0080 (13)
O3	0.129 (3)	0.119 (3)	0.089 (3)	0.042 (3)	−0.034 (2)	−0.044 (2)
N1	0.0388 (15)	0.0357 (15)	0.0473 (15)	0.0007 (13)	0.0204 (13)	0.0018 (13)
N2	0.0401 (15)	0.0323 (14)	0.0452 (15)	0.0015 (12)	0.0185 (13)	0.0009 (12)
N3	0.066 (2)	0.0496 (18)	0.0418 (16)	−0.0036 (15)	0.0270 (16)	0.0034 (15)
N4	0.068 (2)	0.0354 (16)	0.0477 (17)	0.0002 (15)	0.0261 (16)	−0.0028 (14)
S1	0.0704 (7)	0.0682 (7)	0.0519 (6)	−0.0214 (5)	0.0346 (5)	0.0013 (5)
S2	0.0805 (8)	0.0359 (5)	0.0753 (7)	−0.0001 (5)	0.0221 (6)	−0.0013 (5)
C1	0.043 (2)	0.051 (2)	0.077 (3)	0.0035 (18)	0.028 (2)	−0.002 (2)
C2	0.041 (2)	0.053 (3)	0.116 (4)	0.0086 (19)	0.031 (3)	0.011 (3)
C3	0.034 (2)	0.066 (3)	0.093 (3)	0.000 (2)	0.012 (2)	0.028 (3)
C4	0.037 (2)	0.064 (3)	0.059 (2)	−0.0102 (19)	0.0132 (18)	0.011 (2)
C5	0.052 (3)	0.100 (4)	0.052 (3)	−0.017 (3)	0.001 (2)	0.013 (3)
C6	0.074 (3)	0.116 (4)	0.047 (3)	−0.037 (3)	0.015 (2)	−0.020 (3)
C7	0.064 (3)	0.065 (3)	0.059 (2)	−0.015 (2)	0.026 (2)	−0.018 (2)
C8	0.044 (2)	0.047 (2)	0.046 (2)	−0.0124 (17)	0.0198 (16)	−0.0067 (17)
C9	0.0385 (19)	0.0432 (19)	0.0433 (19)	−0.0064 (16)	0.0173 (16)	0.0044 (16)
C10	0.051 (2)	0.0290 (17)	0.057 (2)	−0.0036 (16)	0.0235 (18)	−0.0068 (16)
C11	0.059 (2)	0.050 (2)	0.061 (2)	0.0010 (18)	0.036 (2)	−0.0048 (19)
C12	0.072 (3)	0.051 (2)	0.054 (2)	0.000 (2)	0.039 (2)	0.0027 (19)
C13	0.053 (2)	0.0356 (19)	0.063 (2)	0.0103 (17)	0.0205 (19)	0.0040 (18)

C14	0.052 (2)	0.058 (3)	0.067 (3)	0.013 (2)	0.012 (2)	0.003 (2)
C15	0.0418 (19)	0.0401 (19)	0.0387 (18)	−0.0025 (15)	0.0143 (15)	−0.0036 (15)
C16	0.043 (2)	0.048 (2)	0.0321 (17)	−0.0027 (16)	0.0161 (15)	−0.0015 (16)

Geometric parameters (Å, º)

Ni1—N3	2.011 (3)	C3—C4	1.385 (6)
Ni1—N4	2.018 (3)	C3—H3	0.9300
Ni1—N2	2.061 (3)	C4—C5	1.398 (6)
Ni1—O2	2.067 (2)	C4—C9	1.403 (5)
Ni1—O1	2.089 (2)	C5—C6	1.322 (7)
Ni1—N1	2.093 (3)	C5—H5	0.9300
O1—C12	1.409 (4)	C6—C7	1.399 (6)
O1—H1A	0.9300	C6—H6	0.9300
O2—C14	1.408 (4)	C7—C8	1.362 (5)
O2—H2A	0.9300	C7—H7	0.9300
O3—H31	0.8520	C8—C9	1.406 (5)
O3—H32	0.8520	C8—C10	1.488 (5)
N1—C1	1.305 (4)	C10—H10A	0.9700
N1—C9	1.368 (4)	C10—H10B	0.9700
N2—C10	1.457 (4)	C11—C12	1.486 (5)
N2—C13	1.472 (4)	C11—H11A	0.9700
N2—C11	1.481 (4)	C11—H11B	0.9700
N3—C15	1.139 (4)	C12—H12A	0.9700
N4—C16	1.129 (4)	C12—H12B	0.9700
S1—C15	1.625 (3)	C13—C14	1.499 (5)
S2—C16	1.617 (4)	C13—H13A	0.9700
C1—C2	1.385 (6)	C13—H13B	0.9700
C1—H1	0.9300	C14—H14A	0.9700
C2—C3	1.326 (6)	C14—H14B	0.9700
C2—H2	0.9300		
N3—Ni1—N4	96.64 (12)	C6—C5—H5	119.8
N3—Ni1—N2	97.00 (11)	C4—C5—H5	119.8
N4—Ni1—N2	163.40 (11)	C5—C6—C7	120.8 (4)
N3—Ni1—O2	89.15 (12)	C5—C6—H6	119.6
N4—Ni1—O2	91.29 (11)	C7—C6—H6	119.6
N2—Ni1—O2	79.51 (10)	C8—C7—C6	121.6 (4)
N3—Ni1—O1	177.48 (10)	C8—C7—H7	119.2
N4—Ni1—O1	85.70 (10)	C6—C7—H7	119.2
N2—Ni1—O1	80.54 (10)	C7—C8—C9	117.9 (4)
O2—Ni1—O1	89.84 (10)	C7—C8—C10	119.4 (3)
N3—Ni1—N1	90.10 (12)	C9—C8—C10	122.3 (3)
N4—Ni1—N1	96.35 (11)	N1—C9—C4	120.3 (3)
N2—Ni1—N1	93.04 (10)	N1—C9—C8	119.7 (3)
O2—Ni1—N1	172.36 (10)	C4—C9—C8	120.0 (3)
O1—Ni1—N1	90.59 (10)	N2—C10—C8	115.8 (3)
C12—O1—Ni1	112.29 (19)	N2—C10—H10A	108.3

C12—O1—H1A	123.9	C8—C10—H10A	108.3
Ni1—O1—H1A	123.9	N2—C10—H10B	108.3
C14—O2—Ni1	115.7 (2)	C8—C10—H10B	108.3
C14—O2—H2A	122.1	H10A—C10—H10B	107.4
Ni1—O2—H2A	122.1	N2—C11—C12	112.0 (3)
H31—O3—H32	110.9	N2—C11—H11A	109.2
C1—N1—C9	118.0 (3)	C12—C11—H11A	109.2
C1—N1—Ni1	115.4 (2)	N2—C11—H11B	109.2
C9—N1—Ni1	125.2 (2)	C12—C11—H11B	109.2
C10—N2—C13	108.6 (3)	H11A—C11—H11B	107.9
C10—N2—C11	112.5 (3)	O1—C12—C11	107.5 (3)
C13—N2—C11	110.3 (3)	O1—C12—H12A	110.2
C10—N2—Ni1	110.02 (19)	C11—C12—H12A	110.2
C13—N2—Ni1	104.8 (2)	O1—C12—H12B	110.2
C11—N2—Ni1	110.26 (19)	C11—C12—H12B	110.2
C15—N3—Ni1	171.5 (3)	H12A—C12—H12B	108.5
C16—N4—Ni1	158.8 (3)	N2—C13—C14	111.6 (3)
N1—C1—C2	123.9 (4)	N2—C13—H13A	109.3
N1—C1—H1	118.0	C14—C13—H13A	109.3
C2—C1—H1	118.0	N2—C13—H13B	109.3
C3—C2—C1	118.7 (4)	C14—C13—H13B	109.3
C3—C2—H2	120.7	H13A—C13—H13B	108.0
C1—C2—H2	120.7	O2—C14—C13	108.4 (3)
C2—C3—C4	120.3 (4)	O2—C14—H14A	110.0
C2—C3—H3	119.8	C13—C14—H14A	110.0
C4—C3—H3	119.8	O2—C14—H14B	110.0
C3—C4—C5	122.5 (4)	C13—C14—H14B	110.0
C3—C4—C9	118.3 (4)	H14A—C14—H14B	108.4
C5—C4—C9	119.2 (4)	N3—C15—S1	178.9 (3)
C6—C5—C4	120.3 (4)	N4—C16—S2	178.2 (4)

N3—Ni1—O1—C12	−32 (3)	O1—Ni1—N4—C16	−22.4 (8)
N4—Ni1—O1—C12	169.9 (2)	N1—Ni1—N4—C16	67.7 (8)
N2—Ni1—O1—C12	−19.4 (2)	C9—N1—C1—C2	3.0 (5)
O2—Ni1—O1—C12	−98.8 (2)	Ni1—N1—C1—C2	−163.8 (3)
N1—Ni1—O1—C12	73.5 (2)	N1—C1—C2—C3	3.4 (6)
N3—Ni1—O2—C14	−82.8 (3)	C1—C2—C3—C4	−4.9 (6)
N4—Ni1—O2—C14	−179.4 (3)	C2—C3—C4—C5	−177.1 (4)
N2—Ni1—O2—C14	14.5 (3)	C2—C3—C4—C9	0.2 (6)
O1—Ni1—O2—C14	94.9 (3)	C3—C4—C5—C6	175.3 (4)
N1—Ni1—O2—C14	1.6 (9)	C9—C4—C5—C6	−1.9 (6)
N3—Ni1—N1—C1	−84.8 (3)	C4—C5—C6—C7	−1.1 (7)
N4—Ni1—N1—C1	11.9 (3)	C5—C6—C7—C8	1.7 (7)
N2—Ni1—N1—C1	178.2 (3)	C6—C7—C8—C9	0.8 (6)
O2—Ni1—N1—C1	−169.2 (7)	C6—C7—C8—C10	−172.1 (4)
O1—Ni1—N1—C1	97.6 (3)	C1—N1—C9—C4	−7.9 (5)
N3—Ni1—N1—C9	109.5 (3)	Ni1—N1—C9—C4	157.5 (2)
N4—Ni1—N1—C9	−153.9 (2)	C1—N1—C9—C8	171.4 (3)

N2—Ni1—N1—C9	12.4 (3)	Ni1—N1—C9—C8	−23.2 (4)
O2—Ni1—N1—C9	25.1 (9)	C3—C4—C9—N1	6.4 (5)
O1—Ni1—N1—C9	−68.1 (2)	C5—C4—C9—N1	−176.3 (3)
N3—Ni1—N2—C10	−62.0 (2)	C3—C4—C9—C8	−172.9 (3)
N4—Ni1—N2—C10	153.0 (4)	C5—C4—C9—C8	4.4 (5)
O2—Ni1—N2—C10	−149.8 (2)	C7—C8—C9—N1	176.9 (3)
O1—Ni1—N2—C10	118.6 (2)	C10—C8—C9—N1	−10.4 (5)
N1—Ni1—N2—C10	28.5 (2)	C7—C8—C9—C4	−3.8 (5)
N3—Ni1—N2—C13	54.6 (2)	C10—C8—C9—C4	168.9 (3)
N4—Ni1—N2—C13	−90.4 (4)	C13—N2—C10—C8	−179.4 (3)
O2—Ni1—N2—C13	−33.2 (2)	C11—N2—C10—C8	58.1 (4)
O1—Ni1—N2—C13	−124.8 (2)	Ni1—N2—C10—C8	−65.3 (3)
N1—Ni1—N2—C13	145.1 (2)	C7—C8—C10—N2	−125.4 (3)
N3—Ni1—N2—C11	173.3 (2)	C9—C8—C10—N2	62.1 (4)
N4—Ni1—N2—C11	28.3 (5)	C10—N2—C11—C12	−93.4 (3)
O2—Ni1—N2—C11	85.5 (2)	C13—N2—C11—C12	145.1 (3)
O1—Ni1—N2—C11	−6.1 (2)	Ni1—N2—C11—C12	29.8 (4)
N1—Ni1—N2—C11	−96.2 (2)	Ni1—O1—C12—C11	39.9 (3)
N4—Ni1—N3—C15	53 (2)	N2—C11—C12—O1	−45.8 (4)
N2—Ni1—N3—C15	−117 (2)	C10—N2—C13—C14	166.7 (3)
O2—Ni1—N3—C15	−38 (2)	C11—N2—C13—C14	−69.5 (4)
O1—Ni1—N3—C15	−104 (3)	Ni1—N2—C13—C14	49.1 (3)
N1—Ni1—N3—C15	150 (2)	Ni1—O2—C14—C13	8.5 (4)
N3—Ni1—N4—C16	158.5 (8)	N2—C13—C14—O2	−38.5 (4)
N2—Ni1—N4—C16	−56.4 (10)	Ni1—N3—C15—S1	20 (20)
O2—Ni1—N4—C16	−112.2 (8)	Ni1—N4—C16—S2	−31 (11)