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Structure of Diaquachloro(2,2′:6′,2′′-terpyridyl)nickel(II) Chloride Monohydrate

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Abstract. $[NiCl(C_{15}H_{11}N_3)(H_2O)_2]Cl.H_2O$, $M_r = 416\cdot9$, triclinic, $P\bar{1}$, $a = 6\cdot945\ (1)$, $b = 9\cdot6684\ (9)$, $c = 13\cdot632\ (2)$ Å, $\alpha = 81\cdot74\ (1)$, $\beta = 79\cdot37\ (1)$, $\gamma = 75\cdot73\ (1)^\circ$, $V = 867\cdot2$ Å^3, $Z = 2$, $D_m = 1\cdot60\ (2)$, $D_x = 1\cdot60$ g cm^{-3}, $\lambda(\mathrm{Mo}\ K\alpha) = 0\cdot7107$ Å, $\mu = 14\cdot45$ cm^{-1}, $F(000) = 428$, room temperature, $R = 0\cdot026$ ($wR = 0\cdot030$) for 2309 observed reflections. The crystal consists of discrete monomeric molecules, linked by hydrogen bonds involving the water molecules and the Cl atoms. The Ni atom is hexacoordinated. Bond lengths and angles for the essentially planar terdentate ligand conform to the values given in the literature. Inter- and intramolecular hydrogen bonds are present in the compound. Distortions from an octahedron to a trigonal prism for different terpyridine metal complexes are calculated. The μ_{eff} (room temperature) and g values (3·21 BM; 2·15) are in good agreement with octahedral stereochemistry for the Ni atom.

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Introduction. The structural study of 2,2′:6′,2″-terpyridine (hereafter tpy) complexes of the type $M(tpy)X_2$ [M = bivalent first-row transition metal; X = (pseudo)halide] shows that they are pentacoordinated with a topology intermediate between trigonal bipyramidal (t.b.p.) and regular square pyramidal (s.p.) (Einstein & Penfold, 1966; Goldschmied & Stephenson, 1970).

Recently some structures involving the Cu^{II} ion have been reported (Rojo, Vlasse & Beltran-Porter, 1983; Savariault, Rojo, Arriortua & Galy, 1983; Vlasse, Rojo & Beltran-Porter, 1983). However, spectroscopic and magnetic studies carried out for Co^{II} and Ni^{II} complexes (Judge & Baker, 1967) led to proposals of different topologies for the pentacoordinated complexes. In order to explain the role played by transition metals in adopting different configurations and to provide the first structural information on complexes of Ni^{II} with ligand tpy in 1:1 ratio, we have determined the structure of the title compound.

Experimental. $Ni(tpy)Cl_2.3H_2O$ was prepared by adding a solution of tpy (0·3 g, 1·29 mmol) in acetone to an ethanolic solution of nickel dichloride (0·18 g, 1·89 mmol). Green prisms 0·11 × 0·14 × 0·28 mm were obtained by recrystallization of the resulting precipitate from a water/ethanol mixture. D_m by flotation in bromoform/acetone. Approximate cell parameters determined from oscillation and Weissenberg photographs in agreement with triclinic $P\bar{1}$. Intensity data obtained on an Enraf–Nonius CAD-4 diffractometer, graphite-monochromatized Mo $K\alpha$ radiation; 25 reflections ($3 < \theta < 25°$) for measuring lattice parameters; $\omega/2\theta$-scan mode; ω-scan width $(0{\cdot}80 + 0{\cdot}34\,\mathrm{tg}\theta)°$; 3048 reflections measured with $3 < \theta < 30°$; 2309 independent with $I \geq 2{\cdot}5\sigma(I)$; index range h −8→8, k −11→11, l 0→16; variable scan speed; no systematic loss of intensity of three standard reflections, monitored every hour; correction for Lorentz and polarization effects, but not for absorption or extinction; structure solved by Patterson and Fourier techniques with *SHELX76* (Sheldrick, 1976); least-squares refinement of all non-H atoms treated anisotropically; coordinates of H atoms (from ΔF synthesis) were refined with fixed isotropic temperature factor $U = 0{\cdot}06$ Å^2; $\sum w(|F_o| - |F_c|)^2$ minimized; $w = (\sigma^2|F_o| + 0{\cdot}00145|F_o|^2)^{-1}$; $(\Delta/\sigma)_{max} = 0{\cdot}7$; $(\Delta\rho)_{max} = 0{\cdot}1$ e Å^{-3}; final $R = 0{\cdot}026$, $wR = 0{\cdot}030$; scattering factors from *International Tables for X-ray Crystallography* (1974). Susceptibility measurements were performed with a Faraday-type microbalance between 70–300 K. The ESR spectrum was recorded on a Brucker ER 200tt spectrometer operating at X-band, calibrated by NMR probe for the magnetic field and a HP5342A frequency counter.

Discussion. Fig. 1 shows the title molecule with the numbering system and Fig. 2 the packing of the molecules in the unit cell. Final atomic coordinates for non-H atoms and the equivalent isotropic temperature factors are given in Table 1.* Bond lengths and angles are given in Table 2.

The structure consists of monomeric molecules with Ni hexacoordinated, resulting from bonding to a quasi-planar terdentate ligand [N(1), N(2), N(3)], to a Cl atom and to two water molecules. A second Cl atom acts as counterion and was found to be disordered, being refined as two separate entities [Cl(2,2′)] with site-occupation factors of 0·5; a nearby water molecule also appeared to be disordered and was refined with occupations fixed at 0·5 as derived from a difference map.

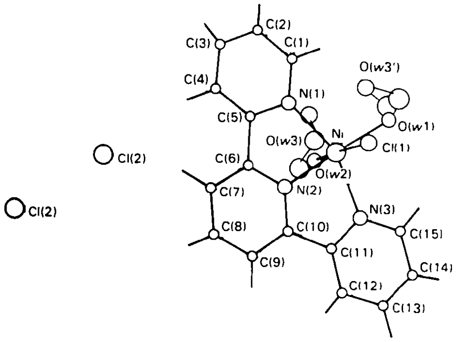

Fig. 1. Molecular conformation of the complex showing the atom numbering.

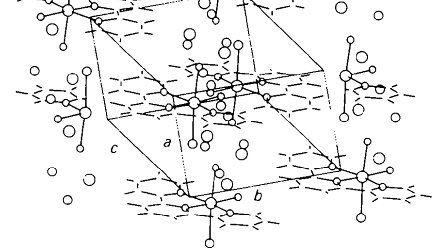

Fig. 2. Packing of the molecules in the unit cell. The larger circles represent Cl, the smaller circles water.

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* Lists of structure factors, anisotropic thermal parameters, H-atom coordinates, bonds and angles involving H atoms and Table 3 have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 42449 (13 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Distortions from octahedral geometry are caused by the terdentate organic ligand which subtends angles of 78·6 and 78·3° at Ni. The average C—C and C—N bond distances in the pyridine rings of the tpy ligand are 1·381 (3) and 1·343 (3) Å respectively. Internal C—C—C and C—N—C angles range from 117·3 to 121·5° and from 117·9 to 121·9°, respectively.

Values obtained for bond distances and angles in tpy are in good agreement with those given in the literature (Kepert, Kucharski & White, 1980; Vlasse *et al.*, 1983).

The Ni—O, Ni—Cl and Ni—N distances in the coordination polyhedron are normal covalent distances.

Table 1. *Atomic coordinates* (×10^4; Ni × 10^5) *and equivalent isotropic thermal parameters for non*-H *atoms*

$$B_{\mathrm{eq}} = \tfrac{8}{3}\pi^2\textstyle\sum_i\sum_j U_{ij}a^*_i a^*_j \mathbf{a}_i.\mathbf{a}_j.$$

	x	*y*	*z*	B_{eq}(Å^2)
Ni	29657 (10)	23077 (5)	22689 (5)	2·41 (2)
N(1)	2724 (4)	1116 (3)	3680 (2)	2·76 (12)
N(2)	2650 (4)	467 (3)	1916 (2)	2·51 (11)
N(3)	2849 (4)	2771 (3)	728 (2)	2·92 (12)
C(1)	2659 (5)	1553 (4)	4586 (3)	3·36 (16)
C(2)	2515 (6)	650 (5)	5460 (3)	4·17 (19)
C(3)	2502 (6)	−743 (5)	5413 (3)	4·30 (19)
C(4)	2563 (6)	−1218 (4)	4500 (3)	3·83 (17)
C(5)	2630 (5)	−255 (4)	3650 (2)	2·77 (13)
C(6)	2543 (5)	−612 (3)	2640 (3)	2·81 (13)
C(7)	2293 (6)	−1913 (4)	2430 (3)	3·78 (17)
C(8)	2157 (7)	−2048 (4)	1448 (3)	4·27 (19)
C(9)	2273 (6)	−928 (4)	696 (3)	3·67 (17)
C(10)	2527 (5)	346 (3)	968 (2)	2·70 (14)
C(11)	2638 (5)	1672 (4)	282 (2)	2·82 (14)
C(12)	2532 (6)	1796 (5)	−737 (3)	3·94 (18)
C(13)	2613 (7)	3094 (5)	−1299 (3)	4·78 (21)
C(14)	2809 (7)	4216 (5)	−842 (3)	4·79 (20)
C(15)	2944 (6)	4021 (4)	167 (3)	3·76 (17)
Cl(1)	6621 (1)	1639 (1)	1965 (1)	3·47 (4)
O(*W*1)	3106 (4)	4269 (3)	2594 (2)	3·44 (11)
O(*W*2)	−189 (4)	3112 (3)	2490 (2)	3·71 (12)
O(*W*3)	300 (10)	−4397 (6)	4040 (5)	4·48 (29)
O(*W*3′)	−4842 (13)	−5243 (10)	3912 (6)	7·20 (48)
Cl(2)	−3781 (4)	5035 (3)	3796 (2)	4·85 (11)
Cl(2′)	889 (4)	4284 (2)	6235 (2)	4·44 (10)

Table 2. *Bond lengths* (Å) *and angles* (°) *with e.s.d.'s in parentheses*

Ni—N(1)	2·097 (3)	N(3)—C(11)	1·347 (4)	C(9)—C(10)	1·396 (5)
Ni—N(2)	1·981 (2)	N(3)—C(15)	1·344 (4)	C(10)—C(11)	1·484 (4)
Ni—N(3)	2·096 (3)	C(1)—C(2)	1·377 (5)	C(11)—C(12)	1·391 (5)
Ni—O(*W*1)	2·037 (2)	C(2)—C(3)	1·360 (6)	C(12)—C(13)	1·381 (6)
Ni—O(*W*2)	2·116 (3)	C(3)—C(4)	1·376 (6)	C(13)—C(14)	1·371 (7)
Ni—Cl(1)	2·432 (1)	C(4)—C(5)	1·379 (5)	C(14)—C(15)	1·378 (6)
N(1)—C(1)	1·350 (4)	C(5)—C(6)	1·482 (5)		
N(1)—C(5)	1·350 (4)	C(6)—C(7)	1·386 (5)		
N(2)—C(6)	1·335 (4)	C(7)—C(8)	1·386 (6)		
N(2)—C(10)	1·334 (4)	C(8)—C(9)	1·388 (6)		

N(1)—Ni—N(2)	78·6 (1)	C(1)—C(2)—C(3)	119·1 (4)
N(1)—Ni—N(3)	156·5 (1)	C(2)—C(3)—C(4)	119·9 (4)
N(1)—Ni—O(*W*1)	103·3 (1)	C(3)—C(4)—C(5)	118·7 (4)
N(1)—Ni—O(*W*2)	89·8 (1)	N(1)—C(5)—C(4)	122·1 (3)
N(1)—Ni—Cl(1)	94·1 (1)	N(1)—C(5)—C(6)	114·3 (3)
N(2)—Ni—N(3)	78·3 (1)	C(4)—C(5)—C(6)	123·5 (3)
N(2)—Ni—O(*W*1)	175·9 (1)	N(2)—C(6)—C(5)	114·1 (3)
N(2)—Ni—O(*W*2)	91·1 (1)	N(2)—C(6)—C(7)	120·8 (3)
N(2)—Ni—Cl(1)	94·1 (1)	C(5)—C(6)—C(7)	125·1 (3)
N(3)—Ni—O(*W*1)	99·5 (1)	C(6)—C(7)—C(8)	117·7 (3)
N(3)—Ni—O(*W*2)	86·6 (1)	C(7)—C(8)—C(9)	121·5 (3)
O(*W*1)—Ni—Cl(1)	89·4 (1)	C(8)—C(9)—C(10)	117·3 (3)
O(*W*2)—Ni—O(*W*1)	85·4 (1)	N(2)—C(10)—C(9)	120·8 (3)
O(*W*2)—Ni—Cl(1)	174·1 (1)	N(2)—C(10)—C(11)	113·7 (3)
Ni—N(1)—C(1)	128·1 (2)	C(9)—C(10)—C(11)	125·5 (3)
Ni—N(1)—C(5)	114·0 (2)	N(3)—C(11)—C(10)	114·3 (3)
C(1)—N(1)—C(5)	117·9 (3)	N(3)—C(11)—C(12)	121·9 (3)
Ni—N(2)—C(6)	118·8 (2)	C(10)—C(11)—C(12)	123·8 (3)
Ni—N(2)—C(10)	119·2 (2)	C(11)—C(12)—C(13)	118·7 (4)
C(6)—N(2)—C(10)	121·9 (3)	C(12)—C(13)—C(14)	119·4 (4)
Ni—N(3)—C(11)	114·4 (2)	C(13)—C(14)—C(15)	119·3 (4)
Ni—N(3)—C(15)	127·1 (2)	N(3)—C(15)—C(14)	122·2 (4)
C(11)—N(3)—C(15)	118·5 (3)	Cl(1)—Ni—N(3)	91·6 (1)
N(1)—C(1)—C(2)	122·2 (4)		

Table 4. *Distortion of six-coordinate terpyridine*–Ni$^{\mathrm{II}}$ *complexes*

$\Delta = [\sum_1^3(|\delta b_{1i} - \delta b_{1\mathrm{oct}}|)/846] + [\sum_1^3(|\delta b_{2i} - \delta b_{2\mathrm{oct}}|)/594] + [\sum_1^6(|\delta_i - \delta_{\mathrm{oct}}|)/234]$. The angles δ refer to the angles formed by the normals to adjacent faces of the coordination polyhedron referenced to its edges b_1, b_2 as defined by Muetterties & Guggenberger (1974).

		Dihedral angles (°)		Distortion
Complex	δ's at b_1	δ's at b_2	Remaining δ's	Δ
Ideal octahedron	70·5, 70·5, 70·5	70·5, 70·5, 70·5	70·5, 70·5, 70·5 70·5, 70·5, 70·5	0
$[\mathrm{Ni(tpy)Cl(H_2O)_2]Cl.H_2O}^{(a)}$	57·0, 61·3, 73·5	73·7, 81·5, 76·9	58·3, 71·5, 77·7 73·0, 87·2, 55·4	0·06
$[\mathrm{Co(tpy)(OH)(CO_3)].4H_2O}^{(b)}$	62·3, 56·3, 77·6	79·3, 73·4, 62·3	61·8, 81·4, 67·9 76·3, 84·8, 60·1	0·06
$[\mathrm{Ni(tpy)(NO_2)(ONO)(H_2O)]}^{(c)}$	59·4, 56·9, 69·4	78·7, 82·8, 73·0	63·9, 76·8, 73·7 74·9, 82·9, 55·4	0·09
$[\mathrm{Co(tpy)_2(NCS)_2].2H_2O}^{(d)}$	56·7, 55·2, 79·6	84·8, 84·6, 72·4	49·7, 84·8, 74·8 72·8, 85·3, 51·5	0·09
$[\mathrm{Co(tpy)_2Br_2].3H_2O}^{(e)}$	55·2, 50·6, 77·8	83·8, 83·1, 74·4	49·0, 84·3, 81·5 76·3, 83·9, 51·7	0·10
$[\mathrm{Cu(tpy)_2](NO_3)_2}^{(f)}$	46·0, 53·5, 78·4	84·3, 89·4, 78·4	46·0, 84·3, 75·2 75·2, 89·4, 53·5	0·11
$[\mathrm{Ni(tpy)_2](PF_6)_2}^{(g)}$	51·3, 52·2, 73·7	85·9, 86·3, 76·6	54·1, 86·2, 72·2 75·3, 85·3, 53·6	0·12
$[\mathrm{Cu(tpy)_2](PF_6)_2}^{(h)}$	48·9, 48·9, 77·2	87·4, 87·4, 77·2	48·9, 87·4, 77·2 77·2, 87·4, 48·9	0·13
Trigonal prism	0, 0, 0	120, 120, 120	90, 90, 90 90, 90, 90	1

References: (*a*) this work; (*b*) Kucharski, Skelton & White (1978); (*c*) Cortés *et al.* (1985); (*d*) Raston & White (1976); (*e*) Maslen, Raston & White (1974); (*f*) Allmann, Henke & Reinen (1978); (*g*) Arriortua, Rojo, Amigo, Germain & Declercq (1982*a*); (*h*) Arriortua, Rojo, Amigo, Germain & Declercq (1982*b*).

The *trans*-chloro-coordinated water molecule forms an intermolecular hydrogen bond with the Cl atom of a second unit of the complex $[O(W2)\cdots Cl(1)(x-1,y,z)$ 3·144 (2), $H(W2)\cdots Cl(1)$ 2·63 (5) Å, $O(W2)-H(W2)\cdots Cl(1)$ 166 (7)°]. Both coordinated water and Cl atoms are involved in intra- and intermolecular hydrogen bonds. The lattice H_2O and Cl counterion also contribute to the packing in this form. Table 3 (deposited) shows the hydrogen-bond parameters. The distortion from octahedral towards trigonal-prismatic geometry was calculated by quantification of the Muetterties & Guggenberger (1974) model (Cortés, Arriortua, Rojo, Solans & Beltran, 1985). The value obtained was $\Delta = 0{\cdot}06$, close to octahedral ($\Delta = 0$). In Table 4 are shown the distortions observed for selected hexacoordinated terpyridine compounds.

As expected, distortion in bis(terpyridine) species is greater than for monoterpyridine ones. In the case of the nitrito complex the distortion is increased by hydrogen bonds between H_2O and NO_2.

Variable-temperature (70–300 K) magnetic-susceptibility data show a paramagnetic behavior (Curie–Weiss law, $\theta = -5$ K) in the complex. The magnetic moment ($\mu_{\rm eff}$) at room temperature is 3·21 BM (1 BM = $9{\cdot}27 \times 10^{-24}$ JT^{-1}). The ESR spectrum shows a quasi-isotropal signal with a g value of 2·15. The results are in good agreement with an octahedral stereochemistry for the Ni atom.

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Structure of Bis(*N*-isopropylidene-1*H*-imidazole-4-ethylamine)nickel(II) Diperchlorate, a Ni^{II}–Schiff-Base Complex Derived from Histamine and Acetone

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Abstract. $[Ni(C_8H_{13}N_3)_2](ClO_4)_2$, $M_r = 560{\cdot}04$, monoclinic, $P2_1/n$, $a = 9{\cdot}471$ (2), $b = 10{\cdot}270$ (1), $c = 12{\cdot}651$ (2) Å, $\beta = 107{\cdot}08$ (2)°, $V = 1176{\cdot}2$ (6) Å^3, $Z = 2$, $D_m = 1{\cdot}57$ (1), $D_x = 1{\cdot}581$ Mg m^{-3}, μ(Mo $K\alpha$, $\lambda = 0{\cdot}71073$ Å) = 1·11 mm^{-1}, $F(000) = 580$, $T = 297$ (1) K, $R_F = 0{\cdot}045$ for 1382 reflections. The structure contains L_2Ni^{II} cations with site symmetry $\bar{1}$. Each Ni^{II} ion is coordinated by two imidazole and two imine N donor atoms to give an approximately square-planar coordination geometry. The Ni—N(imidazole) and Ni—N(imine) distances are 1·881 (3) and 1·911 (4) Å, respectively. The strictly planar NiN_4 unit makes an angle of 42·8 (8)° with the imidazole plane.

Introduction. We have been interested in the electronic, spectroscopic and EPR properties of model Cu^{II}–imidazole chromophores that are useful spectroscopic models for imidazole-containing Cu^{II} protein-binding sites (Bernarducci, Bharadwaj, Krogh-Jespersen, Potenza & Schugar, 1983). Because the imidazole π-electron system as well as the N donor ligand lone pair are involved in metal–ligand bonding, there are spectroscopic consequences of the imidazole-ring orientation relative to that of the Cu^{II} d vacancy (Schugar, 1983). This orientation may be defined precisely only in the solid state. To determine the effects of ligand orientation on the N EPR superhyperfine parameters,

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