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Bis{2,4-dibromo-6-[3-(cyclohexylammonio)propyliminomethyl]phenolato-κ^2N,O}bis(thiocyanato-κN)nickel(II) methanol disolvate

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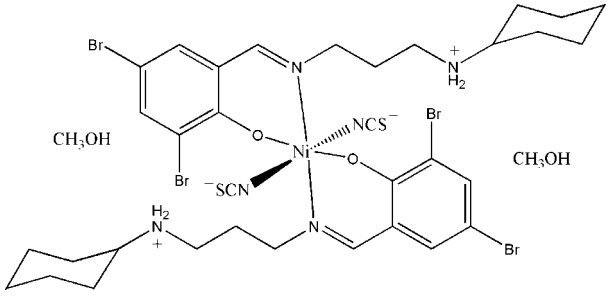
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.007 Å; R factor = 0.045; wR factor = 0.107; data-to-parameter ratio = 18.5.

The title centrosymmetric Schiff base nickel(II) complex, $[Ni(NCS)_2(C_{16}H_{22}Br_2N_2O)_2]\cdot 2CH_3OH$, consists of a mononuclear complex molecule and two solvent methanol molecules. The Ni^{II} atom lies on an inversion centre and is six-coordinated by the imine N and phenolate O atoms of the two Schiff base ligands and by the N atoms of two thiocyanate ligands, in an octahedral coordination geometry. The cyclohexyl rings adopt chair conformations.

Related literature

For related structures, see: Diao (2007); Yuan & Zhang (2005); Yuan *et al.* (2007); Li *et al.* (2007); Li & Wang (2007).



Experimental

Crystal data

$[Ni(NCS)_2(C_{16}H_{22}Br_2N_2O)_2]\cdot 2CH_4O$
M_r = 1075.31
Triclinic, $P\overline{1}$
a = 9.3410 (19) Å
b = 10.957 (2) Å
c = 12.210 (2) Å
α = 108.28 (3)°
β = 104.21 (3)°
γ = 100.80 (3)°
V = 1101.8 (4) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 4.21 mm^{-1}
T = 298 (2) K
0.27 × 0.23 × 0.22 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.397, T_{max} = 0.458
(expected range = 0.343–0.396)
8978 measured reflections
4504 independent reflections
2992 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.107
S = 1.01
4504 reflections
243 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.60 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); 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: SJ2329).

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supplementary materials

Acta Cryst. (2007). E**63**, m2376 [**doi:10.1107/S1600536807040238**]

Bis{2,4-dibromo-6-[3-(cyclohexylammonio)propyliminomethyl]phenolato-κ^2N,O}bis(thiocyanato-κN)nickel(II) methanol disolvate

M. Liu, W.-B. Yuan, H.-W. Xu, Q. Zhang and J.-X. Li

Comment

Recently, we have reported the structures of a few Schiff base copper(II) and zinc(II) complexes (Yuan & Zhang, 2005; Yuan *et al.*, 2007). As an extension of our investigations in this area we report herein the title new mononuclear Schiff base nickel(II) complex.

The complex consists of a mononuclear complex molecule and two lattice methanol molecules (Fig. 1). The Ni^{II} atom, lying on the inversion centre, is six-coordinated by two imine N and two phenolic O atoms from two Schiff base ligands and by two N atoms from two thiocyanate ligands, in octahedral coordination. The bond lengths and angles to the Ni(II) atom are comparable to the values in other similar complexes (Diao, 2007; Li *et al.*, 2007; Li & Wang, 2007). The cyclohexyl rings adopt chair conformations.

Experimental

3,5-Dibromo-2-hydroxybenzaldehyde (1.0 mmol, 280.0 mg), *N*-cyclohexylpropane-1,3-diamine (1.0 mmol, 156.2 mg), and nickel nitrate hexahydrate (0.5 mmol, 145.4 mg) were dissolved in a methanol solution (50 ml). The mixture was stirred at room temperature for 30 min and filtered. After keeping the filtrate in air for 12 days, green block-shaped crystals were formed.

Refinement

All H-atoms were positioned geometrically and refined using a riding model with C—H = 0.93 Å, $U_{iso} = 1.2U_{eq}$ (C) for aromatic 0.97 Å, $U_{iso} = 1.2U_{eq}$ (C) for CH_2, 0.96 Å, $U_{iso} = 1.5U_{eq}$ (C) for CH_3, 0.90 Å, $U_{iso} = 1.2U_{eq}$ (N) for NH and 0.82 Å, $U_{iso} = 1.5U_{eq}$ (O) for OH atoms.

Figures

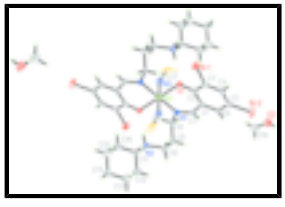


Fig. 1. The structure of (I). Displacement ellipsoids are drawn at the 30% probability level. Labelled atoms are related to unlabelled atoms by the symmetry operation $-x + 2, -y + 1, -z$.

Bis{2,4-dibromo-6-[3-(cyclohexylammonio)propyliminomethyl]phenolato- κ^2N,O}bis(thiocyanato-κN)nickel(II) methanol disolvate

Crystal data

$[Ni(NCS)_2(C_{16}H_{22}Br_2N_2O)_2]\cdot 2CH_4O$	$Z = 1$
$M_r = 1075.31$	$F_{000} = 542$
Triclinic, $P\overline{1}$	$D_x = 1.621$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 9.3410$ (19) Å	Cell parameters from 1932 reflections
$b = 10.957$ (2) Å	$\theta = 2.3$–24.9º
$c = 12.210$ (2) Å	$\mu = 4.21$ mm^{-1}
$\alpha = 108.28$ (3)º	$T = 298$ (2) K
$\beta = 104.21$ (3)º	Block, green
$\gamma = 100.80$ (3)º	0.27 × 0.23 × 0.22 mm
$V = 1101.8$ (4) Å^3	

Data collection

Bruker SMART 1000 CCD area-detector diffractometer	4504 independent reflections
Radiation source: fine-focus sealed tube	2992 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.033$
$T = 298$(2) K	$\theta_{max} = 26.5$º
ω scans	$\theta_{min} = 1.9$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -11\rightarrow11$
$T_{min} = 0.397$, $T_{max} = 0.458$	$k = -13\rightarrow13$
8978 measured reflections	$l = -15\rightarrow15$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.045$	H-atom parameters constrained
$wR(F^2) = 0.107$	$w = 1/[\sigma^2(F_o^2) + (0.048P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.01$	$(\Delta/\sigma)_{max} < 0.001$
4504 reflections	$\Delta\rho_{max} = 0.60$ e Å^{-3}
243 parameters	$\Delta\rho_{min} = -0.32$ 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	1.0000	0.5000	0.0000	0.02932 (18)
Br1	1.51132 (5)	0.62678 (5)	0.30412 (4)	0.05920 (18)
Br2	1.33026 (6)	0.98998 (5)	0.64540 (4)	0.06664 (19)
S1	0.67133 (19)	0.12546 (13)	0.02759 (16)	0.0838 (5)
O1	1.1701 (3)	0.5367 (2)	0.1599 (2)	0.0343 (6)
O2	0.4154 (4)	0.6690 (5)	0.7706 (4)	0.0961 (14)
H2	0.3910	0.7163	0.8256	0.144*
N1	0.8749 (3)	0.5875 (3)	0.1069 (3)	0.0308 (7)
N2	0.7392 (4)	0.6953 (3)	−0.1414 (3)	0.0370 (8)
H2A	0.6383	0.6774	−0.1815	0.044*
H2B	0.7599	0.6164	−0.1507	0.044*
N3	0.8862 (4)	0.3162 (3)	−0.0011 (3)	0.0406 (8)
C1	1.0902 (5)	0.6977 (4)	0.2983 (3)	0.0346 (9)
C2	1.2019 (4)	0.6386 (4)	0.2618 (3)	0.0336 (9)
C3	1.3531 (5)	0.6978 (4)	0.3463 (4)	0.0369 (10)
C4	1.3914 (5)	0.8006 (4)	0.4567 (3)	0.0428 (11)
H4	1.4930	0.8359	0.5086	0.051*
C5	1.2775 (5)	0.8511 (4)	0.4899 (3)	0.0402 (10)
C6	1.1291 (5)	0.8001 (4)	0.4125 (3)	0.0391 (10)
H6	1.0527	0.8340	0.4362	0.047*
C7	0.9310 (5)	0.6557 (4)	0.2211 (4)	0.0357 (9)
H7	0.8612	0.6817	0.2597	0.043*
C8	0.7085 (4)	0.5674 (4)	0.0512 (4)	0.0361 (9)
H8A	0.6524	0.5346	0.0983	0.043*
H8B	0.6724	0.4997	−0.0308	0.043*
C9	0.6743 (5)	0.6966 (4)	0.0459 (4)	0.0430 (10)
H9A	0.5664	0.6750	−0.0007	0.052*
H9B	0.6897	0.7563	0.1283	0.052*
C10	0.7701 (5)	0.7713 (4)	−0.0092 (4)	0.0411 (10)
H10A	0.7485	0.8567	0.0012	0.049*
H10B	0.8784	0.7896	0.0344	0.049*
C11	0.8317 (5)	0.7682 (4)	−0.1982 (4)	0.0402 (10)
H11	0.9403	0.7983	−0.1472	0.048*

C12	0.7835 (9)	0.8882 (6)	−0.2053 (5)	0.106 (3)
H12A	0.7954	0.9484	−0.1240	0.127*
H12B	0.6755	0.8605	−0.2540	0.127*
C13	0.8795 (9)	0.9614 (5)	−0.2620 (5)	0.105 (3)
H13A	0.8441	1.0377	−0.2675	0.125*
H13B	0.9864	0.9949	−0.2099	0.125*
C14	0.8688 (6)	0.8722 (5)	−0.3856 (4)	0.0546 (12)
H14A	0.9368	0.9200	−0.4168	0.066*
H14B	0.7642	0.8467	−0.4406	0.066*
C15	0.9127 (8)	0.7495 (5)	−0.3811 (5)	0.0849 (19)
H15A	1.0213	0.7746	−0.3347	0.102*
H15B	0.8973	0.6894	−0.4633	0.102*
C16	0.8180 (7)	0.6767 (5)	−0.3229 (5)	0.0758 (17)
H16A	0.7106	0.6432	−0.3740	0.091*
H16B	0.8535	0.6005	−0.3174	0.091*
C17	0.7955 (5)	0.2382 (4)	0.0099 (4)	0.0410 (10)
C18	0.2958 (8)	0.6214 (7)	0.6636 (6)	0.101 (2)
H18A	0.2636	0.6950	0.6497	0.151*
H18B	0.2112	0.5605	0.6683	0.151*
H18C	0.3286	0.5753	0.5976	0.151*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0307 (4)	0.0273 (4)	0.0304 (4)	0.0080 (3)	0.0130 (3)	0.0094 (3)
Br1	0.0371 (3)	0.0546 (3)	0.0626 (3)	0.0149 (2)	0.0096 (2)	−0.0039 (2)
Br2	0.0754 (4)	0.0546 (3)	0.0433 (3)	0.0061 (3)	0.0193 (3)	−0.0090 (2)
S1	0.0967 (11)	0.0381 (8)	0.1335 (14)	0.0095 (7)	0.0855 (11)	0.0235 (8)
O1	0.0354 (15)	0.0317 (15)	0.0306 (15)	0.0110 (12)	0.0085 (12)	0.0059 (12)
O2	0.073 (3)	0.122 (4)	0.073 (3)	0.060 (3)	0.012 (2)	0.002 (3)
N1	0.0344 (18)	0.0296 (18)	0.0328 (18)	0.0106 (14)	0.0163 (15)	0.0124 (15)
N2	0.042 (2)	0.0313 (18)	0.0363 (19)	0.0127 (16)	0.0131 (16)	0.0095 (16)
N3	0.040 (2)	0.033 (2)	0.049 (2)	0.0071 (17)	0.0175 (17)	0.0158 (17)
C1	0.043 (2)	0.032 (2)	0.031 (2)	0.0103 (19)	0.0155 (19)	0.0130 (18)
C2	0.038 (2)	0.030 (2)	0.034 (2)	0.0088 (18)	0.0141 (18)	0.0133 (19)
C3	0.034 (2)	0.033 (2)	0.044 (2)	0.0106 (18)	0.0155 (19)	0.012 (2)
C4	0.041 (3)	0.035 (2)	0.035 (2)	0.006 (2)	0.003 (2)	0.002 (2)
C5	0.053 (3)	0.033 (2)	0.028 (2)	0.006 (2)	0.014 (2)	0.0052 (19)
C6	0.049 (3)	0.040 (2)	0.033 (2)	0.016 (2)	0.023 (2)	0.0115 (19)
C7	0.039 (2)	0.034 (2)	0.040 (2)	0.0135 (19)	0.0224 (19)	0.013 (2)
C8	0.034 (2)	0.042 (2)	0.036 (2)	0.0140 (19)	0.0178 (18)	0.0133 (19)
C9	0.042 (2)	0.050 (3)	0.042 (2)	0.023 (2)	0.016 (2)	0.016 (2)
C10	0.054 (3)	0.032 (2)	0.041 (2)	0.016 (2)	0.019 (2)	0.014 (2)
C11	0.043 (2)	0.037 (2)	0.037 (2)	0.009 (2)	0.010 (2)	0.013 (2)
C12	0.228 (8)	0.070 (4)	0.096 (5)	0.090 (5)	0.119 (5)	0.054 (4)
C13	0.216 (8)	0.050 (3)	0.082 (4)	0.043 (4)	0.086 (5)	0.039 (3)
C14	0.061 (3)	0.062 (3)	0.052 (3)	0.019 (3)	0.025 (2)	0.030 (3)
C15	0.131 (6)	0.064 (4)	0.101 (5)	0.040 (4)	0.081 (4)	0.045 (4)

C16	0.126 (5)	0.047 (3)	0.085 (4)	0.033 (3)	0.076 (4)	0.028 (3)
C17	0.042 (3)	0.035 (2)	0.048 (3)	0.016 (2)	0.021 (2)	0.011 (2)
C18	0.105 (5)	0.101 (5)	0.097 (5)	0.054 (4)	0.020 (4)	0.034 (4)

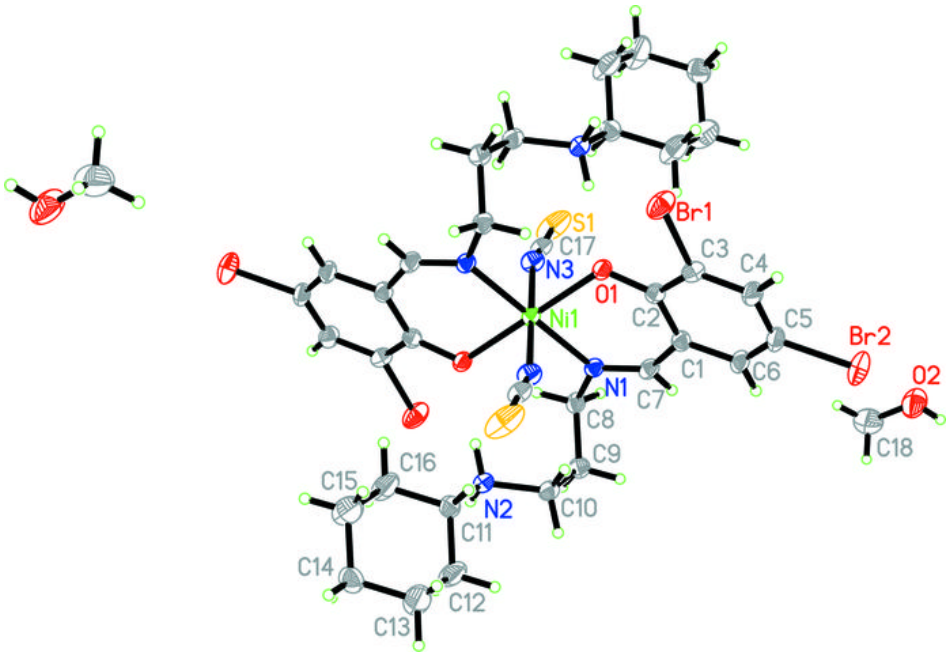
Geometric parameters (Å, °)

Ni1—O1	2.060 (3)	C8—C9	1.525 (6)
Ni1—O1^{i}	2.060 (3)	C8—H8A	0.9700
Ni1—N3^{i}	2.088 (4)	C8—H8B	0.9700
Ni1—N3	2.088 (4)	C9—C10	1.513 (6)
Ni1—N1	2.090 (3)	C9—H9A	0.9700
Ni1—N1^{i}	2.090 (3)	C9—H9B	0.9700
Br1—C3	1.900 (4)	C10—H10A	0.9700
Br2—C5	1.900 (4)	C10—H10B	0.9700
S1—C17	1.635 (5)	C11—C12	1.488 (6)
O1—C2	1.306 (4)	C11—C16	1.496 (6)
O2—C18	1.365 (6)	C11—H11	0.9800
O2—H2	0.8200	C12—C13	1.520 (8)
N1—C7	1.272 (5)	C12—H12A	0.9700
N1—C8	1.479 (5)	C12—H12B	0.9700
N2—C10	1.490 (5)	C13—C14	1.486 (6)
N2—C11	1.500 (5)	C13—H13A	0.9700
N2—H2A	0.9000	C13—H13B	0.9700
N2—H2B	0.9000	C14—C15	1.490 (7)
N3—C17	1.150 (5)	C14—H14A	0.9700
C1—C6	1.398 (5)	C14—H14B	0.9700
C1—C2	1.416 (5)	C15—C16	1.525 (7)
C1—C7	1.447 (5)	C15—H15A	0.9700
C2—C3	1.415 (5)	C15—H15B	0.9700
C3—C4	1.369 (5)	C16—H16A	0.9700
C4—C5	1.376 (5)	C16—H16B	0.9700
C4—H4	0.9300	C18—H18A	0.9600
C5—C6	1.364 (6)	C18—H18B	0.9600
C6—H6	0.9300	C18—H18C	0.9600
C7—H7	0.9300		
O1—Ni1—O1^{i}	180.00 (14)	C10—C9—H9A	108.3
O1—Ni1—N3^{i}	88.72 (12)	C8—C9—H9A	108.3
O1^{i}—Ni1—N3^{i}	91.28 (12)	C10—C9—H9B	108.3
O1—Ni1—N3	91.28 (12)	C8—C9—H9B	108.3
O1^{i}—Ni1—N3	88.72 (12)	H9A—C9—H9B	107.4
N3^{i}—Ni1—N3	180.00 (18)	N2—C10—C9	112.9 (3)
O1—Ni1—N1	87.62 (11)	N2—C10—H10A	109.0
O1^{i}—Ni1—N1	92.38 (11)	C9—C10—H10A	109.0
N3^{i}—Ni1—N1	92.76 (13)	N2—C10—H10B	109.0
N3—Ni1—N1	87.24 (13)	C9—C10—H10B	109.0
O1—Ni1—N1^{i}	92.38 (11)	H10A—C10—H10B	107.8

$O1^{i}$—Ni1—$N1^{i}$	87.62 (11)	C12—C11—C16	109.7 (4)
$N3^{i}$—Ni1—$N1^{i}$	87.24 (13)	C12—C11—N2	111.7 (4)
N3—Ni1—$N1^{i}$	92.76 (13)	C16—C11—N2	110.6 (3)
N1—Ni1—$N1^{i}$	180.00 (15)	C12—C11—H11	108.2
C2—O1—Ni1	124.6 (2)	C16—C11—H11	108.2
C18—O2—H2	109.5	N2—C11—H11	108.2
C7—N1—C8	115.6 (3)	C11—C12—C13	110.9 (5)
C7—N1—Ni1	124.4 (3)	C11—C12—H12A	109.5
C8—N1—Ni1	120.0 (2)	C13—C12—H12A	109.5
C10—N2—C11	113.7 (3)	C11—C12—H12B	109.5
C10—N2—H2A	108.8	C13—C12—H12B	109.5
C11—N2—H2A	108.8	H12A—C12—H12B	108.0
C10—N2—H2B	108.8	C14—C13—C12	111.7 (5)
C11—N2—H2B	108.8	C14—C13—H13A	109.3
H2A—N2—H2B	107.7	C12—C13—H13A	109.3
C17—N3—Ni1	159.1 (3)	C14—C13—H13B	109.3
C6—C1—C2	121.1 (4)	C12—C13—H13B	109.3
C6—C1—C7	116.5 (4)	H13A—C13—H13B	107.9
C2—C1—C7	122.5 (4)	C13—C14—C15	110.4 (4)
O1—C2—C3	121.8 (4)	C13—C14—H14A	109.6
O1—C2—C1	123.8 (4)	C15—C14—H14A	109.6
C3—C2—C1	114.4 (3)	C13—C14—H14B	109.6
C4—C3—C2	124.2 (4)	C15—C14—H14B	109.6
C4—C3—Br1	118.4 (3)	H14A—C14—H14B	108.1
C2—C3—Br1	117.4 (3)	C14—C15—C16	111.7 (4)
C3—C4—C5	119.1 (4)	C14—C15—H15A	109.3
C3—C4—H4	120.5	C16—C15—H15A	109.3
C5—C4—H4	120.5	C14—C15—H15B	109.3
C6—C5—C4	120.1 (4)	C16—C15—H15B	109.3
C6—C5—Br2	121.1 (3)	H15A—C15—H15B	107.9
C4—C5—Br2	118.9 (3)	C11—C16—C15	111.1 (4)
C5—C6—C1	121.1 (4)	C11—C16—H16A	109.4
C5—C6—H6	119.5	C15—C16—H16A	109.4
C1—C6—H6	119.5	C11—C16—H16B	109.4
N1—C7—C1	127.9 (4)	C15—C16—H16B	109.4
N1—C7—H7	116.1	H16A—C16—H16B	108.0
C1—C7—H7	116.1	N3—C17—S1	178.0 (4)
N1—C8—C9	112.1 (3)	O2—C18—H18A	109.5
N1—C8—H8A	109.2	O2—C18—H18B	109.5
C9—C8—H8A	109.2	H18A—C18—H18B	109.5
N1—C8—H8B	109.2	O2—C18—H18C	109.5
C9—C8—H8B	109.2	H18A—C18—H18C	109.5
H8A—C8—H8B	107.9	H18B—C18—H18C	109.5
C10—C9—C8	115.8 (3)		

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

Fig. 1


S1
C17
N3
O1
Ni1
Br1
C3
C4
C2
C5
Br2
C1
C6
O2
N1
C7
C8
C18
C9
C16
C15
N2
C10
C11
C14
C12
C13