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[*N*,*N*′-Bis(6-methoxysalicylidene)-1,3-diaminopropane]nickel(II)

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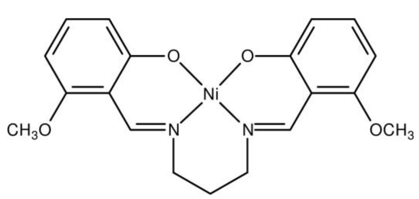
Key indicators: single-crystal X-ray study; T = 150 K; mean σ(C–C) = 0.004 Å; R factor = 0.037; wR factor = 0.101; data-to-parameter ratio = 17.2.

The title compound (systematic name: {3,3′-dimethoxy-2,2′-[propane-1,3-diylbis(nitrilomethylidyne)]diphenolato}nickel(II)), [Ni($C_{19}H_{20}N_2O_4$)], is isostructural with its Cu^{II} analogue. The Ni^{II} ion is coordinated within a distorted square-planar N_2O_2 environment. The dihedral angle between the two $NiNC_3O$ chelate rings is 22.38 (12)°.

Related literature

For the isostructural Cu^{II} compound, see: Habibi *et al.* (2007). For related literature, see: Gosden *et al.* (1981); Healy & Pletcher (1978); Shkol'nikova *et al.* (1970); Akhtar (1981).



Experimental

Crystal data

[Ni($C_{19}H_{20}N_2O_4$)]
M_r = 399.08
Orthorhombic, $Pca2_1$
a = 13.677 (2) Å
b = 12.7319 (18) Å
c = 9.8561 (14) Å
V = 1716.3 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.16 mm^{-1}
T = 150 (2) K
0.34 × 0.30 × 0.30 mm

Data collection

Bruker SMART 1K CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2007) T_{min} = 0.690, T_{max} = 0.725
13065 measured reflections
4083 independent reflections
3384 reflections with $I > 2\sigma(I)$
R_{int} = 0.040

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.101
S = 1.06
4083 reflections
238 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.68 e Å^{-3}
$\Delta\rho_{min}$ = −0.53 e Å^{-3}
Absolute structure: Flack (1983), with 1870 Friedel pairs
Flack parameter: 0.00 (2)

Table 1
Selected geometric parameters (Å, °).

Ni—O2	1.855 (2)	Ni—N1	1.882 (2)
Ni—O3	1.852 (2)	Ni—N2	1.895 (3)
O2—Ni—O3	81.06 (10)	O3—Ni—N1	164.26 (10)
O2—Ni—N1	92.44 (11)	O3—Ni—N2	92.77 (10)
O2—Ni—N2	166.39 (10)	N1—Ni—N2	96.42 (11)

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2005); program(s) used to refine structure: *SHELXTL*; molecular graphics: *DIAMOND* (Brandenburg, 2007); software used to prepare material for publication: *SHELXTL* and local programs.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BI2225).

References

Akhtar, F. (1981). *Acta Cryst.* B**37**, 84–88.
Brandenburg, K. (2007). *DIAMOND*. Version 3.1e. Crystal Impact GbR, Bonn, Germany.
Bruker (2001). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Gosden, C., Kerr, J. B., Pletcher, D. & Rosas, R. (1981). *J. Electroanal. Chem. Interfacial Electrochem.* **117**, 101–107.
Habibi, M. H., Mokhtari, R., Harrington, R. W. & Clegg, W. (2007). *Acta Cryst.* E**63**, m1998.
Healy, K. P. & Pletcher, D. (1978). *J. Organomet. Chem.* **161**, 109–120.
Sheldrick, G. M. (2005). *SHELXTL*. Version 6. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (2007). *SADABS*. University of Göttingen, Germany.
Shkol'nikova, L. M., Yumal, E. M., Shugam, E. A. & Voblikova, V. A. (1970). *Zh. Strukt. Khim.* **11**, 886–890.

supplementary materials

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[*N*,*N*'-Bis(6-methoxysalicylidene)-1,3-diaminopropane]nickel(II)

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Comment

Nickel(II) complexes with N_2O_2 Schiff-base ligands derived from salicylaldehyde have long been used as homogenous catalysts (Gosden *et al.*, 1981; Healy & Pletcher, 1978). Recently we reported the structure of a copper(II) complex with the *N*,*N*'-bis(6-methoxysalicylidene)-1,3-diaminopropane ligand (Habibi *et al.*, 2007). The title compound is isostructural with its Cu^{II} analogue.

In the title compound (Figure 1), the Ni—O and Ni—N distances are larger than the comparable mean distances of 1.829 and 1.859 Å, respectively, in *N*,*N*'-ethylenebis(salicylideneiminato)nickel(II) (Shkol'nikova *et al.*, 1970) and 1.849 (2) and 1.840 (2) Å, respectively, in *N*,*N*'-ethylenebis[(2-hydroxy-1-naphthyl)methaniminato]nickel(II) (Akhtar, 1981).

Experimental

A mixture of 6-methoxysalicylaldehyde (2.0 mmol, 304 mg) and 1,3-diaminopropane (1.0 mmol, 74 mg) was dissolved in methanol (10 ml) with stirring for 10 min at room temperature, to give a clear yellow solution. A methanol solution (10 ml) of $Ni(OAc)_2{\cdot}4H_2O$ (1.0 mmol, 249 mg) was then added. The mixture was refluxed for a further 50 min and then filtered. After keeping the filtrate in air for 5 d, red block-shaped crystals were formed at the bottom of the vessel on slow evaporation of the solvent, in about 70% yield.

Refinement

All H atoms were placed in geometrically idealized positions and allowed to ride on their parent atoms, with C—H distances in the range 0.93–0.97 Å and with U_{iso}(H) = 1.2 or 1.5 times U_{eq}(C).

Figures

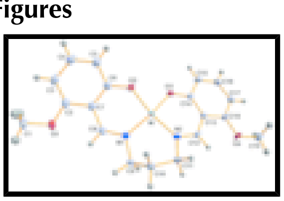


Fig. 1. The molecular structure with atom labels and 50% probability displacement ellipsoids for non-H atoms.

{3,3'-dimethoxy-2,2'-[propane-1,3- diylbis(nitrilomethylidyne)]diphenolato}nickel(II)

Crystal data

$[Ni(C_{19}H_{20}N_2O_4)]$	F_{000} = 832
M_r = 399.08	D_x = 1.544 Mg m^{-3}

Orthorhombic, $Pca2_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2c -2ac	Cell parameters from 7044 reflections
a = 13.677 (2) Å	θ = 2.2–28.3°
b = 12.7319 (18) Å	μ = 1.16 mm^{-1}
c = 9.8561 (14) Å	T = 150 (2) K
V = 1716.3 (4) $Å^3$	Block, red
Z = 4	0.34 × 0.30 × 0.30 mm

Data collection

Bruker SMART 1K CCD diffractometer	4083 independent reflections
Radiation source: sealed tube	3384 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.040
T = 150(2) K	θ_{max} = 28.4°
thin–slice ω scans	θ_{min} = 2.2°
Absorption correction: multi-scan (SADABS; Sheldrick, 2007)	$h = -17 \rightarrow 17$
T_{min} = 0.690, T_{max} = 0.725	$k = -16 \rightarrow 17$
13065 measured reflections	$l = -13 \rightarrow 12$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.037	$w = 1/[\sigma^2(F_o^2) + (0.0578P)^2 + 0.6306P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.101	$(\Delta/\sigma)_{max}$ = 0.001
S = 1.06	$\Delta\rho_{max}$ = 0.68 e $Å^{-3}$
4083 reflections	$\Delta\rho_{min}$ = −0.53 e $Å^{-3}$
238 parameters	Extinction correction: SHELXTL (Sheldrick, 2005), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
1 restraint	Extinction coefficient: 0.0025 (7)
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983), with 1870 Friedel pairs
Secondary atom site location: difference Fourier map	Flack parameter: 0.00 (2)

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ni	0.82396 (2)	0.25163 (3)	0.10277 (8)	0.01355 (10)
O1	0.8627 (2)	−0.12162 (17)	−0.1557 (3)	0.0282 (6)
O2	0.93677 (17)	0.21919 (17)	0.0070 (2)	0.0190 (5)
O3	0.90841 (15)	0.34683 (16)	0.1831 (2)	0.0176 (5)
O4	0.69303 (16)	0.5363 (2)	0.4694 (3)	0.0254 (5)
N1	0.76069 (19)	0.12822 (18)	0.0450 (3)	0.0163 (5)
N2	0.71214 (18)	0.31603 (19)	0.1800 (3)	0.0147 (5)
C1	0.8822 (3)	−0.2066 (3)	−0.2485 (4)	0.0347 (9)
H1A	0.8303	−0.2593	−0.2411	0.052*
H1B	0.9452	−0.2389	−0.2259	0.052*
H1C	0.8844	−0.1794	−0.3414	0.052*
C2	0.9282 (3)	−0.0402 (2)	−0.1530 (3)	0.0208 (7)
C3	1.0159 (3)	−0.0395 (3)	−0.2224 (3)	0.0244 (7)
H3A	1.0353	−0.0979	−0.2761	0.029*
C4	1.0754 (3)	0.0490 (3)	−0.2116 (4)	0.0254 (7)
H4A	1.1356	0.0501	−0.2597	0.031*
C5	1.0507 (2)	0.1349 (3)	−0.1343 (3)	0.0222 (7)
H5A	1.0942	0.1928	−0.1278	0.027*
C6	0.9602 (2)	0.1368 (2)	−0.0644 (3)	0.0178 (6)
C7	0.8979 (2)	0.0481 (3)	−0.0745 (3)	0.0179 (6)
C8	0.8006 (2)	0.0511 (2)	−0.0200 (3)	0.0185 (6)
H8A	0.7615	−0.0098	−0.0331	0.022*
C9	0.6564 (2)	0.1131 (2)	0.0811 (3)	0.0195 (7)
H9A	0.6497	0.1051	0.1806	0.023*
H9B	0.6310	0.0487	0.0373	0.023*
C10	0.5990 (2)	0.2076 (3)	0.0335 (4)	0.0199 (7)
H10A	0.5292	0.1885	0.0243	0.024*
H10B	0.6232	0.2299	−0.0567	0.024*
C11	0.6092 (2)	0.2977 (3)	0.1331 (3)	0.0174 (7)
H11A	0.5845	0.3627	0.0899	0.021*
H11B	0.5676	0.2832	0.2132	0.021*
C12	0.7151 (2)	0.3884 (2)	0.2731 (3)	0.0154 (6)
H12A	0.6537	0.4113	0.3069	0.018*
C13	0.7990 (2)	0.4375 (2)	0.3308 (3)	0.0153 (6)
C14	0.8929 (2)	0.4154 (2)	0.2787 (3)	0.0154 (6)
C15	0.9741 (2)	0.4713 (2)	0.3329 (3)	0.0200 (7)
H15A	1.0382	0.4565	0.3009	0.024*
C16	0.9607 (2)	0.5459 (2)	0.4306 (4)	0.0209 (7)
H16A	1.0160	0.5819	0.4657	0.025*
C17	0.8673 (2)	0.5711 (2)	0.4810 (3)	0.0194 (6)
H17A	0.8594	0.6237	0.5485	0.023*
C18	0.7876 (2)	0.5181 (2)	0.4304 (3)	0.0173 (6)
C19	0.6746 (3)	0.6213 (3)	0.5603 (4)	0.0255 (8)
H19A	0.6041	0.6268	0.5769	0.038*
H19B	0.6984	0.6868	0.5201	0.038*

H19C	0.7085	0.6085	0.6463	0.038*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni	0.01077 (16)	0.01476 (16)	0.01513 (17)	−0.00103 (14)	0.0011 (2)	−0.00126 (15)
O1	0.0344 (14)	0.0200 (11)	0.0301 (14)	0.0000 (10)	0.0024 (11)	−0.0091 (10)
O2	0.0152 (11)	0.0200 (10)	0.0218 (12)	0.0006 (9)	0.0038 (9)	−0.0030 (9)
O3	0.0112 (10)	0.0186 (11)	0.0229 (12)	−0.0027 (8)	0.0008 (9)	−0.0038 (9)
O4	0.0096 (10)	0.0312 (12)	0.0354 (15)	0.0022 (9)	0.0021 (10)	−0.0172 (11)
N1	0.0155 (13)	0.0165 (12)	0.0168 (13)	−0.0028 (10)	0.0004 (10)	−0.0001 (10)
N2	0.0085 (12)	0.0175 (12)	0.0182 (14)	−0.0014 (10)	−0.0017 (10)	−0.0001 (10)
C1	0.043 (2)	0.0250 (18)	0.036 (2)	0.0011 (17)	0.0013 (19)	−0.0158 (16)
C2	0.0258 (18)	0.0209 (15)	0.0156 (16)	0.0046 (13)	−0.0049 (13)	−0.0009 (13)
C3	0.0289 (19)	0.0268 (16)	0.0176 (16)	0.0100 (15)	−0.0004 (14)	−0.0048 (13)
C4	0.0206 (17)	0.0349 (18)	0.0209 (17)	0.0083 (14)	0.0014 (14)	−0.0011 (15)
C5	0.0205 (16)	0.0258 (16)	0.0203 (17)	0.0023 (13)	0.0010 (13)	−0.0003 (13)
C6	0.0177 (15)	0.0201 (14)	0.0155 (15)	0.0026 (12)	−0.0014 (12)	0.0002 (12)
C7	0.0185 (16)	0.0205 (16)	0.0146 (15)	0.0045 (12)	−0.0015 (12)	−0.0004 (12)
C8	0.0210 (16)	0.0168 (14)	0.0177 (16)	0.0005 (12)	−0.0017 (12)	0.0017 (12)
C9	0.0159 (14)	0.0216 (14)	0.0212 (19)	−0.0053 (11)	0.0027 (13)	−0.0013 (12)
C10	0.0150 (15)	0.0225 (15)	0.0223 (17)	−0.0036 (13)	−0.0014 (13)	−0.0048 (13)
C11	0.0059 (13)	0.0240 (15)	0.0222 (19)	−0.0016 (11)	−0.0026 (11)	−0.0030 (12)
C12	0.0076 (13)	0.0209 (14)	0.0176 (15)	0.0027 (11)	0.0009 (11)	−0.0012 (12)
C13	0.0098 (14)	0.0164 (14)	0.0196 (16)	−0.0005 (11)	−0.0004 (12)	−0.0007 (12)
C14	0.0125 (15)	0.0167 (14)	0.0170 (16)	0.0010 (12)	0.0022 (12)	0.0018 (12)
C15	0.0101 (15)	0.0234 (15)	0.0266 (18)	−0.0019 (12)	0.0022 (13)	−0.0025 (13)
C16	0.0146 (15)	0.0210 (15)	0.0270 (18)	−0.0041 (12)	−0.0040 (14)	−0.0034 (14)
C17	0.0163 (15)	0.0201 (14)	0.0218 (16)	−0.0012 (12)	−0.0002 (13)	−0.0060 (12)
C18	0.0100 (14)	0.0204 (15)	0.0214 (16)	0.0028 (11)	0.0004 (12)	−0.0034 (12)
C19	0.0202 (16)	0.0280 (17)	0.028 (2)	0.0039 (13)	0.0039 (13)	−0.0105 (13)

Geometric parameters (Å, °)

Ni—O2	1.855 (2)	C6—C7	1.418 (4)
Ni—O3	1.852 (2)	C7—C8	1.436 (5)
Ni—N1	1.882 (2)	C8—H8A	0.950
Ni—N2	1.895 (3)	C9—H9A	0.990
O1—C1	1.441 (4)	C9—H9B	0.990
O1—C2	1.370 (4)	C9—C10	1.512 (5)
O2—C6	1.303 (4)	C10—H10A	0.990
O3—C14	1.302 (4)	C10—H10B	0.990
O4—C18	1.369 (4)	C10—C11	1.516 (4)
O4—C19	1.427 (4)	C11—H11A	0.990
N1—C8	1.294 (4)	C11—H11B	0.990
N1—C9	1.482 (4)	C12—H12A	0.950
N2—C11	1.500 (4)	C12—C13	1.425 (4)
N2—C12	1.301 (4)	C13—C14	1.411 (4)
C1—H1A	0.980	C13—C18	1.428 (4)

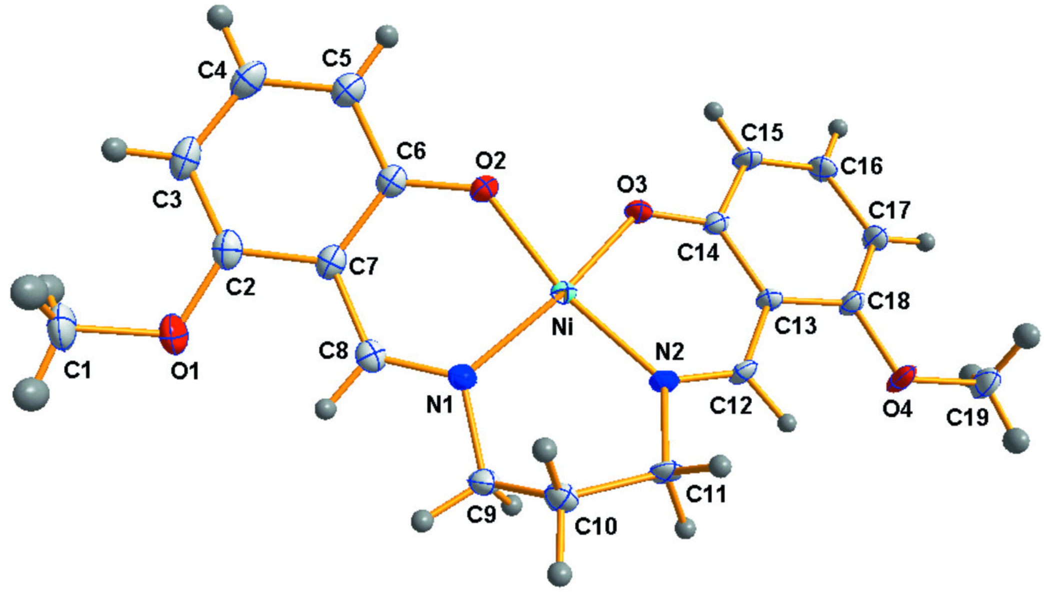
C1—H1B	0.980	C14—C15	1.424 (4)
C1—H1C	0.980	C15—H15A	0.950
C2—C3	1.381 (5)	C15—C16	1.365 (4)
C2—C7	1.427 (4)	C16—H16A	0.950
C3—H3A	0.950	C16—C17	1.408 (4)
C3—C4	1.394 (5)	C17—H17A	0.950
C4—H4A	0.950	C17—C18	1.376 (4)
C4—C5	1.375 (5)	C19—H19A	0.980
C5—H5A	0.950	C19—H19B	0.980
C5—C6	1.416 (4)	C19—H19C	0.980

O2—Ni—O3	81.06 (10)	N1—C9—H9B	109.9
O2—Ni—N1	92.44 (11)	N1—C9—C10	108.8 (2)
O2—Ni—N2	166.39 (10)	H9A—C9—H9B	108.3
O3—Ni—N1	164.26 (10)	H9A—C9—C10	109.9
O3—Ni—N2	92.77 (10)	H9B—C9—C10	109.9
N1—Ni—N2	96.42 (11)	C9—C10—H10A	109.5
C1—O1—C2	117.4 (3)	C9—C10—H10B	109.5
Ni—O2—C6	131.2 (2)	C9—C10—C11	110.7 (3)
Ni—O3—C14	130.3 (2)	H10A—C10—H10B	108.1
C18—O4—C19	118.2 (2)	H10A—C10—C11	109.5
Ni—N1—C8	126.2 (2)	H10B—C10—C11	109.5
Ni—N1—C9	118.56 (19)	N2—C11—C10	113.8 (3)
C8—N1—C9	115.2 (3)	N2—C11—H11A	108.8
Ni—N2—C11	124.5 (2)	N2—C11—H11B	108.8
Ni—N2—C12	124.4 (2)	C10—C11—H11A	108.8
C11—N2—C12	110.9 (3)	C10—C11—H11B	108.8
O1—C1—H1A	109.5	H11A—C11—H11B	107.7
O1—C1—H1B	109.5	N2—C12—H12A	115.9
O1—C1—H1C	109.5	N2—C12—C13	128.1 (3)
H1A—C1—H1B	109.5	H12A—C12—C13	115.9
H1A—C1—H1C	109.5	C12—C13—C14	120.0 (3)
H1B—C1—H1C	109.5	C12—C13—C18	120.1 (3)
O1—C2—C3	124.2 (3)	C14—C13—C18	119.6 (3)
O1—C2—C7	114.7 (3)	O3—C14—C13	123.1 (3)
C3—C2—C7	121.1 (3)	O3—C14—C15	118.7 (3)
C2—C3—H3A	120.9	C13—C14—C15	118.3 (3)
C2—C3—C4	118.3 (3)	C14—C15—H15A	119.7
H3A—C3—C4	120.9	C14—C15—C16	120.5 (3)
C3—C4—H4A	118.6	H15A—C15—C16	119.7
C3—C4—C5	122.8 (3)	C15—C16—H16A	119.0
H4A—C4—C5	118.6	C15—C16—C17	122.0 (3)
C4—C5—H5A	120.1	H16A—C16—C17	119.0
C4—C5—C6	119.9 (3)	C16—C17—H17A	120.7
H5A—C5—C6	120.1	C16—C17—C18	118.6 (3)
O2—C6—C5	119.4 (3)	H17A—C17—C18	120.7
O2—C6—C7	122.1 (3)	O4—C18—C13	114.7 (3)
C5—C6—C7	118.5 (3)	O4—C18—C17	124.3 (3)
C2—C7—C6	119.4 (3)	C13—C18—C17	121.0 (3)
C2—C7—C8	119.5 (3)	O4—C19—H19A	109.5

C6—C7—C8	120.7 (3)	O4—C19—H19B	109.5
N1—C8—C7	126.6 (3)	O4—C19—H19C	109.5
N1—C8—H8A	116.7	H19A—C19—H19B	109.5
C7—C8—H8A	116.7	H19A—C19—H19C	109.5
N1—C9—H9A	109.9	H19B—C19—H19C	109.5

O3—Ni—O2—C6	161.9 (3)	C3—C2—C7—C6	−1.8 (5)
N1—Ni—O2—C6	−3.7 (3)	C3—C2—C7—C8	171.0 (3)
N2—Ni—O2—C6	−134.3 (5)	Ni—N1—C8—C7	−7.3 (5)
O2—Ni—O3—C14	−179.7 (3)	C9—N1—C8—C7	175.7 (3)
N1—Ni—O3—C14	−113.2 (4)	C2—C7—C8—N1	−175.1 (3)
N2—Ni—O3—C14	12.5 (3)	C6—C7—C8—N1	−2.4 (5)
O2—Ni—N1—C8	8.9 (3)	Ni—N1—C9—C10	54.3 (3)
O2—Ni—N1—C9	−174.2 (2)	C8—N1—C9—C10	−128.4 (3)
O3—Ni—N1—C8	−56.2 (6)	N1—C9—C10—C11	−80.6 (3)
O3—Ni—N1—C9	120.8 (4)	Ni—N2—C11—C10	10.4 (4)
N2—Ni—N1—C8	178.5 (3)	C12—N2—C11—C10	−174.9 (3)
N2—Ni—N1—C9	−4.5 (2)	C9—C10—C11—N2	45.3 (4)
O2—Ni—N2—C11	101.5 (5)	Ni—N2—C12—C13	3.4 (5)
O2—Ni—N2—C12	−72.5 (6)	C11—N2—C12—C13	−171.3 (3)
O3—Ni—N2—C11	164.0 (2)	N2—C12—C13—C14	5.6 (5)
O3—Ni—N2—C12	−10.0 (3)	N2—C12—C13—C18	178.4 (3)
N1—Ni—N2—C11	−28.8 (2)	Ni—O3—C14—C13	−7.5 (4)
N1—Ni—N2—C12	157.2 (3)	Ni—O3—C14—C15	172.9 (2)
C1—O1—C2—C3	−7.0 (5)	C12—C13—C14—O3	−3.7 (4)
C1—O1—C2—C7	171.3 (3)	C12—C13—C14—C15	175.9 (3)
O1—C2—C3—C4	179.5 (3)	C18—C13—C14—O3	−176.5 (3)
C7—C2—C3—C4	1.3 (5)	C18—C13—C14—C15	3.0 (4)
C2—C3—C4—C5	0.5 (5)	O3—C14—C15—C16	178.2 (3)
C3—C4—C5—C6	−1.7 (5)	C13—C14—C15—C16	−1.4 (5)
Ni—O2—C6—C5	176.4 (2)	C14—C15—C16—C17	−0.4 (5)
Ni—O2—C6—C7	−3.7 (5)	C15—C16—C17—C18	0.5 (5)
C4—C5—C6—O2	−179.0 (3)	C19—O4—C18—C13	−175.0 (3)
C4—C5—C6—C7	1.1 (5)	C19—O4—C18—C17	5.2 (5)
O2—C6—C7—C2	−179.3 (3)	C16—C17—C18—O4	−179.0 (3)
O2—C6—C7—C8	8.0 (5)	C16—C17—C18—C13	1.2 (5)
C5—C6—C7—C2	0.6 (5)	C12—C13—C18—O4	4.4 (4)
C5—C6—C7—C8	−172.1 (3)	C12—C13—C18—C17	−175.8 (3)
O1—C2—C7—C6	179.8 (3)	C14—C13—C18—O4	177.2 (3)
O1—C2—C7—C8	−7.4 (4)	C14—C13—C18—C17	−3.0 (5)

Fig. 1


C4
C5
C6
O2
O3
C15
C16
C3
C17
C14
C7
C2
C18
C13
Ni
C8
N2
C1
O1
N1
C12
O4
C19
C11
C9
C10