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Bis[2-(pyridin-2-yl)ethanol-κ^2N,O]-bis(thiocyanato-κN)nickel(II)

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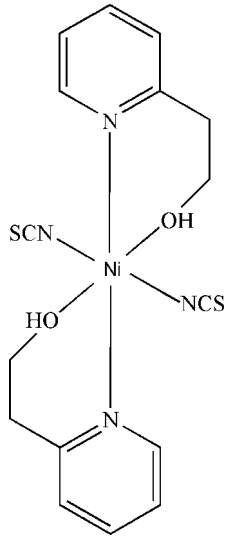
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.027; wR factor = 0.076; data-to-parameter ratio = 14.1.

In the title complex, $[Ni(NCS)_2(C_7H_9NO)_2]$, the Ni^{II} atom is in a distorted octahedral coordination environment defined by two N atoms of the two thiocyanate ions and by the N and O atoms of the two chelating 2-(pyridin-2-yl)ethanol ligands. The complex molecule is located around a crystallographic inversion center. In the crystal, molecules are connected into a two-dimensional polymeric structure parallel to (100) by O—H···S hydrogen bonds.

Related literature

For related structures, see: Pan *et al.* (2007); Yu *et al.* (2010).



Experimental

Crystal data

$[Ni(NCS)_2(C_7H_9NO)_2]$
M_r = 421.17
Monoclinic, $P2_1/c$
a = 8.7197 (9) Å
b = 13.8634 (15) Å
c = 7.8655 (7) Å
β = 105.496 (2)°
V = 916.26 (16) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.30 mm^{-1}
T = 298 K
0.42 × 0.41 × 0.40 mm

Data collection

Bruker SMART 1000 CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.611, T_{max} = 0.624
4493 measured reflections
1616 independent reflections
1408 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.076
S = 1.07
1616 reflections
115 parameters
5 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.55 e Å^{-3}

Table 1
Selected bond lengths (Å).

Ni1—N2	2.052 (2)	Ni1—O1	2.1030 (15)
Ni1—N1	2.1011 (19)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···S1^{i}	0.93	2.66	3.2183 (19)	119

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); 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: GK2318).

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supporting information

Acta Cryst. (2010). E**66**, m1587 [https://doi.org/10.1107/S1600536810046647]

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S1. Comment

Molecular materials with porous coordination frameworks have recently drawn considerable interest because of their attractive properties. The importance of the work in this area is the construction of porous materials from metal ions and organic ligands as building blocks. As a flexible ligand, 2-(hydroxyethyl)pyridine (hepH) can adopt a variety of possible binding modes. As a contribution to this field, we report here the synthesis and structure of the title compound.

In the title complex molecule, $[Ni(SCN)_2(C_7H_9NO)_2]$, the nickel(II) atom displays a distorted octahedral coordination geometry, provided by two N atoms of two thiocyanate ions and by the N and O atoms of two 2-(hydroxyethyl)pyridine ligands. Bond lengths and angles involving the metal centre are typical and comparable with those observed in related $Co^{(II)}$ complexes (Pan *et al.*, 2007; Yu *et al.*, 2010). In the crystal structure, molecules are linked through intermolecular O—H···S hydrogen bonds (Table 1).

S2. Experimental

To a stirred methanol (10 ml) and acetonitrile (10 ml) solution of $NiCl_2.6H_2O$ (1 mmol, 238 mg) was added 2-(pyridyn-2-yl)ethanol (2 mmol, 246 mg) in 5 ml me thanol and tetramethylammonium hydroxide(0.4 mmol, 165 mg, 25% solution in water). After 30 min to the above solution was added KSCN (2 mmol, 194 mg) and the solution was stirred for additional 6 h. The resulting red solution was filtered and was allowed to stand at room temperature for about one week, whereupon blue block crystal, suitable for X-ray diffraction analysis, was obtained.

S3. Refinement

All H atoms were placed in geometrically idealized positions (O–H= 0.93, C—H = 0.93-0.97 Å) and treated as riding on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C). A rigid bond restraints were applied to the Uij values of Ni1, N2, S1 and C8 atoms *via* DELU instruction of SHELXL97 (Sheldrick, 2008).

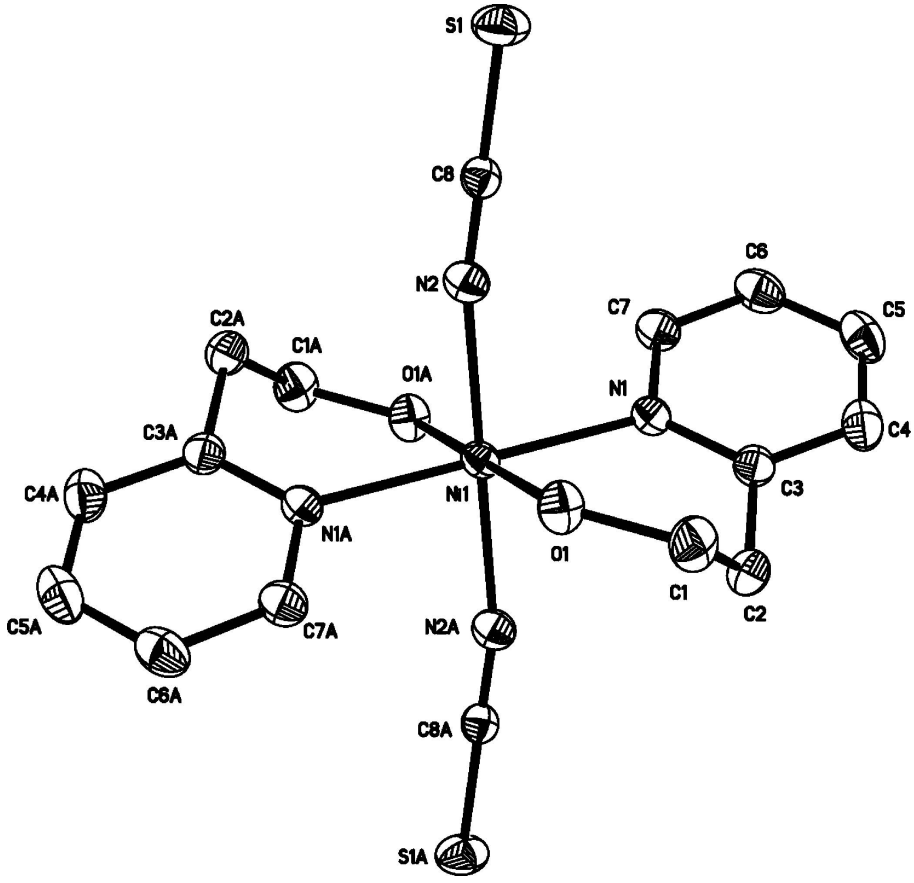

Figure 1

The molecular structure of the title compound, with atom labels and 30% probability displacement ellipsoids. Atoms labelled with the suffix A are generated by the symmetry operation -*x* + 2,-*y*,-*z*.

Bis[2-(pyridin-2-yl)ethanol-κ^2N,O]bis(thiocyanato- κN)nickel(II)

Crystal data

$[Ni(NCS)_2(C_7H_9NO)_2]$
M_r = 421.17
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 8.7197 (9) Å
b = 13.8634 (15) Å
c = 7.8655 (7) Å
β = 105.496 (2)°
V = 916.26 (16) Å^3
Z = 2
$F(000)$ = 436
D_x = 1.527 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2904 reflections
θ = 2.4–28.0°
μ = 1.30 mm^{-1}
T = 298 K
Block, blue
0.42 × 0.41 × 0.40 mm

Data collection

Bruker SMART 1000 CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.611, T_{max} = 0.624
4493 measured reflections
1616 independent reflections
1408 reflections with $I > 2\sigma(I)$

R_{int} = 0.020
θ_{max} = 25.0°, θ_{min} = 2.4°
h = −10→8
k = −16→15
l = −7→9

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.076
S = 1.07
1616 reflections
115 parameters
5 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
$w = 1/[\sigma^2(F_o^2) + (0.0356P)^2 + 0.5792P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.55 e Å^{-3}

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

	x	y	z	U_{iso}*/U_{eq}
Ni1	1.0000	0.5000	0.0000	0.03039 (15)
S1	1.22010 (9)	0.69823 (5)	0.50929 (9)	0.0528 (2)
N1	0.7906 (2)	0.54485 (14)	0.0607 (2)	0.0341 (4)
N2	1.1214 (2)	0.57961 (15)	0.2136 (3)	0.0409 (5)
O1	0.9851 (2)	0.62603 (12)	−0.1523 (2)	0.0415 (4)
H1	1.0793	0.6489	−0.1717	0.050*
C1	0.8438 (3)	0.6798 (2)	−0.2289 (4)	0.0498 (7)
H1A	0.8409	0.6968	−0.3493	0.060*
H1B	0.8448	0.7391	−0.1630	0.060*
C2	0.6971 (3)	0.62185 (19)	−0.2278 (3)	0.0452 (6)
H2A	0.6039	0.6570	−0.2936	0.054*
H2B	0.7005	0.5613	−0.2886	0.054*
C3	0.6788 (3)	0.60033 (17)	−0.0472 (3)	0.0373 (5)
C4	0.5510 (3)	0.6363 (2)	0.0063 (4)	0.0484 (6)
H4	0.4762	0.6754	−0.0692	0.058*
C5	0.5344 (3)	0.6142 (2)	0.1710 (4)	0.0535 (7)
H5	0.4484	0.6374	0.2077	0.064*
C6	0.6478 (3)	0.5570 (2)	0.2799 (4)	0.0499 (7)
H6	0.6397	0.5409	0.3920	0.060*
C7	0.7733 (3)	0.52394 (19)	0.2214 (3)	0.0415 (6)
H7	0.8496	0.4854	0.2963	0.050*
C8	1.1618 (3)	0.62905 (16)	0.3352 (3)	0.0320 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0355 (2)	0.0261 (2)	0.0306 (2)	0.00073 (16)	0.01065 (17)	−0.00126 (16)
S1	0.0696 (5)	0.0394 (4)	0.0428 (4)	−0.0032 (3)	0.0034 (3)	−0.0099 (3)
N1	0.0367 (10)	0.0311 (10)	0.0352 (10)	0.0005 (8)	0.0107 (8)	−0.0025 (8)
N2	0.0445 (11)	0.0363 (11)	0.0409 (10)	−0.0004 (9)	0.0100 (9)	−0.0065 (8)
O1	0.0447 (9)	0.0338 (9)	0.0486 (10)	0.0025 (7)	0.0170 (8)	0.0102 (7)

C1	0.0591 (17)	0.0436 (15)	0.0482 (15)	0.0122 (12)	0.0168 (13)	0.0162 (12)
C2	0.0467 (15)	0.0452 (15)	0.0402 (13)	0.0105 (12)	0.0057 (11)	0.0042 (11)
C3	0.0365 (12)	0.0326 (12)	0.0409 (13)	−0.0014 (10)	0.0070 (10)	−0.0048 (10)
C4	0.0398 (13)	0.0425 (15)	0.0630 (17)	0.0045 (12)	0.0137 (12)	−0.0034 (12)
C5	0.0480 (15)	0.0498 (16)	0.0713 (19)	−0.0007 (13)	0.0310 (14)	−0.0105 (14)
C6	0.0558 (16)	0.0530 (16)	0.0485 (15)	−0.0084 (13)	0.0271 (13)	−0.0068 (13)
C7	0.0453 (14)	0.0429 (14)	0.0393 (13)	−0.0025 (11)	0.0163 (11)	0.0006 (11)
C8	0.0324 (12)	0.0273 (11)	0.0361 (11)	0.0002 (9)	0.0087 (9)	0.0011 (7)

Geometric parameters (Å, º)

Ni1—N2	2.052 (2)	C2—C3	1.501 (3)
Ni1—N1	2.1011 (19)	C2—H2A	0.9700
Ni1—O1	2.1030 (15)	C2—H2B	0.9700
S1—C8	1.637 (2)	C3—C4	1.386 (4)
N1—C7	1.344 (3)	C4—C5	1.375 (4)
N1—C3	1.349 (3)	C4—H4	0.9300
N2—C8	1.153 (3)	C5—C6	1.374 (4)
O1—C1	1.428 (3)	C5—H5	0.9300
O1—H1	0.9300	C6—C7	1.375 (4)
C1—C2	1.513 (4)	C6—H6	0.9300
C1—H1A	0.9700	C7—H7	0.9300
C1—H1B	0.9700		

N2^{i}—Ni1—N2	180.00 (9)	O1—C1—H1B	109.5
N2^{i}—Ni1—N1^{i}	86.82 (8)	C2—C1—H1B	109.5
N2—Ni1—N1^{i}	93.18 (8)	H1A—C1—H1B	108.1
N2^{i}—Ni1—N1	93.18 (8)	C3—C2—C1	114.5 (2)
N2—Ni1—N1	86.82 (8)	C3—C2—H2A	108.6
N1^{i}—Ni1—N1	180.0	C1—C2—H2A	108.6
N2^{i}—Ni1—O1	92.32 (7)	C3—C2—H2B	108.6
N2—Ni1—O1	87.68 (7)	C1—C2—H2B	108.6
N1^{i}—Ni1—O1	92.38 (7)	H2A—C2—H2B	107.6
N1—Ni1—O1	87.62 (7)	N1—C3—C4	121.2 (2)
N2^{i}—Ni1—O1^{i}	87.68 (7)	N1—C3—C2	117.8 (2)
N2—Ni1—O1^{i}	92.32 (7)	C4—C3—C2	120.9 (2)
N1^{i}—Ni1—O1^{i}	87.62 (7)	C5—C4—C3	120.1 (3)
N1—Ni1—O1^{i}	92.38 (7)	C5—C4—H4	119.9
O1—Ni1—O1^{i}	180.00 (5)	C3—C4—H4	119.9
C7—N1—C3	118.1 (2)	C6—C5—C4	118.5 (3)
C7—N1—Ni1	118.18 (16)	C6—C5—H5	120.8
C3—N1—Ni1	123.47 (16)	C4—C5—H5	120.8
C8—N2—Ni1	167.28 (19)	C5—C6—C7	119.2 (3)
C1—O1—Ni1	126.06 (15)	C5—C6—H6	120.4
C1—O1—H1	117.0	C7—C6—H6	120.4
Ni1—O1—H1	117.0	N1—C7—C6	122.8 (3)
O1—C1—C2	110.9 (2)	N1—C7—H7	118.6
O1—C1—H1A	109.5	C6—C7—H7	118.6

C2—C1—H1A	109.5	N2—C8—S1	179.3 (2)
N2^{i}—Ni1—N1—C7	121.90 (18)	N1—Ni1—O1—C1	−23.9 (2)
N2—Ni1—N1—C7	−58.10 (18)	O1—C1—C2—C3	65.5 (3)
O1—Ni1—N1—C7	−145.91 (18)	C7—N1—C3—C4	1.0 (3)
O1^{i}—Ni1—N1—C7	34.09 (18)	Ni1—N1—C3—C4	−173.23 (18)
N2^{i}—Ni1—N1—C3	−63.84 (19)	C7—N1—C3—C2	−178.9 (2)
N2—Ni1—N1—C3	116.16 (19)	Ni1—N1—C3—C2	6.9 (3)
O1—Ni1—N1—C3	28.35 (18)	C1—C2—C3—N1	−63.6 (3)
O1^{i}—Ni1—N1—C3	−151.65 (18)	C1—C2—C3—C4	116.5 (3)
N1^{i}—Ni1—N2—C8	176.2 (9)	N1—C3—C4—C5	−1.2 (4)
N1—Ni1—N2—C8	−3.8 (9)	C2—C3—C4—C5	178.7 (2)
O1—Ni1—N2—C8	84.0 (9)	C3—C4—C5—C6	0.7 (4)
O1^{i}—Ni1—N2—C8	−96.0 (9)	C4—C5—C6—C7	0.0 (4)
N2^{i}—Ni1—O1—C1	69.2 (2)	C3—N1—C7—C6	−0.4 (4)
N2—Ni1—O1—C1	−110.8 (2)	Ni1—N1—C7—C6	174.2 (2)
N1^{i}—Ni1—O1—C1	156.1 (2)	C5—C6—C7—N1	−0.1 (4)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···S1^{ii}	0.93	2.66	3.2183 (19)	119

Symmetry code: (ii) *x*, −*y*+3/2, *z*−1/2.