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(1,2-Disalicyloylhydrazine)hexakis(pyridine)dinickel(II) 1,2-disalicyloylhydrazine solvate

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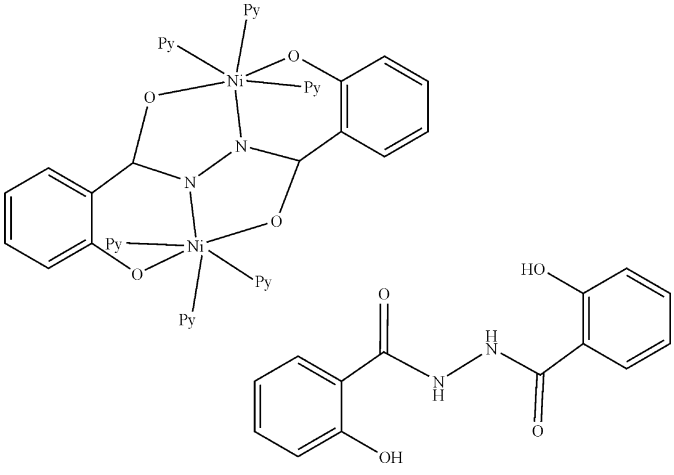
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; R factor = 0.035; wR factor = 0.102; data-to-parameter ratio = 13.2.

The title compound, $[Ni_2(C_{14}H_8N_2O_4)(C_5H_5N)_6]C_{14}H_{12}N_2O_4$, is composed of the complex $[Ni_2(C_{14}H_8N_2O_4)(C_5H_5N)_6]$ and a free ligand. Each nickel(II) coordination environment in the complex exhibits a distorted octahedral geometry. The dinuclear complex is centrosymmetric. The complex molecules are linked into one-dimensional chains *via* intermolecular O—H···O hydrogen bonds.

Related literature

The complex $[Ni_2(C_{14}H_8N_2O_4)(C_5H_5N)_6]\cdot 2C_5H_5N$ with 1,2-disalicyloylhydrazine was reported previously (Chen & Liu, 2005). In that complex, the salicyloylhydrazine ligand functions as a tetranionic hexadentate ligand.



Experimental

Crystal data

$[Ni_2(C_{14}H_8N_2O_4)(C_5H_5N)_6]\cdot C_{14}H_{12}N_2O_4$
M_r = 1132.50
Triclinic, $P\overline{1}$
a = 10.615 (4) Å
b = 11.097 (4) Å
c = 12.094 (5) Å
α = 72.230 (4)°
β = 85.285 (4)°
γ = 82.876 (4)°
V = 1344.7 (9) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 0.77 mm^{-1}
T = 298 (2) K
0.63 × 0.52 × 0.40 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.644, T_{max} = 0.749
6973 measured reflections
4652 independent reflections
3642 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.102
S = 1.00
4652 reflections
352 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.40 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

Table 1
Selected bond angles (°).

N1^i—Ni1—O2^i	90.10 (8)	O1—Ni1—N2	93.90 (9)
N1^i—Ni1—O1	79.56 (8)	N3—Ni1—N2	90.50 (9)
O2^i—Ni1—O1	169.66 (7)	N1^i—Ni1—N4	89.88 (8)
N1^i—Ni1—N3	169.09 (8)	O2^i—Ni1—N4	89.64 (8)
O2^i—Ni1—N3	100.36 (8)	O1—Ni1—N4	90.12 (9)
O1—Ni1—N3	89.96 (8)	N3—Ni1—N4	87.12 (9)
N1^i—Ni1—N2	93.18 (8)	N2—Ni1—N4	175.33 (8)
O2^i—Ni1—N2	86.83 (8)		

Symmetry code: (i) $-x+1, -y+2, -z$.

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

D—H···A	D—H	H···A	D···A	D—H···A
O4—H4···O2^{ii}	0.82	1.72	2.534 (3)	171

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); 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: KJ2063).

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supplementary materials

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(1,2-Disalicyloylhydrazine)hexakis(pyridine)dinickel(II) 1,2-disalicyloylhydrazine solvate

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Comment

A large number of salicylhydrazine complexes have been prepared and studied. However, research on the complex with 1,2-disalicyloylhydrazine is limited to only one complex $[Ni_2(C_{14}H_8N_2O_4)(C_5H_5N)_6]2C_5H_5N$ (Chen & Liu, 2005). We have synthesized another new complex $[Ni_2(C_{14}H_8N_2O_4)(C_5H_5N)_6]C_{14}H_{12}N_2O_4$, which has been characterized by X-ray diffraction and elemental analysis. Here we present the crystal structure of the title complex.

The title compound consists of the complex $[Ni_2(C_{14}H_8N_2O_4)(C_5H_5N)_6]$ and a free ligand (1,2-disalicyloylhydrazine) (Fig. 1). The Ni complex is formed by one chelated ligand, two nickel ions and six pyridine molecules. The ligand is present as the tetranionic hexadentate ligand dsh^{4-} and is linked with two nickel atoms. Both the binuclear nickel complex and the free ligand exhibit crystallographic centrosymmetry. From the data shown in Table 1, we can see that each nickel ion resides in a slightly distorted octahedral coordination environment, consisting of three pyridine N, a phenolate O, a carbonyl O and a hydrazine N of the ligand. which construct the fused five-membered and six-membered rings with each nickel atom. The two unique chelate rings, one five-membered and one six-membered, are near to coplanar with an 3.9 (3) ° dihedral angle.

As illustrated in Fig 2, the alternation of complex and free ligand molecules is linked into one-dimensional chain by intermolecular O4—H4···O2 H-bonds (Table 2) along the [1 − 1 1] axis.

Experimental

A solution of $Ni(OAc)_2H_2O$ (0.0996 g, 0.4 mmol) in methanol (10 ml) was added to 1,2-disalicyloylhydrazine (0.054 g, 0.2 mmol) in pyridine (10 ml). After stirring the solution for four hours at room temperature, a reddish solution was obtained. After the solution had been standing for two weeks, red block crystals suitable for X-ray diffraction appeared. Yield: 0.086 g, 39%. m.p.> 573 K. Anal. for $C_{58}H_{50}N_{10}Ni_2O_8$: Calc. C, 61.46; H, 4.41; N, 11.36; Found: C, 61.42; H, 4.47; N, 11.33%.

Refinement

The H atoms on the ligands were allowed to ride on their parent atoms with C(sp^2)—H distances of 0.93Å [U_{iso}(H)=1.2U_{eq}(C)] and *C*(phenyl)—H distances of 0.93Å [U_{iso}(H)=1.2U_{eq}(C)]. The O—H distance is 0.820Å [U_{iso}(H)=1.5U_{eq}(O)]. All non-hydrogen atoms were refined anisotropically.

Figures

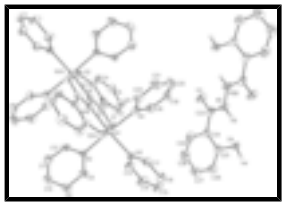

Fig. 1. The molecular structure of the title complex. Displacement ellipsoids are drawn at 30% probability level and H atoms have been omitted for clarity. symm. (A) −*x* + 1, −*y* + 2, −*z*, (B) −*x*, −*y* + 1, −*z* + 1

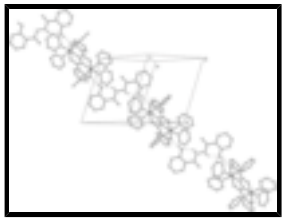

Fig. 2. Crystal packing of the title complex.

(1,2-Disalicyloylhydrazine)hexakis(pyridine)dinickel(II) 1,2-disalicyloylhydrazine solvate

Crystal data

$[Ni_2(C_{14}H_8N_2O_4)(C_5H_5N)_6]\cdot C_{14}H_{12}N_2O_4$	$Z = 1$
$M_r = 1132.50$	$F_{000} = 588$
Triclinic, $P\overline{1}$	$D_x = 1.399$ Mg m^{-3}
$a = 10.615$ (4) Å	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$b = 11.097$ (4) Å	Cell parameters from 2995 reflections
$c = 12.094$ (5) Å	$\theta = 2.2$–25.4º
$\alpha = 72.230$ (4)º	$\mu = 0.77$ mm^{-1}
$\beta = 85.285$ (4)º	$T = 298$ (2) K
$\gamma = 82.876$ (4)º	Block, red
$V = 1344.7$ (9) Å^3	0.63 × 0.52 × 0.40 mm

Data collection

Bruker SMART CCD area-detector diffractometer	4652 independent reflections
Radiation source: fine-focus sealed tube	3642 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.024$
$T = 298$(2) K	$\theta_{max} = 25.0$º
φ and ω scans	$\theta_{min} = 1.8$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -12\rightarrow12$
$T_{min} = 0.644$, $T_{max} = 0.749$	$k = -9\rightarrow13$
6973 measured reflections	$l = -13\rightarrow14$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.035$

$wR(F^2) = 0.102$

$S = 1.00$

4652 reflections

352 parameters

Primary atom site location: structure-invariant direct methods

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.048P)^2 + 0.4895P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 0.40$ e Å^{-3}

$\Delta\rho_{min} = -0.27$ e Å^{-3}

Extinction correction: none

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 $F^2 > 2$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	0.58655 (3)	0.85566 (3)	0.16798 (3)	0.03193 (12)
N1	0.45229 (19)	1.05133 (19)	−0.00523 (17)	0.0279 (5)
N2	0.7511 (2)	0.9521 (2)	0.16127 (19)	0.0371 (5)
N3	0.5968 (2)	0.7776 (2)	0.34846 (18)	0.0381 (5)
N4	0.4278 (2)	0.7424 (2)	0.18095 (19)	0.0388 (5)
N5	0.0379 (3)	0.5115 (3)	0.5385 (2)	0.0567 (7)
H5	0.0788	0.4495	0.5882	0.068*
O1	0.46160 (17)	1.00370 (17)	0.19156 (14)	0.0366 (4)
O2	0.29489 (17)	1.27700 (16)	−0.11339 (15)	0.0358 (4)
O3	−0.0127 (2)	0.7197 (2)	0.4626 (2)	0.0711 (7)
O4	0.1637 (2)	0.43717 (19)	0.73076 (18)	0.0514 (5)
H4	0.2054	0.3913	0.7850	0.077*
C1	0.4151 (2)	1.0710 (2)	0.0945 (2)	0.0285 (6)
C2	0.3100 (2)	1.1727 (2)	0.0950 (2)	0.0306 (6)
C3	0.2541 (2)	1.2639 (2)	−0.0030 (2)	0.0327 (6)
C4	0.1496 (3)	1.3461 (3)	0.0180 (3)	0.0449 (7)
H4A	0.1106	1.4054	−0.0452	0.054*
C5	0.1028 (3)	1.3425 (3)	0.1281 (3)	0.0528 (8)
H5A	0.0329	1.3981	0.1381	0.063*
C6	0.1585 (3)	1.2572 (3)	0.2234 (3)	0.0506 (8)
H6	0.1284	1.2558	0.2982	0.061*
C7	0.2595 (3)	1.1742 (3)	0.2060 (2)	0.0419 (7)

H7	0.2965	1.1159	0.2708	0.050*
C8	0.8504 (3)	0.8988 (3)	0.2266 (3)	0.0517 (8)
H8	0.8428	0.8217	0.2839	0.062*
C9	0.9626 (3)	0.9511 (3)	0.2139 (3)	0.0656 (10)
H9	1.0285	0.9113	0.2627	0.079*
C10	0.9763 (3)	1.0626 (3)	0.1285 (3)	0.0642 (10)
H10	1.0528	1.0987	0.1157	0.077*
C11	0.8747 (3)	1.1202 (3)	0.0620 (3)	0.0642 (10)
H11	0.8801	1.1976	0.0046	0.077*
C12	0.7657 (3)	1.0625 (3)	0.0812 (3)	0.0488 (8)
H12	0.6974	1.1028	0.0355	0.059*
C13	0.5915 (3)	0.8589 (3)	0.4115 (3)	0.0541 (8)
H13	0.5839	0.9457	0.3730	0.065*
C14	0.5965 (4)	0.8199 (4)	0.5297 (3)	0.0730 (11)
H14	0.5928	0.8792	0.5704	0.088*
C15	0.6072 (4)	0.6928 (4)	0.5873 (3)	0.0803 (12)
H15	0.6117	0.6640	0.6677	0.096*
C16	0.6112 (4)	0.6085 (4)	0.5247 (3)	0.0689 (10)
H16	0.6187	0.5213	0.5619	0.083*
C17	0.6040 (3)	0.6544 (3)	0.4060 (3)	0.0485 (8)
H17	0.6042	0.5966	0.3642	0.058*
C18	0.3257 (3)	0.7548 (3)	0.2496 (3)	0.0502 (8)
H18	0.3233	0.8124	0.2920	0.060*
C19	0.2233 (3)	0.6862 (4)	0.2606 (3)	0.0644 (10)
H19	0.1534	0.6978	0.3094	0.077*
C20	0.2254 (4)	0.6018 (4)	0.2000 (4)	0.0723 (11)
H20	0.1574	0.5543	0.2065	0.087*
C21	0.3297 (4)	0.5875 (3)	0.1286 (3)	0.0666 (10)
H21	0.3337	0.5300	0.0861	0.080*
C22	0.4284 (3)	0.6599 (3)	0.1209 (3)	0.0499 (8)
H22	0.4984	0.6506	0.0716	0.060*
C23	0.0469 (3)	0.6322 (3)	0.5347 (3)	0.0493 (8)
C24	0.1349 (3)	0.6538 (3)	0.6131 (2)	0.0451 (7)
C25	0.1928 (3)	0.5585 (3)	0.7058 (3)	0.0442 (7)
C26	0.2772 (3)	0.5909 (3)	0.7717 (3)	0.0585 (9)
H26	0.3158	0.5283	0.8330	0.070*
C27	0.3040 (4)	0.7143 (4)	0.7470 (4)	0.0746 (11)
H27	0.3618	0.7347	0.7905	0.090*
C28	0.2452 (4)	0.8086 (4)	0.6577 (4)	0.0819 (12)
H28	0.2619	0.8926	0.6422	0.098*
C29	0.1627 (4)	0.7781 (3)	0.5924 (3)	0.0674 (10)
H29	0.1240	0.8422	0.5323	0.081*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0359 (2)	0.0282 (2)	0.02966 (19)	0.00429 (14)	−0.00713 (14)	−0.00721 (14)
N1	0.0280 (11)	0.0233 (11)	0.0314 (11)	0.0056 (8)	−0.0071 (9)	−0.0081 (9)

N2	0.0397 (13)	0.0301 (12)	0.0389 (12)	0.0012 (10)	−0.0122 (10)	−0.0058 (10)
N3	0.0445 (14)	0.0332 (13)	0.0328 (12)	−0.0011 (11)	−0.0077 (10)	−0.0040 (11)
N4	0.0379 (14)	0.0361 (13)	0.0397 (13)	−0.0001 (10)	−0.0056 (10)	−0.0076 (11)
N5	0.0685 (19)	0.0425 (15)	0.0532 (16)	0.0106 (14)	−0.0261 (13)	−0.0059 (13)
O1	0.0453 (11)	0.0360 (10)	0.0267 (9)	0.0095 (8)	−0.0078 (8)	−0.0106 (8)
O2	0.0401 (11)	0.0291 (10)	0.0345 (10)	0.0082 (8)	−0.0055 (8)	−0.0076 (8)
O3	0.0887 (19)	0.0464 (14)	0.0629 (15)	0.0190 (13)	−0.0272 (13)	0.0024 (12)
O4	0.0591 (14)	0.0373 (12)	0.0513 (12)	0.0072 (10)	−0.0215 (10)	−0.0036 (10)
C1	0.0285 (14)	0.0281 (14)	0.0303 (14)	−0.0005 (11)	−0.0041 (11)	−0.0108 (11)
C2	0.0300 (14)	0.0292 (14)	0.0348 (14)	−0.0016 (11)	−0.0051 (11)	−0.0125 (11)
C3	0.0321 (14)	0.0283 (14)	0.0387 (15)	−0.0009 (11)	−0.0028 (11)	−0.0123 (12)
C4	0.0406 (17)	0.0380 (17)	0.0510 (18)	0.0116 (13)	−0.0040 (14)	−0.0115 (14)
C5	0.0441 (18)	0.0492 (19)	0.064 (2)	0.0144 (15)	0.0028 (15)	−0.0234 (17)
C6	0.0505 (19)	0.057 (2)	0.0478 (17)	0.0094 (16)	0.0045 (14)	−0.0284 (16)
C7	0.0441 (17)	0.0445 (17)	0.0385 (15)	0.0057 (14)	−0.0060 (13)	−0.0172 (14)
C8	0.0464 (19)	0.0376 (17)	0.063 (2)	−0.0010 (14)	−0.0196 (16)	−0.0007 (15)
C9	0.048 (2)	0.052 (2)	0.091 (3)	−0.0017 (17)	−0.0284 (19)	−0.007 (2)
C10	0.050 (2)	0.062 (2)	0.083 (3)	−0.0165 (18)	−0.0067 (18)	−0.020 (2)
C11	0.074 (3)	0.049 (2)	0.062 (2)	−0.0234 (19)	−0.0175 (19)	0.0038 (17)
C12	0.054 (2)	0.0391 (17)	0.0490 (18)	−0.0059 (15)	−0.0206 (15)	−0.0022 (15)
C13	0.077 (2)	0.0435 (18)	0.0432 (17)	0.0012 (16)	−0.0187 (16)	−0.0131 (15)
C14	0.105 (3)	0.075 (3)	0.0423 (19)	0.002 (2)	−0.0203 (19)	−0.0234 (19)
C15	0.100 (3)	0.096 (3)	0.0348 (18)	−0.010 (3)	−0.0134 (19)	−0.001 (2)
C16	0.081 (3)	0.054 (2)	0.054 (2)	−0.009 (2)	−0.0116 (19)	0.0109 (19)
C17	0.0482 (19)	0.0418 (18)	0.0493 (18)	−0.0016 (14)	−0.0078 (14)	−0.0041 (15)
C18	0.0499 (19)	0.0480 (19)	0.0465 (17)	0.0000 (15)	0.0034 (15)	−0.0081 (15)
C19	0.050 (2)	0.061 (2)	0.067 (2)	−0.0070 (18)	0.0094 (17)	0.0012 (19)
C20	0.056 (2)	0.057 (2)	0.095 (3)	−0.0221 (19)	−0.008 (2)	−0.002 (2)
C21	0.071 (3)	0.053 (2)	0.084 (3)	−0.0117 (19)	−0.018 (2)	−0.026 (2)
C22	0.0498 (19)	0.0480 (19)	0.0546 (18)	−0.0010 (15)	−0.0078 (15)	−0.0195 (16)
C23	0.056 (2)	0.0427 (18)	0.0397 (16)	0.0099 (15)	0.0018 (14)	−0.0052 (14)
C24	0.0491 (18)	0.0384 (17)	0.0428 (16)	0.0048 (14)	0.0024 (14)	−0.0096 (14)
C25	0.0435 (17)	0.0400 (17)	0.0458 (17)	0.0075 (14)	0.0005 (13)	−0.0130 (14)
C26	0.059 (2)	0.054 (2)	0.063 (2)	0.0058 (17)	−0.0104 (17)	−0.0201 (18)
C27	0.077 (3)	0.067 (3)	0.092 (3)	−0.008 (2)	−0.011 (2)	−0.040 (2)
C28	0.094 (3)	0.049 (2)	0.105 (3)	−0.015 (2)	−0.004 (3)	−0.023 (2)
C29	0.084 (3)	0.042 (2)	0.069 (2)	−0.0011 (18)	−0.002 (2)	−0.0088 (18)

Geometric parameters (Å, °)

Ni1—N1^{i}	1.974 (2)	C9—C10	1.364 (5)
Ni1—O2^{i}	2.0455 (18)	C9—H9	0.9300
Ni1—O1	2.0549 (18)	C10—C11	1.370 (5)
Ni1—N3	2.095 (2)	C10—H10	0.9300
Ni1—N2	2.142 (2)	C11—C12	1.360 (4)
Ni1—N4	2.192 (2)	C11—H11	0.9300
N1—C1	1.312 (3)	C12—H12	0.9300
N1—N1^{i}	1.410 (4)	C13—C14	1.365 (4)

N1—Ni1^{i}	1.974 (2)	C13—H13	0.9300
N2—C12	1.327 (3)	C14—C15	1.365 (5)
N2—C8	1.335 (4)	C14—H14	0.9300
N3—C17	1.328 (4)	C15—C16	1.367 (5)
N3—C13	1.341 (4)	C15—H15	0.9300
N4—C18	1.330 (4)	C16—C17	1.374 (4)
N4—C22	1.331 (4)	C16—H16	0.9300
N5—C23	1.341 (4)	C17—H17	0.9300
N5—N5^{ii}	1.378 (5)	C18—C19	1.378 (5)
N5—H5	0.8600	C18—H18	0.9300
O1—C1	1.284 (3)	C19—C20	1.352 (5)
O2—C3	1.339 (3)	C19—H19	0.9300
O2—Ni1^{i}	2.0455 (18)	C20—C21	1.370 (5)
O3—C23	1.235 (3)	C20—H20	0.9300
O4—C25	1.356 (3)	C21—C22	1.378 (4)
O4—H4	0.8200	C21—H21	0.9300
C1—C2	1.485 (4)	C22—H22	0.9300
C2—C7	1.409 (4)	C23—C24	1.473 (4)
C2—C3	1.419 (4)	C24—C29	1.389 (4)
C3—C4	1.404 (4)	C24—C25	1.407 (4)
C4—C5	1.373 (4)	C25—C26	1.394 (4)
C4—H4A	0.9300	C26—C27	1.370 (5)
C5—C6	1.372 (4)	C26—H26	0.9300
C5—H5A	0.9300	C27—C28	1.382 (5)
C6—C7	1.371 (4)	C27—H27	0.9300
C6—H6	0.9300	C28—C29	1.362 (5)
C7—H7	0.9300	C28—H28	0.9300
C8—C9	1.366 (4)	C29—H29	0.9300
C8—H8	0.9300		
N1^{i}—Ni1—O2^{i}	90.10 (8)	C9—C10—C11	118.3 (3)
N1^{i}—Ni1—O1	79.56 (8)	C9—C10—H10	120.8
O2^{i}—Ni1—O1	169.66 (7)	C11—C10—H10	120.8
N1^{i}—Ni1—N3	169.09 (8)	C12—C11—C10	119.1 (3)
O2^{i}—Ni1—N3	100.36 (8)	C12—C11—H11	120.5
O1—Ni1—N3	89.96 (8)	C10—C11—H11	120.5
N1^{i}—Ni1—N2	93.18 (8)	N2—C12—C11	123.8 (3)
O2^{i}—Ni1—N2	86.83 (8)	N2—C12—H12	118.1
O1—Ni1—N2	93.90 (9)	C11—C12—H12	118.1
N3—Ni1—N2	90.50 (9)	N3—C13—C14	123.0 (3)
N1^{i}—Ni1—N4	89.88 (8)	N3—C13—H13	118.5
O2^{i}—Ni1—N4	89.64 (8)	C14—C13—H13	118.5
O1—Ni1—N4	90.12 (9)	C15—C14—C13	119.1 (4)
N3—Ni1—N4	87.12 (9)	C15—C14—H14	120.5
N2—Ni1—N4	175.33 (8)	C13—C14—H14	120.5
C1—N1—N1^{i}	113.2 (2)	C14—C15—C16	118.8 (3)
C1—N1—Ni1^{i}	133.30 (17)	C14—C15—H15	120.6

N1^{i}—N1—Ni1^{i}	113.25 (19)	C16—C15—H15	120.6
C12—N2—C8	116.2 (3)	C15—C16—C17	119.0 (3)
C12—N2—Ni1	120.89 (18)	C15—C16—H16	120.5
C8—N2—Ni1	122.46 (19)	C17—C16—H16	120.5
C17—N3—C13	117.2 (3)	N3—C17—C16	122.9 (3)
C17—N3—Ni1	125.4 (2)	N3—C17—H17	118.6
C13—N3—Ni1	117.38 (19)	C16—C17—H17	118.6
C18—N4—C22	117.2 (3)	N4—C18—C19	122.9 (3)
C18—N4—Ni1	120.6 (2)	N4—C18—H18	118.6
C22—N4—Ni1	122.2 (2)	C19—C18—H18	118.6
C23—N5—N5^{ii}	119.0 (3)	C20—C19—C18	119.4 (3)
C23—N5—H5	120.5	C20—C19—H19	120.3
N5^{ii}—N5—H5	120.5	C18—C19—H19	120.3
C1—O1—Ni1	110.36 (15)	C19—C20—C21	118.8 (3)
C3—O2—Ni1^{i}	124.83 (16)	C19—C20—H20	120.6
C25—O4—H4	109.5	C21—C20—H20	120.6
O1—C1—N1	123.2 (2)	C20—C21—C22	118.9 (3)
O1—C1—C2	118.8 (2)	C20—C21—H21	120.5
N1—C1—C2	118.0 (2)	C22—C21—H21	120.5
C7—C2—C3	117.7 (2)	N4—C22—C21	122.8 (3)
C7—C2—C1	115.1 (2)	N4—C22—H22	118.6
C3—C2—C1	127.3 (2)	C21—C22—H22	118.6
O2—C3—C4	118.1 (2)	O3—C23—N5	119.3 (3)
O2—C3—C2	124.4 (2)	O3—C23—C24	123.0 (3)
C4—C3—C2	117.5 (2)	N5—C23—C24	117.5 (3)
C5—C4—C3	122.5 (3)	C29—C24—C25	118.2 (3)
C5—C4—H4A	118.7	C29—C24—C23	116.8 (3)
C3—C4—H4A	118.7	C25—C24—C23	125.0 (3)
C6—C5—C4	120.5 (3)	O4—C25—C26	121.1 (3)
C6—C5—H5A	119.8	O4—C25—C24	119.5 (3)
C4—C5—H5A	119.8	C26—C25—C24	119.4 (3)
C7—C6—C5	118.5 (3)	C27—C26—C25	120.5 (3)
C7—C6—H6	120.8	C27—C26—H26	119.7
C5—C6—H6	120.8	C25—C26—H26	119.7
C6—C7—C2	123.4 (3)	C26—C27—C28	120.2 (4)
C6—C7—H7	118.3	C26—C27—H27	119.9
C2—C7—H7	118.3	C28—C27—H27	119.9
N2—C8—C9	123.7 (3)	C29—C28—C27	119.8 (4)
N2—C8—H8	118.1	C29—C28—H28	120.1
C9—C8—H8	118.1	C27—C28—H28	120.1
C10—C9—C8	118.9 (3)	C28—C29—C24	121.8 (4)
C10—C9—H9	120.6	C28—C29—H29	119.1
C8—C9—H9	120.6	C24—C29—H29	119.1

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*

O4—H4···O2^{iii}	0.82	1.72	2.534 (3)	171

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

Fig. 1

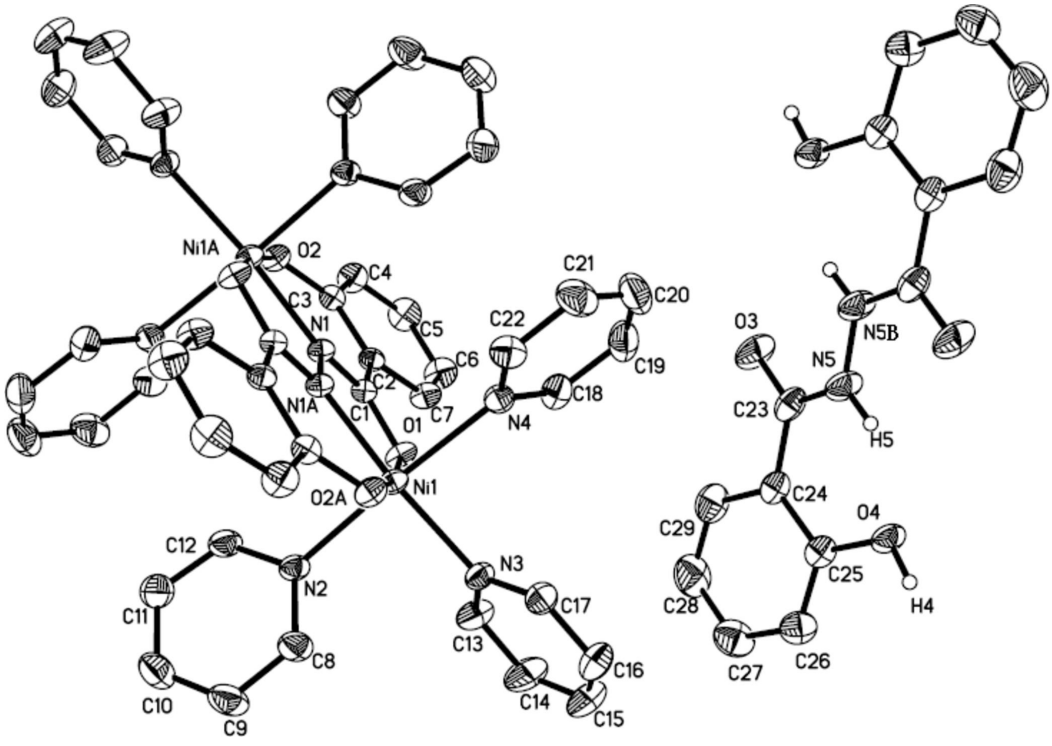

Fig. 2