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Di-μ-thiocyanato-κ^4N:N-bis({2,4-dibromo-6-[2-(methylamino)ethyliminomethyl]phenolato-κ^3N,N',O}nickel(II))

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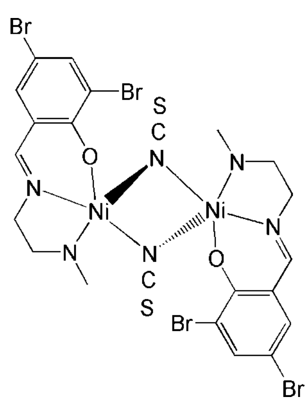
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.012 Å; R factor = 0.067; wR factor = 0.151; data-to-parameter ratio = 20.1.

The title complex, $[Ni_2(C_{11}H_{11}Br_2N_2O)_2(NCS)_2]$, is a thiocyanate-bridged dinuclear nickel(II) complex. The asymmetric unit contains two molecules. Both Ni atoms in each molecule have a square-pyramidal coordination geometry, and each center is bound by one O and two N atoms of one Schiff base ligand and by one N atom of a bridging thiocyanate ligand, which define the basal planes. N atoms from the bridging thiocyanate ligands occupy the apical positions.

Related literature

For related literature, see: Arıcı *et al.* (2005); Hebbachi & Benali-Cherif (2005); Henkel & Krebs (2004); Salmon *et al.* (2005); Sarı *et al.* (2006); Tshuva & Lippard (2004); Weston (2005).



Experimental

Crystal data

$[Ni_2(C_{10}H_{11}Br_2N_2O)_2(NCS)_2]$
M_r = 451.82
Monoclinic, $P2_1/n$
a = 9.2040 (18) Å
b = 19.833 (4) Å
c = 16.319 (3) Å
β = 100.71 (3)°
V = 2927.0 (10) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 6.92 mm^{-1}
T = 293 (2) K
0.43 × 0.40 × 0.38 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.155, T_{max} = 0.178 (expected range = 0.063–0.072)
25095 measured reflections
6938 independent reflections
2858 reflections with $I > 2\sigma(I)$
R_{int} = 0.139

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.066
$wR(F^2)$ = 0.150
S = 0.94
6938 reflections
345 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.65 e Å^{-3}
$\Delta\rho_{min}$ = −0.77 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O2^i	0.91	2.48	3.269 (9)	146
N5—H5A···O1^i	0.91	2.15	3.012 (9)	158
N5—H5A···Br2^i	0.91	2.86	3.500 (7)	129

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; 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: RN2034).

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supplementary materials

Acta Cryst. (2008). E**64**, m295 [**doi:10.1107/S1600536807068146**]

Di-μ-thiocyanato-κ^4N:N-bis({2,4-dibromo-6-[2-(methylamino)ethyliminomethyl]phenolato-κ^3N,N',O}nickel(II))

H.-W. Lin

Comment

The design of multidentate ligands and their metallosupramolecular chemistry are of great interest (Henkel & Krebs, 2004; Tshuva & Lippard, 2004; Weston, 2005). Schiff base ligands readily lead to the formation of diverse complexes with most metal ions (Arıcı *et al.*, 2005; Salmon *et al.*, 2005; Hebbachi & Benali-Cherif, 2005; Sarı *et al.*, 2006).

The two Ni centers in the title dinuclear nickel(II) complex are doubly-bridged by thiocyanato ligands. Both Ni atoms are five-coordinate and have square pyramidal geometry but both thiocyanate bridges are asymmetric where the distances are 2.643 (8) and 1.973 (8)Å for Ni1···N6 and Ni1—N3 respectively and 2.589 (8) and 1.978 (7)Å for Ni2···N3 and Ni2—N6 respectively. The Ni···Ni distance is 3.268 (3) Å.

Experimental

3,5-Dibromosalicylaldehyde (1.0 mmol, 280.0 mg), *N*-methylethane-1,2-diamine (1.0 mmol, 74.0 mg), NH_4NCS (1.0 mmol, 76.0 mg), and $Ni(NO_3)_2.6H_2O$ (1.0 mmol, 290.8 mg) were dissolved in a 50 ml me thanol solution. The mixture was stirred at reflux for half an hour to give a green solution. After keeping the solution in air for 15 days to allow slow evaporation, green block-like crystals were formed.

Refinement

H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.97 Å, N—H distances of 0.91 Å, and with U_{iso}(H) values set to 1.2U_{eq}(C,N) and 1.5U_{eq}(methyl C).

Figures

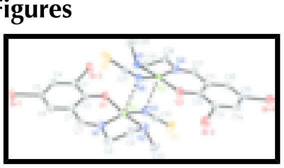


Fig. 1. The structure of (I) with displacement ellipsoids drawn at the 30% probability level. H atoms have been omitted for clarity.

Di-μ-thiocyanato-κ^4*N*:*N*-bis({2,4-dibromo-6-[2- (methylamino)ethyliminomethyl]phenolato-κ^3*N*,*N*',*O*}nickel(II))

Crystal data

$[Ni_2(C_{10}H_{11}Br_2N_2O)_2(NCS)_2]$	F_{000} = 1760

$M_r = 451.82$	$D_x = 2.051$ Mg m^{-3}
Monoclinic, $P21/n$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 9.2040$ (18) Å	Cell parameters from 1344 reflections
$b = 19.833$ (4) Å	$\theta = 2.4$–24.5°
$c = 16.319$ (3) Å	$\mu = 6.92$ mm^{-1}
$\beta = 100.71$ (3)°	$T = 293$ (2) K
$V = 2927.0$ (10) Å^3	Block, green
$Z = 8$	0.43 × 0.40 × 0.38 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer	6938 independent reflections
Radiation source: fine-focus sealed tube	2858 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.139$
$T = 293(2)$ K	$\theta_{max} = 28.3°$
ω scans	$\theta_{min} = 1.6°$
Absorption correction: multi-scan (SADABS; Bruker, 2000)	$h = -12 \rightarrow 12$
$T_{min} = 0.155$, $T_{max} = 0.178$	$k = -25 \rightarrow 25$
25095 measured reflections	$l = -21 \rightarrow 21$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.066$	H-atom parameters constrained
$wR(F^2) = 0.151$	$w = 1/[\sigma^2(F_o^2) + (0.0506P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.94$	$(\Delta/\sigma)_{max} < 0.001$
6938 reflections	$\Delta\rho_{max} = 0.65$ e Å^{-3}
345 parameters	$\Delta\rho_{min} = -0.77$ 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 $F^2 > \sigma(F^2)$ 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	0.59997 (12)	0.01132 (5)	0.24264 (7)	0.0378 (3)
Ni2	0.61799 (12)	0.12004 (5)	0.77631 (7)	0.0349 (3)
Br1	0.41051 (12)	0.33151 (5)	0.43009 (7)	0.0685 (4)
Br2	0.31619 (12)	0.05315 (5)	0.46208 (6)	0.0564 (3)
Br3	0.36394 (13)	0.17932 (5)	1.00163 (7)	0.0669 (4)
Br4	0.37706 (12)	0.45174 (5)	0.90757 (7)	0.0644 (3)
S1	0.8160 (4)	−0.18127 (14)	0.37004 (19)	0.0779 (10)
S2	0.8415 (4)	−0.07194 (15)	0.8944 (2)	0.0851 (10)
O1	0.4903 (6)	0.0452 (3)	0.3223 (4)	0.0440 (16)
O2	0.5198 (6)	0.1600 (3)	0.8571 (3)	0.0468 (16)
N1	0.6349 (8)	0.1003 (3)	0.2016 (4)	0.045 (2)
N2	0.6704 (8)	−0.0212 (4)	0.1394 (4)	0.050 (2)
H2A	0.6074	−0.0543	0.1164	0.060*
N3	0.6368 (8)	−0.0765 (4)	0.2996 (5)	0.049 (2)
N4	0.6322 (8)	0.2040 (3)	0.7179 (5)	0.047 (2)
N5	0.6960 (8)	0.0799 (3)	0.6800 (4)	0.0449 (19)
H5A	0.6473	0.0404	0.6660	0.054*
N6	0.6537 (9)	0.0353 (4)	0.8409 (5)	0.049 (2)
C1	0.5295 (10)	0.1639 (4)	0.3041 (5)	0.041 (2)
C2	0.4755 (10)	0.1078 (4)	0.3426 (5)	0.041 (2)
C3	0.3982 (9)	0.1240 (4)	0.4082 (5)	0.040 (2)
C4	0.3789 (10)	0.1898 (4)	0.4331 (6)	0.047 (2)
H4	0.3275	0.1986	0.4759	0.056*
C5	0.4366 (10)	0.2416 (4)	0.3938 (6)	0.045 (2)
C6	0.5112 (10)	0.2302 (4)	0.3303 (6)	0.052 (3)
H6	0.5497	0.2662	0.3046	0.062*
C7	0.6038 (10)	0.1557 (4)	0.2333 (6)	0.048 (3)
H7	0.6311	0.1950	0.2088	0.057*
C8	0.7089 (11)	0.0998 (5)	0.1295 (6)	0.057 (3)
H8A	0.8153	0.0975	0.1475	0.068*
H8B	0.6848	0.1403	0.0963	0.068*
C9	0.6515 (11)	0.0371 (5)	0.0789 (6)	0.060 (3)
H9A	0.5482	0.0426	0.0537	0.072*
H9B	0.7076	0.0293	0.0351	0.072*
C10	0.7144 (10)	−0.1202 (5)	0.3285 (6)	0.045 (2)
C11	0.5255 (9)	0.2750 (4)	0.8123 (6)	0.041 (2)
C12	0.4913 (9)	0.2237 (4)	0.8649 (5)	0.037 (2)
C13	0.4210 (10)	0.2452 (4)	0.9302 (5)	0.045 (2)
C14	0.3902 (10)	0.3114 (4)	0.9432 (6)	0.048 (3)
H14	0.3449	0.3234	0.9875	0.057*
C15	0.4267 (9)	0.3604 (4)	0.8902 (6)	0.043 (2)
C16	0.4953 (10)	0.3435 (4)	0.8254 (6)	0.047 (2)
H16	0.5216	0.3766	0.7906	0.057*
C17	0.5928 (10)	0.2625 (5)	0.7395 (6)	0.052 (3)
H17	0.6081	0.2992	0.7066	0.062*

C18	0.6914 (11)	0.1982 (4)	0.6398 (6)	0.059 (3)
H18A	0.7973	0.2059	0.6502	0.071*
H18B	0.6442	0.2305	0.5987	0.071*
C19	0.6558 (11)	0.1265 (4)	0.6100 (6)	0.056 (3)
H19A	0.5510	0.1226	0.5872	0.067*
H19B	0.7103	0.1153	0.5664	0.067*
C20	0.8556 (10)	0.0652 (5)	0.6983 (6)	0.061 (3)
H20A	0.8725	0.0239	0.7293	0.091*
H20B	0.9068	0.1014	0.7305	0.091*
H20C	0.8914	0.0607	0.6469	0.091*
C21	0.7334 (10)	−0.0092 (5)	0.8631 (6)	0.044 (2)
C22	0.8217 (10)	−0.0497 (5)	0.1533 (6)	0.071 (3)
H22A	0.8432	−0.0657	0.1013	0.107*
H22B	0.8283	−0.0865	0.1921	0.107*
H22C	0.8917	−0.0154	0.1755	0.107*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0465 (8)	0.0318 (6)	0.0374 (7)	0.0009 (5)	0.0140 (6)	0.0000 (5)
Ni2	0.0449 (7)	0.0264 (6)	0.0357 (7)	0.0005 (5)	0.0140 (6)	−0.0007 (5)
Br1	0.0776 (8)	0.0362 (6)	0.0944 (9)	0.0020 (5)	0.0229 (7)	−0.0143 (6)
Br2	0.0783 (8)	0.0426 (6)	0.0560 (7)	−0.0078 (5)	0.0329 (6)	−0.0048 (5)
Br3	0.0927 (9)	0.0551 (7)	0.0637 (7)	0.0114 (6)	0.0426 (7)	0.0071 (6)
Br4	0.0686 (8)	0.0395 (6)	0.0873 (9)	0.0079 (5)	0.0202 (7)	−0.0125 (6)
S1	0.101 (2)	0.0635 (19)	0.069 (2)	0.0369 (18)	0.0174 (19)	0.0090 (16)
S2	0.088 (2)	0.068 (2)	0.106 (3)	0.0307 (18)	0.034 (2)	0.0328 (19)
O1	0.056 (4)	0.031 (3)	0.048 (4)	−0.004 (3)	0.017 (3)	−0.003 (3)
O2	0.063 (4)	0.037 (4)	0.046 (4)	0.005 (3)	0.023 (3)	0.001 (3)
N1	0.059 (5)	0.036 (4)	0.043 (5)	0.003 (4)	0.015 (4)	−0.001 (4)
N2	0.051 (5)	0.047 (5)	0.053 (5)	0.008 (4)	0.014 (4)	−0.003 (4)
N3	0.053 (6)	0.034 (4)	0.058 (6)	0.003 (4)	0.009 (4)	−0.006 (4)
N4	0.066 (6)	0.032 (4)	0.050 (5)	−0.007 (4)	0.027 (4)	0.001 (4)
N5	0.052 (5)	0.043 (5)	0.043 (5)	−0.003 (4)	0.018 (4)	−0.002 (4)
N6	0.064 (6)	0.038 (5)	0.044 (5)	0.003 (4)	0.012 (4)	0.008 (4)
C1	0.047 (6)	0.035 (5)	0.041 (6)	−0.004 (4)	0.006 (5)	−0.005 (4)
C2	0.045 (6)	0.042 (6)	0.032 (6)	−0.002 (5)	−0.003 (5)	0.001 (4)
C3	0.048 (6)	0.029 (5)	0.043 (6)	−0.007 (4)	0.009 (5)	0.005 (4)
C4	0.048 (6)	0.043 (6)	0.049 (6)	0.005 (5)	0.008 (5)	−0.006 (5)
C5	0.051 (6)	0.029 (5)	0.052 (7)	0.014 (5)	−0.001 (5)	0.005 (5)
C6	0.052 (7)	0.038 (6)	0.064 (7)	−0.007 (5)	0.004 (6)	0.002 (5)
C7	0.056 (7)	0.039 (6)	0.048 (7)	−0.001 (5)	0.010 (5)	0.002 (5)
C8	0.073 (8)	0.055 (6)	0.049 (7)	−0.002 (5)	0.031 (6)	0.008 (5)
C9	0.077 (8)	0.058 (7)	0.047 (7)	−0.006 (6)	0.015 (6)	0.008 (6)
C10	0.040 (6)	0.053 (6)	0.043 (6)	−0.009 (5)	0.012 (5)	−0.007 (5)
C11	0.038 (6)	0.033 (5)	0.052 (6)	−0.004 (4)	0.007 (5)	−0.011 (5)
C12	0.040 (6)	0.034 (5)	0.035 (6)	−0.008 (4)	−0.001 (5)	0.000 (4)
C13	0.054 (6)	0.046 (6)	0.036 (6)	0.007 (5)	0.014 (5)	0.003 (4)

C14	0.065 (7)	0.038 (6)	0.044 (6)	0.001 (5)	0.019 (5)	−0.012 (5)
C15	0.033 (6)	0.039 (5)	0.057 (7)	0.006 (4)	0.009 (5)	−0.018 (5)
C16	0.056 (7)	0.032 (5)	0.052 (7)	0.000 (5)	0.007 (5)	0.005 (5)
C17	0.072 (7)	0.040 (6)	0.046 (6)	0.001 (5)	0.017 (6)	0.012 (5)
C18	0.086 (8)	0.044 (6)	0.055 (7)	−0.007 (5)	0.032 (6)	−0.003 (5)
C19	0.069 (7)	0.045 (6)	0.059 (7)	−0.006 (5)	0.025 (6)	0.003 (5)
C20	0.055 (7)	0.063 (7)	0.070 (8)	−0.003 (6)	0.025 (6)	−0.017 (6)
C21	0.046 (6)	0.046 (6)	0.039 (6)	−0.008 (5)	0.010 (5)	0.005 (5)
C22	0.056 (7)	0.078 (8)	0.089 (9)	0.018 (6)	0.040 (7)	0.002 (7)

Geometric parameters (Å, °)

Ni1—O1	1.911 (6)	C2—C3	1.428 (11)
Ni1—N1	1.934 (7)	C3—C4	1.388 (11)
Ni1—N2	2.019 (7)	C4—C5	1.370 (11)
Ni1—N3	1.973 (8)	C4—H4	0.9300
Ni1—N6^{i}	2.643 (8)	C5—C6	1.365 (12)
Ni2—O2	1.904 (5)	C6—H6	0.9300
Ni2—N3^{i}	2.589 (8)	C7—H7	0.9300
Ni2—N4	1.935 (7)	C8—C9	1.532 (12)
Ni2—N6	1.978 (7)	C8—H8A	0.9700
Ni2—N5	2.010 (7)	C8—H8B	0.9700
Br1—C5	1.907 (8)	C9—H9A	0.9700
Br2—C3	1.888 (8)	C9—H9B	0.9700
Br3—C13	1.889 (9)	C11—C12	1.404 (11)
Br4—C15	1.902 (8)	C11—C16	1.410 (11)
S1—C10	1.602 (10)	C11—C17	1.460 (12)
S2—C21	1.617 (10)	C12—C13	1.412 (11)
O1—C2	1.299 (9)	C13—C14	1.369 (11)
O2—C12	1.301 (9)	C14—C15	1.383 (11)
N1—C7	1.270 (10)	C14—H14	0.9300
N1—C8	1.466 (10)	C15—C16	1.372 (11)
N2—C22	1.481 (10)	C16—H16	0.9300
N2—C9	1.509 (10)	C17—H17	0.9300
N2—H2A	0.9100	C18—C19	1.519 (11)
N3—C10	1.166 (10)	C18—H18A	0.9700
N4—C17	1.283 (10)	C18—H18B	0.9700
N4—C18	1.481 (10)	C19—H19A	0.9700
N5—C19	1.462 (10)	C19—H19B	0.9700
N5—C20	1.472 (10)	C20—H20A	0.9600
N5—H5A	0.9100	C20—H20B	0.9600
N6—C21	1.161 (10)	C20—H20C	0.9600
C1—C6	1.403 (11)	C22—H22A	0.9600
C1—C2	1.412 (11)	C22—H22B	0.9600
C1—C7	1.457 (11)	C22—H22C	0.9600
O1—Ni1—N1	93.3 (3)	N1—C7—H7	116.8
O1—Ni1—N3	93.2 (3)	C1—C7—H7	116.8
N1—Ni1—N3	160.5 (3)	N1—C8—C9	105.8 (7)

O1—Ni1—N2	166.4 (3)	N1—C8—H8A	110.6
N1—Ni1—N2	84.4 (3)	C9—C8—H8A	110.6
N3—Ni1—N2	93.3 (3)	N1—C8—H8B	110.6
O1—Ni1—N6^{i}	86.9 (3)	C9—C8—H8B	110.6
N1—Ni1—N6^{i}	109.2 (3)	H8A—C8—H8B	108.7
N2—Ni1—N6^{i}	81.3 (3)	N2—C9—C8	106.5 (8)
N3—Ni1—N6^{i}	89.5 (3)	N2—C9—H9A	110.4
O2—Ni2—N4	93.9 (3)	C8—C9—H9A	110.4
O2—Ni2—N6	92.2 (3)	N2—C9—H9B	110.4
N4—Ni2—N6	166.8 (3)	C8—C9—H9B	110.4
O2—Ni2—N5	172.3 (3)	H9A—C9—H9B	108.6
N4—Ni2—N5	83.6 (3)	N3—C10—S1	177.8 (9)
N6—Ni2—N5	91.8 (3)	C12—C11—C16	122.2 (8)
O2—Ni2—N3^{i}	88.0 (3)	C12—C11—C17	123.5 (8)
N4—Ni2—N3^{i}	101.0 (3)	C16—C11—C17	114.4 (8)
N5—Ni2—N3^{i}	85.2 (3)	O2—C12—C11	124.9 (8)
N6—Ni2—N3^{i}	91.0 (3)	O2—C12—C13	119.7 (8)
C2—O1—Ni1	127.1 (6)	C11—C12—C13	115.4 (8)
C12—O2—Ni2	127.0 (5)	C14—C13—C12	123.0 (8)
C7—N1—C8	120.3 (8)	C14—C13—Br3	118.6 (7)
C7—N1—Ni1	125.8 (6)	C12—C13—Br3	118.4 (6)
C8—N1—Ni1	113.8 (6)	C13—C14—C15	119.7 (8)
C22—N2—C9	112.5 (7)	C13—C14—H14	120.1
C22—N2—Ni1	115.6 (6)	C15—C14—H14	120.1
C9—N2—Ni1	106.6 (5)	C16—C15—C14	120.7 (8)
C22—N2—H2A	107.2	C16—C15—Br4	120.4 (7)
C9—N2—H2A	107.2	C14—C15—Br4	118.9 (6)
Ni1—N2—H2A	107.2	C15—C16—C11	119.0 (8)
C10—N3—Ni1	152.4 (7)	C15—C16—H16	120.5
C17—N4—C18	118.3 (7)	C11—C16—H16	120.5
C17—N4—Ni2	126.4 (6)	N4—C17—C11	124.1 (8)
C18—N4—Ni2	115.2 (6)	N4—C17—H17	117.9
C19—N5—C20	112.4 (7)	C11—C17—H17	117.9
C19—N5—Ni2	106.6 (5)	N4—C18—C19	104.9 (7)
C20—N5—Ni2	114.1 (6)	N4—C18—H18A	110.8
C19—N5—H5A	107.9	C19—C18—H18A	110.8
C20—N5—H5A	107.9	N4—C18—H18B	110.8
Ni2—N5—H5A	107.9	C19—C18—H18B	110.8
C21—N6—Ni2	147.6 (7)	H18A—C18—H18B	108.9
C6—C1—C2	122.1 (8)	N5—C19—C18	109.5 (8)
C6—C1—C7	116.5 (8)	N5—C19—H19A	109.8
C2—C1—C7	121.4 (8)	C18—C19—H19A	109.8
O1—C2—C1	125.3 (8)	N5—C19—H19B	109.8
O1—C2—C3	119.8 (8)	C18—C19—H19B	109.8
C1—C2—C3	115.0 (8)	H19A—C19—H19B	108.2
C4—C3—C2	122.7 (8)	N5—C20—H20A	109.5
C4—C3—Br2	118.6 (7)	N5—C20—H20B	109.5

C2—C3—Br2	118.7 (6)	H20A—C20—H20B	109.5
C5—C4—C3	119.1 (8)	N5—C20—H20C	109.5
C5—C4—H4	120.4	H20A—C20—H20C	109.5
C3—C4—H4	120.4	H20B—C20—H20C	109.5
C6—C5—C4	121.6 (8)	N6—C21—S2	178.9 (9)
C6—C5—Br1	120.1 (7)	N2—C22—H22A	109.5
C4—C5—Br1	118.3 (7)	N2—C22—H22B	109.5
C5—C6—C1	119.5 (9)	H22A—C22—H22B	109.5
C5—C6—H6	120.2	N2—C22—H22C	109.5
C1—C6—H6	120.2	H22A—C22—H22C	109.5
N1—C7—C1	126.3 (8)	H22B—C22—H22C	109.5

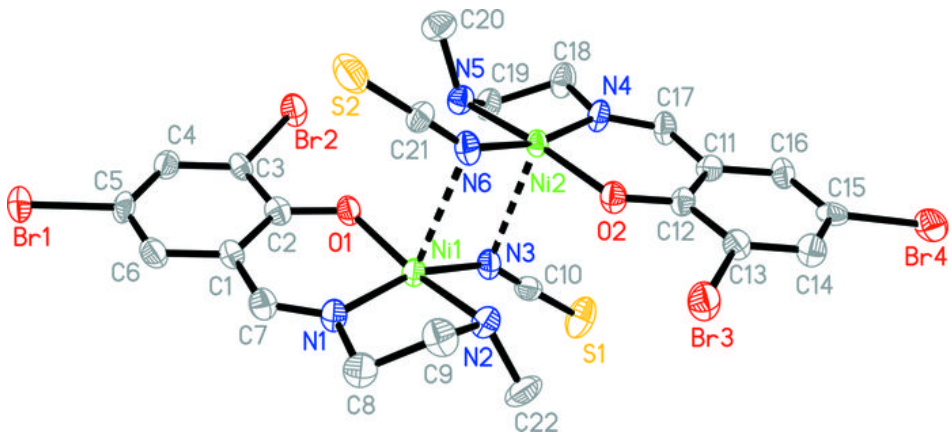
Symmetry codes: (i) $-x+1$, $-y$, $-z+1$.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2A···O2^{i}	0.91	2.48	3.269 (9)	146
N5—H5A···O1^{i}	0.91	2.15	3.012 (9)	158
N5—H5A···Br2^{i}	0.91	2.86	3.500 (7)	129

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

Fig. 1


C20
C18
N5
C19
N4
C17
S2
Br2
C4
C21
C11
C16
C3
N6
Ni2
C15
C5
Br1
C2
O1
O2
C12
Br4
Ni1
N3
C6
C1
C10
C13
C14
C7
N1
C9
N2
S1
Br3
C8
C22