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**Key indicators**

Single-crystal X-ray study  
 T = 110 K  
 Mean  $\sigma(\text{C}-\text{C}) = 0.003 \text{ \AA}$   
 Disorder in main residue  
 R factor = 0.042  
 wR factor = 0.072  
 Data-to-parameter ratio = 22.0

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

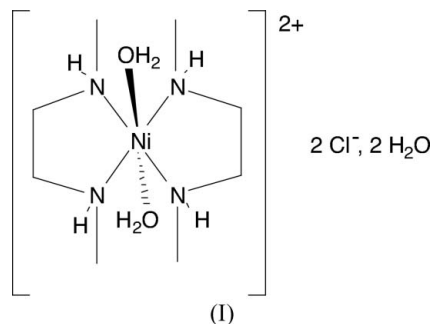
***trans*-Diaquabis(*N,N'*-dimethylethane-1,2-  
 diamine- $\kappa^2N,N'$ )nickel(II) dichloride dihydrate**

The title complex,  $[\text{Ni}(\text{C}_4\text{H}_{12}\text{N}_2)_2(\text{H}_2\text{O})_2]\text{Cl}_2 \cdot 2\text{H}_2\text{O}$ , consists of two chloride ions, two water molecules and a complex dication. The nickel(II) center is pseudo-octahedral six-coordinate, with a *trans* geometry and is located on an inversion center. The coordinated water molecule hydrogen bonds to two chloride ions, as does the uncoordinated water molecule. The uncoordinated water molecule also accepts a hydrogen bond from one of the secondary amines.

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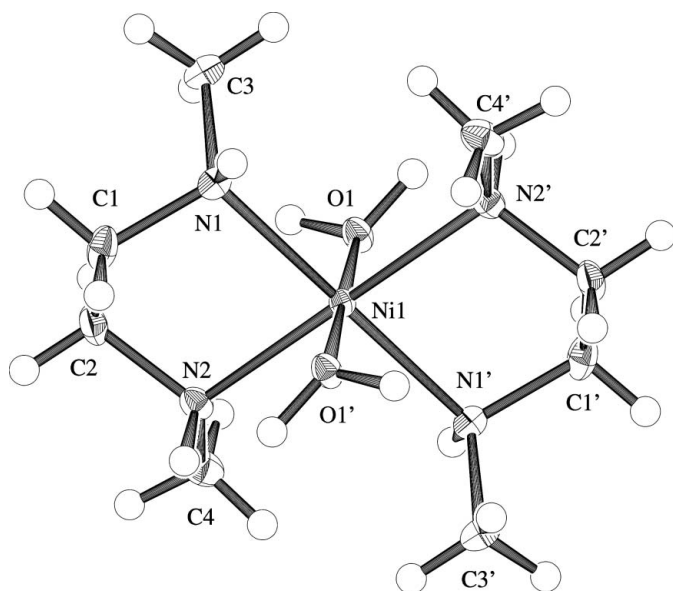
**Comment**

We have reported magneto-structural studies of nickel(II) dimers containing the  $\{\text{Ni}X\}_2$  core, where *X* is Cl and Br (Tong *et al.*, 1999, 2000; Xie & Norman, 2006), and observed that a bridging bromide mediates stronger ferromagnetic coupling between six-coordinate nickel(II) centers than does a bridging chloride for the same effective ferromagnetic coupling pathway. Consequently, we have been attempting the synthesis and structural characterization of additional examples. In this context, the title compound, (I), was prepared and characterized.

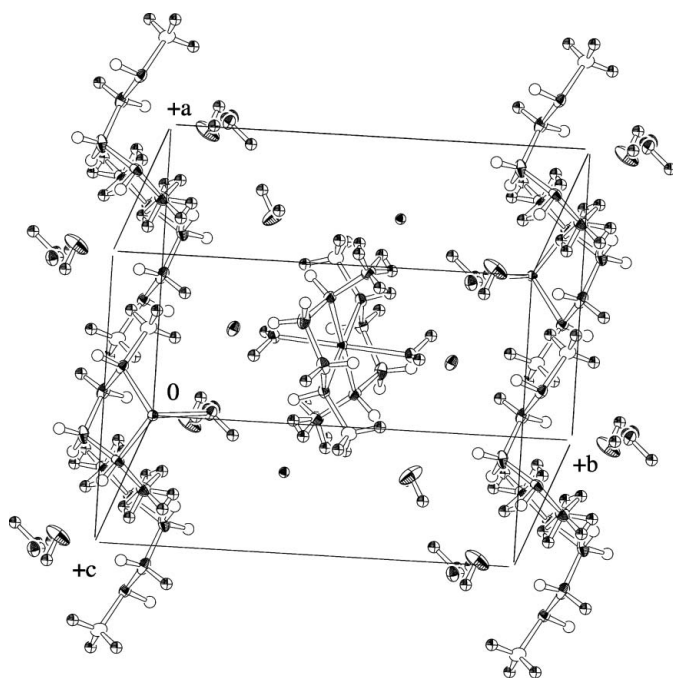


The title compound contains a dicationic nickel(II) complex, two chloride counter-ions and two solvent water molecules. The dication is a centrosymmetric pseudo-octahedral nickel(II) complex of *trans* geometry with two dimethylethylenediamine ligands providing four N atoms that serve as an equatorial plane for the octahedral arrangement. The axial positions are occupied by water molecules.

It is somewhat surprising that all of the nickel(II)-to-ligand atom distances are somewhat long. The median value for six-coordinate secondary amine Ni–N distances reported by Orpen *et al.* (1989) is 2.098 Å while the upper quartile distance is 2.121 Å. One of the Ni–N distances falls at the median [2.098 (2) Å], while the other [2.123 (1) Å] falls in the upper quartile, as does the Ni–O distance of 2.135 (1) Å (upper quartile of similar distances 2.105 Å; Orpen *et al.*, 1989). Not



**Figure 1**  
View of the dication of (I), with displacement ellipsoids drawn at the 50% probability level. Atoms with the suffix a are at the symmetry position  $(1-x, 1-y, 1-z)$ . The minor set of disordered methyl H atoms has been omitted.



**Figure 2**  
Packing diagram of (I).

only are the nickel(II)-to-ligand atom distances long in the title complex, the similar *trans*-dibromobis(*N,N'*-dimethylethane-1,2-diamine- $\kappa^2N,N'$ )nickel(II) (Ariyananda & Norman, 2006a) and analogous chloride complex (Ariyananda & Norman, 2006b) also exhibit long nickel(II)-to-ligand atom distances. The observation that all of the distances are somewhat long suggests crowding about the nickel(II) center.

The title compound exhibits extensive hydrogen bonding. The axial water molecule hydrogen bonds to the chloride ion in the same asymmetric unit through H13 and to an adjacent chloride ion at  $(\frac{1}{2}-x, \frac{1}{2}-y, \frac{1}{2}-z)$ . The solvent water molecule also hydrogen bonds to two adjacent chloride ions, *i.e.* at  $(\frac{1}{2}-x, \frac{1}{2}+y, \frac{3}{2}-z)$  and  $(1-x, 1-y, 2-z)$ , and accepts a hydrogen bond from atom N1.

It should be noted that the title compound is a kinetic product which recrystallizes over several days to give *trans*-dichlorobis(*N,N'*-dimethylethane-1,2-diamine- $\kappa^2N,N'$ )nickel(II) (Ariyanada & Norman, 2006b).

## Experimental

*N,N'*-Dimethylethane-1,2-diamine (0.545 ml, 5.12 mmol) was dissolved in 25 ml methanol. Nickel(II) chloride hexahydrate (0.6010 g, 2.53 mmol) was dissolved separately in 25 ml methanol giving a green solution. The two methanol solutions were mixed, producing a blue solution that was allowed to stand at room temperature. Crystals began to form after several hours. If the crystals are allowed to sit, they redissolve and recrystallize to give *trans*-dichlorobis(*N,N'*-dimethylethane-1,2-diamine- $\kappa^2N,N'$ )nickel(II).

### Crystal data

$[\text{Ni}(\text{C}_4\text{H}_{12}\text{N}_2)_2(\text{H}_2\text{O})_2]\text{Cl}_2 \cdot 2\text{H}_2\text{O}$   
 $M_r = 377.97$   
 Monoclinic,  $P2_1/n$   
 $a = 8.7402(15) \text{ \AA}$   
 $b = 12.788(3) \text{ \AA}$   
 $c = 9.011(2) \text{ \AA}$   
 $\beta = 116.703(13)^\circ$   
 $V = 899.7(3) \text{ \AA}^3$

$Z = 2$   
 $D_x = 1.395 \text{ Mg m}^{-3}$   
 Mo  $K\alpha$  radiation  
 $\mu = 1.39 \text{ mm}^{-1}$   
 $T = 110 \text{ K}$   
 Block, light purple  
 $0.30 \times 0.15 \times 0.10 \text{ mm}$

### Data collection

Nonius KappaCCD diffractometer  
 with an Oxford Cryosystems  
 Cryostream cooler  
 $\omega$  scans with  $\kappa$  offsets  
 Absorption correction: multi-scan  
 (SCALEPACK; Otwinowski &

Minor, 1997)  
 $T_{\min} = 0.734$ ,  $T_{\max} = 0.874$   
 13820 measured reflections  
 2774 independent reflections  
 1978 reflections with  $I > 3.00\sigma(I)$   
 $R_{\text{int}} = 0.031$   
 $\theta_{\max} = 30.8^\circ$

### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.042$   
 $wR(F^2) = 0.072$   
 $S = 0.96$   
 1978 reflections  
 90 parameters  
 H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o) + 0.0004|F_o|^2]$

$(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 0.36 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\min} = -0.42 \text{ e \AA}^{-3}$   
 Extinction correction: Zachariasen  
 (1967)  
 Extinction coefficient:  
 $1.5(3) \times 10^{-6}$

**Table 1**

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

Ni1—O1	2.135 (1)	Ni1—N1 <sup>i</sup>	2.098 (2)
Ni1—O1 <sup>i</sup>	2.135 (1)	Ni1—N2	2.123 (1)
Ni1—N1	2.098 (2)	Ni1—N2 <sup>i</sup>	2.123 (1)
O1—Ni1—N1	95.46 (6)	O1—Ni1—N2 <sup>i</sup>	90.63 (5)
O1—Ni1—N1 <sup>i</sup>	84.54 (6)	N1—Ni1—N2	83.92 (6)
O1—Ni1—N2	89.37 (5)	N1—Ni1—N2 <sup>i</sup>	96.08 (6)

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

**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>
O1—H13···Cl1	0.94	2.22	3.144 (2)	168
O1—H14···Cl1 <sup>iii</sup>	0.95	2.14	3.080 (1)	170
O2—H15···Cl1 <sup>iii</sup>	0.89	2.37	3.250 (2)	172
O2—H16···Cl1 <sup>iv</sup>	0.88	2.39	3.266 (2)	175
N1—H1···O2	0.95	2.12	2.952 (2)	146
N2—H2···Cl1 <sup>v</sup>	0.95	2.49	3.430 (2)	170

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

With the exception of the water molecules, the H atoms were placed in calculated positions (C—H = N—H = 0.95 Å) and assigned displacement parameters 1.2 times larger than the atoms to which they are bound. The H atoms of the water molecules were located in difference maps, and were also assigned displacement parameters 1.2 times larger than the O atoms to which they are bound. During refinement it became apparent that the *N*-methyl group associated with C3 is disordered. A second set of three H atoms was placed in calculated positions using electron density in a difference map to orient the group. The occupancy of one of the H atoms (H7) was refined. The occupancy of H8 and H9 (the remaining two H atoms of that methyl group) were constrained to the occupancy of H7. The occupancies of the H atoms of the other orientation of the methyl group (H17, H18 and H19) were constrained to one minus the refined occupancy. Displacement parameters for these H atoms were assigned to be the occupancy times 1.2 times the C3 displacement parameter. This gave a model with a methyl orientation of greater occupancy (H17–H19 = 0.79) and a methyl orientation of lesser occupancy (H7–H9 = 0.21).

Data collection: *COLLECT* (Nonius, 2000); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK* and *DENZO* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *TEXSAN for Windows* (Molecular Structure Corporation, 1999); molecular graphics: *ORTEPII* (Johnson, 1976) in *TEXSAN*; software used to prepare material for publication: *TEXSAN for Windows*.

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