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Key indicators

Single-crystal X-ray study
 T = 298 K
 Mean $\sigma(\text{C}-\text{C}) = 0.006 \text{ \AA}$
 Disorder in main residue
 R factor = 0.035
 wR factor = 0.092
 Data-to-parameter ratio = 13.8

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

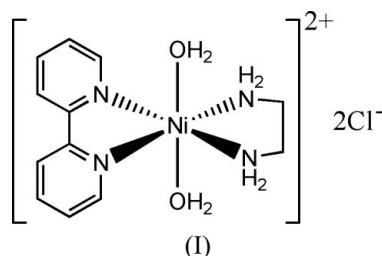
Diaqua(2,2'-bipyridine)(ethylenediamine)-
 nickel(II) dichloride

The Ni^{II} ion of the title compound, [Ni(C₂H₈N₂)(C₁₀H₈N₂)(H₂O)₂]Cl₂, is coordinated by four N atoms and two water molecules in a distorted octahedral geometry. $\pi-\pi$ Stacking of pyridine rings from adjacent complexes leads to a one-dimensional supramolecular ribbon along the *b* axis. The chloride anions are hydrogen bonded with complex cations, resulting in a three-dimensional supramolecular architecture.

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Comment

Diamine complexes as hydrogenation catalysts or precatalysts have attracted a lot of interest in recent years (Noyori & Ohkuma, 2001; Haack *et al.*, 1997; Doucet *et al.*, 1998; Ohkuma *et al.*, 2002). However, much less is known about phosphine-free diamine complexes as catalysts for the hydrogenation of ketones (Hedberg *et al.*, 2005; Ito *et al.*, 2001). In this work, we report the synthesis and crystal structure of the title phosphine-free diamine complex, (I).



The molecular structure of (I) is shown in Fig. 1. The Ni^{II} ion is six-coordinated in a distorted octahedral geometry by two bipyridine N atoms and two ethylenediamine N atoms

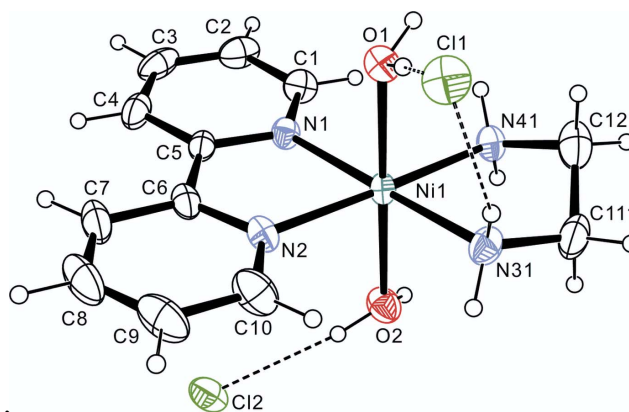


Figure 1
 The molecular structure of (I), with 30% probability displacement ellipsoids (arbitrary spheres for H atoms). Thin dashed lines indicate hydrogen bonds. One disordered component of ethylenediamine has been omitted for clarity.

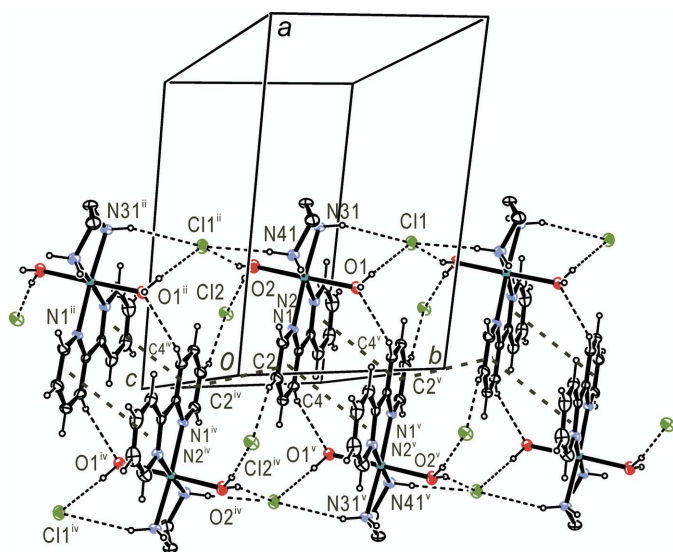


Figure 2

The infinite one-dimensional supramolecular ribbon extended along the *b* axis. Dashed lines indicate hydrogen bonds. For clarity, H atoms on the C atoms of ethylenediamine have been omitted and one disordered component of ethylenediamine is not drawn. [Symmetry codes: (ii) $x, y - 1, z$; (iv) $-x, -y, -z$; (v) $-x, 1 - y, -z$.]

chelated in the equatorial positions and two water molecules coordinating in the axial positions (Table 1).

π - π Stacking is observed between parallel N1-pyridine and N1^{iv}-pyridine rings [symmetry code: (iv) $-x, -y, -z$], the centroid-to-centroid separation being 3.884 (2) Å. π - π Stacking is also observed between the N1-pyridine and N2^v-pyridyl rings [symmetry code: (v) $-x, 1 - y, -z$], the centroid-to-centroid separation being 3.998 (3) Å. These two π - π stacking interactions lead to the formation of an infinite one-dimensional supramolecular ribbon extended along the *b* axis (Fig. 2).

The chloride anions are linked with complex cations *via* hydrogen bonding (Table 2), which connects the one-dimensional supramolecular ribbons into a three-dimensional supramolecular architecture.

Experimental

To an ethanol solution (10 ml) of NiCl₂·6H₂O (0.238 g, 1 mmol) was slowly added an ethanol solution (6 ml) of 2,2'-bipyridine (0.156 g, 1 mmol) and ethylenediamine (0.07 ml, 1 mmol). The mixture was stirred for 24 h at room temperature, then filtered. Single crystals of (I) were obtained from the filtrate after 3 d. Elemental analysis calculated for C₁₂H₂₀Cl₂N₄NiO₂: C 37.74, H 5.28, N 14.67%; found: C 37.33, H 6.09, N 14.72%.

Crystal data

[Ni(C ₂ H ₈ N ₂)(C ₁₀ H ₈ N ₂)(H ₂ O) ₂]Cl ₂	$Z = 4$
$M_r = 381.93$	$D_x = 1.541 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 14.132$ (5) Å	$\mu = 1.51 \text{ mm}^{-1}$
$b = 8.371$ (3) Å	$T = 298$ (2) K
$c = 15.454$ (6) Å	Block, grey
$\beta = 115.734$ (5)°	$0.50 \times 0.48 \times 0.37 \text{ mm}$
$V = 1646.8$ (11) Å ³	

Data collection

Bruker SMART CCD area-detector diffractometer	8258 measured reflections
φ and ω scans	2889 independent reflections
Absorption correction: multi-scan (SADABS; Bruker, 1998)	2219 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.490, T_{\max} = 0.572$	$R_{\text{int}} = 0.043$
	$\theta_{\max} = 25.0^\circ$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0433P)^2 + 0.2675P]$
$R[F^2 > 2\sigma(F^2)] = 0.035$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.092$	$(\Delta/\sigma)_{\max} < 0.001$
$S = 1.04$	$\Delta\rho_{\max} = 0.42 \text{ e \AA}^{-3}$
2889 reflections	$\Delta\rho_{\min} = -0.39 \text{ e \AA}^{-3}$
209 parameters	
H-atom parameters constrained	

Table 1

Selected geometric parameters (Å, °).

Ni1—N1	2.078 (2)	Ni1—N41	2.090 (2)
Ni1—N2	2.078 (2)	Ni1—O1	2.111 (2)
Ni1—N31	2.087 (2)	Ni1—O2	2.097 (2)
N1—Ni1—N2	78.65 (10)	N31—Ni1—O2	89.49 (9)
N1—Ni1—N31	176.22 (10)	N41—Ni1—O2	90.36 (9)
N2—Ni1—N31	99.28 (10)	N1—Ni1—O1	87.51 (9)
N1—Ni1—N41	98.42 (10)	N2—Ni1—O1	89.62 (9)
N2—Ni1—N41	177.07 (10)	N31—Ni1—O1	89.32 (9)
N31—Ni1—N41	83.65 (10)	N41—Ni1—O1	90.36 (9)
N1—Ni1—O2	93.64 (9)	O2—Ni1—O1	178.54 (9)
N2—Ni1—O2	89.72 (9)		

Table 2

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O1—H13 \cdots Cl2 ⁱ	0.85	2.20	3.025 (2)	164
O1—H14 \cdots Cl1	0.85	2.24	3.090 (2)	174
O2—H15 \cdots Cl2	0.85	2.25	3.099 (2)	172
O2—H16 \cdots Cl1 ⁱⁱ	0.85	2.32	3.137 (2)	162
N31—H3A \cdots Cl1	0.90	2.76	3.628 (3)	162
N31—H3B \cdots Cl1 ⁱⁱⁱ	0.90	2.61	3.425 (3)	151
N32—H3C \cdots Cl1	0.90	2.88	3.628 (3)	142
N32—H3D \cdots Cl1 ⁱⁱⁱ	0.90	2.59	3.425 (3)	154
N41—H4A \cdots Cl1 ⁱⁱ	0.90	2.56	3.444 (3)	169
N41—H4B \cdots Cl2 ⁱ	0.90	2.66	3.416 (3)	143
N42—H4C \cdots Cl1 ⁱⁱ	0.90	2.71	3.444 (3)	139
N42—H4D \cdots Cl2 ⁱ	0.90	2.55	3.416 (3)	161
C2—H2 \cdots Cl2 ^{iv}	0.93	2.75	3.613 (4)	154
C4—H4 \cdots O1 ^v	0.93	2.46	3.191 (4)	135

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

The CH₂ groups of ethylenediamine are disordered over two sites; occupancies were set at 0.5 for each component. H atoms of water molecules were located in a difference Fourier map and refined as riding; O—H = 0.85 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{O})$. Other H atoms were placed in calculated positions, with C—H = 0.93 Å and N—H = 0.90 Å, and refined in riding mode, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C}, \text{N})$.

Data collection: SMART (Bruker, 1998); cell refinement: SAINT (Bruker, 1998); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics:

SHELXTL (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

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