

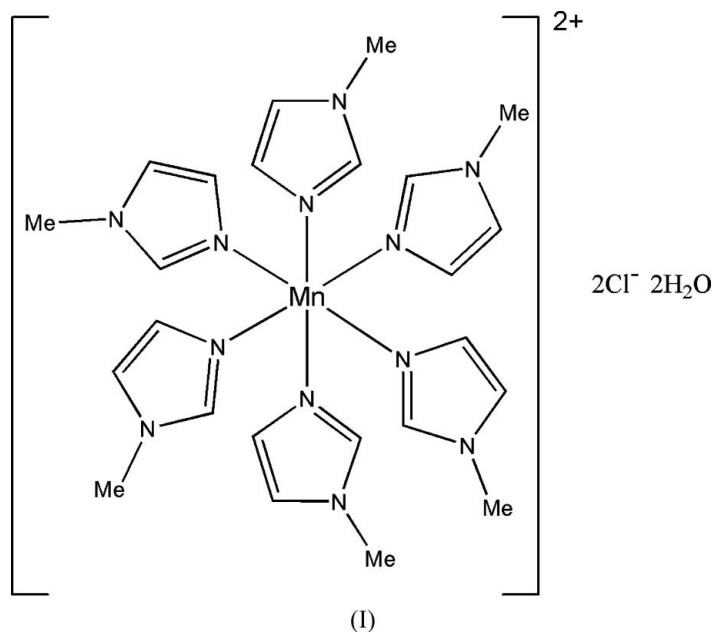
Chong-Min Zhong,^{a*} Ya-Jie Zuo,^b Hua-Shu Jin,^a Tian-Chi Wang^a and Shuang-Quan Liu^a^aDepartment of Chemistry, Harbin Normal University, Harbin 150080, People's Republic of China, and ^bLibrary, Harbin Normal University, Harbin 150080, People's Republic of China

Correspondence e-mail: zhong_cm@yahoo.co

Key indicators

Single-crystal X-ray study
 $T = 294$ K
Mean $\sigma(\text{C}-\text{C}) = 0.002$ Å
 R factor = 0.030
 wR factor = 0.087
Data-to-parameter ratio = 20.2For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.Hexakis(1-methyl-1*H*-imidazole- κN^3)manganese(II) dichloride dihydrateIn the title compound, $[\text{Mn}(\text{C}_4\text{H}_6\text{N}_2)_6]\text{Cl}_2 \cdot 2\text{H}_2\text{O}$, the Mn^{II} ion is located on an inversion center and is coordinated by six 1-methylimidazole molecules in a distorted octahedral geometry.Received 30 August 2006
Accepted 11 September 2006

Comment

As part of an investigation on Mn complexes with nitrogen donor ligands, we present here the crystal structure of the title compound, (I). The crystal structure of (I) consists of Mn^{II} complex cations, Cl^- anions and solvent water molecules. The Mn^{II} ion is located on an inversion center and is coordinated by six 1-methylimidazole molecules in a distorted octahedral geometry (Table 1).The Cl^- anions and water molecules are linked together by $\text{O}-\text{H}\cdots\text{Cl}$ hydrogen bonds (Table 2), forming a planar quadrilateral. This quadrilateral links with 1-methylimidazole ligands *via* weak $\text{C}-\text{H}\cdots\text{O}$ and $\text{C}-\text{H}\cdots\text{Cl}$ interactions.A packing diagram of (I) is presented in Fig. 2. The Mn^{II} complex cations form a three-dimensional network with a hollow mesh along the a axis, in which lie the quadrilaterals formed by Cl^- anions and solvent molecules.

Experimental

 $\text{MnCl}_2 \cdot 4\text{H}_2\text{O}$ (80 mg, 0.40 mmol) was added to 1-methylimidazole (1.000 g, 12.18 mmol) in 2.0 ml acetonitrile. The resulting white

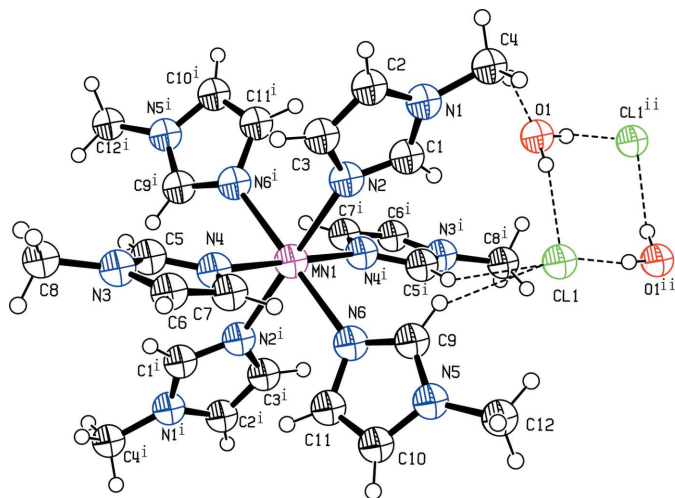


Figure 1
The molecular structure of (I) with 50% probability displacement ellipsoids (arbitrary spheres for H atoms). Dashed lines indicate hydrogen bonds. [Symmetry codes: (i) $-x, -y, 2 - z$; (ii) $-x, 1 - y, 2 - z$]

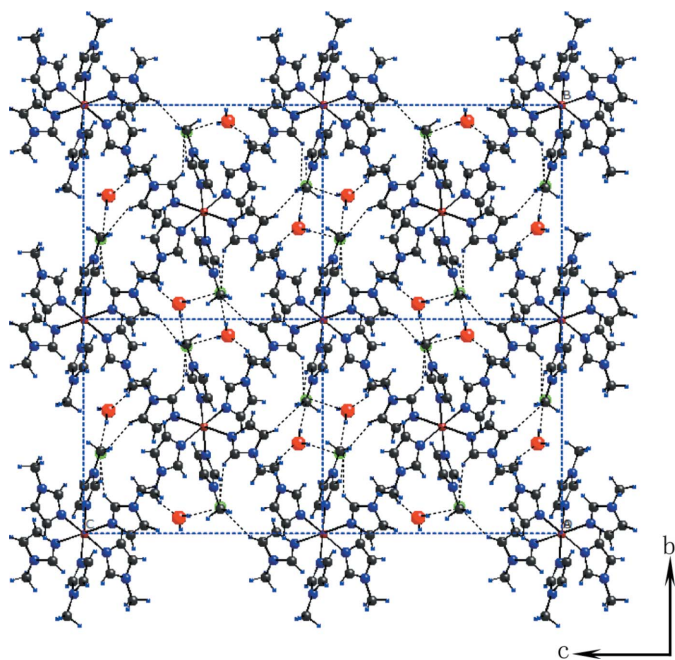


Figure 2
The packing of (I), viewed along the a axis. Dashed lines indicate hydrogen bonds.

precipitate was dissolved in a suitable quantity of hot acetonitrile and then filtered. Single crystals of (I) were obtained from the filtrate.

Crystal data

[Mn(C₄H₆N₂)₆]Cl₂·2H₂O
 $M_r = 654.52$
 Monoclinic, $P2_1/n$
 $a = 8.1645$ (2) Å
 $b = 13.4135$ (4) Å
 $c = 15.1186$ (4) Å
 $\beta = 97.994$ (11)°
 $V = 1639.62$ (9) Å³

$Z = 2$
 $D_x = 1.326$ Mg m⁻³
 Mo $K\alpha$ radiation
 $\mu = 0.61$ mm⁻¹
 $T = 294$ (2) K
 Block, colorless
 $0.32 \times 0.25 \times 0.24$ mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 2005)
 $T_{\min} = 0.768$, $T_{\max} = 0.864$

11514 measured reflections
 4028 independent reflections
 3529 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.014$
 $\theta_{\max} = 28.3^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.030$
 $wR(F^2) = 0.087$
 $S = 1.06$
 4028 reflections
 199 parameters
 H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.044P)^2 + 0.3715P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.24$ e Å⁻³
 $\Delta\rho_{\min} = -0.23$ e Å⁻³
 Extinction correction: SHELXL97
 Extinction coefficient: 0.0058 (11)

Table 1

Selected bond lengths (Å).

Mn1—N2	2.2755 (11)	Mn1—N6	2.2585 (11)
Mn1—N4	2.3197 (11)		

Table 2

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O1—H13 \cdots Cl1	0.78 (3)	2.42 (3)	3.1972 (18)	172 (3)
O1—H14 \cdots Cl1 ⁱ	0.80 (3)	2.42 (3)	3.2059 (19)	167 (3)
C4—H4C \cdots O1	0.96	2.42	3.342 (3)	161
C5—H5 \cdots Cl1 ⁱⁱ	0.93	2.83	3.6714 (15)	150
C9—H9 \cdots Cl1	0.93	2.71	3.4920 (14)	142
C10—H10 \cdots Cl1 ⁱⁱⁱ	0.93	2.76	3.6318 (16)	156

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

The methyl H atoms were constrained to an ideal geometry, with $C-H = 0.96$ Å and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$; each methyl group was allowed to rotate freely about its N—C bond. The water H atoms were located in a difference Fourier map and refined isotropically. Other H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with $C-H = 0.93$ Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Data collection: SMART (Bruker, 2005); cell refinement: SAINT (Bruker, 2005); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEP-3 for Windows (Farrugia, 1997); software used to prepare material for publication: SHELXTL (Bruker, 2000).

This study was sponsored by the Scientific Research Foundation for Returned Overseas Chinese Scholars of the Education Office of Heilongjiang Province (No. 1151hq018).

References

- Bruker (2000). SHELXTL. Bruker AXS Inc., Madison, Wisconsin, USA.
 Bruker (2005). SMART and SAINT. Bruker AXS Inc., Madison, Wisconsin, USA.
 Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
 Sheldrick, G. M. (1997). SHELXS97 and SHELXL97. University of Göttingen, Germany.
 Sheldrick, G. M. (2005). SADABS (Version 2.10). University of Göttingen, Germany.