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Bis{2-[({[3-(dimethylazaniumyl)propyl]imino}-methyl)phenyl]sulfanido}nickel(II) tetraphenylborate

Alexandra Meloccaro, Joshua R. Zimmerman and David M. Eichhorn*

Department of Chemistry, Wichita State University, 1845 Fairmount, Wichita, KS 67260-0051, USA. *Correspondence e-mail: david.eichhorn@wichita.edu

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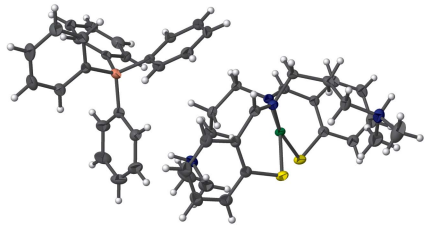
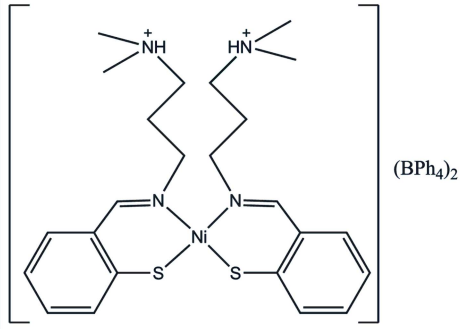
In the title compound, $[Ni(C_{12}H_{18}N_2S)_2](C_{24}H_{20}B)_2$, the Ni^{II} atom is coordinated by two ligands *via* the thiolate S and the imine N atoms. The amine N atoms are protonated and interact with the phenyl rings of the BPh_4 anions.

3D view



Chemical scheme



Structure description

We have previously published the reaction of 2,2′-dithiodibenzaldehyde with $NiCl_2$ and *N*,*N*-dimethylethylenediamine to produce a nickel complex of a tridentate ligand in which the Ni is coordinated by the three potential donor atoms (imine N, amine N, and thiolate S) of the ligand with the square-planar Ni coordination sphere completed by a Cl ligand. When $Ni(BPh_4)_2$ was used as the nickel source, a related species was isolated in which the fourth coordination site is occupied by a thiolate derived from the tridentate ligand. (Zimmerman, *et al.*, 2011) In an analogous reaction using *N*,*N*-dimethylpropylenediamine, the title complex was isolated in which the potentially tridentate ligand utilizes only the imine N and thiolate S atoms to bind to Ni (Table 1).

Two ligands coordinate to the Ni atom, related to each other by a crystallographic twofold rotation axis (Fig. 1). The coordination around Ni deviates somewhat from ideal square planar, with the chelate rings of the two ligands rotated by 19.40 (9)° with respect to each other. The amine N atoms are protonated, with each proton participating in a hydrogen bond with a phenyl ring of one BPh_4^- anion (Fig. 2, Table 2).

Synthesis and crystallization

The title compound was synthesized and crystallized by layering a solution of 0.10 g (0.90 mmol) of *N*,*N*-dimethylpropylenediamine and 0.701 g (1.0 mmol) of $[Ni(BPh_4)_2]$ in 20 mL of ethyl acetate on top of a solution of 0.123 g (0.45 mmol) of 2,2′-dithiodibenzaldehyde in 10 mL of dichloromethane.

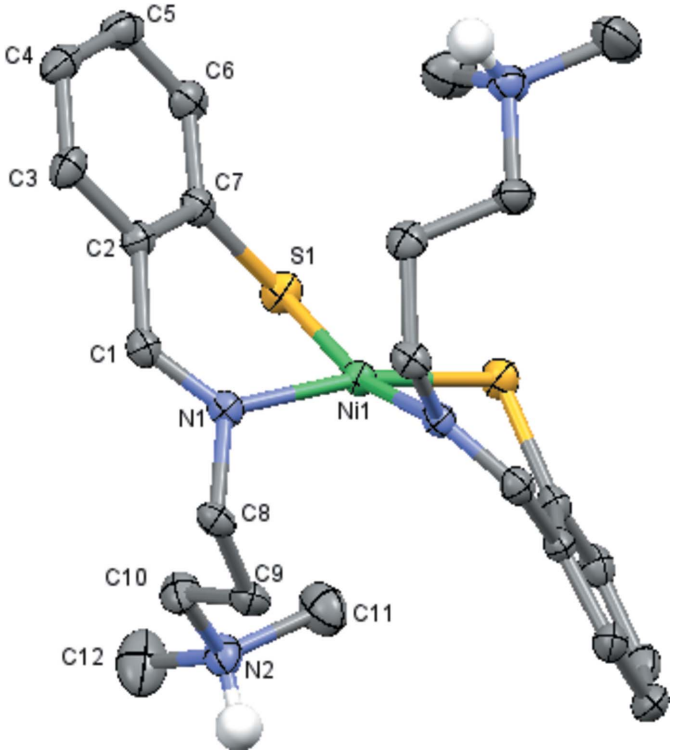


Figure 1
The molecular structure of the cation in the title compound, with displacement ellipsoids drawn at the 50% probability level. H atoms have been omitted for clarity.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3.

Acknowledgements

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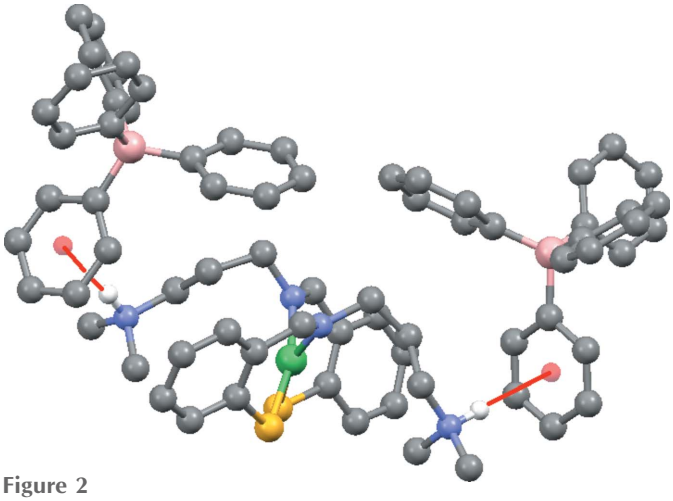

Figure 2
Part of the crystal structure of the title compound showing interactions between the protonated amine groups on the cation and the BPh_4 anions, indicated by red lines connecting the N—H hydrogen atom and the orange sphere representing the centroid of the phenyl ring.

Table 1
Selected geometric parameters (Å, °).

Ni1—S1	2.1665 (8)	Ni1—N1	1.922 (2)
S1—Ni1—S1^{i}	86.93 (4)	N1—Ni1—S1	91.85 (7)
N1—Ni1—S1^{i}	165.78 (7)	N1^{i}—Ni1—S1^{i}	91.85 (7)
N1^{i}—Ni1—S1	165.78 (7)	N1^{i}—Ni1—N1	92.73 (13)

Symmetry code: (i) $-x+1, y, -z+\frac{3}{2}$.

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

Cg is the centroid of the C25–C30 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···*Cg*	0.98	2.54	3.510 (3)	171

Table 3
Experimental details.

Crystal data	
Chemical formula	$[Ni(C_{12}H_{18}N_2S)_2](C_{24}H_{20}B)_2$
M_r	1141.81
Crystal system, space group	Monoclinic, *C*2/*c*
Temperature (K)	150
a, *b*, *c* (Å)	16.376 (2), 9.9864 (14), 36.605 (5)
β (°)	99.419 (4)
V (Å^3)	5905.6 (14)
Z	4
Radiation type	Mo *K*α
μ (mm^{-1})	0.45
Crystal size (mm)	0.63 × 0.60 × 0.34
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Numerical (*SADABS*; Bruker, 2012)
T_{min}, T_{max}	0.599, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	30373, 6401, 4454
R_{int}	0.076
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.641
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.054, 0.109, 1.05
No. of reflections	6401
No. of parameters	368
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.30, −0.71

Computer programs: *APEX2* (Bruker, 2013), *SAINT* (Bruker, 2013), *SHELXT* (Sheldrick, 2015), *XL* (Sheldrick, 2008), *OLEX2* (Dolomanov *et al.*, 2009).

Funding information

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References

Bruker (2012). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.

Bruker (2013). *APEX* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Sheldrick, G. M. (2015). *Acta Cryst.* A**71**, 3–8.
Zimmerman, J. R., Smucker, B. W., Dain, R. P., Van Stipdonk, M. J. & Eichhorn, D. M. (2011). *Inorg. Chim. Acta*, **373**, 54–61.

full crystallographic data

IUCrData (2017). **2**, x171067 [https://doi.org/10.1107/S2414314617010677]

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Crystal data

$[Ni(C_{12}H_{18}N_2S_2)_2](C_{24}H_{20}B)_2$
M_r = 1141.81
Monoclinic, $C2/c$
a = 16.376 (2) Å
b = 9.9864 (14) Å
c = 36.605 (5) Å
β = 99.419 (4)°
V = 5905.6 (14) Å^3
Z = 4
$F(000)$ = 2424
D_x = 1.284 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 4652 reflections
θ = 2.6–24.3°
μ = 0.45 mm^{-1}
T = 150 K
Block, violet
0.63 × 0.60 × 0.34 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: sealed X-ray tube
Graphite monochromator
Detector resolution: 5.6 pixels mm^{-1}
φ and ω scans
Absorption correction: numerical (SADABS; Bruker, 2012)
T_{min} = 0.599, T_{max} = 0.746
30373 measured reflections
6401 independent reflections
4454 reflections with $I > 2\sigma(I)$
R_{int} = 0.076
θ_{max} = 27.1°, θ_{min} = 3.1°
h = −20→20
k = −12→12
l = −46→46

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.109
S = 1.05
6401 reflections
368 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.029P)^2 + 11.6381P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.71 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. 1. Fixed Uiso
At 1.2 times of:
All C(H) groups, All C(H,H) groups, All N(H) groups
At 1.5 times of:
All C(H,H,H) groups
2.a Ternary CH refined with riding coordinates:
N2(H2)
2.b Secondary CH2 refined with riding coordinates:
C8(H8A,H8B), C9(H9A,H9B), C10(H10A,H10B)
2.c Aromatic/amide H refined with riding coordinates:
C18(H18), C3(H3), C17(H17), C15(H15), C1(H1), C16(H16), C14(H14), C6(H6), C32(H32), C5(H5), C4(H4), C33(H33), C34(H34), C36(H36), C35(H35), C24(H24), C26(H26), C23(H23), C20(H20), C21(H21), C30(H30), C22(H22), C29(H29), C27(H27), C28(H28)
2.d Idealised Me refined as rotating group:
C11(H11A,H11B,H11C), C12(H12A,H12B,H12C)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ni1	0.5000	0.94419 (5)	0.7500	0.01869 (13)
S1	0.40969 (4)	1.10165 (7)	0.75171 (2)	0.02515 (18)
N1	0.41471 (13)	0.8114 (2)	0.73848 (6)	0.0198 (5)
N2	0.40986 (14)	0.9765 (2)	0.62926 (6)	0.0281 (6)
H2	0.4357	0.9225	0.6120	0.034*
C18	0.50475 (16)	0.4326 (3)	0.66288 (7)	0.0220 (6)
H18	0.4515	0.4090	0.6518	0.026*
C3	0.26569 (17)	0.8453 (3)	0.80122 (8)	0.0271 (7)
H3	0.2463	0.7577	0.7984	0.033*
C2	0.32047 (16)	0.8932 (3)	0.77834 (7)	0.0211 (6)
C17	0.52741 (18)	0.4125 (3)	0.70094 (8)	0.0275 (7)
H17	0.4896	0.3758	0.7145	0.033*
C15	0.66161 (19)	0.4988 (3)	0.69757 (8)	0.0285 (7)
H15	0.7149	0.5210	0.7089	0.034*
C13	0.55877 (17)	0.4869 (2)	0.64052 (7)	0.0209 (6)
C1	0.34617 (17)	0.8015 (3)	0.75121 (7)	0.0218 (6)
H1	0.3107	0.7315	0.7426	0.026*
C31	0.45004 (16)	0.4282 (3)	0.57731 (7)	0.0208 (6)
C16	0.60599 (19)	0.4470 (3)	0.71857 (8)	0.0281 (6)
H16	0.6211	0.4356	0.7440	0.034*
C14	0.63840 (17)	0.5177 (3)	0.65982 (8)	0.0253 (6)
H14	0.6773	0.5526	0.6465	0.030*
C6	0.31900 (17)	1.1093 (3)	0.80796 (8)	0.0274 (7)
H6	0.3353	1.1985	0.8102	0.033*
C19	0.61271 (16)	0.4398 (3)	0.57707 (7)	0.0209 (6)
C32	0.37278 (16)	0.4651 (3)	0.58659 (8)	0.0247 (6)
H32	0.3711	0.5340	0.6035	0.030*
C5	0.26801 (18)	1.0579 (3)	0.83128 (8)	0.0318 (7)
H5	0.2522	1.1123	0.8495	0.038*
C25	0.52708 (16)	0.6677 (3)	0.58324 (8)	0.0215 (6)

C8	0.42913 (17)	0.7166 (3)	0.70892 (7)	0.0226 (6)
H8A	0.3794	0.6643	0.7011	0.027*
H8B	0.4734	0.6555	0.7186	0.027*
C7	0.34641 (16)	1.0285 (3)	0.78095 (7)	0.0223 (6)
C4	0.24024 (17)	0.9263 (3)	0.82782 (8)	0.0303 (7)
H4	0.2050	0.8932	0.8432	0.036*
C33	0.29891 (18)	0.4027 (3)	0.57146 (8)	0.0303 (7)
H33	0.2496	0.4292	0.5788	0.036*
C34	0.29856 (18)	0.3015 (3)	0.54565 (8)	0.0297 (7)
H34	0.2494	0.2591	0.5356	0.036*
C36	0.44618 (18)	0.3265 (3)	0.55081 (7)	0.0241 (6)
H36	0.4952	0.2989	0.5434	0.029*
C35	0.37274 (18)	0.2643 (3)	0.53491 (8)	0.0292 (7)
H35	0.3735	0.1980	0.5171	0.035*
C24	0.64779 (17)	0.3167 (3)	0.59048 (8)	0.0253 (6)
H24	0.6304	0.2786	0.6111	0.030*
C26	0.57679 (17)	0.7696 (3)	0.60160 (8)	0.0261 (6)
H26	0.6133	0.7481	0.6230	0.031*
C23	0.70681 (19)	0.2500 (3)	0.57433 (8)	0.0337 (7)
H23	0.7279	0.1686	0.5840	0.040*
C20	0.64204 (17)	0.4912 (3)	0.54601 (7)	0.0252 (6)
H20	0.6209	0.5721	0.5361	0.030*
C9	0.45220 (17)	0.7912 (3)	0.67557 (7)	0.0253 (6)
H9A	0.5018	0.8436	0.6835	0.030*
H9B	0.4645	0.7266	0.6574	0.030*
C21	0.70175 (18)	0.4253 (3)	0.52945 (8)	0.0337 (7)
H21	0.7194	0.4624	0.5088	0.040*
C30	0.47271 (19)	0.7095 (3)	0.55167 (8)	0.0328 (7)
H30	0.4379	0.6462	0.5385	0.039*
C22	0.7346 (2)	0.3050 (3)	0.54369 (8)	0.0371 (8)
H22	0.7749	0.2614	0.5329	0.045*
C10	0.38377 (18)	0.8832 (3)	0.65759 (8)	0.0294 (7)
H10A	0.3378	0.8291	0.6457	0.035*
H10B	0.3644	0.9360	0.6767	0.035*
C29	0.4683 (2)	0.8411 (3)	0.53907 (10)	0.0410 (8)
H29	0.4311	0.8639	0.5180	0.049*
C27	0.57369 (19)	0.9017 (3)	0.58911 (9)	0.0346 (8)
H27	0.6086	0.9654	0.6019	0.042*
C28	0.5191 (2)	0.9386 (3)	0.55781 (9)	0.0386 (8)
H28	0.5165	1.0267	0.5495	0.046*
C11	0.4715 (2)	1.0792 (3)	0.64582 (9)	0.0417 (8)
H11A	0.4503	1.1264	0.6651	0.063*
H11B	0.4813	1.1413	0.6270	0.063*
H11C	0.5225	1.0357	0.6560	0.063*
C12	0.3369 (2)	1.0444 (4)	0.60779 (10)	0.0535 (10)
H12A	0.2976	0.9785	0.5970	0.080*
H12B	0.3542	1.0973	0.5885	0.080*
H12C	0.3119	1.1014	0.6239	0.080*

B1	0.53614 (19)	0.5067 (3)	0.59512 (9)	0.0214 (7)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0205 (3)	0.0140 (2)	0.0217 (3)	0.000	0.0037 (2)	0.000
S1	0.0272 (4)	0.0168 (3)	0.0323 (4)	0.0024 (3)	0.0072 (3)	0.0020 (3)
N1	0.0215 (12)	0.0168 (11)	0.0205 (12)	0.0004 (9)	0.0020 (10)	0.0006 (9)
N2	0.0271 (14)	0.0309 (14)	0.0257 (14)	−0.0052 (11)	0.0028 (11)	0.0043 (11)
C18	0.0215 (14)	0.0193 (13)	0.0264 (15)	−0.0002 (11)	0.0080 (12)	0.0000 (12)
C3	0.0209 (15)	0.0306 (15)	0.0304 (17)	0.0036 (12)	0.0057 (13)	0.0045 (13)
C2	0.0198 (14)	0.0234 (13)	0.0197 (15)	0.0043 (11)	0.0019 (12)	0.0027 (11)
C17	0.0355 (17)	0.0231 (15)	0.0268 (16)	0.0032 (12)	0.0140 (14)	0.0013 (12)
C15	0.0333 (17)	0.0238 (14)	0.0265 (16)	−0.0030 (13)	−0.0005 (13)	−0.0022 (13)
C13	0.0249 (15)	0.0148 (13)	0.0235 (15)	0.0011 (11)	0.0058 (12)	−0.0006 (11)
C1	0.0216 (15)	0.0202 (13)	0.0227 (15)	−0.0010 (11)	0.0009 (12)	0.0008 (12)
C31	0.0238 (14)	0.0189 (13)	0.0195 (14)	0.0005 (11)	0.0033 (11)	0.0046 (11)
C16	0.0443 (18)	0.0236 (14)	0.0162 (14)	0.0084 (14)	0.0040 (13)	0.0005 (12)
C14	0.0261 (16)	0.0234 (15)	0.0269 (16)	−0.0033 (12)	0.0055 (13)	0.0032 (12)
C6	0.0253 (16)	0.0261 (15)	0.0294 (17)	0.0058 (12)	0.0007 (13)	−0.0009 (13)
C19	0.0200 (14)	0.0239 (14)	0.0182 (14)	−0.0049 (12)	0.0014 (11)	−0.0020 (12)
C32	0.0271 (16)	0.0226 (15)	0.0243 (15)	0.0015 (12)	0.0044 (12)	−0.0014 (12)
C5	0.0281 (16)	0.0417 (18)	0.0258 (16)	0.0114 (15)	0.0051 (13)	−0.0018 (14)
C25	0.0188 (14)	0.0219 (14)	0.0247 (15)	0.0015 (11)	0.0066 (12)	0.0012 (12)
C8	0.0278 (16)	0.0179 (13)	0.0210 (15)	−0.0010 (11)	0.0011 (12)	−0.0029 (11)
C7	0.0204 (14)	0.0223 (14)	0.0228 (15)	0.0040 (11)	−0.0001 (12)	0.0020 (11)
C4	0.0257 (16)	0.0400 (18)	0.0275 (16)	0.0073 (13)	0.0107 (13)	0.0057 (14)
C33	0.0210 (15)	0.0350 (16)	0.0346 (18)	0.0023 (13)	0.0036 (13)	0.0070 (14)
C34	0.0267 (16)	0.0303 (16)	0.0290 (17)	−0.0076 (13)	−0.0047 (13)	0.0062 (13)
C36	0.0264 (15)	0.0236 (14)	0.0228 (15)	0.0014 (12)	0.0056 (12)	0.0024 (12)
C35	0.0368 (18)	0.0244 (15)	0.0246 (16)	−0.0023 (13)	−0.0005 (14)	−0.0016 (12)
C24	0.0279 (16)	0.0264 (15)	0.0227 (15)	0.0027 (12)	0.0072 (13)	0.0028 (12)
C26	0.0264 (16)	0.0244 (15)	0.0274 (16)	−0.0002 (12)	0.0045 (13)	−0.0011 (12)
C23	0.0368 (19)	0.0320 (17)	0.0325 (18)	0.0129 (14)	0.0062 (15)	0.0018 (14)
C20	0.0232 (15)	0.0291 (15)	0.0226 (15)	0.0021 (12)	0.0018 (12)	0.0022 (12)
C9	0.0274 (16)	0.0258 (15)	0.0231 (16)	−0.0010 (12)	0.0050 (13)	−0.0060 (12)
C21	0.0340 (17)	0.0462 (19)	0.0227 (16)	−0.0015 (15)	0.0093 (13)	0.0014 (14)
C30	0.0345 (18)	0.0277 (16)	0.0337 (18)	−0.0060 (14)	−0.0011 (14)	0.0044 (14)
C22	0.0356 (18)	0.050 (2)	0.0288 (18)	0.0124 (16)	0.0132 (15)	−0.0058 (15)
C10	0.0286 (17)	0.0350 (16)	0.0246 (16)	−0.0058 (13)	0.0045 (13)	0.0067 (13)
C29	0.038 (2)	0.0376 (18)	0.045 (2)	0.0018 (15)	−0.0015 (16)	0.0166 (16)
C27	0.0342 (18)	0.0243 (15)	0.047 (2)	−0.0066 (13)	0.0123 (16)	−0.0037 (14)
C28	0.0411 (19)	0.0229 (15)	0.054 (2)	0.0015 (15)	0.0138 (17)	0.0105 (15)
C11	0.047 (2)	0.0361 (18)	0.042 (2)	−0.0135 (16)	0.0049 (16)	0.0022 (15)
C12	0.043 (2)	0.063 (2)	0.051 (2)	−0.0031 (19)	−0.0010 (17)	0.029 (2)
B1	0.0221 (17)	0.0225 (15)	0.0198 (17)	−0.0004 (13)	0.0043 (13)	0.0031 (13)

Geometric parameters (Å, º)

Ni1—S1	2.1665 (8)	C25—C30	1.402 (4)
Ni1—S1^{i}	2.1665 (8)	C25—B1	1.665 (4)
Ni1—N1^{i}	1.922 (2)	C8—H8A	0.9700
Ni1—N1	1.922 (2)	C8—H8B	0.9700
S1—C7	1.765 (3)	C8—C9	1.529 (4)
N1—C1	1.287 (3)	C4—H4	0.9300
N1—C8	1.485 (3)	C33—H33	0.9300
N2—H2	0.9800	C33—C34	1.383 (4)
N2—C10	1.507 (3)	C34—H34	0.9300
N2—C11	1.496 (4)	C34—C35	1.387 (4)
N2—C12	1.482 (4)	C36—H36	0.9300
C18—H18	0.9300	C36—C35	1.393 (4)
C18—C17	1.396 (4)	C35—H35	0.9300
C18—C13	1.409 (4)	C24—H24	0.9300
C3—H3	0.9300	C24—C23	1.383 (4)
C3—C2	1.408 (4)	C26—H26	0.9300
C3—C4	1.381 (4)	C26—C27	1.394 (4)
C2—C1	1.463 (4)	C23—H23	0.9300
C2—C7	1.414 (4)	C23—C22	1.391 (4)
C17—H17	0.9300	C20—H20	0.9300
C17—C16	1.385 (4)	C20—C21	1.396 (4)
C15—H15	0.9300	C9—H9A	0.9700
C15—C16	1.385 (4)	C9—H9B	0.9700
C15—C14	1.385 (4)	C9—C10	1.513 (4)
C13—C14	1.412 (4)	C21—H21	0.9300
C13—B1	1.654 (4)	C21—C22	1.384 (4)
C1—H1	0.9300	C30—H30	0.9300
C31—C32	1.411 (4)	C30—C29	1.391 (4)
C31—C36	1.399 (4)	C22—H22	0.9300
C31—B1	1.651 (4)	C10—H10A	0.9700
C16—H16	0.9300	C10—H10B	0.9700
C14—H14	0.9300	C29—H29	0.9300
C6—H6	0.9300	C29—C28	1.386 (4)
C6—C5	1.387 (4)	C27—H27	0.9300
C6—C7	1.406 (4)	C27—C28	1.383 (4)
C19—C24	1.411 (4)	C28—H28	0.9300
C19—C20	1.402 (4)	C11—H11A	0.9600
C19—B1	1.651 (4)	C11—H11B	0.9600
C32—H32	0.9300	C11—H11C	0.9600
C32—C33	1.392 (4)	C12—H12A	0.9600
C5—H5	0.9300	C12—H12B	0.9600
C5—C4	1.390 (4)	C12—H12C	0.9600
C25—C26	1.404 (4)		
S1—Ni1—S1^{i}	86.93 (4)	C32—C33—H33	119.8
N1—Ni1—S1^{i}	165.78 (7)	C34—C33—C32	120.3 (3)

N1^{i}—Ni1—S1	165.78 (7)	C34—C33—H33	119.8
N1—Ni1—S1	91.85 (7)	C33—C34—H34	120.6
N1^{i}—Ni1—S1^{i}	91.85 (7)	C33—C34—C35	118.9 (3)
N1^{i}—Ni1—N1	92.73 (13)	C35—C34—H34	120.6
C7—S1—Ni1	100.86 (9)	C31—C36—H36	118.3
C1—N1—Ni1	128.23 (19)	C35—C36—C31	123.4 (3)
C1—N1—C8	117.8 (2)	C35—C36—H36	118.3
C8—N1—Ni1	113.76 (16)	C34—C35—C36	119.9 (3)
C10—N2—H2	107.8	C34—C35—H35	120.1
C11—N2—H2	107.8	C36—C35—H35	120.1
C11—N2—C10	113.2 (2)	C19—C24—H24	118.5
C12—N2—H2	107.8	C23—C24—C19	123.0 (3)
C12—N2—C10	110.7 (2)	C23—C24—H24	118.5
C12—N2—C11	109.5 (3)	C25—C26—H26	118.6
C17—C18—H18	118.5	C27—C26—C25	122.8 (3)
C17—C18—C13	123.1 (3)	C27—C26—H26	118.6
C13—C18—H18	118.5	C24—C23—H23	120.0
C2—C3—H3	119.5	C24—C23—C22	119.9 (3)
C4—C3—H3	119.5	C22—C23—H23	120.0
C4—C3—C2	121.0 (3)	C19—C20—H20	118.7
C3—C2—C1	118.2 (2)	C21—C20—C19	122.5 (3)
C3—C2—C7	119.9 (2)	C21—C20—H20	118.7
C7—C2—C1	121.8 (2)	C8—C9—H9A	109.1
C18—C17—H17	119.9	C8—C9—H9B	109.1
C16—C17—C18	120.3 (3)	H9A—C9—H9B	107.9
C16—C17—H17	119.9	C10—C9—C8	112.4 (2)
C16—C15—H15	119.8	C10—C9—H9A	109.1
C16—C15—C14	120.5 (3)	C10—C9—H9B	109.1
C14—C15—H15	119.8	C20—C21—H21	119.9
C18—C13—C14	114.2 (2)	C22—C21—C20	120.2 (3)
C18—C13—B1	124.8 (2)	C22—C21—H21	119.9
C14—C13—B1	120.9 (2)	C25—C30—H30	118.4
N1—C1—C2	124.2 (2)	C29—C30—C25	123.1 (3)
N1—C1—H1	117.9	C29—C30—H30	118.4
C2—C1—H1	117.9	C23—C22—H22	120.4
C32—C31—B1	121.5 (2)	C21—C22—C23	119.2 (3)
C36—C31—C32	114.6 (2)	C21—C22—H22	120.4
C36—C31—B1	123.9 (2)	N2—C10—C9	113.7 (2)
C17—C16—H16	120.7	N2—C10—H10A	108.8
C15—C16—C17	118.6 (3)	N2—C10—H10B	108.8
C15—C16—H16	120.7	C9—C10—H10A	108.8
C15—C14—C13	123.3 (3)	C9—C10—H10B	108.8
C15—C14—H14	118.3	H10A—C10—H10B	107.7
C13—C14—H14	118.3	C30—C29—H29	119.8
C5—C6—H6	119.5	C28—C29—C30	120.3 (3)
C5—C6—C7	120.9 (3)	C28—C29—H29	119.8
C7—C6—H6	119.5	C26—C27—H27	119.7
C24—C19—B1	120.4 (2)	C28—C27—C26	120.5 (3)

C20—C19—C24	115.3 (2)	C28—C27—H27	119.7
C20—C19—B1	124.1 (2)	C29—C28—H28	120.8
C31—C32—H32	118.6	C27—C28—C29	118.5 (3)
C33—C32—C31	122.8 (3)	C27—C28—H28	120.8
C33—C32—H32	118.6	N2—C11—H11A	109.5
C6—C5—H5	119.5	N2—C11—H11B	109.5
C6—C5—C4	121.0 (3)	N2—C11—H11C	109.5
C4—C5—H5	119.5	H11A—C11—H11B	109.5
C26—C25—B1	123.7 (2)	H11A—C11—H11C	109.5
C30—C25—C26	114.8 (2)	H11B—C11—H11C	109.5
C30—C25—B1	121.3 (2)	N2—C12—H12A	109.5
N1—C8—H8A	109.4	N2—C12—H12B	109.5
N1—C8—H8B	109.4	N2—C12—H12C	109.5
N1—C8—C9	111.1 (2)	H12A—C12—H12B	109.5
H8A—C8—H8B	108.0	H12A—C12—H12C	109.5
C9—C8—H8A	109.4	H12B—C12—H12C	109.5
C9—C8—H8B	109.4	C13—B1—C25	112.0 (2)
C2—C7—S1	123.6 (2)	C31—B1—C13	112.1 (2)
C6—C7—S1	118.4 (2)	C31—B1—C25	108.8 (2)
C6—C7—C2	118.0 (2)	C19—B1—C13	107.1 (2)
C3—C4—C5	119.1 (3)	C19—B1—C31	107.8 (2)
C3—C4—H4	120.5	C19—B1—C25	109.1 (2)
C5—C4—H4	120.5		

Symmetry code: (i) $-x+1, y, -z+3/2$.

Hydrogen-bond geometry (Å, º)

Cg is the centroid of the C25–C30 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···*Cg*	0.98	2.54	3.510 (3)	171