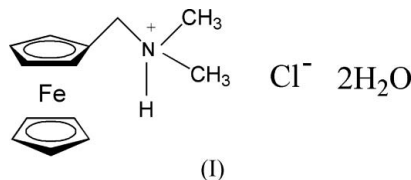


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of ChinaCorrespondence e-mail:
guohongxu919@yahoo.com.cn**Key indicators**Single-crystal X-ray study
 $T = 293$ K
Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å
 R factor = 0.032
 wR factor = 0.071
Data-to-parameter ratio = 19.2For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.**(*N*-Ferrocenylmethyl)dimethylammonium
chloride dihydrate**In the title compound, $[\text{Fe}(\text{C}_5\text{H}_5)(\text{C}_8\text{H}_{13}\text{N})]\text{Cl}\cdot 2\text{H}_2\text{O}$, Fe—C bond lengths lie in the range 2.020 (2)–2.047 (2) Å. Intermolecular N—H···Cl, O—H···Cl and O—H···O hydrogen bonds link the cations, chloride anions and water molecules into a three-dimensional hydrogen-bonded network, which stabilizes the crystal packing.Received 19 June 2006
Accepted 3 July 2006**Comment**The search for ferrocene derivatives has attracted considerable attention over the last decades owing to their biological activity and applications in electrochemistry and materials science (Hall *et al.*, 1998; Li *et al.*, 2001; Welipitiya *et al.*, 1996). (Ferrocenylmethyl)dimethylamine serves as an intermediate in the syntheses of many ferrocene derivatives (Gibbons & Trotter, 1971; Winter & Wolmershäuser, 1998). In this communication, we report the crystal structure of the title compound, (I) (Fig. 1), which is a new (ferrocenylmethyl)-dimethylammonium salt.In (I), the Fe atom is bonded to the two five-membered carbon rings with Fe—C bond lengths in the range 2.020 (2)–2.047 (2) Å (Table 1). The two rings, C1–C5 and C6–C10, are nearly parallel with a dihedral angle between their mean planes of 3.3 (1)° and exhibit a nearly eclipsed conformation, as is usually found in other ferrocene derivatives (Ye *et al.*, 2005; Todd *et al.*, 2006; Guo *et al.*, 2006).In the crystal structure, classical intermolecular N—H···Cl, O—H···Cl and O—H···O hydrogen bonds are observed (Table 2), which link the ammonium cations, chloride anions and uncoordinated water molecules into a three-dimensional hydrogen-bonded network and stabilize the crystal packing (Fig. 2). The N—H···Cl hydrogen bond is similar to that found in the anhydrous compound $[\text{Fe}(\text{C}_5\text{H}_5)(\text{C}_8\text{H}_{13}\text{N})]^+\cdot\text{Cl}^-$ with an (N—)H···Cl distance of 2.18 Å (Winter & Wolmershäuser, 1998).**Experimental**

A solution of NaCl (0.0292 g, 0.5 mmol) in methanol (10 ml) was added to a solution of (ferrocenylmethyl)dimethylamine (0.1214 g, 0.5 mmol) in methanol (10 ml). To this solution, dichloromethane (1.5 ml) was added dropwise and the mixture shaken for 3 h and

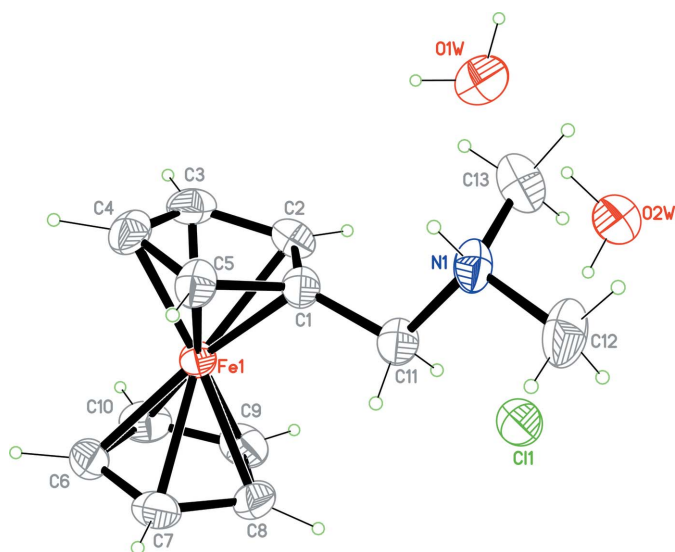


Figure 1
View of (I) showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

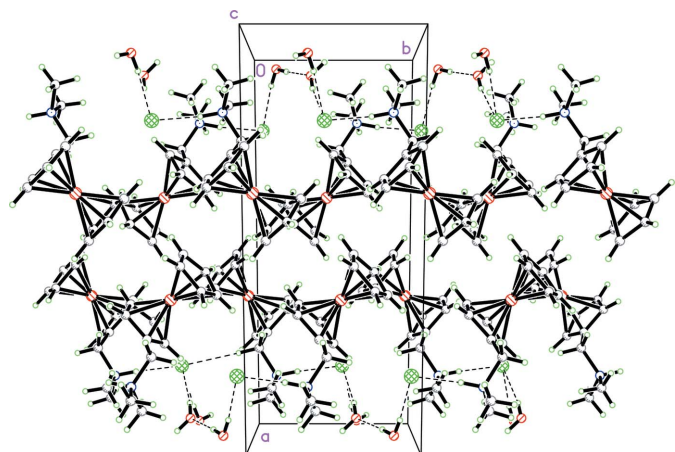


Figure 2
The crystal packing viewed along the *c*-axis direction. The intermolecular N—H...Cl, N—H...O and O—H...O hydrogen bonds are shown as dashed lines.

concentrated under vacuum to a volume of 10 ml. Brown prism-shaped crystals of (I) were obtained by slow evaporation of the solvent in air.

Crystal data

[Fe(C₅H₅)(C₈H₁₃N)]Cl·2H₂O
 $M_r = 315.62$
 Monoclinic, $P2_1/c$
 $a = 18.116$ (4) Å
 $b = 7.3783$ (15) Å
 $c = 11.799$ (2) Å
 $\beta = 105.17$ (3)°
 $V = 1522.2$ (6) Å³

$Z = 4$
 $D_x = 1.377$ Mg m⁻³
 Mo $K\alpha$ radiation
 $\mu = 1.16$ mm⁻¹
 $T = 293$ (2) K
 Prism, brown
 $0.51 \times 0.35 \times 0.34$ mm

Data collection

Rigaku Weissenberg IP
 diffractometer
 ω scans
 Absorption correction: multi-scan
 (RAPID-AUTO; Rigaku, 1998)
 $T_{\min} = 0.620$, $T_{\max} = 0.674$

13908 measured reflections
 3501 independent reflections
 2484 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.035$
 $\theta_{\text{max}} = 27.5^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.032$
 $wR(F^2) = 0.071$
 $S = 1.01$
 3501 reflections
 182 parameters

H atoms treated by a mixture of independent and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.032P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.46$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.26$ e Å⁻³

Table 1

Selected bond lengths (Å).

Fe1—C9	2.020 (2)	Fe1—C5	2.0347 (18)
Fe1—C1	2.0248 (18)	Fe1—C3	2.044 (2)
Fe1—C8	2.027 (2)	Fe1—C7	2.044 (2)
Fe1—C2	2.0305 (19)	Fe1—C4	2.046 (2)
Fe1—C10	2.034 (2)	Fe1—C6	2.047 (2)

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>
O2W—H2WA...Cl1	0.84 (2)	2.32 (2)	3.161 (2)	174 (3)
O2W—H2WB...O1W	0.85 (2)	1.87 (2)	2.712 (3)	176 (3)
N1—HM1...Cl1 ⁱ	0.96	2.13	3.0783 (18)	168
O1W—H1WA...O2W ⁱⁱ	0.84 (2)	1.91 (2)	2.744 (3)	175 (3)
O1W—H1WB...Cl1 ⁱⁱⁱ	0.84 (2)	2.36 (2)	3.195 (3)	171 (2)
O2W—H2WA...Cl1	0.84 (2)	2.32 (2)	3.161 (2)	174 (3)
O2W—H2WB...O1W	0.84 (2)	1.87 (2)	2.712 (3)	176 (3)

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

The C-bound H atoms were positioned geometrically, with C—H = 0.98, 0.97 and 0.96 Å for those on cyclopentadienyl, methylene and methyl C atoms, respectively, and refined as riding with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ or $1.5U_{\text{eq}}(\text{methyl C})$. Atom H1N was positioned geometrically and allowed to ride on N1, with N—H = 0.96 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{N})$. Water H atoms were located in a difference map and refined with O—H and H...H distance restraints of 0.85 (1) and 1.39 (1) Å, respectively, and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$.

Data collection: RAPID-AUTO (Rigaku, 1998); cell refinement: RAPID-AUTO; data reduction: TEXSAN (Molecular Structure Corporation, 1999); program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: PLATON (Spek, 2003); software used to prepare material for publication: SHELXL97.

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References

- Gibbons, C. S. & Trotter, J. (1971). *J. Chem. Soc. A*, pp. 2659–2662.
 Guo, H.-X., Yang, L.-M. & Zhang, S.-D. (2006). *Acta Cryst. E* **62**, m1338–m1339.
 Hall, C. D., Sachsingher, N., Nyburg, S. C. & Steed, J. W. (1998). *J. Organomet. Chem.* **561**, 209–219.
 Li, M., Bai, Y.-J. & Lu, J. (2001). *J. Organomet. Chem.* **637–639**, 738–741.
 Molecular Structure Corporation (1999). TEXSAN. MSC, The Woodlands, Texas, USA.
 Rigaku (1998). RAPID-AUTO. PC Version. Rigaku Corporation, Tokyo, Japan.

- Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
- Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
- Todd, M. H., Motevalli, M., El-Fayyoumy, S. & Richards, C. (2006). *Acta Cryst.* **E62**, m719–m720.
- Welipitiya, D., Dowben, P. A., Zhang, J., Pai, W. W. & Wendelken, J. F. (1996). *Surf. Sci.* **367**, 20–32.
- Winter, R. F. & Wolmershäuser, G. (1998). *J. Organomet. Chem.* **570**, 201–218.
- Ye, B.-X., Xu, Y., Wang, F., Fu, Y. & Song, M.-P. (2005). *Inorg. Chem. Commun.* **8**, 44–47.