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Dichlorotetrakis(3-hydroxypyridine-*κN*)nickel(II)

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Key indicators

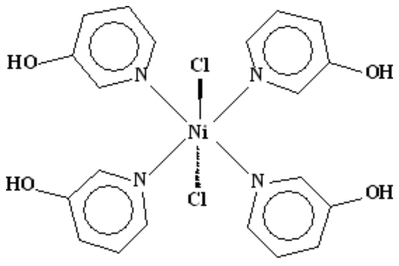
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.047
wR factor = 0.105
Data-to-parameter ratio = 17.3

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

In the title complex, $[NiCl_2(C_5H_5NO)_4]$, the Ni^{II} atom lies on a special position with twofold rotation symmetry and assumes an elongated octahedral NiN_4Cl_2 configuration defined by two Cl^- ions occupying the axial sites [Ni—Cl = 2.4953 (8) Å] and four N atoms of 3-hydroxypyridine ligands in the equatorial plane [average Ni—N = 2.119 (2) Å]. A two-dimensional hydrogen-bonding framework is formed by O—H···Cl interactions.

Comment

3-Hydroxypyridine (3-PyOH), which is known as an important medical intermediate, is a potential bifunctional ligand with versatile binding modes (Breeze & Wang, 1993). However, in contrast to the numerous complexes containing 2-PyOH or its tautomer, the lactam 2-pyridone (Maity *et al.*, 2002; Chattopadhyay *et al.*, 2004), only a few complexes with the 3-PyOH ligand have been structurally characterized (Kawata *et al.*, 1997; Castillo *et al.*, 2001). Recently, a novel hydrogen-bonding layer architecture has been reported for the complex $[CoCl_2(3\text{-PyOH})_4]$ (Gao *et al.*, 2004), and under similar reaction conditions we obtained the title complex, $[NiCl_2(3\text{-PyOH})_4]$, (I), which is isomorphous with the Co^{II} analog. Similar structural descriptions of the Co^{II} complex apply to the present isomorphous complex (Fig. 1).



(I)

The mononuclear Ni^{II} units are linked *via* O—H···Cl hydrogen bonds between the uncoordinated hydroxyl O atoms of 3-PyOH and the Cl^- ions, forming a layer structure (Table 2 and Fig. 2).

Experimental

The title complex was prepared by the addition of $NiCl_2\cdot 6H_2O$ (2 mmol) to an ethanol solution of 3-PyOH (8 mmol). The mixed solution was allowed to evaporate at room temperature and green single crystals were isolated from the solution after 10 d. Analysis calculated for $C_{20}H_{20}Cl_2N_4NiO_4$: C 47.10, H 3.95, N 10.99%; found: C 47.21, H 3.82, N 10.83%.

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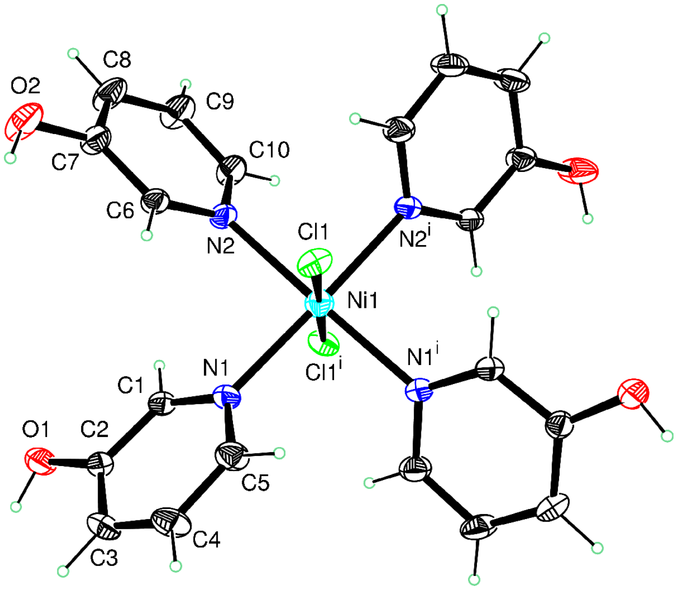

Figure 1
*ORTEP*II (Johnson, 1976) plot of (I), drawn with 30% probability displacement ellipsoids [symmetry code: (i) $\frac{3}{2} - x, -y, z$].

Crystal data

$[NiCl_2(C_5H_5NO)_4]$
$M_r = 509.99$
Orthorhombic, *Pcca*
$a = 15.701$ (3) Å
$b = 7.6110$ (15) Å
$c = 18.606$ (4) Å
$V = 2223.4$ (8) Å^3
$Z = 4$
$D_x = 1.524$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 11124 reflections
$\theta = 3.4–27.5°$
$\mu = 1.15$ mm^{-1}
$T = 293$ (2) K
Prism, green
0.42 × 0.32 × 0.24 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.638$, $T_{max} = 0.762$
19465 measured reflections
2539 independent reflections
1944 reflections with $I > 2\sigma(I)$
$R_{int} = 0.064$
$\theta_{max} = 27.5°$
$h = -20 \rightarrow 20$
$k = -9 \rightarrow 9$
$l = -24 \rightarrow 23$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.105$
$S = 1.08$
2539 reflections
147 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0482P)^2 + 1.2106P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.48$ e Å^{-3}
$\Delta\rho_{min} = -0.29$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ni1—Cl1	2.4935 (8)	O1—C2	1.365 (3)
Ni1—N1	2.113 (2)	O2—C7	1.351 (4)
Ni1—N2	2.126 (2)		
Cl1—Ni1—Cl1^i	178.36 (3)	N1^i—Ni1—Cl1	90.83 (6)
N1^i—Ni1—N1	91.67 (11)	N1—Ni1—Cl1	88.02 (6)
N1—Ni1—N2	89.85 (8)	N2^i—Ni1—Cl1	90.42 (6)
N1—Ni1—N2^i	177.84 (9)	N2—Ni1—Cl1	90.76 (6)
N2^i—Ni1—N2	88.68 (11)		

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

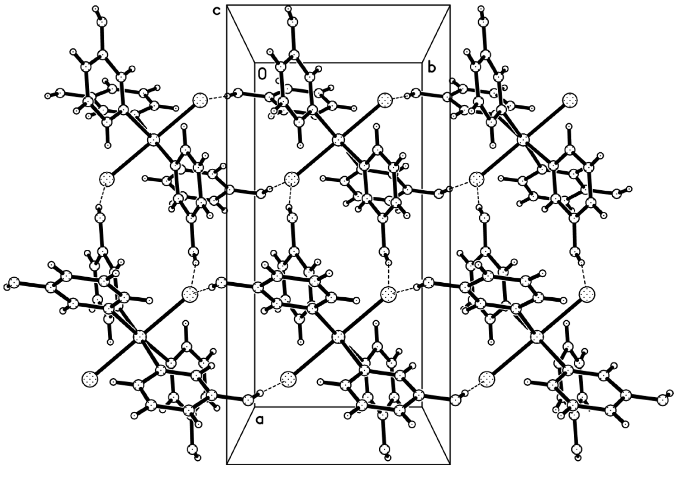

Figure 2
The packing of (I), with the O—H···Cl hydrogen bonds denoted by dashed lines.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H11···Cl1^{ii}	0.85 (3)	2.20 (3)	3.034 (2)	168 (4)
O2—H12···Cl1^{iii}	0.85 (3)	2.20 (3)	3.050 (2)	177 (4)

Symmetry codes: (ii) $x - \frac{1}{2}, y, 1 - z$; (iii) $\frac{3}{2} - x, 1 - y, z$.

H atoms on oxygen were located in difference Fourier synthesis maps and refined with an O—H distance restraint of 0.85 (1) Å and $U_{iso}(H) = 1.5U_{eq}(O)$. Other H atoms were placed in calculated positions and were allowed to ride on their parent C atoms [C—H = 0.93 Å (aromatic) and $U_{iso}(H) = 1.2U_{eq}(C)$].

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *SHELXL*97.

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References

Breeze, S. R. & Wang, S. (1993). *Inorg. Chem.* **32**, 5981–5989.
Castillo, O., Luque, A., Julve, M., Lloret, F. & Román, P. (2001). *Inorg. Chim. Acta*, **315**, 9–17.
Chattopadhyay, S., Fanwick, P. E. & Walton, R. A. (2004). *Inorg. Chim. Acta*, **357**, 764–768.
Gao, S., Zhang, X.-F., Huo, L.-H., Lu, Z.-Z., Zhao, H. & Zhao, J.-G. (2004). *Acta Cryst.* E**60**, m1128–m1130.
Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
Johnson, C. K. (1976). *ORTEP*II. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
Kawata, S., Breeze, S. R., Wang, S., Greedan, J. E. & Raju, N. P. (1997). *Chem. Commun.* pp. 717–718.
Maity, S., Roy, R., Sinha, C., Sheen, W. J., Panneerselvam, K. & Lu, T. H. (2002). *J. Organomet. Chem.* **650**, 202–209.

Rigaku (1998). *RAPID-AUTO*. Rigaku Corporation, Tokyo, Japan.

Rigaku/MSC (2002). *CrystalStructure*. Rigaku/MSC Inc., 9009 New Trails Drive, The Woodlands, TX 77381, USA.

Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.