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Diaquabis(*N*-ethyl-*N*′,*N*′-dimethylethylenediamine-κ^2N,N')nickel(II) dichloride

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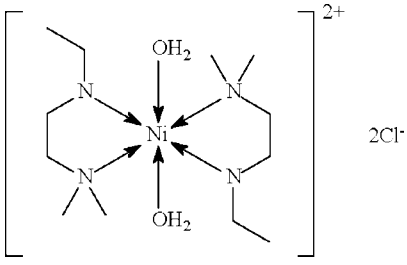
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.003 Å; R factor = 0.030; wR factor = 0.078; data-to-parameter ratio = 20.2.

In the title compound, $[Ni(C_6H_{16}N_2)_2(H_2O)_2]Cl_2$, the Ni^{II} cation (site symmetry $\overline{1}$) is coordinated by two *N*,*N*-bidentate ligands and two water molecules, resulting in a slightly distorted *trans*-NiO_2N_4 octahedron. The complex cations and chloride anions are linked by N—H···Cl and O—H···Cl hydrogen bonds into a chain.

Related literature

For other nickel dichloride complexes of substituted ethylenediamines, see Ide & Norman (2007) and Ihara *et al.* (1991).



Experimental

Crystal data

$[Ni(C_6H_{16}N_2)_2(H_2O)_2]Cl_2$
M_r = 398.06
Monoclinic, $P2_1/n$
a = 7.802 (1) Å
b = 12.550 (1) Å
c = 9.935 (1) Å
β = 95.750 (1)°
V = 967.9 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.29 mm^{-1}
T = 295 (2) K
0.20 × 0.20 × 0.15 mm

Data collection

Bruker APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.856, T_{max} = 1.000
(expected range = 0.706–0.824)
5912 measured reflections
2203 independent reflections
1843 reflections with $I > 2\sigma(I)$
R_{int} = 0.019

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.078
S = 1.04
2203 reflections
109 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.47 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

Table 1
Selected bond lengths (Å).

Ni1—O1*W*	2.103 (1)	Ni1—N2	2.231 (2)
Ni1—N1	2.122 (2)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*W*1···Cl1	0.84 (1)	2.26 (1)	3.095 (2)	174 (2)
O1*W*—H1*W*2···Cl1^{i}	0.84 (1)	2.26 (1)	3.090 (2)	169 (2)
N1—H1N···Cl1	0.84 (1)	2.58 (1)	3.349 (2)	154 (2)

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2007).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2461).

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supplementary materials

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Diaquabis(*N*-ethyl-*N*',*N*'-dimethylethylenediamine-κ^2N,N')nickel(II) dichloride

Y.-N. Liang, Z.-L. Chen, Y.-Z. Zhang and S. W. Ng

Comment

A number of nickel dichloride complexes of substituted ethylenediamines have been characterized by X-ray diffraction; these have the nickel atom chelated by two ligands. The octahedral geometry is completed by two water molecules. Such aquanickel salts are exemplified by the *N*,*N*-dimethylethylenediamine and *N*,*N*-diethylethylenediamine complexes (Ide & Norman, 2007; Ihara *et al.*, 1991). The title compound, (I), shows a similar metal geometry (Fig. 1, Table 1). and the bite angle of the ligand is also similar to those found in such compounds. The components interact by way of N—H···Cl and O—H···Cl hydrogen bonds (Table 2).

Experimental

To an ethanol solution (5 ml) of nickel chloride hexahydrate (0.119 g, 0.5 mmol) was added an ethanol solution (5 ml) of *N*,*N*-dimethyl-*N*'-ethyl-ethylenediamine (1.6 ml, 1 mmol). The solution was filtered. Ether was diffused into the filtrate; light blue crystals of (I) were isolated after a week.

Refinement

The C-bound hydrogen atoms were placed at calculated positions in the riding model approximation [C—H = 0.93–0.98 Å, U(H) = 1.2–1.5 U_{eq}(C)]. The water and amino H atoms were located in a difference Fourier map, and were refined with a distance restraint of O–H = N–H = 0.85±0.01 Å and free refinement of their U_{iso} values.

Figures

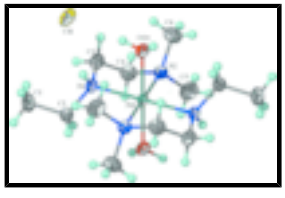

Fig. 1. **Figure 1**. View of part of a chain in (I) showing 50% displacement ellipsoids for the non-hydrogen atoms.

Diaquabis[*N*,*N*-dimethyl-*N*'-ethylethylenediamine-κ^2N,N']nickel(II) dichloride

Crystal data

$[Ni(C_6H_{16}N_2)_2(H_2O)_2]Cl_2$	F_{000} = 428
M_r = 398.06	D_x = 1.366 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 2782 reflections

a = 7.802 (1) Å	θ = 2.6–27.5º
b = 12.550 (1) Å	μ = 1.29 mm^{-1}
c = 9.935 (1) Å	T = 295 (2) K
β = 95.750 (1)º	Block, light blue
V = 967.9 (2) Å^3	0.20 × 0.20 × 0.15 mm
Z = 2	

Data collection

Bruker APEX CCD diffractometer	2203 independent reflections
Radiation source: fine-focus sealed tube	1843 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.019
T = 295(2) K	θ_{max} = 27.5º
φ and ω scans	θ_{min} = 2.6º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -9 \rightarrow 9$
T_{min} = 0.856, T_{max} = 1.000	$k = -12 \rightarrow 16$
5912 measured reflections	$l = -12 \rightarrow 12$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.030	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.078	$w = 1/[\sigma^2(F_o^2) + (0.0399P)^2 + 0.2921P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.04	$(\Delta/\sigma)_{max}$ = 0.001
2203 reflections	$\Delta\rho_{max}$ = 0.47 e Å^{-3}
109 parameters	$\Delta\rho_{min}$ = −0.35 e Å^{-3}
3 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Ni1	0.5000	0.5000	0.5000	0.02374 (11)
Cl1	0.02304 (6)	0.31615 (4)	0.44701 (7)	0.05183 (18)
O1W	0.23497 (17)	0.52469 (12)	0.44802 (15)	0.0353 (3)
N1	0.4525 (2)	0.33584 (12)	0.46081 (17)	0.0303 (3)
N2	0.5432 (2)	0.50319 (12)	0.28146 (16)	0.0340 (4)
C1	0.4882 (3)	0.14532 (19)	0.5352 (3)	0.0565 (6)
H1A	0.5675	0.0980	0.5854	0.085*
H1B	0.4670	0.1206	0.4436	0.085*
H1C	0.3818	0.1470	0.5760	0.085*

C2	0.5644 (3)	0.25613 (15)	0.5361 (2)	0.0415 (5)
H2A	0.5879	0.2796	0.6291	0.050*
H2B	0.6734	0.2531	0.4971	0.050*
C3	0.4438 (3)	0.32060 (16)	0.3122 (2)	0.0431 (5)
H3A	0.3294	0.3387	0.2712	0.052*
H3B	0.4655	0.2464	0.2922	0.052*
C4	0.5748 (3)	0.38971 (18)	0.2536 (2)	0.0441 (5)
H4A	0.6894	0.3701	0.2927	0.053*
H4B	0.5689	0.3785	0.1567	0.053*
C5	0.6964 (3)	0.5649 (2)	0.2497 (2)	0.0560 (6)
H5A	0.7056	0.5622	0.1541	0.084*
H5B	0.7981	0.5347	0.2973	0.084*
H5C	0.6846	0.6376	0.2771	0.084*
C6	0.3960 (3)	0.5413 (2)	0.1889 (2)	0.0508 (6)
H6A	0.4261	0.5397	0.0976	0.076*
H6B	0.3681	0.6130	0.2125	0.076*
H6C	0.2983	0.4960	0.1966	0.076*
H1W1	0.170 (3)	0.4708 (13)	0.448 (3)	0.055 (8)*
H1W2	0.177 (3)	0.5738 (14)	0.478 (2)	0.056 (8)*
H1N	0.3539 (16)	0.3279 (16)	0.486 (2)	0.034 (6)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.01999 (17)	0.02258 (17)	0.02879 (18)	0.00071 (11)	0.00310 (12)	−0.00120 (12)
Cl1	0.0282 (3)	0.0379 (3)	0.0903 (5)	−0.0015 (2)	0.0104 (3)	−0.0152 (3)
O1W	0.0237 (7)	0.0315 (8)	0.0510 (9)	0.0016 (6)	0.0045 (6)	−0.0039 (6)
N1	0.0249 (8)	0.0259 (8)	0.0403 (9)	0.0000 (6)	0.0038 (6)	−0.0011 (6)
N2	0.0353 (9)	0.0365 (9)	0.0304 (8)	−0.0016 (7)	0.0047 (7)	0.0004 (7)
C1	0.0533 (15)	0.0329 (12)	0.0823 (18)	−0.0003 (10)	0.0025 (13)	0.0111 (11)
C2	0.0350 (11)	0.0296 (10)	0.0581 (14)	0.0022 (8)	−0.0045 (9)	0.0015 (9)
C3	0.0523 (13)	0.0337 (11)	0.0427 (12)	−0.0035 (9)	0.0016 (10)	−0.0100 (9)
C4	0.0495 (13)	0.0461 (13)	0.0377 (12)	0.0050 (10)	0.0099 (9)	−0.0077 (9)
C5	0.0536 (14)	0.0733 (18)	0.0436 (13)	−0.0183 (13)	0.0171 (11)	0.0022 (12)
C6	0.0577 (15)	0.0583 (14)	0.0351 (12)	0.0045 (12)	−0.0010 (10)	0.0042 (10)

Geometric parameters (Å, °)

Ni1—O1W	2.103 (1)	C1—H1B	0.9600
Ni1—O1W^{i}	2.103 (1)	C1—H1C	0.9600
Ni1—N1	2.122 (2)	C2—H2A	0.9700
Ni1—N1^{i}	2.122 (2)	C2—H2B	0.9700
Ni1—N2	2.231 (2)	C3—C4	1.501 (3)
Ni1—N2^{i}	2.231 (2)	C3—H3A	0.9700
O1W—H1W1	0.84 (1)	C3—H3B	0.9700
O1W—H1W2	0.84 (1)	C4—H4A	0.9700
N1—C2	1.480 (2)	C4—H4B	0.9700
N1—C3	1.484 (3)	C5—H5A	0.9600

N1—H1N	0.84 (1)	C5—H5B	0.9600
N2—C4	1.476 (3)	C5—H5C	0.9600
N2—C6	1.477 (3)	C6—H6A	0.9600
N2—C5	1.484 (3)	C6—H6B	0.9600
C1—C2	1.512 (3)	C6—H6C	0.9600
C1—H1A	0.9600		
O1W^{i}—Ni1—O1W	180.0	C2—C1—H1C	109.5
O1W^{i}—Ni1—N1	92.95 (6)	H1A—C1—H1C	109.5
O1W—Ni1—N1	87.05 (6)	H1B—C1—H1C	109.5
O1W^{i}—Ni1—N1^{i}	87.05 (6)	N1—C2—C1	114.00 (17)
O1W—Ni1—N1^{i}	92.95 (6)	N1—C2—H2A	108.8
N1—Ni1—N1^{i}	180.0	C1—C2—H2A	108.8
O1W^{i}—Ni1—N2	90.05 (6)	N1—C2—H2B	108.8
O1W—Ni1—N2	89.95 (6)	C1—C2—H2B	108.8
N1—Ni1—N2	83.08 (6)	H2A—C2—H2B	107.6
N1^{i}—Ni1—N2	96.92 (6)	N1—C3—C4	110.26 (16)
O1W^{i}—Ni1—N2^{i}	89.95 (6)	N1—C3—H3A	109.6
O1W—Ni1—N2^{i}	90.05 (6)	C4—C3—H3A	109.6
N1—Ni1—N2^{i}	96.92 (6)	N1—C3—H3B	109.6
N1^{i}—Ni1—N2^{i}	83.08 (6)	C4—C3—H3B	109.6
N2—Ni1—N2^{i}	180.0	H3A—C3—H3B	108.1
Ni1—O1W—H1W1	116.9 (18)	N2—C4—C3	110.61 (17)
Ni1—O1W—H1W2	125.3 (17)	N2—C4—H4A	109.5
H1W1—O1W—H1W2	104 (3)	C3—C4—H4A	109.5
C2—N1—C3	112.42 (16)	N2—C4—H4B	109.5
C2—N1—Ni1	118.68 (13)	C3—C4—H4B	109.5
C3—N1—Ni1	107.30 (12)	H4A—C4—H4B	108.1
C2—N1—H1N	106.3 (14)	N2—C5—H5A	109.5
C3—N1—H1N	109.3 (15)	N2—C5—H5B	109.5
Ni1—N1—H1N	102.1 (14)	H5A—C5—H5B	109.5
C4—N2—C6	109.24 (17)	N2—C5—H5C	109.5
C4—N2—C5	108.09 (17)	H5A—C5—H5C	109.5
C6—N2—C5	106.93 (18)	H5B—C5—H5C	109.5
C4—N2—Ni1	102.09 (12)	N2—C6—H6A	109.5
C6—N2—Ni1	115.32 (13)	N2—C6—H6B	109.5
C5—N2—Ni1	114.83 (13)	H6A—C6—H6B	109.5
C2—C1—H1A	109.5	N2—C6—H6C	109.5
C2—C1—H1B	109.5	H6A—C6—H6C	109.5
H1A—C1—H1B	109.5	H6B—C6—H6C	109.5
O1W^{i}—Ni1—N1—C2	29.32 (15)	N1^{i}—Ni1—N2—C6	−80.96 (15)
O1W—Ni1—N1—C2	−150.68 (15)	O1W^{i}—Ni1—N2—C5	−42.98 (16)
N2—Ni1—N1—C2	119.01 (15)	O1W—Ni1—N2—C5	137.02 (16)
N2^{i}—Ni1—N1—C2	−60.99 (15)	N1—Ni1—N2—C5	−135.94 (16)
O1W^{i}—Ni1—N1—C3	−99.41 (13)	N1^{i}—Ni1—N2—C5	44.06 (16)
O1W—Ni1—N1—C3	80.59 (13)	N2^{i}—Ni1—N2—C5	114 (100)

N2—Ni1—N1—C3	−9.72 (13)	C3—N1—C2—C1	−72.2 (2)
N2^{i}—Ni1—N1—C3	170.28 (13)	Ni1—N1—C2—C1	161.47 (17)
O1W^{i}—Ni1—N2—C4	73.70 (13)	C2—N1—C3—C4	−94.2 (2)
O1W—Ni1—N2—C4	−106.30 (13)	Ni1—N1—C3—C4	38.0 (2)
N1—Ni1—N2—C4	−19.27 (12)	C6—N2—C4—C3	−76.6 (2)
N1^{i}—Ni1—N2—C4	160.74 (12)	C5—N2—C4—C3	167.39 (18)
O1W^{i}—Ni1—N2—C6	−168.00 (15)	Ni1—N2—C4—C3	45.94 (19)
O1W—Ni1—N2—C6	12.00 (15)	N1—C3—C4—N2	−59.9 (2)
N1—Ni1—N2—C6	99.04 (15)		

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*W*1···Cl1	0.84 (1)	2.26 (1)	3.095 (2)	174 (2)
O1*W*—H1*W*2···Cl1^{ii}	0.84 (1)	2.26 (1)	3.090 (2)	169 (2)
N1—H1N···Cl1	0.84 (1)	2.58 (1)	3.349 (2)	154 (2)

Symmetry codes: (ii) −*x*, −*y*+1, −*z*+1.

Fig. 1