

Feng-Wu Wang

Department of Chemistry, Huainan Normal  
 College, Huainan 232001, People's Republic of  
 China

Correspondence e-mail: fengwuwang@163.com

Key indicators

Single-crystal X-ray study  
 T = 298 K  
 Mean  $\sigma(C-C)$  = 0.003 Å  
 Disorder in solvent or counterion  
 R factor = 0.043  
 wR factor = 0.113  
 Data-to-parameter ratio = 18.9

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

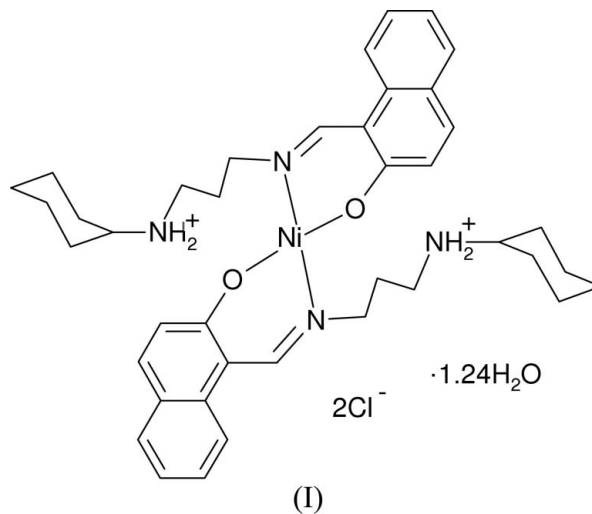
Bis{1-[3-(cyclohexylaminio)propyliminomethyl]-  
 2-naphtholato}nickel(II) dichloride 1.24-hydrate

The title complex,  $[Ni(C_{20}H_{26}N_2O)_2]Cl_2 \cdot 1.24H_2O$ , is a mono-  
 nuclear nickel(II) compound. The  $Ni^{II}$  atom, lying on an  
 inversion centre, is four-coordinated in a square-planar  
 geometry by two imine N and two phenolate O atoms from  
 two Schiff bases.

Received 17 August 2005  
 Accepted 12 September 2005  
 Online 17 September 2005

Comment

Schiff base complexes have been studied extensively, due to  
 their excellent biological activities (Ren *et al.*, 2002;  
 Deschamps *et al.*, 2003; Pal *et al.*, 2003). Nickel(II) complexes  
 are very important in coordination chemistry (Dey *et al.*, 2004;  
 Christensen *et al.*, 1997). The structures of a large number of  
 mono-, di- and polynuclear Schiff base nickel(II) complexes  
 have been reported (Vance *et al.*, 1997; Carbonaro *et al.*, 1999;  
 Rybak-Akimova *et al.*, 1998). The title new nickel(II)  
 complex, (I), is reported here.



Complex (I) is a mononuclear nickel(II) compound, with  
 the  $Ni^{II}$  atom lying on an inversion centre (Fig. 1). The  
 structural unit contains an  $[Ni(C_{20}H_{26}N_2O)_2]^{2+}$  cation, two  $Cl^-$   
 anions and two water molecules, each with site occupancy of  
 0.62. The  $Ni^{II}$  atom is four-coordinated in a square-planar  
 geometry by two imine N and two phenolate O atoms from  
 two Schiff bases. All bond angles (Table 1) subtended at the  
 $Ni^{II}$  centre are comparable with the values observed in other  
 Schiff base nickel(II) complexes (Gomes *et al.*, 2000; Chak-  
 raborty *et al.*, 2004).

In the crystal structure, the molecules are linked through  
 intermolecular O—H...Cl and N—H...Cl hydrogen bonds  
 (Table 2), forming layers parallel to the *bc* plane (Fig. 2).

## Experimental

*N*-Cyclohexyl-1,3-diaminopropane (0.1 mmol, 15.6 mg) and 2-hydroxy-1-naphthaldehyde (0.1 mmol, 8.6 mg) were dissolved in MeOH (10 ml). The mixture was stirred at room temperature for 10 min to give a clear yellow solution, to which was added an aqueous solution (5 ml) of NiCl<sub>2</sub>·4H<sub>2</sub>O (0.1 mmol, 20.2 mg) with stirring. The mixture was stirred for another 10 min at room temperature and filtered. After keeping the filtrate in air for 9 d, green block crystals of (I) separated. The crystals were isolated, washed three times with MeOH and dried in a vacuum desiccator using anhydrous CaCl<sub>2</sub> (yield 51.3%). Analysis, found: C 60.89, H 7.27, N 7.30%; calculated for C<sub>40</sub>H<sub>54.49</sub>Cl<sub>2</sub>N<sub>4</sub>NiO<sub>3.245</sub>: C 62.16, H 7.11, N 7.25%.

### Crystal data

[Ni(C <sub>20</sub> H <sub>26</sub> N <sub>2</sub> O) <sub>2</sub> ]Cl <sub>2</sub> ·1.24H <sub>2</sub> O	<i>D<sub>x</sub></i> = 1.299 Mg m <sup>-3</sup>
<i>M<sub>r</sub></i> = 772.79	Mo <i>K</i> α radiation
Monoclinic, <i>P</i> 2 <sub>1</sub> / <i>c</i>	Cell parameters from 3936 reflections
<i>a</i> = 11.179 (1) Å	<i>θ</i> = 2.4–26.8°
<i>b</i> = 7.431 (1) Å	<i>μ</i> = 0.67 mm <sup>-1</sup>
<i>c</i> = 23.683 (2) Å	<i>T</i> = 298 (2) K
<i>β</i> = 92.53 (1)°	Block, green
<i>V</i> = 1965.5 (4) Å <sup>3</sup>	0.20 × 0.13 × 0.12 mm
<i>Z</i> = 2	

### Data collection

Bruker SMART CCD area-detector diffractometer	4490 independent reflections
<i>ω</i> scans	3546 reflections with <i>I</i> > 2σ( <i>I</i> )
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	<i>R</i> <sub>int</sub> = 0.036
<i>T</i> <sub>min</sub> = 0.878, <i>T</i> <sub>max</sub> = 0.924	<i>θ</i> <sub>max</sub> = 27.5°
16272 measured reflections	<i>h</i> = -14 → 14
	<i>k</i> = -9 → 9
	<i>l</i> = -29 → 30

### Refinement

Refinement on <i>F</i> <sup>2</sup>	$w = 1/[\sigma^2(F_o^2) + (0.0602P)^2 + 0.2608P]$
<i>R</i> [ <i>F</i> <sup>2</sup> > 2σ( <i>F</i> <sup>2</sup> )] = 0.043	where $P = (F_o^2 + 2F_c^2)/3$
<i>wR</i> ( <i>F</i> <sup>2</sup> ) = 0.114	(Δ/σ) <sub>max</sub> < 0.001
<i>S</i> = 1.02	Δρ <sub>max</sub> = 0.41 e Å <sup>-3</sup>
4490 reflections	Δρ <sub>min</sub> = -0.24 e Å <sup>-3</sup>
238 parameters	
H atoms treated by a mixture of independent and constrained refinement	

**Table 1**

Selected geometric parameters (Å, °).

Ni1–O1	1.827 (2)	Ni1–N1	1.915 (2)
O1–Ni1–O1 <sup>i</sup>	180	O1–Ni1–N1 <sup>i</sup>	88.34 (7)
O1–Ni1–N1	91.66 (7)	N1–Ni1–N1 <sup>i</sup>	180

Symmetry code: (i)  $-x + 1, -y, -z + 2$ .

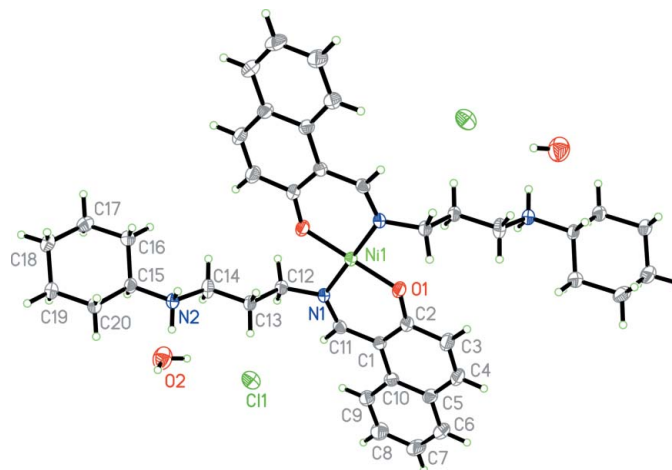
**Table 2**

Hydrogen-bond geometry (Å, °).

<i>D</i> –H... <i>A</i>	<i>D</i> –H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> –H... <i>A</i>
N2–H2A...Cl1 <sup>ii</sup>	0.90	2.24	3.133 (2)	172
N2–H2B...Cl1 <sup>iii</sup>	0.90	2.32	3.208 (2)	171
O2–H2C...Cl1	0.83 (1)	2.36 (2)	3.170 (4)	164 (5)
O2–H2D...Cl1 <sup>iii</sup>	0.84 (1)	2.56 (2)	3.362 (4)	161 (4)

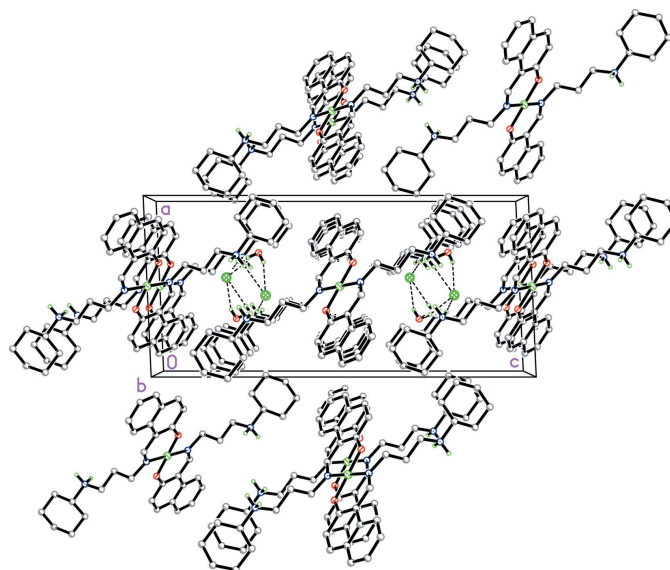
Symmetry codes: (ii)  $x, y - 1, z$ ; (iii)  $-x + 1, y - \frac{1}{2}, -z + \frac{3}{2}$ .

Attempts to refine the water O atom (O2) with full occupancy resulted in a high *U*<sub>iso</sub> value, and hence it was refined with partial occupancy; this was initially refined to 0.623 (8) and later fixed at 0.62.



**Figure 1**

The structure of (I). Displacement ellipsoids are drawn at the 30% probability level. Unlabelled atoms are at the symmetry position ( $1 - x, -y, 2 - z$ ).



**Figure 2**

The crystal packing of (I), viewed along the *b* axis. Dashed lines indicate hydrogen bonds. Only the H atoms involved in hydrogen bonding are shown.

Atoms H2C and H2D were located in a difference Fourier map and refined isotropically, with the O–H and H...H distances restrained to 0.84 (1) and 1.37 (2) Å, respectively, and with a fixed *U*<sub>iso</sub>(H) value of 0.08 Å<sup>2</sup>. All other H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with N–H = 0.90 Å and C–H distances in the range 0.93–0.98 Å, and with *U*<sub>iso</sub>(H) = 1.2–1.5*U*<sub>eq</sub>(C,*N*).

Data collection: SMART (Bruker, 1998); cell refinement: SAINT (Bruker, 1998); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997a); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997a); molecular graphics: SHELXTL (Sheldrick, 1997b); software used to prepare material for publication: SHELXTL.

The author acknowledges Huainan Normal College for financial support.

## References

- Bruker (1998). *SMART* (Version 5.628) and *SAINT* (Version 6.02). Bruker AXS Inc., Madison, Wisconsin, USA.
- Carbonaro, L., Isola, M., Pegna, P. L. & Senatore, L. (1999). *Inorg. Chem.* **38**, 5519–5525.
- Chakraborty, S., Samanta, B., Chowdhury, C. R., Mitra, S. & Mukherjee, A. K. (2004). *Acta Cryst.* **C60**, m578–m580.
- Christensen, A., Jensen, H. S., McKee, V., McKenzie, C. & Munch, M. (1997). *Inorg. Chem.* **36**, 6080–6085.
- Deschamps, P., Kulkarni, P. P. & Sarkar, B. (2003). *Inorg. Chem.* **42**, 7366–7368.
- Dey, S. K., Mondal, N., El Fallah, M. S., Vicente, R., Escuer, A., Solans, X., Font-Bardia, M., Matsushita, T., Gramlich, V. & Mitra, S. (2004). *Inorg. Chem.* **43**, 2427–2434.
- Gomes, L., Sousa, C., Freire, C. & de Castro, B. (2000). *Acta Cryst.* **C56**, 1201–1203.
- Pal, B., Ikeda, S. & Ohtani, B. (2003). *Inorg. Chem.* **42**, 1518–1524.
- Ren, S., Wang, R., Komatsu, K., Bonaz-Krause, P., Zyrianov, Y., McKenna, C. E., Csipke, C., Tokes, Z. A. & Lien, E. J. (2002). *J. Med. Chem.* **45**, 410–419.
- Rybak-Akimova, E. V., Alcock, N. W. & Busch, D. H. (1998). *Inorg. Chem.* **37**, 1563–1574.
- Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
- Sheldrick, G. M. (1997a). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
- Sheldrick, G. M. (1997b). *SHELXTL*. Version 5.10. Bruker AXS, Inc., Madison, Wisconsin, USA.
- Vance, A. L., Alcock, N. W., Busch, D. H. & Heppert, J. A. (1997). *Inorg. Chem.* **36**, 5132–5134.