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[μ-1,2-Disalicyloylhydrazine(2–)-$\kappa^3N,O,O':\kappa^3N',O'',O'''$]bis[tripyridinenickel(II)] pyridine disolvate

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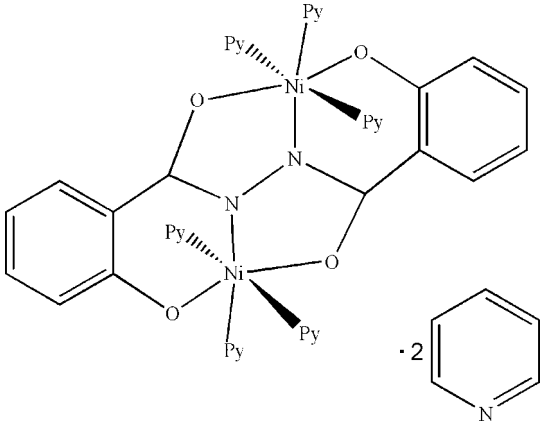
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.010 Å; R factor = 0.053; wR factor = 0.152; data-to-parameter ratio = 14.6.

The title complex, $[Ni_2(C_{14}H_8N_2O_4)(C_5H_5N)_6]\cdot 2C_5H_5N$, is a polymorph of a previously reported compound [Chen & Liu (2005). *Chin. J. Inorg. Chem.* **21**, 15–20]. The 1,2-disalicyloylhydrazine ligand lies on an inversion center and coordinates to two Ni^{II} atoms. Each Ni^{II} atom is octahedrally coordinated by a phenolate O atom, a carbonyl O atom and a hydrazine N atom of the ligand and three pyridine N atoms.

Related literature

For related literature, see: Chen & Liu (2005); Dou *et al.* (2006); Kwak *et al.* (2000).



Experimental

Crystal data

$[Ni_2(C_{14}H_8N_2O_4)(C_5H_5N)_6]\cdot 2C_5H_5N$
M_r = 1018.44
Tetragonal, $I4_1/a$
a = 27.040 (2) Å
c = 14.3178 (18) Å
V = 10468.6 (17) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.77 mm^{-1}
T = 298 (2) K
0.34 × 0.23 × 0.20 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.779, T_{max} = 0.861
21466 measured reflections
4609 independent reflections
2743 reflections with $I > 2\sigma(I)$
R_{int} = 0.064

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.152
S = 1.02
4609 reflections
316 parameters
102 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.43 e Å^{-3}

Table 1
Selected bond lengths (Å).

Ni1—N1	1.955 (3)	Ni1—N4	2.083 (3)
Ni1—O2	1.989 (3)	Ni1—N2	2.196 (4)
Ni1—O1^{i}	2.060 (3)	Ni1—N3	2.201 (3)

Symmetry code: (i) $-x+1, -y, -z$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Siemens, 1996); 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: HY2070).

References

Chen, X. H. & Liu, S. X. (2005). *Chin. J. Inorg. Chem.* **21**, 15–20.
Dou, J. M., Liu, M. L., Li, D. C. & Wang, D. Q. (2006). *Eur. J. Inorg. Chem.* **23**, 4866–4871.
Kwak, B., Rhee, H. & Lah, M. S. (2000). *Polyhedron*, **19**, 1985–1994.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Siemens (1996). *SMART*, *SAINT* and *SHELXTL*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.

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supplementary materials

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[μ-1,2-Disalicyloylhydrazine(2-)-$\kappa^3N,O,O':\kappa^3N',O'',O'''$]bis[tripyridinenickel(II)] pyridine disolvate

Y.-T. Chen, J.-M. Dou, D.-C. Li, D.-Q. Wang and Y.-H. Zhu

Comment

Recently, we have synthesized two metallacrowns using *N*-acyl-3-hydroxy-2-naphthalenecarbohydrazide (Dou *et al.*, 2006). As an extension of our work on the structural characterization of naphthalenecarbohydrazide compounds, the title complex, (I), was synthesized and characterized by X-ray diffraction.

The complex (I) (space group $I4_1/a$) is a polymorph of the compound (space group $P2_1/c$) previously reported by Chen & Liu (2005), with the same formula $[Ni_2(C_{14}H_8N_2O_4)(C_5H_5N)_6]\cdot 2C_5H_5N$. The complex molecule of (I) lies on an inversion center (Fig. 1). The 1,2-disalicyloylhydrazine molecule acts as a hexadentate tetravalent anionic ligand linking two Ni^{II} atoms. The iminophenolate group (O2 and N1) and the iminoacyl group ($O1^i$ and N1; symmetry code: (i) $1-x, -y, -z$) of the ligand are coordinated to the Ni1 atom to form six-membered and five-membered chelating rings, respectively, with a dihedral angle of 1.7 (4)°. Besides the above three atoms coordinated to the Ni1 atom, there are other three pyridine N atoms bonded to the Ni1 atom. So the coordination geometry of the Ni1 atom can be described as an N_4O_2 octahedron. As shown in Table 1, the axial Ni—N distances are longer than the equatorial Ni—N and Ni—O distances, which shows the Ni^{II} atom in a distorted octahedral geometry. This typical Jahn-Teller elongation has been observed in the other complexes (Kwak *et al.*, 2000).

Experimental

A solution of $Ni(CH_3CO_2)_2\cdot H_2O$ (0.100 g, 0.4 mmol) in methanol (10 ml) was added to the mixture of 1,2-disalicyloylhydrazine (0.054 g, 0.2 mmol) and sodium hydroxide (0.032 g, 0.8 mmol) in pyridine (10 ml). A red solution was generated after stirring for 2 h at room temperature. The solution was allowed to stand for 2 weeks, whereupon red needle crystals were obtained (0.070 g, yield 34%).

Refinement

All H atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93Å and $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures

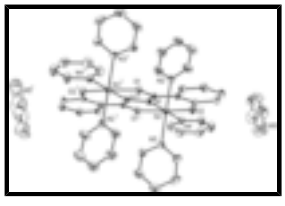

Fig. 1. The molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted for clarity. [Symmetry code: (i) $1-x, -y, -z$.]

[μ-1,2-Disalicyloylhydrazine(2-)- $\kappa^3N,O,O':\kappa^3N',O'',O'''$]bis[tripyridinenickel(II)] pyridine disolvate

Crystal data

$[Ni_2(C_{14}H_8N_2O_4)(C_5H_5N)_6]\cdot 2C_5H_5N$	$Z = 8$
$M_r = 1018.44$	$F_{000} = 4240$
Tetragonal, $I4_1/a$	$D_x = 1.292$ Mg m^{-3}
Hall symbol: -I 4ad	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 27.040$ (2) Å	Cell parameters from 3046 reflections
$b = 27.040$ (2) Å	$\theta = 2.2$–21.5º
$c = 14.3178$ (18) Å	$\mu = 0.77$ mm^{-1}
$\alpha = 90$º	$T = 298$ (2) K
$\beta = 90$º	Block, red
$\gamma = 90$º	0.34 × 0.23 × 0.20 mm
$V = 10468.6$ (17) Å^3	

Data collection

Bruker SMART 1000 CCD area-detector diffractometer	4609 independent reflections
Radiation source: fine-focus sealed tube	2743 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.064$
$T = 298$(2) K	$\theta_{max} = 25.0$º
φ and ω scans	$\theta_{min} = 1.5$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -13\rightarrow32$
$T_{min} = 0.779$, $T_{max} = 0.861$	$k = -32\rightarrow30$
21466 measured reflections	$l = -17\rightarrow17$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.053$	H-atom parameters constrained
$wR(F^2) = 0.152$	$w = 1/[\sigma^2(F_o^2) + (0.07P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.02$	$(\Delta/\sigma)_{max} < 0.001$
4609 reflections	$\Delta\rho_{max} = 0.31$ e Å^{-3}
316 parameters	$\Delta\rho_{min} = -0.43$ e Å^{-3}
102 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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}
Ni1	0.547168 (18)	0.061356 (19)	0.07264 (4)	0.0430 (2)
N1	0.50175 (11)	0.00672 (11)	0.0474 (2)	0.0402 (8)
N2	0.49003 (13)	0.11803 (14)	0.0520 (3)	0.0576 (9)
N3	0.61032 (12)	0.01068 (13)	0.0880 (3)	0.0498 (9)
N4	0.59618 (12)	0.12023 (12)	0.0881 (2)	0.0465 (9)
N5	0.7088 (6)	0.3732 (4)	0.3455 (7)	0.175 (4)
O1	0.44541 (9)	−0.05583 (9)	0.07017 (18)	0.0443 (7)
O2	0.53200 (10)	0.05767 (9)	0.2084 (2)	0.0492 (7)
C1	0.47284 (14)	−0.02083 (14)	0.1014 (3)	0.0384 (9)
C2	0.47115 (14)	−0.00872 (14)	0.2032 (3)	0.0381 (9)
C3	0.49896 (14)	0.02951 (14)	0.2477 (3)	0.0420 (10)
C4	0.48975 (16)	0.03587 (16)	0.3447 (3)	0.0501 (11)
H4	0.5068	0.0607	0.3761	0.060*
C5	0.45740 (16)	0.00756 (17)	0.3939 (3)	0.0533 (11)
H5	0.4528	0.0135	0.4572	0.064*
C6	0.43109 (17)	−0.03022 (17)	0.3502 (3)	0.0565 (12)
H6	0.4094	−0.0502	0.3836	0.068*
C7	0.43824 (14)	−0.03701 (16)	0.2565 (3)	0.0468 (10)
H7	0.4203	−0.0617	0.2266	0.056*
C8	0.4812 (2)	0.1372 (2)	−0.0297 (5)	0.0941 (16)
H8	0.4977	0.1238	−0.0807	0.113*
C9	0.4494 (2)	0.1757 (3)	−0.0462 (5)	0.1082 (17)
H9	0.4458	0.1884	−0.1062	0.130*
C10	0.4239 (2)	0.1948 (2)	0.0245 (5)	0.1061 (17)
H10	0.4014	0.2204	0.0154	0.127*
C11	0.4319 (3)	0.1754 (3)	0.1097 (5)	0.1206 (19)
H11	0.4149	0.1876	0.1613	0.145*
C12	0.4651 (2)	0.1376 (2)	0.1203 (5)	0.1042 (17)
H12	0.4702	0.1251	0.1801	0.125*
C13	0.61964 (19)	−0.02483 (18)	0.0272 (4)	0.0725 (15)
H13	0.5992	−0.0278	−0.0247	0.087*
C14	0.6578 (2)	−0.0574 (2)	0.0369 (5)	0.0954 (19)
H14	0.6626	−0.0819	−0.0077	0.115*
C15	0.6881 (2)	−0.0543 (3)	0.1102 (6)	0.101 (2)
H15	0.7142	−0.0763	0.1176	0.121*
C16	0.6796 (2)	−0.0176 (3)	0.1742 (5)	0.109 (2)
H16	0.6998	−0.0140	0.2264	0.131*
C17	0.6407 (2)	0.0136 (2)	0.1591 (4)	0.0812 (17)

H17	0.6354	0.0388	0.2023	0.097*
C18	0.62427 (18)	0.13505 (18)	0.0177 (4)	0.0663 (14)
H18	0.6214	0.1184	−0.0389	0.080*
C19	0.65742 (19)	0.17364 (19)	0.0229 (4)	0.0746 (15)
H19	0.6760	0.1828	−0.0289	0.090*
C20	0.66227 (19)	0.19768 (18)	0.1045 (4)	0.0708 (15)
H20	0.6844	0.2239	0.1104	0.085*
C21	0.6339 (2)	0.18282 (19)	0.1793 (4)	0.0796 (16)
H21	0.6365	0.1987	0.2368	0.096*
C22	0.60200 (19)	0.14440 (18)	0.1675 (3)	0.0679 (14)
H22	0.5831	0.1345	0.2185	0.081*
C23	0.6591 (6)	0.3744 (4)	0.3440 (8)	0.159 (4)
H23	0.6407	0.3514	0.3775	0.191*
C24	0.6371 (4)	0.4087 (7)	0.2945 (11)	0.185 (6)
H24	0.6029	0.4119	0.2979	0.223*
C25	0.6630 (7)	0.4396 (4)	0.2384 (10)	0.166 (6)
H25	0.6465	0.4614	0.1990	0.199*
C26	0.7111 (7)	0.4387 (4)	0.2398 (8)	0.177 (5)
H26	0.7291	0.4609	0.2036	0.213*
C27	0.7346 (3)	0.4057 (5)	0.2934 (11)	0.156 (4)
H27	0.7690	0.4053	0.2948	0.187*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0436 (3)	0.0457 (3)	0.0396 (3)	−0.0082 (2)	−0.0003 (2)	−0.0042 (2)
N1	0.0420 (18)	0.048 (2)	0.0302 (17)	−0.0042 (16)	0.0010 (15)	−0.0027 (15)
N2	0.056 (2)	0.060 (2)	0.058 (2)	0.0037 (18)	0.0054 (18)	−0.0014 (18)
N3	0.047 (2)	0.049 (2)	0.053 (2)	−0.0053 (17)	−0.0005 (18)	0.0004 (18)
N4	0.049 (2)	0.044 (2)	0.047 (2)	−0.0061 (16)	−0.0016 (17)	−0.0021 (17)
N5	0.249 (13)	0.146 (8)	0.131 (8)	0.039 (9)	−0.048 (8)	−0.037 (6)
O1	0.0460 (16)	0.0466 (16)	0.0402 (17)	−0.0145 (13)	0.0017 (12)	−0.0025 (13)
O2	0.0572 (18)	0.0501 (17)	0.0403 (17)	−0.0147 (15)	0.0006 (13)	−0.0016 (13)
C1	0.037 (2)	0.041 (2)	0.037 (2)	0.0008 (18)	0.0024 (17)	0.0012 (18)
C2	0.039 (2)	0.041 (2)	0.034 (2)	0.0028 (18)	−0.0001 (17)	0.0000 (17)
C3	0.041 (2)	0.044 (2)	0.041 (2)	0.0062 (19)	−0.0039 (19)	−0.0007 (19)
C4	0.056 (3)	0.055 (3)	0.039 (3)	0.002 (2)	0.000 (2)	−0.010 (2)
C5	0.057 (3)	0.069 (3)	0.034 (2)	0.004 (2)	0.006 (2)	0.000 (2)
C6	0.055 (3)	0.064 (3)	0.050 (3)	−0.006 (2)	0.012 (2)	0.003 (2)
C7	0.041 (2)	0.055 (3)	0.045 (3)	−0.005 (2)	0.0049 (19)	−0.001 (2)
C8	0.105 (3)	0.096 (3)	0.081 (3)	0.040 (3)	0.003 (3)	0.006 (3)
C9	0.119 (4)	0.110 (4)	0.096 (4)	0.045 (3)	−0.003 (3)	0.010 (3)
C10	0.111 (4)	0.104 (4)	0.104 (4)	0.046 (3)	0.003 (3)	0.010 (3)
C11	0.133 (4)	0.125 (4)	0.105 (4)	0.058 (3)	0.022 (3)	0.004 (3)
C12	0.113 (4)	0.114 (4)	0.086 (4)	0.056 (3)	0.020 (3)	0.013 (3)
C13	0.085 (4)	0.067 (3)	0.066 (4)	0.023 (3)	−0.008 (3)	−0.007 (3)
C14	0.112 (5)	0.091 (4)	0.083 (5)	0.044 (4)	0.014 (4)	0.005 (3)
C15	0.071 (4)	0.114 (6)	0.118 (6)	0.035 (4)	0.003 (4)	0.026 (5)

C16	0.085 (5)	0.109 (5)	0.133 (7)	0.011 (4)	−0.054 (4)	0.001 (5)
C17	0.075 (4)	0.075 (4)	0.093 (4)	0.008 (3)	−0.031 (3)	−0.009 (3)
C18	0.070 (3)	0.070 (3)	0.059 (3)	−0.021 (3)	0.012 (3)	−0.006 (3)
C19	0.070 (3)	0.072 (4)	0.082 (4)	−0.025 (3)	0.011 (3)	0.002 (3)
C20	0.063 (3)	0.055 (3)	0.094 (4)	−0.020 (3)	−0.011 (3)	0.004 (3)
C21	0.088 (4)	0.071 (4)	0.080 (4)	−0.033 (3)	−0.006 (3)	−0.019 (3)
C22	0.076 (3)	0.071 (3)	0.056 (3)	−0.028 (3)	0.007 (3)	−0.012 (3)
C23	0.184 (11)	0.172 (11)	0.121 (9)	0.005 (10)	0.069 (9)	0.017 (7)
C24	0.128 (9)	0.245 (17)	0.184 (14)	0.104 (11)	−0.004 (8)	−0.064 (11)
C25	0.223 (15)	0.094 (7)	0.181 (13)	0.054 (9)	−0.090 (12)	−0.019 (7)
C26	0.257 (16)	0.071 (6)	0.204 (12)	−0.036 (9)	−0.035 (11)	0.032 (6)
C27	0.131 (8)	0.101 (7)	0.235 (14)	−0.010 (7)	−0.024 (9)	−0.058 (8)

Geometric parameters (Å, °)

Ni1—N1	1.955 (3)	C9—H9	0.9300
Ni1—O2	1.989 (3)	C10—C11	1.346 (9)
Ni1—O1^{i}	2.060 (3)	C10—H10	0.9300
Ni1—N4	2.083 (3)	C11—C12	1.369 (8)
Ni1—N2	2.196 (4)	C11—H11	0.9300
Ni1—N3	2.201 (3)	C12—H12	0.9300
N1—C1	1.328 (5)	C13—C14	1.363 (7)
N1—N1^{i}	1.409 (6)	C13—H13	0.9300
N2—C12	1.300 (6)	C14—C15	1.335 (8)
N2—C8	1.301 (6)	C14—H14	0.9300
N3—C17	1.310 (6)	C15—C16	1.371 (9)
N3—C13	1.320 (6)	C15—H15	0.9300
N4—C22	1.320 (5)	C16—C17	1.366 (8)
N4—C18	1.325 (5)	C16—H16	0.9300
N5—C23	1.345 (11)	C17—H17	0.9300
N5—C27	1.348 (11)	C18—C19	1.378 (6)
O1—C1	1.283 (4)	C18—H18	0.9300
O1—Ni1^{i}	2.060 (3)	C19—C20	1.344 (7)
O2—C3	1.302 (4)	C19—H19	0.9300
C1—C2	1.495 (5)	C20—C21	1.378 (7)
C2—C7	1.399 (5)	C20—H20	0.9300
C2—C3	1.428 (5)	C21—C22	1.361 (6)
C3—C4	1.421 (5)	C21—H21	0.9300
C4—C5	1.359 (5)	C22—H22	0.9300
C4—H4	0.9300	C23—C24	1.310 (11)
C5—C6	1.393 (6)	C23—H23	0.9300
C5—H5	0.9300	C24—C25	1.354 (12)
C6—C7	1.368 (6)	C24—H24	0.9300
C6—H6	0.9300	C25—C26	1.30 (3)
C7—H7	0.9300	C25—H25	0.9300
C8—C9	1.371 (7)	C26—C27	1.337 (10)
C8—H8	0.9300	C26—H26	0.9300
C9—C10	1.329 (8)	C27—H27	0.9300

N1—Ni1—O2	90.75 (11)	C8—C9—H9	120.4
N1—Ni1—O1^{i}	79.81 (11)	C9—C10—C11	117.1 (7)
O2—Ni1—O1^{i}	170.55 (10)	C9—C10—H10	121.4
N1—Ni1—N4	175.46 (13)	C11—C10—H10	121.4
O2—Ni1—N4	93.76 (12)	C10—C11—C12	119.8 (7)
O1^{i}—Ni1—N4	95.68 (12)	C10—C11—H11	120.1
N1—Ni1—N2	93.47 (13)	C12—C11—H11	120.1
O2—Ni1—N2	91.23 (13)	N2—C12—C11	124.1 (6)
O1^{i}—Ni1—N2	89.17 (13)	N2—C12—H12	118.0
N4—Ni1—N2	85.91 (13)	C11—C12—H12	118.0
N1—Ni1—N3	92.03 (13)	N3—C13—C14	123.2 (5)
O2—Ni1—N3	91.77 (12)	N3—C13—H13	118.4
O1^{i}—Ni1—N3	88.77 (12)	C14—C13—H13	118.4
N4—Ni1—N3	88.37 (12)	C15—C14—C13	120.3 (6)
N2—Ni1—N3	173.70 (13)	C15—C14—H14	119.8
C1—N1—N1^{i}	112.1 (4)	C13—C14—H14	119.8
C1—N1—Ni1	133.4 (3)	C14—C15—C16	117.9 (6)
N1^{i}—N1—Ni1	114.5 (3)	C14—C15—H15	121.1
C12—N2—C8	114.8 (5)	C16—C15—H15	121.1
C12—N2—Ni1	123.2 (4)	C17—C16—C15	118.1 (6)
C8—N2—Ni1	121.9 (4)	C17—C16—H16	120.9
C17—N3—C13	115.9 (4)	C15—C16—H16	120.9
C17—N3—Ni1	121.8 (3)	N3—C17—C16	124.6 (6)
C13—N3—Ni1	122.3 (3)	N3—C17—H17	117.7
C22—N4—C18	115.9 (4)	C16—C17—H17	117.7
C22—N4—Ni1	123.1 (3)	N4—C18—C19	124.1 (5)
C18—N4—Ni1	121.0 (3)	N4—C18—H18	117.9
C23—N5—C27	119.5 (9)	C19—C18—H18	117.9
C1—O1—Ni1^{i}	110.1 (2)	C20—C19—C18	118.5 (5)
C3—O2—Ni1	126.4 (2)	C20—C19—H19	120.7
O1—C1—N1	123.5 (4)	C18—C19—H19	120.7
O1—C1—C2	118.9 (3)	C19—C20—C21	118.7 (5)
N1—C1—C2	117.6 (3)	C19—C20—H20	120.6
C7—C2—C3	119.2 (4)	C21—C20—H20	120.6
C7—C2—C1	115.5 (3)	C22—C21—C20	118.6 (5)
C3—C2—C1	125.3 (3)	C22—C21—H21	120.7
O2—C3—C4	118.2 (4)	C20—C21—H21	120.7
O2—C3—C2	126.3 (4)	N4—C22—C21	124.1 (5)
C4—C3—C2	115.5 (4)	N4—C22—H22	117.9
C5—C4—C3	123.4 (4)	C21—C22—H22	117.9
C5—C4—H4	118.3	C24—C23—N5	118.7 (9)
C3—C4—H4	118.3	C24—C23—H23	120.6
C4—C5—C6	120.6 (4)	N5—C23—H23	120.6
C4—C5—H5	119.7	C23—C24—C25	121.5 (10)
C6—C5—H5	119.7	C23—C24—H24	119.3
C7—C6—C5	117.8 (4)	C25—C24—H24	119.3
C7—C6—H6	121.1	C26—C25—C24	119.8 (10)

C5—C6—H6	121.1	C26—C25—H25	120.1
C6—C7—C2	123.4 (4)	C24—C25—H25	120.1
C6—C7—H7	118.3	C25—C26—C27	119.7 (9)
C2—C7—H7	118.3	C25—C26—H26	120.1
N2—C8—C9	124.9 (6)	C27—C26—H26	120.1
N2—C8—H8	117.5	C26—C27—N5	120.4 (9)
C9—C8—H8	117.5	C26—C27—H27	119.8
C10—C9—C8	119.3 (7)	N5—C27—H27	119.8
C10—C9—H9	120.4		

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

Fig. 1