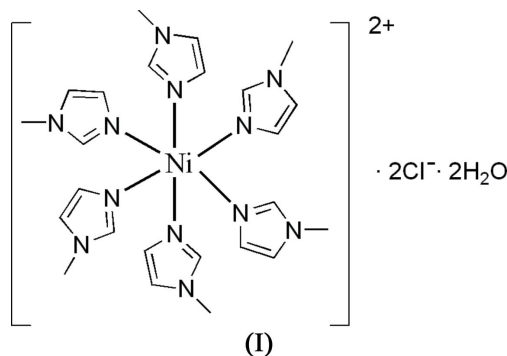


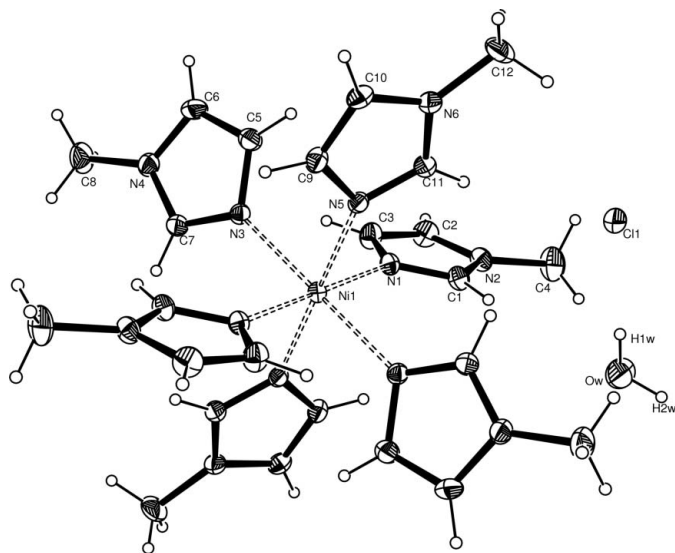
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schemorg@mail.sc.cninfo.net**Key indicators**Single-crystal X-ray study  
 $T = 290$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.006$  Å  
 $R$  factor = 0.043  
 $wR$  factor = 0.115  
Data-to-parameter ratio = 14.0For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.**Hexakis(1-methyl-1*H*-imidazole- $\kappa\text{N}^3$ )-  
nickel(II) dichloride dihydrate**The title complex,  $[\text{Ni}(\text{C}_4\text{H}_6\text{N}_2)_6]\text{Cl}_2 \cdot 2\text{H}_2\text{O}$ , is a mononuclear complex in which the  $\text{Ni}^{\text{II}}$  ion, lying on a centre of inversion, is coordinated by six 1-methylimidazole ligands that define an octahedral geometry.

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**Comment**The use of organic ligands and suitable metal salts to construct supramolecular architectures has attracted considerable interest because of their potential applications as functional materials (Tong *et al.*, 1999; Kitagawa *et al.*, 2004). Several complexes containing 1-methylimidazole have been prepared (Liu *et al.*, 2005), as 1-methylimidazole is a good ligand for a range of metals. We report here the crystal structure of the title complex, (I), as a continuation of our studies in this field.The molecular structure of the cation in (I) is shown in Fig. 1. Each Ni atom, lying on a centre of inversion, displays a slightly distorted octahedral coordination defined by six 1-methylimidazole ligands that define an  $\text{N}_6$  donor set. The Ni–N bond lengths are in the range 2.115 (3)–2.160 (3) Å (Table 1) and agree well with other  $\text{Ni}^{\text{II}}$  complexes described in the literature (*e.g.* Gao *et al.*, 2004). Interestingly, two chloride anions and two water molecules associate to form a ring *via* O–H...Cl hydrogen bonds, as shown in Fig. 2 and detailed in Table 2.**Experimental**

Nickel(II) chloride hexahydrate (1 mmol, 0.24 g) and 1-methylimidazole (6 mmol, 0.49 g) were mixed in chloroform (15 ml) and the mixture was stirred for 5 h at room temperature. After filtration, the solid was dissolved in methanol (8 ml). Blue crystals suitable for X-ray analysis were obtained by slow evaporation of this solution over a period of 6 d.



**Figure 1**  
The structure of (I), showing 30% probability displacement ellipsoids and the atomic numbering. Unlabelled atoms are related to labelled atoms by the symmetry operator  $(-x, -y, -z)$ .

*Crystal data*

$[\text{Ni}(\text{C}_4\text{H}_6\text{N}_2)_6]\text{Cl}_2 \cdot 2\text{H}_2\text{O}$	$D_x = 1.376 \text{ Mg m}^{-3}$
$M_r = 658.29$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 27 reflections
$a = 8.065 (4) \text{ \AA}$	$\theta = 4.5\text{--}7.4^\circ$
$b = 13.238 (5) \text{ \AA}$	$\mu = 0.82 \text{ mm}^{-1}$
$c = 15.029 (7) \text{ \AA}$	$T = 290 (2) \text{ K}$
$\beta = 98.07 (4)^\circ$	Block, blue
$V = 1588.7 (12) \text{ \AA}^3$	$0.25 \times 0.25 \times 0.23 \text{ mm}$
$Z = 2$	

*Data collection*

Enraf–Nonius CAD-4 diffractometer	$\theta_{\text{max}} = 25.0^\circ$
$\omega/2\theta$ scans	$h = -8 \rightarrow 9$
Absorption correction: none	$k = 0 \rightarrow 15$
2860 measured reflections	$l = -9 \rightarrow 17$
2714 independent reflections	3 standard reflections
1829 reflections with $I > 2\sigma(I)$	every 300 reflections
$R_{\text{int}} = 0.012$	intensity decay: 1.0%

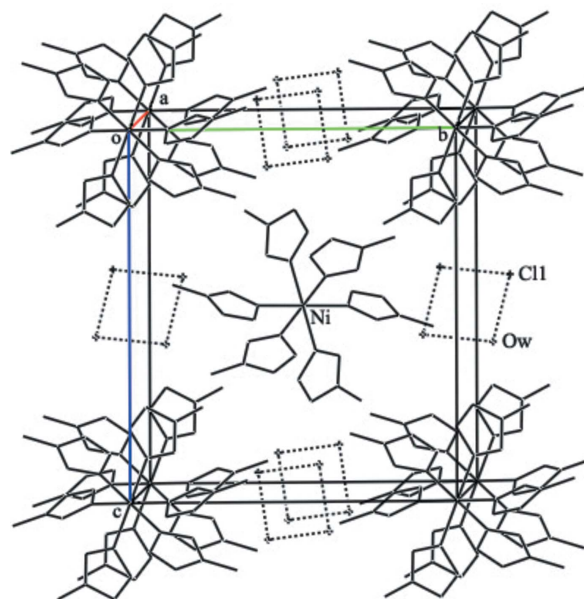
*Refinement*

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.061P)^2 + 0.0104P]$
$R[F^2 > 2\sigma(F^2)] = 0.043$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.115$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.02$	$\Delta\rho_{\text{max}} = 0.35 \text{ e \AA}^{-3}$
2714 reflections	$\Delta\rho_{\text{min}} = -0.39 \text{ e \AA}^{-3}$
194 parameters	
H atoms treated by a mixture of independent and constrained refinement	

**Table 1**  
Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ).

Ni1–N1	2.126 (3)	Ni1–N5	2.115 (3)
Ni1–N3	2.160 (3)		
N1–Ni1–N3	88.57 (11)	N5–Ni1–N1 <sup>i</sup>	87.93 (11)
N1–Ni1–N3 <sup>i</sup>	91.43 (11)	N5–Ni1–N3	87.23 (10)
N5–Ni1–N1	92.07 (11)	N5–Ni1–N3 <sup>i</sup>	92.77 (10)

Symmetry code: (i)  $-x, -y, -z$ .



**Figure 2**  
The packing in (I), viewed approximately down the  $a$  axis. Dashed lines indicate hydrogen bonds but H atoms have been omitted for clarity.

**Table 2**  
Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ).

$D\text{--}H\cdots A$	$D\text{--}H$	$H\cdots A$	$D\cdots A$	$D\text{--}H\cdots A$
OW–H1W $\cdots$ Cl1	0.92	2.29	3.187 (3)	166
OW–H2W $\cdots$ Cl1 <sup>ii</sup>	0.89	2.35	3.205 (3)	162

Symmetry code: (ii)  $-x, -y + 1, -z$ .

The O-bound H atoms were located in a difference Fourier map and fixed at those sites with  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$  (see Table 2 for distances). The remaining H atoms were placed in calculated positions and refined in the riding-model approximation, with C–H = 0.93 (aromatic H) and 0.96 Å (methyl H), and with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{aromatic C})$  and  $1.5U_{\text{eq}}(\text{methyl C})$ .

Data collection: *DIFRAC* (Gabe & White, 1993); cell refinement: *DIFRAC*; data reduction: *NRCVAX* (Gabe *et al.*, 1989); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *MERCURY* (Version 1.2; Bruno *et al.*, 2002); software used to prepare material for publication: *SHELXL97*.

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**References**

Bruno, I. J., Cole, J. C., Edgington, P. R., Kessler, M. K., Macrae, C. F., McCabe, P., Pearson, J. & Taylor, R. (2002). *Acta Cryst.* **B58**, 389–397.  
 Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.  
 Gabe, E. J., Le Page, Y., Charland, J.-P., Lee, F. L. & White, P. S. (1989). *J. Appl. Cryst.* **22**, 384–387.  
 Gabe, E. J. & White, P. S. (1993). *DIFRAC*. American Crystallographic Association, Pittsburgh meeting. Abstract PA104.  
 Gao, S., Liu, J.-W., Dong, Y., Huo, L.-H. & Zhao, H. (2004). *Acta Cryst.* **E60**, m778–m780.

Kitagawa, S., Kitaura, R. & Noro, S. I. (2004). *Angew. Chem. Int. Ed.* **43**, 2334–2375.

Liu, F.-Q., Jian, F.-F., Liu, G.-Y., Lu, L.-D., Yang, X.-J. & Wang, X. (2005). *Acta Cryst.* **E61**, m1568–1570.

Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

Tong, M. L., Chen, X. X., Ye, B. H. & Ji, L. N. (1999). *Angew. Chem. Int. Ed.* **38**, 2237–2240.