Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# *cis*-Bis(2,2-bipyridine)dichloronickel(II) methanol solvate

**Frédéric Georges Fontaine**

Département de Chimie, Université de Montréal, CP 6128, Succ. Centre-ville, Montréal, Québec, Canada H3C 3J7

Correspondence e-mail: fontaifr@yahoo.ca

Received 8 May 2001
Accepted 11 May 2001
Online 15 June 2001

**Key indicators**

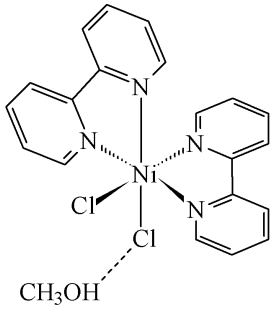
Single-crystal X-ray study
$T$ = 293 K
Mean $\sigma$(C–C) = 0.007 Å
$R$ factor = 0.047
$wR$ factor = 0.101
Data-to-parameter ratio = 14.7

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

The title complex, $[NiCl_2(bipy)_2].CH_3OH$, where bipy is 2,2-bipyridine ($C_{10}H_8N_2$), consists of an Ni atom coordinated to two *cis* chlorides and two bidentate bipyridines. One molecule of methanol is hydrogen bonded to one of the two inequivalent chlorides.

## Comment

In the course of our studies, the synthesis of $[Ni(bipy)_2Cl_2].CH_3OH$, (I), was carried out using a method previously reported for the synthesis of $Ni(pyridine)_4Cl_2$ (Long & Clarke, 1978). The molecule adopts a pseudo-octahedral geometry with N—Ni—N bite angles of 77.75 (14) and 78.00 (14) Å, and *cis* angles between 87.84 (10) and 97.58 (13) Å; *trans* angles are close to linearity. The structure of this complex (Fig. 1) is similar to the two structures of $Ni(bipy)_2Cl_2$ previously reported.




(I)

If $CH_3CN$ is used for recrystallization (Ferbinteanu *et al.*, 1998), two water molecules make strong hydrogen bonds with the chlorides. The structure of the dimethylformamide (DMF) solvate was also published the same year (Hipler *et al.*, 1998). In both published structures, a $C_2$ axis is observed on the nickel making both chlorides and bipy ligands equivalent by symmetry. Our studies revealed that the Ni—Cl bond lengths are quite different (more than 20$\sigma$) from one another. We believe that this is due to a methanol being hydrogen bonded only to Cl1 [3.276 (3) *versus* 3.467 (3) Å]. Also unexpected is that one of the bipy shows both of its Ni—N lengths [2.073 (3) and 2.077 (3) Å] shorter than the other bipy [2.084 (3) and 2.100 (4) Å].

## Experimental

A solution of $NiCl_2.6H_2O$ (2 g) in methanol (25 ml) was added to a solution of 2,2-bipyridine (2.75 g) in methanol. This mixture was agitated for 1 h and concentrated under vacuum to a volume of 10 ml.

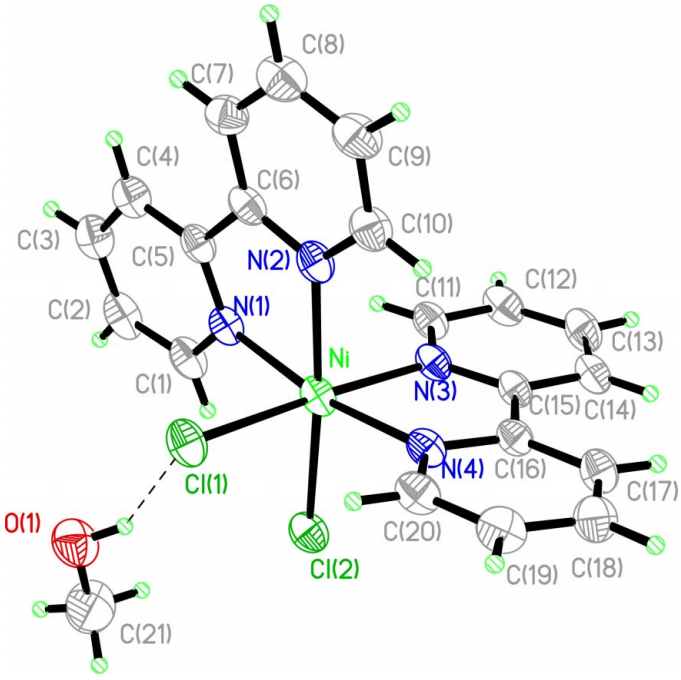



**Figure 1**
The structure of the title complex showing 30% probability displacement ellipsoids and the atom-numbering scheme.

Slow evaporation of the solvent in air allowed the formation of green crystals.

*Crystal data*

$[NiCl_2(C_{10}H_8N_2)_2]\cdot CH_4O$
$M_r$ = 474.02
Orthorhombic, *Pbca*
$a$ = 10.455 (3) Å
$b$ = 13.830 (4) Å
$c$ = 28.548 (10) Å
$V$ = 4128 (2) Å$^3$
$Z$ = 8
$D_x$ = 1.526 Mg m$^{-3}$
Cu $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta$ = 20.0–23.0°
$\mu$ = 3.90 mm$^{-1}$
$T$ = 293 (2) K
Block, dark green
0.23 × 0.23 × 0.16 mm

*Data collection*

Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: by integration (*ABSORP* in *NRCVAX*; Gabe *et al.*, 1989)
$T_{min}$ = 0.432, $T_{max}$ = 0.593
22 288 measured reflections
3908 independent reflections
2054 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.073
$\theta_{max}$ = 69.9°
$h = 0 \rightarrow 12$
$k = 0 \rightarrow 16$
$l = 0 \rightarrow 34$
5 standard reflections
frequency: 60 min
intensity decay: none

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.101
$S$ = 1.01
3908 reflections
265 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.04P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.31 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.65 e Å$^{-3}$
Extinction correction: *SHELXL*96 (Sheldrick, 1996)
Extinction coefficient: 0.00066 (5)

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| Ni—N4 | 2.073 (3) | Ni—N2 | 2.100 (4) |
| Ni—N3 | 2.077 (3) | Ni—Cl1 | 2.3940 (13) |
| Ni—N1 | 2.084 (3) | Ni—Cl2 | 2.4213 (13) |
| | | | |
| N4—Ni—N3 | 78.00 (14) | N1—Ni—Cl1 | 88.60 (10) |
| N4—Ni—N1 | 170.07 (14) | N2—Ni—Cl1 | 87.84 (10) |
| N3—Ni—N1 | 97.58 (13) | N4—Ni—Cl2 | 94.06 (10) |
| N4—Ni—N2 | 93.37 (14) | N3—Ni—Cl2 | 88.70 (10) |
| N3—Ni—N2 | 91.44 (13) | N1—Ni—Cl2 | 94.73 (11) |
| N1—Ni—N2 | 77.75 (14) | N2—Ni—Cl2 | 172.43 (11) |
| N4—Ni—Cl1 | 95.58 (10) | Cl1—Ni—Cl2 | 92.87 (5) |
| N3—Ni—Cl1 | 173.48 (10) | | |

**Table 2**
Hydrogen-bonding geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1—H1$A$···Cl1 | 0.82 | 2.63 | 3.276 (3) | 137 |
| O1—H1$A$···Cl2 | 0.82 | 2.78 | 3.467 (3) | 143 |

H atoms were constrained to the parent site using a riding model (C—H 0.93–0.96 and O—H 0.82 Å). The isotropic displacement parameters, $U_{iso}$, were adjusted to a value 50% higher than that of the parent site (methyl and OH) and 20% higher (others).

Data collection: *CAD*-4 *Software* (Enraf–Nonius, 1989); cell refinement: *CAD*-4 *Software*; data reduction: *NRC*-2 and *NRC*-2*A* (Ahmed *et al.*, 1973); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*96 (Sheldrick, 1996); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXL*96.

The financial support from the Natural Sciences and Engineering Research Council of Canada and from the Fonds FCAR du Ministère de l'Éducation du Québec is gratefully acknowledged.

## References

Ahmed, F. R., Hall, S. R., Pippy, M. E. & Huber, C. P. (1973). *NRC Crystallographic Computer Programs for the IBM*/360. Accession Nos. 133–147. *J. Appl. Cryst.* **6**, 309–346.
Bruker (1997). *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Enraf–Nonius (1989). *CAD*-4 *Software*. Version 5.0. Enraf–Nonius, Delft, The Netherlands.
Ferbinteanu, M., Cimpoesu, F., Andruh, M. & Rochon, F. D. (1998). *Polyhedron*, **21**, 3671–3679.
Gabe, E. J., Le Page, Y., Charland, J.-P., Lee, F. L. & White, P. S. (1989). *J. Appl. Cryst.* **22**, 384–387.
Hipler, B., Doring, M., Dubs, C., Gorls, H., Hubler, T. & Uhlig, E. (1998). *Z. Anorg. Allg. Chem.* **624**, 1329–1335.
Long, G. J. & Clarke, P. J. (1978). *Inorg. Chem.* **17**, 1394–1401.
Sheldrick, G. M. (1996). *SHELXL*96. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS*97. University of Göttingen, Germany.