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Dihistaminedisaccharinatonickel(II)

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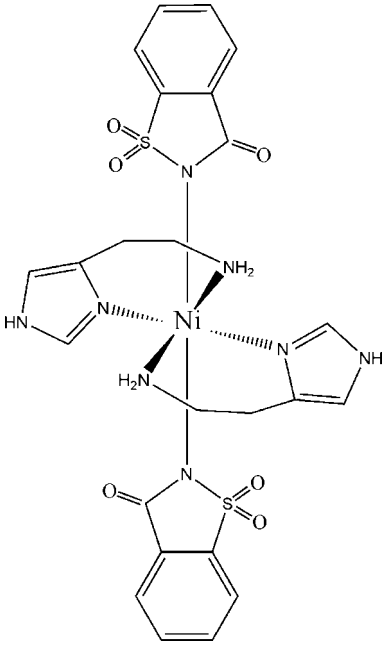
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.004 Å; disorder in main residue; R factor = 0.036; wR factor = 0.104; data-to-parameter ratio = 10.5.

The title complex, bis[2-(1*H*-imidazol-4-yl)ethanamine]disaccharinatonickel(II), $[Ni(C_7H_4NO_3S)_2(C_5H_9N_3)_2]$, has an octahedral coordination around the nickel(II) ion, and the Ni atom lies on a center of symmetry. The histamine ligands and sulfonyl group of the saccharinate ligands show disorder, and the two conformations (*A* and *B*, with almost equal occupancy) are inversion isomers. The molecular packing is stabilized by intra- and intermolecular hydrogen bonds between imidazole N atoms and sulfonyl O atoms. In the extended stucture, intermolecular N—H···O hydogen bonds constitute a chain structure parallel to the direction [110].

Related literature

For a related structure, see: Bulut *et al.* (2007); Bernstein *et al.* (1995).



Experimental

Crystal data

$[Ni(C_7H_4NO_3S)_2(C_5H_9N_3)_2]$
M_r = 645.36
Triclinic, $P\overline{1}$
a = 7.7508 (8) Å
b = 8.9840 (9) Å
c = 10.8167 (11) Å
α = 93.728 (8)°
β = 103.541 (8)°
γ = 109.994 (8)°
V = 679.40 (13) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 0.92 mm^{-1}
T = 296 K
0.52 × 0.47 × 0.28 mm

Data collection

Stoe IPDS II diffractometer
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
T_{min} = 0.629, T_{max} = 0.878
9525 measured reflections
2667 independent reflections
2420 reflections with $I > 2\sigma(I)$
R_{int} = 0.050

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.104
S = 1.01
2667 reflections
255 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.92 e Å^{-3}
$\Delta\rho_{min}$ = −0.76 e Å^{-3}

Table 1
Selected bond lengths (Å).

Ni1—N1	2.2874 (19)	Ni1—N3	2.094 (2)
Ni1—N2	2.0944 (19)		

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O3	0.90	2.09	2.927 (3)	153
N2—H2B···O1A^{i}	0.90	2.32	2.936 (10)	126
N2—H2B···S1A^{i}	0.90	2.84	3.409 (5)	122
N4—H4A···O2A^{ii}	0.79 (3)	2.12 (4)	2.801 (9)	144 (3)
N4—H4A···O2B^{ii}	0.79 (3)	2.04 (4)	2.794 (9)	159 (3)
N2—H2B···O3^{iii}	0.90	2.66	3.123 (4)	113

Symmetry codes: (i) $-x, -y, -z$; (ii) $-x+1, -y+1, -z$; (iii) $-x-1, -y, -z$.

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BR2052).

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supplementary materials

Acta Cryst. (2007). E**63**, m2409-m2410 [**doi:10.1107/S1600536807040780**]

Dihistaminedisaccharinatonickel(II)

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Comment

The title compound, (I), is composed of discrete [$C_{24}H_{26}N_8NiO_6S_2$] molecules. As shown in Figure 1, the nickel atom lies on a center of symmetry and is coordinated by four N atoms of two bidentate histamine ligands and monodentate saccharinato ligands. The geometry around the Ni(II) ion is an elongated octahedron. Related bond distances and angles are given in Table 1. The equatorial plane (N2/N3/N2i/N3i) is formed by N atoms of histamine ligands while the axial positions are occupied by saccharinate N atoms. It is observed that the apical Ni–N bond distance is longer than the basal Ni–N bond distances. The intraligand bond distances are comparable to those observed in the complex [$C_{24}H_{26}N_8CuO_6S_2$] (Bulut *et al.*, 2007).

Histamine ligand and sulfonyl group of saccharinato ligand show disorder, which is modelled as two different orientations with the occupancy factors of 0.493 (8) for conformer A and 0.507 (8) for conformer B. Both conformers, being inversion isomers, have similiar bond angles and distances. These values are also in good agreement with those found in [$C_{24}H_{26}N_8CuO_6S_2$] (Bulut *et al.*, 2007).

The molecular packing is stabilized by intra- and inter-molecular hydrogen bonds (Table 2). The neutral complexes are linked by N—H···O hydrogen bonding interactions between the imidazole N atoms of histamine and sacchatinate sulfonyl O atoms. As is seen from Figure 2, imidazol atom N4 acts as a donor atom, *via* H4a, to atom O2a, producing a chain C(8) (Bernstein *et al.*, 1995) running parallel to the direction [110] and centrosymmetric [$R_2^2(16)$] rings centered at (n+1/2, n+1/2, 0) (n=zero or integer).

Experimental

A solution of histamine (2 mmol, 0.222 g) in water (10 ml) was added dropwise upon stirring to the mixture of sodium saccharinate (2 mmol, 0.412 g) and $NiCl_2{\cdot}H_2O$ (1 mmol, 0.238 g) in distilled water (30 ml). The solution was heated to 60°C in a temperature-controlled bath and stirred for 8 h at 60°C and then filtered. The blue filtrates were left about two weaks at room temperature, and then the blue crystals of title complex suitable for *x*-ray diffraction analyses were collected.

Refinement

The sulfonyl group of sacharinate ligand and the histamine ligand show disorder, which is modelled as two different orientations (C8A—C11A, C8B—C11B; S1A—S1B; O1A—O2A, O1B—O2B) with occupancy factors of 0.507 (8) and 0.493 (8). All H atoms except those bonded to N4 atom were placed in geometricaly idealized positions, [N—H = 0.90 Å; C—H = 0.93 − 0.97 Å], and refined as riding atoms.

Figures

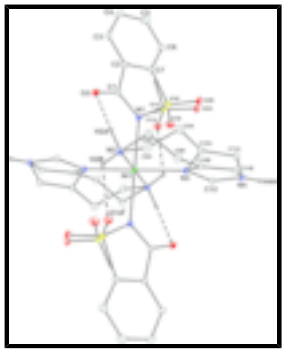

Fig. 1. The molecular structure of (I), with atom labels and 30% probability displacement ellipsoids. H atoms not involved in hydrogen bonding have been omitted for clarity.

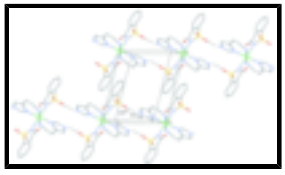

Fig. 2. A view of the complex showing the chain structure parallel to direction [110].

bis[2-(1*H*-imidazol-4-yl)ethanamine]disaccharinatonickel(II)

Crystal data

$[Ni(C_7H_4N_1O_3S_1)_2(C_5H_9N_3)_2]$	$Z = 1$
$M_r = 645.36$	$F_{000} = 334$
Triclinic, $P\overline{1}$	$D_x = 1.577$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 7.7508$ (8) Å	Cell parameters from 25242 reflections
$b = 8.9840$ (9) Å	$\theta = 2.0$–28.1º
$c = 10.8167$ (11) Å	$\mu = 0.92$ mm^{-1}
$\alpha = 93.728$ (8)º	$T = 296$ K
$\beta = 103.541$ (8)º	Prism, grey
$\gamma = 109.994$ (8)º	0.52 × 0.47 × 0.28 mm
$V = 679.40$ (13) Å^3	

Data collection

Stoe IPDS II diffractometer	2667 independent reflections
Radiation source: fine-focus sealed tube	2420 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.050$
$T = 296$ K	$\theta_{max} = 26.0$º
rotation method scans	$\theta_{min} = 2.0$º
Absorption correction: integration (X-RED32; Stoe & Cie, 2002)	$h = -8 \rightarrow 9$
$T_{min} = 0.629$, $T_{max} = 0.878$	$k = -11 \rightarrow 11$
9525 measured reflections	$l = -13 \rightarrow 13$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.036$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.104$	$w = 1/[\sigma^2(F_o^2) + (0.0852P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.01$	$(\Delta/\sigma)_{max} < 0.001$
2667 reflections	$\Delta\rho_{max} = 0.92$ e Å^{-3}
255 parameters	$\Delta\rho_{min} = -0.76$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	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}	Occ. (<1)
Ni1	0.0000	0.0000	0.0000	0.03453 (14)	
S1A	−0.0051 (8)	0.1787 (6)	−0.2688 (4)	0.0409 (7)	0.493 (8)
O1A	0.0482 (13)	0.0628 (9)	−0.3309 (8)	0.0616 (17)	0.493 (8)
O2A	0.1427 (12)	0.3296 (11)	−0.2139 (9)	0.0681 (18)	0.493 (8)
S1B	−0.0059 (9)	0.2164 (7)	−0.2538 (6)	0.0552 (10)	0.507 (8)
O1B	0.0969 (14)	0.1302 (12)	−0.3034 (11)	0.086 (3)	0.507 (8)
O2B	0.1140 (13)	0.3761 (10)	−0.1841 (10)	0.081 (2)	0.507 (8)
O3	−0.4308 (2)	0.0515 (2)	−0.14797 (16)	0.0563 (4)	
N1	−0.1265 (2)	0.1088 (2)	−0.16691 (16)	0.0415 (4)	
N2	−0.1652 (2)	0.0732 (2)	0.10049 (17)	0.0436 (4)	
H2A	−0.2647	0.0790	0.0412	0.052*	
H2B	−0.2134	−0.0065	0.1435	0.052*	
N3	0.2278 (2)	0.21908 (19)	0.07337 (16)	0.0424 (4)	
N4	0.5050 (3)	0.4154 (2)	0.1223 (2)	0.0558 (5)	
H4A	0.610 (5)	0.466 (4)	0.120 (3)	0.063 (8)*	
C1	−0.3102 (3)	0.1008 (2)	−0.20708 (19)	0.0407 (4)	
C2	−0.3531 (3)	0.1607 (2)	−0.33201 (19)	0.0432 (4)	

C3	−0.5258 (4)	0.1636 (3)	−0.4027 (2)	0.0565 (6)	
H3	−0.6357	0.1240	−0.3753	0.068*	
C4	−0.5279 (5)	0.2278 (4)	−0.5159 (3)	0.0742 (8)	
H4	−0.6418	0.2314	−0.5651	0.089*	
C5	−0.3669 (6)	0.2860 (5)	−0.5571 (3)	0.0812 (9)	
H5	−0.3740	0.3276	−0.6338	0.097*	
C6	−0.1946 (5)	0.2844 (4)	−0.4874 (3)	0.0709 (7)	
H6	−0.0847	0.3246	−0.5147	0.085*	
C7	−0.1933 (3)	0.2200 (3)	−0.3749 (2)	0.0489 (5)	
C8A	−0.0828 (13)	0.2245 (12)	0.1936 (8)	0.064 (2)	0.507 (8)
H8A1	0.0066	0.2144	0.2690	0.077*	0.507 (8)
H8A2	−0.1835	0.2462	0.2211	0.077*	0.507 (8)
C9A	0.0179 (9)	0.3599 (6)	0.1310 (6)	0.069 (2)	0.507 (8)
H9A1	−0.0636	0.3532	0.0461	0.083*	0.507 (8)
H9A2	0.0387	0.4608	0.1815	0.083*	0.507 (8)
C10A	0.2042 (9)	0.3590 (7)	0.1182 (7)	0.0509 (13)	0.507 (8)
C11A	0.3791 (13)	0.4790 (9)	0.1533 (8)	0.0593 (18)	0.507 (8)
H11A	0.4081	0.5837	0.1911	0.071*	0.507 (8)
C8B	−0.1115 (12)	0.2479 (9)	0.1411 (8)	0.0513 (17)	0.493 (8)
H8B1	−0.2045	0.2656	0.1805	0.062*	0.493 (8)
H8B2	−0.1106	0.3021	0.0664	0.062*	0.493 (8)
C9B	0.0827 (7)	0.3149 (6)	0.2356 (5)	0.0582 (16)	0.493 (8)
H9B1	0.1016	0.4193	0.2793	0.070*	0.493 (8)
H9B2	0.0886	0.2451	0.2999	0.070*	0.493 (8)
C10B	0.2398 (8)	0.3316 (6)	0.1739 (7)	0.0466 (13)	0.493 (8)
C11B	0.4107 (13)	0.4534 (10)	0.1985 (9)	0.0583 (19)	0.493 (8)
H11B	0.4538	0.5466	0.2580	0.070*	0.493 (8)
C12	0.4010 (3)	0.2674 (3)	0.0614 (2)	0.0508 (5)	
H12	0.4465	0.2052	0.0155	0.061*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0241 (2)	0.0339 (2)	0.0429 (2)	0.00635 (14)	0.01269 (14)	−0.00122 (12)
S1A	0.0276 (10)	0.0488 (17)	0.0456 (8)	0.0100 (10)	0.0132 (6)	0.0131 (9)
O1A	0.059 (4)	0.082 (4)	0.062 (2)	0.033 (3)	0.036 (2)	0.017 (3)
O2A	0.038 (3)	0.070 (4)	0.069 (3)	−0.011 (3)	0.010 (2)	0.009 (3)
S1B	0.0346 (11)	0.059 (2)	0.083 (2)	0.0180 (15)	0.0297 (13)	0.0301 (16)
O1B	0.074 (6)	0.122 (7)	0.118 (7)	0.066 (5)	0.071 (5)	0.069 (5)
O2B	0.042 (3)	0.069 (5)	0.100 (6)	−0.010 (3)	0.002 (3)	0.027 (4)
O3	0.0347 (8)	0.0821 (11)	0.0600 (9)	0.0226 (8)	0.0235 (7)	0.0210 (8)
N1	0.0282 (8)	0.0472 (9)	0.0481 (9)	0.0101 (7)	0.0140 (7)	0.0094 (7)
N2	0.0326 (9)	0.0499 (9)	0.0497 (9)	0.0144 (7)	0.0167 (7)	0.0022 (7)
N3	0.0310 (9)	0.0375 (8)	0.0518 (9)	0.0061 (7)	0.0102 (7)	0.0007 (7)
N4	0.0352 (11)	0.0477 (10)	0.0655 (12)	−0.0025 (9)	0.0035 (9)	0.0148 (9)
C1	0.0319 (10)	0.0424 (9)	0.0465 (10)	0.0117 (8)	0.0125 (8)	0.0027 (7)
C2	0.0379 (11)	0.0458 (10)	0.0433 (9)	0.0143 (8)	0.0101 (8)	−0.0004 (8)
C3	0.0438 (13)	0.0724 (14)	0.0528 (12)	0.0253 (11)	0.0088 (10)	0.0011 (10)

C4	0.0726 (19)	0.103 (2)	0.0531 (13)	0.0495 (18)	0.0033 (13)	0.0105 (13)
C5	0.096 (2)	0.109 (2)	0.0520 (14)	0.050 (2)	0.0213 (15)	0.0295 (15)
C6	0.0681 (19)	0.0895 (19)	0.0634 (15)	0.0288 (16)	0.0291 (14)	0.0299 (14)
C7	0.0429 (12)	0.0527 (11)	0.0488 (11)	0.0136 (9)	0.0141 (9)	0.0090 (9)
C8A	0.059 (5)	0.079 (5)	0.058 (4)	0.028 (3)	0.025 (4)	−0.017 (4)
C9A	0.066 (4)	0.049 (3)	0.092 (4)	0.024 (3)	0.023 (3)	−0.013 (2)
C10A	0.049 (3)	0.042 (2)	0.053 (3)	0.011 (2)	0.010 (3)	−0.006 (2)
C11A	0.063 (5)	0.036 (3)	0.059 (4)	0.002 (3)	0.008 (4)	−0.004 (3)
C8B	0.043 (3)	0.055 (3)	0.058 (4)	0.023 (3)	0.013 (3)	−0.005 (3)
C9B	0.050 (3)	0.061 (3)	0.057 (3)	0.020 (2)	0.008 (2)	−0.014 (2)
C10B	0.040 (3)	0.040 (2)	0.052 (3)	0.0142 (19)	0.002 (2)	−0.001 (2)
C11B	0.054 (4)	0.037 (3)	0.062 (5)	0.006 (2)	−0.006 (4)	0.002 (3)
C12	0.0336 (11)	0.0471 (11)	0.0647 (13)	0.0067 (9)	0.0133 (9)	0.0081 (9)

Geometric parameters (Å, °)

Ni1—N1	2.2874 (19)	C2—C3	1.387 (3)
Ni1—N2	2.0944 (19)	C3—C4	1.385 (4)
Ni1—N3	2.094 (2)	C3—H3	0.9300
S1A—O2A	1.421 (9)	C4—C5	1.369 (5)
S1A—O1A	1.428 (8)	C4—H4	0.9300
S1A—N1	1.632 (6)	C5—C6	1.377 (5)
S1A—C7	1.796 (5)	C5—H5	0.9300
S1B—O1B	1.445 (9)	C6—C7	1.379 (3)
S1B—O2B	1.453 (9)	C6—H6	0.9300
S1B—N1	1.613 (6)	C8A—C9A	1.501 (12)
S1B—C7	1.725 (6)	C8A—H8A1	0.9700
O3—C1	1.230 (3)	C8A—H8A2	0.9700
N1—C1	1.363 (3)	C9A—C10A	1.485 (9)
N2—C8A	1.483 (8)	C9A—H9A1	0.9700
N2—C8B	1.486 (8)	C9A—H9A2	0.9700
N2—H2A	0.9000	C10A—C11A	1.360 (10)
N2—H2B	0.9000	C11A—H11A	0.9300
N3—C12	1.303 (3)	C8B—C9B	1.501 (10)
N3—C10B	1.399 (6)	C8B—H8B1	0.9700
N3—C10A	1.403 (6)	C8B—H8B2	0.9700
N4—C11B	1.322 (11)	C9B—C10B	1.490 (8)
N4—C12	1.325 (3)	C9B—H9B1	0.9700
N4—C11A	1.379 (10)	C9B—H9B2	0.9700
N4—H4A	0.79 (3)	C10B—C11B	1.352 (11)
C1—C2	1.495 (3)	C11B—H11B	0.9300
C2—C7	1.373 (3)	C12—H12	0.9300
N3—Ni1—N3^{i}	180.00 (7)	C4—C3—C2	117.3 (3)
N3—Ni1—N2	90.30 (10)	C4—C3—H3	121.4
N3^{i}—Ni1—N2	89.70 (10)	C2—C3—H3	121.4
N3—Ni1—N2^{i}	89.70 (10)	C5—C4—C3	121.7 (3)
N3^{i}—Ni1—N2^{i}	90.30 (10)	C5—C4—H4	119.1
N2—Ni1—N2^{i}	180.00 (8)	C3—C4—H4	119.1

N3—Ni1—N1^{i}	89.27 (9)	C4—C5—C6	121.4 (3)
N3^{i}—Ni1—N1^{i}	90.73 (9)	C4—C5—H5	119.3
N2—Ni1—N1^{i}	93.59 (8)	C6—C5—H5	119.3
N2^{i}—Ni1—N1^{i}	86.41 (8)	C5—C6—C7	116.6 (3)
N3—Ni1—N1	90.73 (9)	C5—C6—H6	121.7
N3^{i}—Ni1—N1	89.27 (9)	C7—C6—H6	121.7
N2—Ni1—N1	86.41 (8)	C2—C7—C6	122.9 (2)
N2^{i}—Ni1—N1	93.59 (8)	C2—C7—S1B	106.1 (3)
N1^{i}—Ni1—N1	180.00 (7)	C6—C7—S1B	130.6 (3)
O2A—S1A—O1A	116.3 (5)	C2—C7—S1A	107.5 (2)
O2A—S1A—N1	111.0 (4)	C6—C7—S1A	129.3 (3)
O1A—S1A—N1	113.5 (5)	N2—C8A—C9A	109.4 (6)
O2A—S1A—C7	106.4 (5)	N2—C8A—H8A1	109.8
O1A—S1A—C7	112.2 (5)	C9A—C8A—H8A1	109.8
N1—S1A—C7	95.3 (3)	N2—C8A—H8A2	109.8
O1B—S1B—O2B	114.1 (6)	C9A—C8A—H8A2	109.8
O1B—S1B—N1	109.1 (5)	H8A1—C8A—H8A2	108.2
O2B—S1B—N1	111.5 (5)	C10A—C9A—C8A	113.2 (6)
O1B—S1B—C7	110.6 (5)	C10A—C9A—H9A1	108.9
O2B—S1B—C7	111.7 (5)	C8A—C9A—H9A1	108.9
N1—S1B—C7	98.8 (3)	C10A—C9A—H9A2	108.9
C1—N1—S1B	108.4 (2)	C8A—C9A—H9A2	108.9
C1—N1—S1A	112.1 (2)	H9A1—C9A—H9A2	107.8
C1—N1—Ni1	127.06 (13)	C11A—C10A—N3	107.5 (6)
S1B—N1—Ni1	124.5 (2)	C11A—C10A—C9A	129.8 (6)
S1A—N1—Ni1	120.0 (2)	N3—C10A—C9A	122.5 (4)
C8A—N2—Ni1	121.5 (4)	C10A—C11A—N4	106.8 (6)
C8B—N2—Ni1	118.1 (3)	C10A—C11A—H11A	126.6
C8A—N2—H2A	106.9	N4—C11A—H11A	126.6
C8B—N2—H2A	86.0	N2—C8B—C9B	109.7 (5)
Ni1—N2—H2A	106.9	N2—C8B—H8B1	109.7
C8A—N2—H2B	106.9	C9B—C8B—H8B1	109.7
C8B—N2—H2B	127.1	N2—C8B—H8B2	109.7
Ni1—N2—H2B	106.9	C9B—C8B—H8B2	109.7
H2A—N2—H2B	106.7	H8B1—C8B—H8B2	108.2
C12—N3—C10B	103.1 (3)	C10B—C9B—C8B	113.0 (5)
C12—N3—C10A	105.0 (3)	C10B—C9B—H9B1	109.0
C12—N3—Ni1	130.02 (15)	C8B—C9B—H9B1	109.0
C10B—N3—Ni1	125.2 (3)	C10B—C9B—H9B2	109.0
C10A—N3—Ni1	123.2 (3)	C8B—C9B—H9B2	109.0
C11B—N4—C12	107.2 (4)	H9B1—C9B—H9B2	107.8
C12—N4—C11A	106.3 (4)	C11B—C10B—N3	108.2 (6)
C11B—N4—H4A	126 (2)	C11B—C10B—C9B	128.4 (6)
C12—N4—H4A	126 (2)	N3—C10B—C9B	123.4 (4)
C11A—N4—H4A	125 (2)	N4—C11B—C10B	107.3 (7)
O3—C1—N1	124.7 (2)	N4—C11B—H11B	126.4
O3—C1—C2	122.09 (19)	C10B—C11B—H11B	126.4

N1—C1—C2	113.15 (17)	N3—C12—N4	112.3 (2)
C7—C2—C3	120.0 (2)	N3—C12—H12	123.9
C7—C2—C1	111.53 (19)	N4—C12—H12	123.9
C3—C2—C1	128.4 (2)		

Symmetry codes: (i) −*x*, −*y*, −*z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2A···O3	0.90	2.09	2.927 (3)	153
N2—H2B···O1A^{i}	0.90	2.32	2.936 (10)	126
N2—H2B···S1A^{i}	0.90	2.84	3.409 (5)	122
N4—H4A···O2A^{ii}	0.79 (3)	2.12 (4)	2.801 (9)	144 (3)
N4—H4A···O2B^{ii}	0.79 (3)	2.04 (4)	2.794 (9)	159 (3)
N2—H2B···O3^{iii}	0.90	2.66	3.123 (4)	113

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

Fig. 1

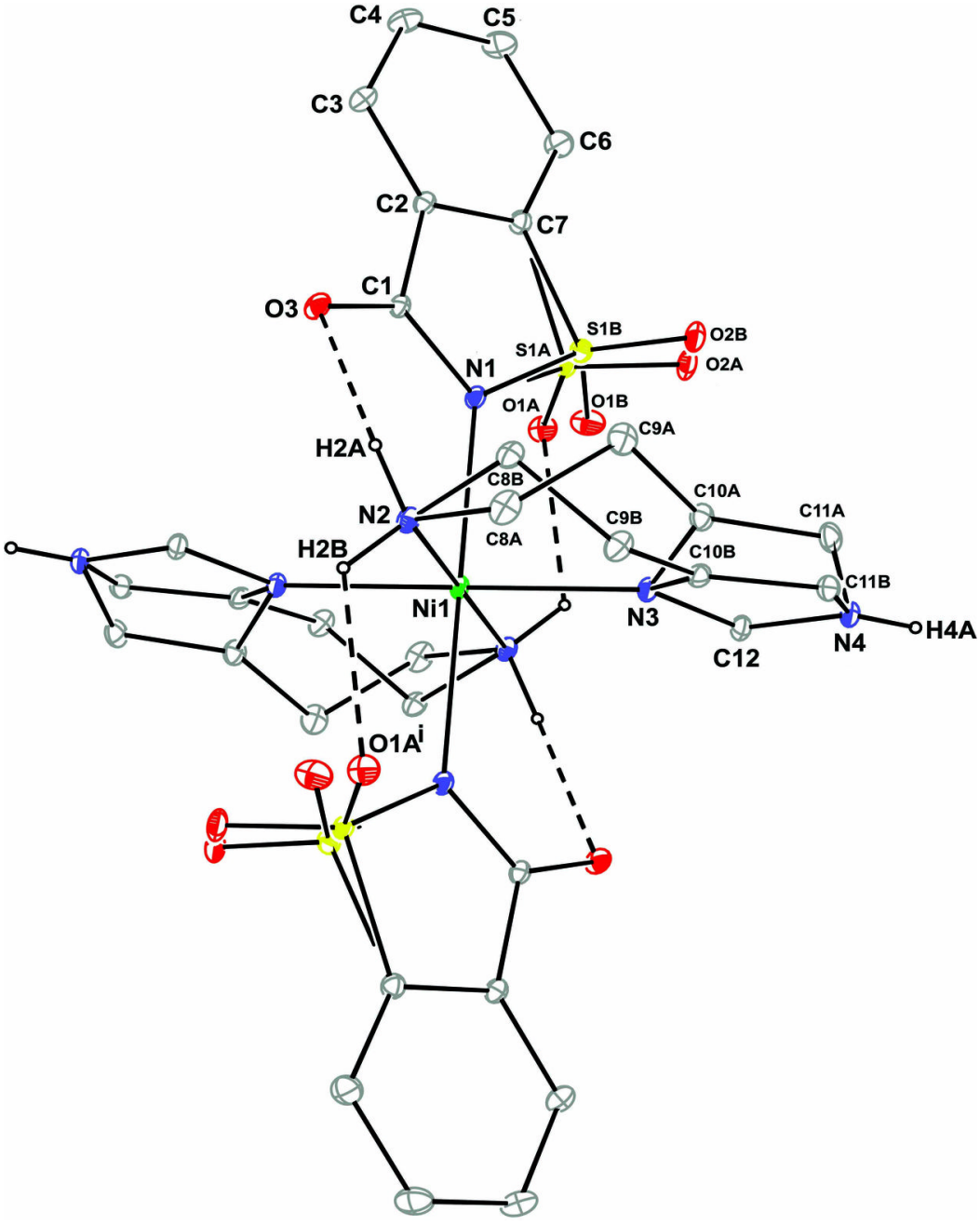
C4
C5
C3
C6
C2
C7
C1
O3
S1B
O2B
S1A
O2A
N1
O1A
O1B
C9A
H2A
C8B
C10A
C11A
N2
C9B
C8A
H2B
C10B
C11B
Ni1
N3
N4
H4A
C12
O1A^{i}

Fig. 2