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(Methanol-κO)bis(thiocyanato-κN)[2,4,6-tris-(pyridin-2-yl)-1,3,5-triazine-κ^3N^2,N^1,N^6]nickel(II) methanol monosolvate

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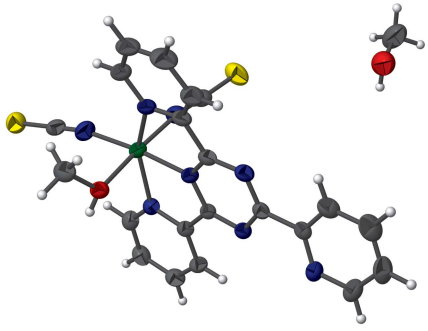
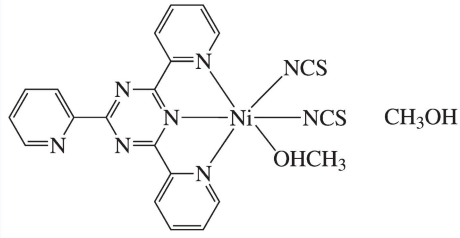
Structural data: full structural data are available from iucrdata.iucr.org

In the structure of the title compound, $[Ni(NCS)_2(C_{18}H_{12}N_6)(CH_3OH)]\cdot CH_3OH$, the Ni^{II} ion is six-coordinated in an octahedral coordination environment defined by three N atoms from a 2,4,6-tris(pyridin-2-yl)-1,3,5-triazine ligand, two N atoms from two mutually *cis*-positioned SCN^- anions and one O atom from a methanol ligand. The complex and methanol solvent molecules are linked by intermolecular hydrogen bonds. In the crystal, the complex molecules are stacked in columns parallel to the *b* axis.

3D view



Chemical scheme



Structure description

With reference to the title compound, $[Ni(NCS)_2(tptz)(CH_3OH)]\cdot CH_3OH$, the crystal structures of related tptz-Ni^{II} [tptz = 2,4,6-tris(pyridin-2-yl)-1,3,5-triazine] complexes $[NiCl_2(tptz)(CH_3OH)]$ (Hadadzadeh *et al.*, 2012), $[NiBr(\mu\text{-}Br)(tptz)]_2$ and $[Ni(tptz)_2](I_3)_2$ (Aragoni *et al.*, 2007) have previously been determined.

In the structure of the title complex, the central Ni^{II} ion is six-coordinated in a distorted octahedral coordination environment defined by three N atoms from a tridentate tptz ligand, two N atoms derived from two mutually *cis*-positioned SCN^- anions and one O atom from a methanol ligand (Fig. 1). The acute N—Ni—N chelating angles of N1—Ni1—N4 = 76.33 (7)° and N1—Ni1—N6 = 76.39 (7)° contribute to the distortion of the octahedron. The axial O1—Ni1—N7, N1—Ni1—N8, and N4—Ni1—N6 bond angles are 175.85 (8), 174.35 (8) and 152.19 (7)°, respectively. The Ni—N(pyridyl) bonds [2.1623 (18) and 2.165 (2) Å] are considerably longer than the Ni—N(triazine, NCS) bonds [1.9943 (18)-2.049 (2) Å].

The two pyridyl rings coordinating to the Ni^{II} atom are positioned approximately parallel to their carrier triazine ring, making dihedral angles of 3.9 (1) and 8.2 (1)°. The

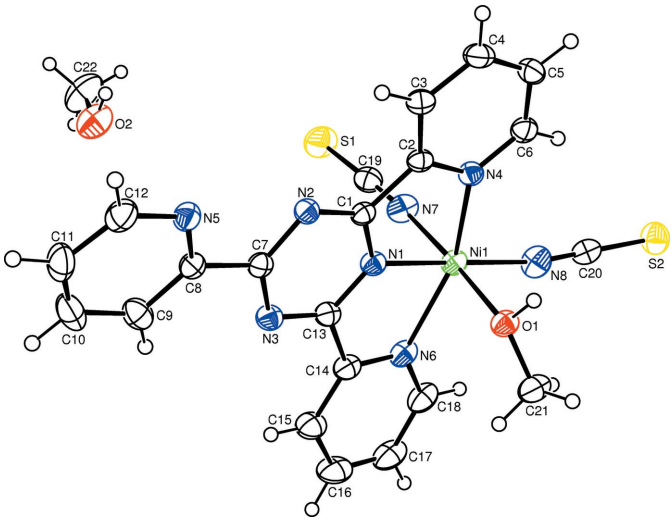


Figure 1
The molecular entities in the crystal structure of the title compound, showing the atom labelling and displacement ellipsoids drawn at the 50% probability level for non-H atoms.

dihedral angle between the non-coordinating pyridyl and triazine rings is 10.5 (1)°. The thiocyanato ligands are almost linear, displaying N—C—S bond angles of 178.3 (2) and 179.6 (2)°; the Ni—N—C(NCS) bond angles are slightly bent with 170.6 (2) and 166.7 (2)°, characteristic of an N-bonded conformation (Ha, 2017). The complex and additional methanol solvent molecules display intermolecular O—H···N and O—H···S hydrogen bonds (Table 1, Fig. 2). In the crystal structure, the complex molecules are stacked in columns parallel to the *b* axis. In the columns, numerous intermolecular π–π interactions between adjacent six-membered rings are present. For *Cg*1 (the centroid of ring N1–N3/C1/C7/C13) and *Cg*2^{i} [the centroid of ring N4/C2–C6; symmetry code: (i) $2-x$, y, $1-z$], the centroid-to-centroid distance is 3.658 (1) Å, and the dihedral angle between the ring planes is 3.7 (1)°.

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N2^{i}	0.83	2.61	3.154 (2)	124
O1—H1···N5^{i}	0.83	1.97	2.784 (2)	165
O2—H2···S1^{ii}	0.83	2.63	3.403 (2)	156

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

Table 2
Experimental details.

Crystal data	
Chemical formula	[Ni(NCS)$_2$(C$_{18}$H$_{12}$N$_6$)(CH$_4$O)]·CH$_4$O
M_r	551.29
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	223
a, b, c (Å)	10.5022 (3), 11.1772 (4), 20.8084 (7)
β (°)	95.1737 (12)
V (Å^3)	2432.65 (14)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	1.01
Crystal size (mm)	0.25 × 0.14 × 0.09
Data collection	
Diffractometer	PHOTON 100 CMOS detector
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.677, 0.745
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	66153, 4809, 3788
R_{int}	0.075
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.619
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.036, 0.083, 1.06
No. of reflections	4809
No. of parameters	320
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.31, −0.27

Computer programs: *APEX2* and *SAINT* (Bruker, 2016), *SHELXT2014/7* (Sheldrick, 2015*a*), *SHELXL2014/7* (Sheldrick, 2015*b*), *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2009).

Synthesis and crystallization

To a solution of Ni(NCS)$_2$·4H$_2$O (0.1829 g, 0.741 mmol) in acetone (20 ml) was added 2,4,6-tris(pyridin-2-yl)-1,3,5-triazine (0.2332 g, 0.747 mmol) and stirred for 3 h at room temperature. The formed precipitate was separated by filtration, washed with acetone, and dried at 323 K, to give a green–yellow powder (0.2501 g). Green crystals suitable for X-ray analysis were obtained by slow evaporation from a methanol solution at room temperature.

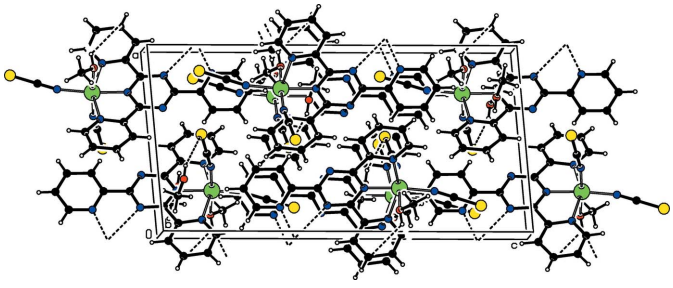


Figure 2
The packing in the crystal structure of the title compound, viewed approximately along the *b* axis. Hydrogen-bonding interactions are drawn as dashed lines.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

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full crystallographic data

IUCrData (2019). **4**, x190169 [https://doi.org/10.1107/S2414314619001690X]

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Crystal data

$[Ni(NCS)_2(C_{18}H_{12}N_6)(CH_4O)]\cdot CH_4O$
M_r = 551.29
Monoclinic, $P2_1/c$
a = 10.5022 (3) Å
b = 11.1772 (4) Å
c = 20.8084 (7) Å
β = 95.1737 (12)°
V = 2432.65 (14) Å^3
Z = 4
$F(000)$ = 1136
D_x = 1.505 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9985 reflections
θ = 2.6–25.9°
μ = 1.01 mm^{-1}
T = 223 K
Block, green
0.25 × 0.14 × 0.09 mm

Data collection

PHOTON 100 CMOS detector diffractometer
Radiation source: sealed tube
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2016)
T_{min} = 0.677, T_{max} = 0.745
66153 measured reflections
4809 independent reflections
3788 reflections with $I > 2\sigma(I)$
R_{int} = 0.075
θ_{max} = 26.1°, θ_{min} = 2.6°
h = −12→12
k = −13→13
l = −25→25

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.083
S = 1.06
4809 reflections
320 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0342P)^2 + 1.4276P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 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. Hydrogen atoms were positioned geometrically and allowed to ride on their respective parent atoms: C—H = 0.94 Å (CH) or 0.97 Å (CH_3), O—H = 0.83 Å and U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C, O). The remaining maximum electron density (0.31 e^- Å^{-3}) and the minimum electron density (-0.27 e^- Å^{-3}) in the difference Fourier map are located 0.64 Å and 0.71 Å, respectively, from the atoms N1 and Ni1.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Ni1	0.76420 (3)	0.04297 (3)	0.35072 (2)	0.03224 (10)
S1	0.47633 (7)	0.37353 (7)	0.37185 (4)	0.0615 (2)
S2	0.85612 (7)	0.08721 (7)	0.13357 (3)	0.05033 (19)
N1	0.76531 (16)	0.02980 (16)	0.44635 (9)	0.0298 (4)
N2	0.85785 (17)	0.08124 (16)	0.54915 (9)	0.0289 (4)
N3	0.67864 (17)	−0.05148 (17)	0.53620 (9)	0.0332 (4)
N4	0.92575 (17)	0.15144 (16)	0.38653 (9)	0.0297 (4)
N5	0.86950 (18)	0.04978 (17)	0.67830 (9)	0.0348 (4)
N6	0.61519 (17)	−0.08624 (18)	0.36378 (10)	0.0360 (5)
N7	0.6425 (2)	0.1862 (2)	0.35067 (10)	0.0450 (5)
N8	0.7806 (2)	0.0500 (2)	0.25666 (10)	0.0471 (5)
C1	0.85167 (19)	0.08808 (19)	0.48540 (10)	0.0268 (5)
C2	0.9443 (2)	0.15844 (19)	0.45141 (10)	0.0279 (5)
C3	1.0426 (2)	0.2232 (2)	0.48358 (11)	0.0329 (5)
H3	1.0519	0.2269	0.5289	0.039*
C4	1.1265 (2)	0.2823 (2)	0.44732 (12)	0.0388 (6)
H4	1.1949	0.3266	0.4675	0.047*
C5	1.1085 (2)	0.2755 (2)	0.38089 (12)	0.0390 (6)
H5	1.1647	0.3149	0.3553	0.047*
C6	1.0073 (2)	0.2101 (2)	0.35257 (11)	0.0352 (5)
H6	0.9953	0.2067	0.3073	0.042*
C7	0.7682 (2)	0.01166 (19)	0.57226 (11)	0.0288 (5)
C8	0.7681 (2)	0.0024 (2)	0.64301 (11)	0.0299 (5)
C9	0.6692 (2)	−0.0542 (2)	0.67030 (12)	0.0417 (6)
H9	0.6021	−0.0900	0.6442	0.050*
C10	0.6708 (3)	−0.0572 (3)	0.73660 (14)	0.0530 (7)
H10	0.6032	−0.0925	0.7564	0.064*
C11	0.7721 (3)	−0.0080 (3)	0.77305 (13)	0.0506 (7)
H11	0.7753	−0.0086	0.8183	0.061*
C12	0.8699 (3)	0.0428 (2)	0.74214 (12)	0.0443 (6)
H12	0.9406	0.0740	0.7676	0.053*
C13	0.6837 (2)	−0.0412 (2)	0.47331 (11)	0.0304 (5)
C14	0.6000 (2)	−0.1117 (2)	0.42620 (12)	0.0346 (5)
C15	0.5189 (2)	−0.1993 (2)	0.44523 (14)	0.0452 (6)
H15	0.5120	−0.2152	0.4891	0.054*

C16	0.4479 (2)	−0.2632 (3)	0.39732 (16)	0.0560 (8)
H16	0.3919	−0.3240	0.4083	0.067*
C17	0.4602 (2)	−0.2369 (3)	0.33408 (15)	0.0533 (8)
H17	0.4117	−0.2786	0.3012	0.064*
C18	0.5446 (2)	−0.1484 (2)	0.31875 (13)	0.0455 (7)
H18	0.5525	−0.1315	0.2750	0.055*
C19	0.5753 (2)	0.2647 (2)	0.35972 (12)	0.0396 (6)
C20	0.8120 (2)	0.0659 (2)	0.20530 (12)	0.0366 (6)
O1	0.88931 (14)	−0.10777 (14)	0.35803 (8)	0.0349 (4)
H1	0.9647	−0.0883	0.3545	0.052*
C21	0.8602 (2)	−0.2147 (2)	0.32201 (13)	0.0466 (6)
H21A	0.8044	−0.2648	0.3452	0.070*
H21B	0.9387	−0.2575	0.3163	0.070*
H21C	0.8177	−0.1942	0.2801	0.070*
O2	0.2762 (2)	0.45232 (19)	0.56669 (11)	0.0695 (6)
H2	0.3492	0.4799	0.5749	0.104*
C22	0.1909 (4)	0.5459 (3)	0.54825 (16)	0.0794 (11)
H22A	0.1064	0.5132	0.5366	0.119*
H22B	0.2203	0.5877	0.5115	0.119*
H22C	0.1872	0.6012	0.5839	0.119*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.03140 (17)	0.03424 (17)	0.03000 (16)	0.00026 (13)	−0.00313 (11)	−0.00294 (13)
S1	0.0502 (4)	0.0488 (4)	0.0865 (6)	0.0127 (3)	0.0110 (4)	−0.0049 (4)
S2	0.0542 (4)	0.0564 (4)	0.0406 (4)	0.0048 (3)	0.0055 (3)	0.0057 (3)
N1	0.0258 (9)	0.0306 (10)	0.0323 (10)	−0.0014 (8)	−0.0009 (8)	−0.0033 (8)
N2	0.0263 (9)	0.0298 (10)	0.0305 (10)	−0.0006 (8)	0.0022 (8)	−0.0013 (8)
N3	0.0256 (10)	0.0332 (11)	0.0406 (11)	−0.0018 (8)	0.0030 (8)	−0.0022 (9)
N4	0.0312 (10)	0.0269 (10)	0.0309 (10)	0.0009 (8)	0.0024 (8)	0.0005 (8)
N5	0.0399 (11)	0.0347 (11)	0.0298 (10)	0.0004 (9)	0.0040 (8)	−0.0023 (9)
N6	0.0258 (10)	0.0393 (11)	0.0414 (12)	0.0016 (8)	−0.0048 (8)	−0.0111 (9)
N7	0.0395 (12)	0.0422 (13)	0.0516 (14)	0.0048 (10)	−0.0047 (10)	−0.0033 (10)
N8	0.0516 (13)	0.0529 (14)	0.0355 (12)	0.0061 (11)	−0.0044 (10)	0.0001 (11)
C1	0.0252 (11)	0.0248 (11)	0.0302 (12)	0.0015 (9)	0.0010 (9)	−0.0031 (9)
C2	0.0278 (11)	0.0223 (11)	0.0332 (12)	0.0022 (9)	0.0006 (9)	0.0004 (9)
C3	0.0322 (12)	0.0304 (12)	0.0352 (13)	−0.0030 (10)	−0.0014 (10)	−0.0020 (10)
C4	0.0346 (13)	0.0298 (13)	0.0518 (15)	−0.0055 (10)	0.0033 (11)	−0.0029 (11)
C5	0.0408 (14)	0.0298 (13)	0.0481 (15)	−0.0036 (11)	0.0140 (11)	0.0036 (11)
C6	0.0443 (14)	0.0275 (12)	0.0343 (13)	0.0027 (11)	0.0060 (10)	0.0024 (10)
C7	0.0258 (11)	0.0263 (12)	0.0343 (12)	0.0040 (9)	0.0036 (9)	−0.0007 (9)
C8	0.0282 (12)	0.0271 (11)	0.0348 (12)	0.0058 (9)	0.0048 (10)	0.0003 (9)
C9	0.0345 (13)	0.0441 (15)	0.0469 (15)	0.0014 (11)	0.0064 (11)	0.0077 (12)
C10	0.0545 (17)	0.0574 (18)	0.0502 (17)	0.0020 (14)	0.0215 (14)	0.0175 (14)
C11	0.0686 (19)	0.0524 (17)	0.0329 (14)	0.0106 (15)	0.0156 (13)	0.0072 (12)
C12	0.0554 (16)	0.0422 (15)	0.0344 (13)	0.0025 (13)	−0.0001 (11)	−0.0044 (12)
C13	0.0236 (11)	0.0292 (12)	0.0381 (13)	0.0005 (10)	0.0012 (9)	−0.0019 (10)

C14	0.0229 (11)	0.0341 (13)	0.0462 (14)	−0.0001 (10)	−0.0005 (10)	−0.0078 (11)
C15	0.0334 (13)	0.0432 (15)	0.0589 (17)	−0.0075 (11)	0.0033 (12)	−0.0070 (13)
C16	0.0361 (15)	0.0472 (17)	0.084 (2)	−0.0138 (13)	0.0011 (14)	−0.0133 (16)
C17	0.0324 (14)	0.0535 (18)	0.071 (2)	−0.0040 (13)	−0.0091 (13)	−0.0270 (16)
C18	0.0347 (14)	0.0499 (16)	0.0497 (16)	0.0032 (12)	−0.0076 (11)	−0.0175 (13)
C19	0.0377 (14)	0.0399 (15)	0.0401 (14)	−0.0040 (12)	−0.0021 (11)	0.0017 (11)
C20	0.0375 (13)	0.0325 (13)	0.0375 (14)	0.0044 (10)	−0.0085 (11)	−0.0018 (10)
O1	0.0303 (8)	0.0350 (9)	0.0388 (9)	−0.0011 (7)	−0.0008 (7)	−0.0054 (7)
C21	0.0422 (15)	0.0376 (15)	0.0590 (17)	0.0015 (12)	0.0001 (12)	−0.0123 (13)
O2	0.0694 (14)	0.0655 (14)	0.0724 (15)	0.0098 (12)	0.0000 (12)	−0.0137 (12)
C22	0.095 (3)	0.078 (2)	0.060 (2)	0.025 (2)	−0.0200 (19)	−0.0141 (18)

Geometric parameters (Å, º)

Ni1—N8	1.982 (2)	C6—H6	0.9400
Ni1—N1	1.9943 (18)	C7—C8	1.476 (3)
Ni1—N7	2.049 (2)	C8—C9	1.381 (3)
Ni1—O1	2.1336 (16)	C9—C10	1.379 (4)
Ni1—N4	2.1623 (18)	C9—H9	0.9400
Ni1—N6	2.165 (2)	C10—C11	1.365 (4)
S1—C19	1.634 (3)	C10—H10	0.9400
S2—C20	1.620 (3)	C11—C12	1.381 (4)
N1—C13	1.329 (3)	C11—H11	0.9400
N1—C1	1.332 (3)	C12—H12	0.9400
N2—C1	1.324 (3)	C13—C14	1.483 (3)
N2—C7	1.343 (3)	C14—C15	1.379 (3)
N3—C13	1.320 (3)	C15—C16	1.388 (4)
N3—C7	1.348 (3)	C15—H15	0.9400
N4—C6	1.331 (3)	C16—C17	1.366 (4)
N4—C2	1.349 (3)	C16—H16	0.9400
N5—C12	1.330 (3)	C17—C18	1.384 (4)
N5—C8	1.346 (3)	C17—H17	0.9400
N6—C18	1.336 (3)	C18—H18	0.9400
N6—C14	1.353 (3)	O1—C21	1.429 (3)
N7—C19	1.152 (3)	O1—H1	0.8300
N8—C20	1.160 (3)	C21—H21A	0.9700
C1—C2	1.479 (3)	C21—H21B	0.9700
C2—C3	1.383 (3)	C21—H21C	0.9700
C3—C4	1.379 (3)	O2—C22	1.407 (4)
C3—H3	0.9400	O2—H2	0.8300
C4—C5	1.380 (3)	C22—H22A	0.9700
C4—H4	0.9400	C22—H22B	0.9700
C5—C6	1.378 (3)	C22—H22C	0.9700
C5—H5	0.9400		

N8—Ni1—N1	174.35 (8)	N5—C8—C7	116.4 (2)
N8—Ni1—N7	94.50 (9)	C9—C8—C7	120.7 (2)
N1—Ni1—N7	90.32 (8)	C10—C9—C8	118.7 (2)

N8—Ni1—O1	89.64 (8)	C10—C9—H9	120.6
N1—Ni1—O1	85.55 (7)	C8—C9—H9	120.6
N7—Ni1—O1	175.85 (8)	C11—C10—C9	119.0 (3)
N8—Ni1—N4	100.53 (8)	C11—C10—H10	120.5
N1—Ni1—N4	76.33 (7)	C9—C10—H10	120.5
N7—Ni1—N4	91.83 (8)	C10—C11—C12	118.8 (2)
O1—Ni1—N4	87.66 (6)	C10—C11—H11	120.6
N8—Ni1—N6	106.18 (8)	C12—C11—H11	120.6
N1—Ni1—N6	76.39 (7)	N5—C12—C11	123.6 (3)
N7—Ni1—N6	93.64 (8)	N5—C12—H12	118.2
O1—Ni1—N6	84.94 (7)	C11—C12—H12	118.2
N4—Ni1—N6	152.19 (7)	N3—C13—N1	123.8 (2)
C13—N1—C1	117.65 (19)	N3—C13—C14	122.3 (2)
C13—N1—Ni1	121.29 (14)	N1—C13—C14	113.9 (2)
C1—N1—Ni1	121.00 (15)	N6—C14—C15	123.6 (2)
C1—N2—C7	114.80 (18)	N6—C14—C13	114.1 (2)
C13—N3—C7	114.70 (19)	C15—C14—C13	122.2 (2)
C6—N4—C2	117.47 (19)	C14—C15—C16	117.7 (3)
C6—N4—Ni1	128.00 (16)	C14—C15—H15	121.1
C2—N4—Ni1	114.53 (14)	C16—C15—H15	121.1
C12—N5—C8	116.9 (2)	C17—C16—C15	119.3 (3)
C18—N6—C14	117.2 (2)	C17—C16—H16	120.4
C18—N6—Ni1	128.38 (19)	C15—C16—H16	120.4
C14—N6—Ni1	114.20 (14)	C16—C17—C18	119.6 (2)
C19—N7—Ni1	170.6 (2)	C16—C17—H17	120.2
C20—N8—Ni1	166.7 (2)	C18—C17—H17	120.2
N2—C1—N1	123.5 (2)	N6—C18—C17	122.4 (3)
N2—C1—C2	122.32 (19)	N6—C18—H18	118.8
N1—C1—C2	114.14 (19)	C17—C18—H18	118.8
N4—C2—C3	123.3 (2)	N7—C19—S1	178.3 (2)
N4—C2—C1	113.97 (18)	N8—C20—S2	179.6 (2)
C3—C2—C1	122.7 (2)	C21—O1—Ni1	121.43 (14)
C4—C3—C2	118.1 (2)	C21—O1—H1	109.5
C4—C3—H3	120.9	Ni1—O1—H1	111.9
C2—C3—H3	120.9	O1—C21—H21A	109.5
C3—C4—C5	119.0 (2)	O1—C21—H21B	109.5
C3—C4—H4	120.5	H21A—C21—H21B	109.5
C5—C4—H4	120.5	O1—C21—H21C	109.5
C6—C5—C4	119.2 (2)	H21A—C21—H21C	109.5
C6—C5—H5	120.4	H21B—C21—H21C	109.5
C4—C5—H5	120.4	C22—O2—H2	109.5
N4—C6—C5	122.9 (2)	O2—C22—H22A	109.5
N4—C6—H6	118.6	O2—C22—H22B	109.5
C5—C6—H6	118.6	H22A—C22—H22B	109.5
N2—C7—N3	125.5 (2)	O2—C22—H22C	109.5
N2—C7—C8	117.47 (19)	H22A—C22—H22C	109.5
N3—C7—C8	117.1 (2)	H22B—C22—H22C	109.5
N5—C8—C9	122.9 (2)		

C7—N2—C1—N1	−1.0 (3)	N2—C7—C8—C9	171.4 (2)
C7—N2—C1—C2	−178.66 (19)	N3—C7—C8—C9	−9.2 (3)
C13—N1—C1—N2	−1.8 (3)	N5—C8—C9—C10	3.4 (4)
Ni1—N1—C1—N2	−179.04 (16)	C7—C8—C9—C10	−177.8 (2)
C13—N1—C1—C2	176.00 (18)	C8—C9—C10—C11	−2.3 (4)
Ni1—N1—C1—C2	−1.2 (2)	C9—C10—C11—C12	−0.3 (4)
C6—N4—C2—C3	0.2 (3)	C8—N5—C12—C11	−1.1 (4)
Ni1—N4—C2—C3	179.87 (17)	C10—C11—C12—N5	2.1 (4)
C6—N4—C2—C1	−178.40 (18)	C7—N3—C13—N1	−3.3 (3)
Ni1—N4—C2—C1	1.3 (2)	C7—N3—C13—C14	174.84 (19)
N2—C1—C2—N4	177.72 (19)	C1—N1—C13—N3	4.2 (3)
N1—C1—C2—N4	−0.2 (3)	Ni1—N1—C13—N3	−178.65 (16)
N2—C1—C2—C3	−0.9 (3)	C1—N1—C13—C14	−174.09 (18)
N1—C1—C2—C3	−178.8 (2)	Ni1—N1—C13—C14	3.1 (3)
N4—C2—C3—C4	−0.8 (3)	C18—N6—C14—C15	1.7 (3)
C1—C2—C3—C4	177.7 (2)	Ni1—N6—C14—C15	−173.79 (19)
C2—C3—C4—C5	0.6 (3)	C18—N6—C14—C13	178.6 (2)
C3—C4—C5—C6	0.1 (4)	Ni1—N6—C14—C13	3.1 (2)
C2—N4—C6—C5	0.6 (3)	N3—C13—C14—N6	177.7 (2)
Ni1—N4—C6—C5	−179.05 (17)	N1—C13—C14—N6	−4.0 (3)
C4—C5—C6—N4	−0.7 (4)	N3—C13—C14—C15	−5.3 (3)
C1—N2—C7—N3	1.9 (3)	N1—C13—C14—C15	172.9 (2)
C1—N2—C7—C8	−178.67 (18)	N6—C14—C15—C16	−1.1 (4)
C13—N3—C7—N2	0.1 (3)	C13—C14—C15—C16	−177.7 (2)
C13—N3—C7—C8	−179.32 (19)	C14—C15—C16—C17	−0.3 (4)
C12—N5—C8—C9	−1.7 (3)	C15—C16—C17—C18	1.0 (4)
C12—N5—C8—C7	179.5 (2)	C14—N6—C18—C17	−1.0 (3)
N2—C7—C8—N5	−9.8 (3)	Ni1—N6—C18—C17	173.78 (18)
N3—C7—C8—N5	169.66 (19)	C16—C17—C18—N6	−0.3 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N2^{i}	0.83	2.61	3.154 (2)	124
O1—H1···N5^{i}	0.83	1.97	2.784 (2)	165
O2—H2···S1^{ii}	0.83	2.63	3.403 (2)	156

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