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The Structure of *N,N'*-Ethylenebis[(2-hydroxy-1-naphthyl)methaniminato]nickel(II)

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Abstract

$C_{24}H_{18}N_2NiO_2$ is monoclinic, space group $P2_1/a$, with $a = 12.982$ (2), $b = 8.197$ (1), $c = 17.721$ (2) Å, $\beta = 79.93$ (1)°, $V = 1857.1$ Å³, $d_c = 1.455$ Mg m⁻³, $Z = 4$; $\lambda(Mo K\alpha) = 0.71069$ Å. The final $R = 0.033$ for 2601 counter reflexions. The structure is made up of centrosymmetric dimers with Ni–Ni = 3.3244 (4) Å. The Ni atom is situated in a nearly square-planar environment with Ni–O = 1.849, Ni–N = 1.840 Å. One of the six-membered rings is folded by $\sim 13^\circ$, while the other is folded by $\sim 15^\circ$ about the N···O line, presumably owing to steric interaction. The ethylenediamine group has an unsymmetrical *gauche* form, the C atoms deviating from the NNiN plane by +0.118 and –0.416 Å.

Introduction

Metal complexes of the quadridentate *N,N'*-ethylenebis(salicylideneimine) ligand have been investigated fairly well and the crystal structures of the Cu^{II} (Shkol'nikova, 1967) and Ni^{II} (Shkol'nikova, Yumal, Shugam & Voblikova, 1970) complexes have been reported. However, relatively little attention has been paid to the complexes of *N,N'*-ethylenebis[(2-hydroxy-1-naphthyl)methanimine], and several metal com-

plexes of this ligand have been prepared to study their characteristics compared with the corresponding salicylideneimine complexes. The title compound is a representative of this series and in the present paper the crystal structure is discussed.

Experimental

The title compound was prepared (Ahmed, 1977) by refluxing an equimolar mixture of Ni(NO₃)₂ and *N,N'*-ethylenebis[(2-hydroxy-1-naphthyl)methanimine] (prepared from 2-hydroxynaphthaldehyde and ethylenediamine). Single crystals were grown from dimethylformamide as wine-red prisms. A crystal was placed in an argon-filled glass capillary. The crystalline quality was checked and preliminary cell constants and the space group were obtained from rotation and Weissenberg photographs. The crystal was transferred to an automated CAD-4 diffractometer equipped with a Mo source and a graphite monochromator. An orientation matrix was calculated before data collection from the setting angles of 25 centred reflections. At the end of data collection, precise cell constants were obtained by least squares from the Bragg angles of 74 reflections in the range $6 \leq \theta \leq 20^\circ$. Intensities were collected within the range $0.5 \leq \theta \leq 25^\circ$ with the $\theta/2\theta$ scan technique. Before each measurement a fast

scan of the reflection at $20^\circ \text{ min}^{-1}$ was used to determine the final scanning speed. Moving-crystal-moving-counter background scans were made by scanning a quarter of the peak width before the start and at the end of each peak scan. The variation of the intensities of three check reflections was $<2\%$. The intensities were corrected for check-reflection fluctuation and reduced to $|F_o|$'s. Doubly measured reflections were averaged to yield 3609 data. Of these, 2601 obeyed the condition $I \geq 2\sigma(I)$ and were considered observed. Here $I = K[P - 2(\text{BG1} + \text{BG2})]$ and $\sigma(I) = K[P + 4(\text{BG1} + \text{BG2})]^{1/2}$ where P is the peak intensity, BG1 and BG2 are the background intensities, and K is a constant which depends on the scanning speed. Each observed reflection was assigned a standard deviation $\sigma(|F_o|)$ where $\sigma(|F_o|) = [\sigma^2(I) + (0.04I)^2]^{1/2}/2F$. A check on the list of $|F_o|$'s revealed that the conditions limiting the reflections are hkl : no condition; $h0l$: $h = 2n$; $0k0$: $k = 2n$, which correspond to $P2_1/a$.

Determination and refinement of the structure

The structure was solved by the heavy-atom method. The position of the Ni atom was obtained from the Patterson map. Least-squares refinement of the Ni atom and a scale factor resulted in $R = \sum \Delta / \sum |F_o| = 0.502$ and $R_w = \sum w\Delta^2 / \sum w|F_o|^2 = 0.504$ where $\Delta = ||F_o| - |F_c||$ and $w = 1/\sigma^2$ for observed and $w = 0$ for unobserved reflections. The structure was refined first isotropically then anisotropically by full-matrix and large-block least squares. In both processes the function minimized was $\sum \Delta^2$. Relativistic Hartree-Fock scattering factors (Cromer & Waber, 1965) were used for Ni, O, N, C and the best spherical scattering factors (Stewart, Davidson & Simpson, 1965) for the H atoms. A difference map yielded 14 lighter atoms. Isotropic refinement yielded $R = 0.404$ and $R_w = 0.400$. The next difference map showed the positions of most of the remaining C atoms. Isotropic refinement gave $R = 0.105$ and $R_w = 0.113$ and anisotropic refinement $R = 0.0506$ and $R_w = 0.0559$. All the H atoms were located from a subsequent difference map. Final refinement (H atoms isotropic) yielded $R = 0.0329$ and $R_w = 0.0383$.* The positional parameters are given in Table 1, selected bond distances and angles in Tables 2 and 3. A perspective drawing of the molecule is shown in Fig. 1 (the H atoms are numbered after the C atoms to which they are attached). Fig. 2 gives a stereoscopic view of the cell contents down **b**. Tables 4 and 5 give best planes and selected intermolecular contacts respectively.

* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 35642 (14 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. Final atomic coordinates (for Ni $\times 10^5$; for C, N, O $\times 10^4$; for H $\times 10^3$) and isotropic thermal parameters ($\times 10^4$)

For the non-hydrogen atoms $U_{eq} = \frac{1}{3}(U_{11} + U_{22} + U_{33})$.

	<i>x</i>	<i>y</i>	<i>z</i>	U_{eq}/U (\AA^2)
Ni	7300 (2)	16520 (4)	47704 (2)	3150
O(1)	1413 (1)	666 (2)	5483 (1)	379
O(2)	1768 (1)	792 (2)	4032 (1)	392
N(1)	-341 (1)	2406 (2)	5505 (1)	353
N(2)	69 (1)	2683 (2)	4064 (1)	357
C(1)	354 (2)	1668 (3)	6640 (1)	344
C(2)	1193 (2)	770 (3)	6228 (1)	349
C(3)	1856 (2)	-126 (3)	6650 (1)	430
C(4)	1695 (2)	-104 (3)	7422 (1)	498
C(5)	878 (2)	816 (3)	7862 (1)	467
C(6)	712 (3)	828 (4)	8674 (2)	629
C(7)	-71 (3)	1695 (4)	9087 (2)	719
C(8)	-727 (2)	2630 (4)	8710 (2)	670
C(9)	-593 (2)	2653 (4)	7924 (2)	537
C(10)	202 (2)	1732 (3)	7473 (1)	402
C(11)	-408 (2)	2364 (3)	6243 (1)	364
C(12)	1209 (2)	1821 (3)	2896 (1)	357
C(13)	1864 (2)	889 (3)	3284 (1)	363
C(14)	2699 (2)	-19 (3)	2844 (1)	438
C(15)	2899 (2)	59 (3)	2070 (1)	500
C(16)	2290 (2)	1048 (3)	1656 (1)	472
C(17)	2528 (2)	1172 (4)	845 (2)	637
C(18)	1939 (3)	2104 (4)	453 (2)	757
C(19)	1076 (3)	2944 (4)	848 (2)	681
C(20)	823 (2)	2846 (3)	1631 (1)	553
C(21)	1423 (2)	1911 (3)	2064 (1)	409
C(22)	334 (2)	2668 (3)	3322 (1)	371
C(23)	-858 (2)	3647 (3)	4404 (1)	435
C(24)	-1261 (2)	2959 (3)	5187 (1)	433
H(3)	239 (2)	-78 (3)	636 (1)	529
H(4)	210 (2)	-79 (3)	771 (1)	644
H(6)	117 (2)	13 (3)	893 (1)	623
H(7)	-17 (3)	169 (3)	965 (1)	811
H(8)	-129 (2)	326 (3)	901 (1)	687
H(9)	-105 (2)	336 (3)	769 (1)	510
H(11)	-105 (2)	281 (3)	656 (1)	474
H(14)	308 (2)	-73 (3)	312 (1)	435
H(15)	347 (2)	-55 (3)	177 (1)	524
H(17)	312 (2)	61 (3)	59 (1)	652
H(18)	215 (2)	224 (4)	-10 (1)	817
H(19)	59 (2)	362 (3)	57 (1)	846
H(20)	24 (2)	343 (3)	191 (1)	534
H(22)	-11 (1)	332 (2)	304 (1)	370
H(23A)	-66 (2)	480 (3)	445 (1)	418
H(23B)	-138 (2)	358 (2)	406 (1)	398
H(24A)	-163 (2)	378 (3)	553 (1)	335
H(24B)	-168 (2)	199 (3)	513 (1)	471

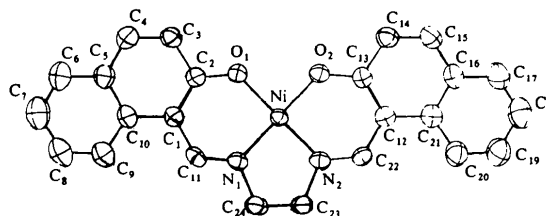


Fig. 1. A perspective drawing of the title compound. H atoms have been omitted for clarity.

Table 2. Selected bond distances (Å)

Ni—O(1)	1.852 (2)	C(6)—C(7)	1.348 (5)
Ni—O(2)	1.847 (2)	C(7)—C(8)	1.400 (5)
Ni—N(1)	1.839 (2)	C(8)—C(9)	1.374 (4)
Ni—N(2)	1.842 (2)	C(9)—C(10)	1.410 (4)
O(1)—C(2)	1.306 (3)	C(12)—C(13)	1.410 (3)
O(2)—C(13)	1.312 (3)	C(12)—C(21)	1.455 (3)
N(1)—C(11)	1.295 (3)	C(12)—C(22)	1.430 (3)
N(1)—C(24)	1.480 (3)	C(13)—C(14)	1.430 (3)
N(2)—C(22)	1.300 (3)	C(14)—C(15)	1.353 (4)
N(2)—C(23)	1.478 (3)	C(15)—C(16)	1.423 (4)
C(1)—C(2)	1.409 (3)	C(16)—C(17)	1.420 (4)
C(1)—C(10)	1.455 (3)	C(16)—C(21)	1.414 (4)
C(1)—C(11)	1.431 (3)	C(17)—C(18)	1.356 (5)
C(2)—C(3)	1.437 (3)	C(18)—C(19)	1.395 (5)
C(3)—C(4)	1.348 (4)	C(19)—C(20)	1.371 (4)
C(4)—C(5)	1.419 (4)	C(20)—C(21)	1.412 (4)
C(5)—C(6)	1.417 (4)	C(23)—C(24)	1.506 (4)
C(5)—C(10)	1.422 (4)		

Table 3. Selected bond angles (°)

O(1)NiN(1)	93.3 (1)	C(8)C(9)C(10)	121.3 (3)
O(2)NiN(2)	93.6 (1)	C(5)C(10)C(1)	119.2 (2)
O(1)NiO(2)	86.5 (1)	C(9)C(10)C(1)	123.5 (2)
N(1)NiN(2)	86.7 (1)	C(9)C(10)C(5)	117.4 (2)
NiO(1)C(2)	128.0 (1)	C(1)C(11)N(1)	125.2 (2)
NiO(2)C(13)	128.4 (1)	C(13)C(12)C(21)	119.9 (2)
NiN(1)C(11)	128.0 (2)	C(13)C(12)C(22)	119.8 (2)
NiN(1)C(24)	113.2 (2)	C(21)C(12)C(22)	120.3 (2)
C(11)N(1)C(24)	118.4 (2)	O(2)C(13)C(12)	124.6 (2)
NiN(2)C(22)	127.6 (2)	O(2)C(13)C(14)	116.7 (2)
NiN(2)C(23)	114.4 (2)	C(12)C(13)C(14)	118.7 (2)
C(22)N(2)C(23)	118.0 (2)	C(13)C(14)C(15)	121.4 (2)
C(2)C(1)C(10)	120.0 (2)	C(14)C(15)C(16)	121.7 (2)
C(2)C(1)C(11)	119.5 (2)	C(15)C(16)C(17)	121.4 (2)
C(10)C(1)C(11)	120.2 (2)	C(15)C(16)C(21)	119.0 (2)
O(1)C(2)C(1)	124.9 (1)	C(17)C(16)C(21)	119.6 (2)
O(1)C(2)C(3)	116.6 (2)	C(16)C(17)C(18)	121.1 (2)
C(1)C(2)C(3)	118.5 (2)	C(17)C(18)C(19)	119.8 (2)
C(2)C(3)C(4)	121.4 (2)	C(18)C(19)C(20)	120.6 (3)
C(3)C(4)C(5)	122.3 (2)	C(19)C(20)C(21)	121.6 (3)
C(4)C(5)C(6)	121.9 (3)	C(12)C(21)C(16)	119.1 (2)
C(4)C(5)C(10)	118.6 (2)	C(12)C(21)C(20)	123.6 (2)
C(6)C(5)C(10)	119.5 (3)	C(16)C(21)C(20)	117.3 (2)
C(5)C(6)C(7)	121.5 (3)	C(12)C(22)N(2)	125.8 (2)
C(6)C(7)C(8)	119.6 (3)	C(24)C(23)N(2)	107.6 (2)
C(7)C(8)C(9)	120.8 (3)	C(23)C(24)N(1)	107.0 (2)

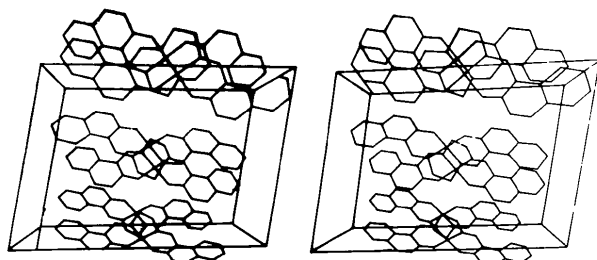
Fig. 2. A stereoscopic view of the cell contents down *b*.

Table 4. Equations of least-squares planes with deviations (Å) of atoms from them

Plane 1: Ni, O(1), N(1), N(2), O(2)	$-0.5544X - 0.8297Y - 0.0648Z = 2.9981$
Ni—0.009 (1); N(1) 0.039 (1); O(2) 0.038 (1); O(1) —0.033 (1); N(2) —0.034 (1)	
Plane 2: Ni, O(1), C(2), C(1), C(11), N(1)	$-0.5321X - 0.8465Y + 0.0166Z = 2.2299$
Ni —0.068 (1); C(2) 0.025 (1); C(11) 0.024 (1); O(1) 0.047 (1); C(1) —0.074 (1); N(1) 0.048 (1)	
Plane 3: Ni, O(2), C(13), C(12), C(22), N(2)	$0.5848X + 0.8103Y + 0.0376Z = -2.8390$
Ni —0.01 (1); C(13) —0.022 (1); C(22) 0.006 (1); O(2) 0.025 (1); C(12) 0.003 (1); N(2) —0.002 (1)	
Plane 4: C(1), C(2), C(3), C(4), C(5), C(6), C(7), C(8), C(9), C(10)	$0.6160X + 0.7872Y - 0.0302Z = -2.3092$
C(1) —0.033 (1); C(4) 0.004 (1); C(7) —0.018 (1); C(2) 0.003 (1); C(5) 0.006 (1); C(8) 0.009 (1); C(3) 0.012 (1); C(6) —0.008 (1); C(9) 0.023 (1); C(10) 0.002 (1)	
Plane 5: C(12), C(13), C(14), C(15), C(16), C(17), C(18), C(19), C(20), C(21)	$-0.6146X - 0.7862Y - 0.0647Z = 3.0126$
C(12) —0.005 (1); C(16) 0.007 (1); C(19) —0.001 (1); C(13) —0.045 (1); C(17) —0.016 (1); C(20) 0.027 (1); C(14) 0.008 (1); C(18) —0.029 (1); C(21) 0.019 (1); C(15) 0.033 (1)	

Table 5. Selected intermolecular contacts (Å)

Ni...Ni	3.3244 (4)	C _{ar} ...O	3.175 (3)
Ni...O	3.463 (2)	C _{ar} ...O	3.218 (3)
Ni...N	3.414 (2)	C _{ar} ...N	3.356 (3)
N...O	3.233 (3)		

Discussion of the structure

The molecule is virtually planar with the two C atoms in the ethylenediamine group out of the plane. The *cis* configuration of the molecule is due to the geometry of the quadridentate ligand. The Ni atom has square-planar coordination with average angles of 93.4° in the six-membered metallocycles and 86.7° in the five-membered metallocycle. The average values Ni—O = 1.849 and Ni—N = 1.840 Å are close to the sums of the covalent radii (Shkol'nikova, 1967). The structure is thus analogous to that of *N,N'*-ethylenebis(salicylideneiminato)nickel which has a *cis* structure with Ni—O and Ni—N = 1.82, and 1.85, Å respectively (Shkol'nikova, Yumal, Shugam & Voblikova, 1970). In bis(salicylideneiminato)nickel(II) (Stewart & Lingafelter, 1959), which also consists of essentially planar molecules, both the Ni—O and Ni—N distances are 1.840 Å. The Ni—O and Ni—N distances in the present

structure agree satisfactorily with the distances reported for other diamagnetic Ni^{II} complexes [1.83 and 1.86 Å respectively in the nickel–salicylaldehyde oxime complex (Merritt, Guare & Lessor, 1956); 1.87 and 1.90 Å respectively in the nickel–dimethylglyoxime complex (Godycki & Rundle, 1953)], and are shorter than the distances found in paramagnetic Ni^{II} compounds [Ni–O = 2.10 Å in nickel(II) acetate tetrahydrate (van Niekerk & Schoening, 1953), Ni–O = 2.08 and Ni–N = 2.09 Å in nickel(II) glycinate dihydrate (Stosick, 1945), Ni–O = 2.03 Å in di-aquabis(salicylaldehydato)nickel (Stewart, Lingafelter & Breazeale, 1961)]. In the present structure, however, the Ni–O bond is a little longer than the Ni–N bonds and a similar trend has been observed in some compounds of Pd; e.g. [Pd{*N*-hydroxysalicylideneimine(1–)}₂], [Pd{5-chloro-*N*-hydroxysalicylideneimine(1–)}₂] (Lingafelter & Braun, 1966), and [Pd{*N*-ethylsalicylideneimine(1–)}₂] (Frasson & Panattoni, 1962), where the Pd–O and Pd–N bonds are 1.99 and 1.94; 2.02 and 1.90; 1.94 and 1.86 Å respectively. The average values of the other bond lengths in the six-membered metalocycles are C–O = 1.308, C–N = 1.297 and C–C = 1.429 and 1.409 Å, and correspond closely to the values reported for *N,N'*-ethylenbis(salicylideneiminato)nickel (Shkol'nikova, Yumal, Shugam & Voblikova, 1970) and for related inner complexes of salicylideneimine (Lingafelter & Braun, 1966). The slightly shorter C–C lengths here must be due to greater resonance stabilisation in the naphthalene system. The average interatomic distances in the two naphthyl rings are found to be the same, 1.403 Å. The valence angles in the molecule have normal values. The sums of the valence angles at the N atoms are about 360°, which is consistent with a planar configuration corresponding to *sp*² hybridization. The angles at the C atoms of the ethylenediamine groups are 107.6 and 107.0° respectively, indicating almost regular tetrahedral configurations. C(13) and C(12) deviate from the NiO(1)–N(1)N(2)O(2) plane by –0.416 and +0.118 Å respectively and the ethylenediamine bridge is thus in the unsymmetrical *gauche* form similar to that observed in many other ethylenediamine complexes (Shkol'nikova, Yumal, Shugam & Voblikova, 1970; Llewellyn & Waters, 1960; Scouloudi, 1953). The closest Ni–Ni distance is 3.3244 (4) Å, which is close to the metal–metal distance of 3.33 Å in bis(*N*-methylsalicylideneiminato)copper (Lingafelter, Simmons, Morosin, Scheringer & Freiburg, 1961), 3.25 Å in bis(dimethylglyoximato)nickel (Godycki & Rundle, 1953) and 3.21 Å in *N,N'*-ethylenbis(salicylideneiminato)nickel (Shkol'nikova, Yumal, Shugam & Voblikova, 1970). In the first two cases the metal–metal interaction leads to structures containing Cu–Cu and Ni–Ni chains respectively. In the last compound, however, the short Ni–Ni bond is the result of the formation of

centrosymmetric dimers and the direction of the Ni–Ni bond makes an angle of 75° with the Ni(NO)₂ coordination plane. The present structure is similar and formation of centrosymmetric dimers leads to the formation of a short Ni–Ni bond which makes an angle of 76° with the Ni(NO)₂ coordination plane. The shift of the molecules in the dimer relative to each other is found to be small, and they lie almost one above another, as shown in Fig. 2. The two metalocycles NiO(1)C(2)C(1)C(11)N(1) and NiO(2)C(13)C(12)–C(22)N(2) are nearly planar, the largest deviations of the atoms from the best plane passing through the molecule being C(1) 0.074 and C(13) 0.022 Å. The angle between the planes is 4.8°. The two metalocycles are also found to have slightly different structures. Both the rings are buckled around the N···O line with the plane of the ring NiO(1)C(2)C(1)C(11)N(1) folded by ~13° about the N(1)···O(1) line and the plane of the ring NiO(2)C(13)C(12)C(22)N(2) folded by ~15° about the N(2)···O(2) line. Compared to this, one of the metalocycle rings in *N,N'*-ethylenbis(salicylideneiminato)nickel (Shkol'nikova, Yumal, Shugam, & Voblikova, 1970) is found to be planar and the other folded by 9° about the N···O line. The observed difference may be due to the greater steric influence of the bulkier naphthyl rings compared to the phenyl rings.

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The Structures of High- and Low-Spin Nickel Chloride Complexes Containing the Macrocyclic Ligand [7*R*(*S*),14*S*(*R*)]-5,5,7,12,12,14-Hexamethyl-1,4,8,11-tetraazacyclotetradecane

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Abstract

The crystal and molecular structures of the low-spin complex $[\text{Ni}(\textit{meso}\text{-Me}_6[14]\text{aneN}_4)]\text{Cl}_2 \cdot 2\text{H}_2\text{O}$ and the high-spin complex $[\text{NiCl}_2(\textit{meso}\text{-Me}_6[14]\text{aneN}_4)] \cdot 2\text{CHCl}_3$, where $\textit{meso}\text{-Me}_6[14]\text{aneN}_4$ is the title macrocyclic ligand, have been determined by single-crystal X-ray diffraction. [Low-spin form: $P\bar{1}$, $a = 8.833(1)$, $b = 8.721(1)$, $c = 8.213(1)$ Å, $\alpha = 86.79(1)$, $\beta = 100.41(1)$, $\gamma = 118.61(1)^\circ$; $R = 0.031$, $R_w = 0.040$ for 3018 observed reflexions. High-spin form: $P\bar{1}$, $a = 9.656(2)$, $b = 11.253(3)$, $c = 6.787(1)$ Å, $\alpha = 93.98(2)$, $\beta = 91.29(2)$, $\gamma = 90.32(2)^\circ$; $R = 0.047$, $R_w = 0.047$ for 2623 observed reflexions.] In the orange low-spin form, the Ni^{II} ion is surrounded by four N atoms of the macrocyclic ligand with an average Ni–N distance of 1.959(2) Å, yielding a square-planar four-coordinate complex. The strong hydrogen-bond networks prevent the coordination of the Cl^- ions and water molecules. In the violet high-spin complex, the Ni^{II} ion is surrounded pseudo-octahedrally by four N atoms of the ligand in a single plane with two independent Ni–N distances of 2.102(3) and 2.060(3) Å, and by two Cl^- ions occupying the axial positions with a Ni–Cl separation of 2.562(1) Å.

$[14]\text{aneN}_4)]\text{Cl}_2 \cdot 2\text{H}_2\text{O}$, and a violet high-spin complex, $[\text{NiCl}_2(\textit{meso}\text{-Me}_6[14]\text{aneN}_4)]$ (Busch, 1967). The macrocyclic ligand $\textit{meso}\text{-Me}_6[14]\text{aneN}_4$ is constrained by steric requirements to coordinate in a single plane. From their electronic spectra and magnetic properties, it has been shown that the orange dihydrate is a square-planar four-coordinate complex having a singlet ground state, whereas the violet anhydride is a pseudo-octahedral six-coordinate complex having a triplet ground state (Busch, 1967). Our recent study revealed that the solid, orange diamagnetic dihydrate is converted upon heating to a violet paramagnetic anhydride (Ito, Hiratsuka, Tsutsumi, Imamura & Fujimoto, 1978). Conversely, the solid, violet paramagnetic anhydrous complex readily reverts to $[\text{Ni}(\textit{meso}\text{-Me}_6[14]\text{aneN}_4)]\text{Cl}_2 \cdot 2\text{H}_2\text{O}$ when moisture is available (Busch, 1967). Of particular interest is the fact that two molecules of water are taken up to produce a diamagnetic Ni^{II} complex. Although water has considerable coordinating ability as compared with the Cl^- ion, the incorporated water molecules are not involved in coordination in the dihydrate.

In an attempt to determine the role played by water in the high-spin–low-spin interconversion and for comparison of the structures with different spin states, the present study has been carried out.

Introduction

Nickel(II) chloride and the title macrocyclic ligand form an orange low-spin complex, $[\text{Ni}(\textit{meso}\text{-Me}_6$

Experimental

The orange dihydrate $[\text{Ni}(\textit{meso}\text{-Me}_6[14]\text{aneN}_4)]\text{Cl}_2 \cdot 2\text{H}_2\text{O}$ was prepared from the corresponding