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Diaquabis(isothiocyanato)bis(4-methylpyridine *N*-oxide)nickel(II) monohydrate

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The title compound, $[Ni(NCS)_2(C_6H_7NO)_2(H_2O)_2]\cdot H_2O$, consists of a mononuclear complex and an uncoordinated water molecule. The nickel(II) ion has a distorted octahedral coordination, formed by two N atoms from two thiocyanate anions and four O atoms from two water molecules and two 4-methylpyridine *N*-oxide molecules. The uncoordinated water molecules and the complex are connected by O—H···O and O—H···S hydrogen bonds.

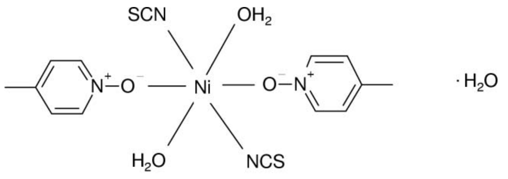
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.035
wR factor = 0.094
Data-to-parameter ratio = 14.1

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

Fig. 1 shows the title compound, (I), in which Ni1 is coordinated by two N atoms from thiocyanate anions and four O atoms from two water molecules and two 4-methylpyridine *N*-oxide molecules. As indicated in Table 1 and Fig. 1, Ni1 has a distorted octahedral coordination. Each of the three independent ligands is *trans* to its chemical equivalent.



(I)

Various hydrogen bonds (Table 2) help to stabilize the crystal packing. The coordinated water molecule O3 makes O—H···O and O—H···S bonds, the acceptor O atom being the uncoordinated water molecule, O5. The coordinated water molecule O4 makes two O—H···O bonds to *N*-oxide O-atom acceptors. The uncoordinated water molecule O5 makes a hydrogen bond to an *N*-oxide acceptor.

Experimental

4-Methylpyridine *N*-oxide (0.0615 g, 0.564 mmol) was added to a 10 ml aqueous solution containing $Ni(ClO_4)_2\cdot 6H_2O$ (0.1034 g, 0.283 mmol) and sodium thiocyanate (0.0468 g, 0.577 mmol) and the solution was stirred for a few minutes. Blue single crystals of (I) were obtained after the solution was allowed to stand at room temperature for three weeks.

Crystal data

$[Ni(C_6H_7NO)_2(NCS)_2(H_2O)_2]\cdot H_2O$
M_r = 447.17
Triclinic, $P\overline{1}$
a = 7.5665 (16) Å
b = 9.701 (2) Å
c = 14.129 (3) Å
α = 103.820 (3)°
β = 98.958 (3)°
γ = 91.721 (3)°
V = 992.4 (4) Å^3

Z = 2
D_x = 1.496 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2545 reflections
θ = 2.3–27.1°
μ = 1.22 mm^{-1}
T = 293 (2) K
Prism, blue
0.14 × 0.09 × 0.08 mm

Data collection

Bruker SMART CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\rm min} = 0.848$, $T_{\rm max} = 0.909$
5120 measured reflections
3426 independent reflections
3069 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.018$
$\theta_{\rm max} = 25.0°$
$h = -8 \rightarrow 8$
$k = -11 \rightarrow 11$
$l = -10 \rightarrow 16$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.094$
$S = 1.06$
3426 reflections
243 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0493P)^2 + 0.2162P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} = 0.001$
$\Delta\rho_{\rm max} = 0.31$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.30$ e Å^{-3}

Table 1
Selected bond lengths (Å).

Ni1—N3	2.014 (2)	Ni1—O4	2.0970 (18)
Ni1—N4	2.020 (2)	Ni1—O2	2.1082 (18)
Ni1—O3	2.0859 (18)	Ni1—O1	2.1109 (18)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3*WA*···S2$^{\rm i}$	0.82	2.66	3.337 (2)	140
O3—H3*WB*···O5$^{\rm i}$	0.76	1.98	2.690 (3)	157
O4—H4*WA*···O2$^{\rm ii}$	0.82	2.07	2.811 (2)	151
O4—H4*WB*···O1$^{\rm iii}$	0.74	2.17	2.892 (3)	165
O5—H5*A*···O2$^{\rm iv}$	0.88	2.00	2.879 (3)	174

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

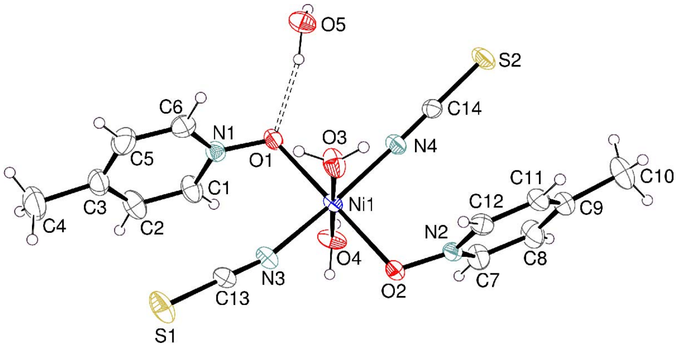


Figure 1
view of (I), showing 30% displacement ellipsoids (H atoms are shown as spheres of arbitrary radius). The broken lines indicates a hydrogen bond.

H atoms bonded to C and the coordinated water H atoms H3*WA* and H4*WA* were included in calculated positions. Other H atoms were located in a difference map. All H atoms were refined as riding [d(C—H) = 0.93–0.96 Å; $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C) or 1.5$U_{\rm eq}$(methyl C); d(O—H) = 0.74–0.88 Å, $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(O)].

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 2001); software used to prepare material for publication: *SHELXTL*.

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