

Hui Zhang,^{a,b*} Yan-Mei Wu^b and
Liang Fang^a^aKey Laboratory of Nonferrous Materials and
New Processing Technology, Ministry of
Education, Guilin University of Technology,
Guilin 541004, People's Republic of China, and^bDepartment of Applied Chemistry, Wuhan
University of Technology, Wuhan 430070,
People's Republic of China

Correspondence e-mail: huizhangac@126.com

Key indicators

Single-crystal X-ray study

T = 293 K

Mean $\sigma(\text{C}-\text{C}) = 0.004 \text{ \AA}$

R factor = 0.019

wR factor = 0.046

Data-to-parameter ratio = 24.5

For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.**catena-Poly[imidazolium [[diaquadichloro-
manganese(II)]- μ -chloro]]**

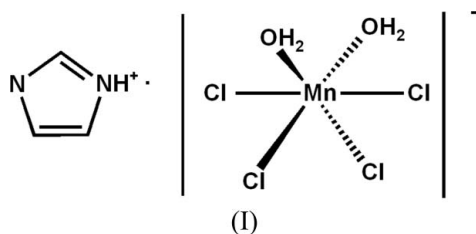
The structure of the title compound, $\{(\text{C}_3\text{H}_5\text{N}_2)[\text{MnCl}_3(\text{H}_2\text{O})_2]\}_n$, is composed of discrete imidazolium cations and an $[\text{MnCl}_3(\text{H}_2\text{O})_2]_n$ infinite-chain anion. The structure is stabilized by $\text{N}-\text{H}\cdots\text{Cl}$ and $\text{O}-\text{H}\cdots\text{Cl}$ hydrogen bonds, forming a three-dimensional network.

Received 11 February 2006

Accepted 24 May 2006

Comment

Some manganese chloride complexes with imidazole as ligands have been investigated, such as $[\text{Mn}(\text{Im})_6]\text{Cl}_2\cdot 4\text{H}_2\text{O}$ (where Im is imidazole) and $[\text{Mn}(\text{Im})_4(\text{H}_2\text{O})_2]\text{Cl}_2$ (Garrett *et al.*, 1983*a,b*). $[\text{Mn}(\text{N}_3)_2(\text{bim})_2]$ [where bim is 1,2-bis(imidazol-1-yl)ethane] (Li *et al.*, 2004) has also been investigated.



In the title compound, (I), the Mn atom is octahedrally coordinated by four Cl atoms and two O atoms. The $[\text{MnCl}_4(\text{H}_2\text{O})_2]$ groups form a distorted octahedral chain

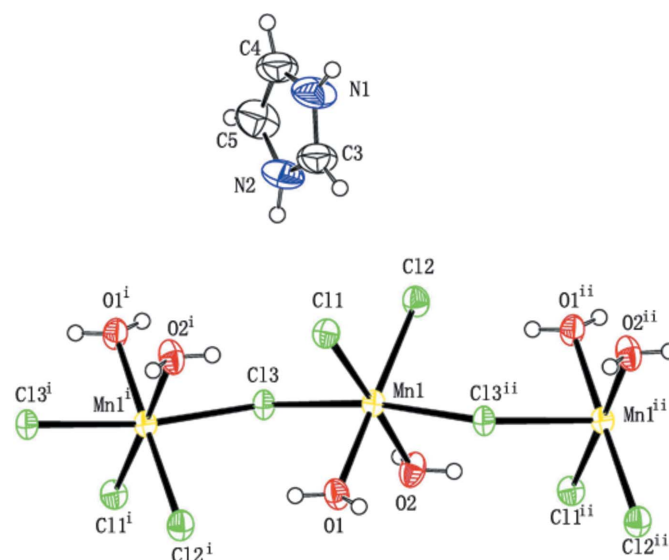


Figure 1

Drawing of (I) showing one cation and three units of the anion chain. Displacement ellipsoids are drawn at the 50% probability level [symmetry codes: (i) $2 - x, 1 - y, \frac{1}{2} + z$; (ii) $2 - x, 1 - y, -\frac{1}{2} + z$]. H atoms are drawn as circles with arbitrary radii.

along the *c* axis, in which the octahedra share common Cl atoms. The coordination environment of Mn corresponds to that observed in Cs[MnCl₃(H₂O)₂], (II) (Jensen *et al.*, 1962), and Rb[MnCl₃(H₂O)₂], (III) (Jensen, 1967). However, (II) and (III) crystallize in the space group *Pcca*. The bond distances and angles around the Mn atom of the title compound are not significantly different from those in (II) or (III).

In (I), the potentially active H atoms, *viz.* the imidazole N—H and aqua H atoms, are engaged in hydrogen bonds with Cl atoms, forming a three-dimensional hydrogen-bonded network (Table 2).

Experimental

The title complex crystallized from a solution of MnCl₂·4H₂O (6 mmol) and imidazole (6 mmol) in HCl (1 N, 20 ml) upon slow evaporation at room temperature. Pink crystals of block shape were obtained after several weeks.

Crystal data

(C ₃ H ₅ N ₂)[MnCl ₃ (H ₂ O) ₂]	Z = 4
<i>M_r</i> = 266.41	<i>D_x</i> = 1.786 Mg m ⁻³
Orthorhombic, <i>Pca</i> 2 ₁	Mo <i>Kα</i> radiation
<i>a</i> = 11.623 (6) Å	μ = 2.10 mm ⁻¹
<i>b</i> = 9.354 (5) Å	<i>T</i> = 293 (2) K
<i>c</i> = 9.114 (5) Å	Block, pink
<i>V</i> = 990.9 (9) Å ³	0.52 × 0.31 × 0.29 mm

Data collection

Bruker APEX CCD diffractometer	12930 measured reflections
ω scans	2471 independent reflections
Absorption correction: multi-scan	2301 reflections with <i>I</i> > 2 σ (<i>I</i>)
(<i>SADABS</i> ; Sheldrick, 2002)	<i>R</i> _{int} = 0.053
<i>T</i> _{min} = 0.46, <i>T</i> _{max} = 0.54	θ _{max} = 28.3°

Refinement

Refinement on <i>F</i> ²	(Δ/σ) _{max} = 0.001
<i>R</i> [<i>F</i> ² > 2 σ (<i>F</i> ²)] = 0.019	$\Delta\rho$ _{max} = 0.18 e Å ⁻³
<i>wR</i> (<i>F</i> ²) = 0.046	$\Delta\rho$ _{min} = -0.26 e Å ⁻³
<i>S</i> = 1.01	Extinction correction: <i>SHELXTL</i>
2471 reflections	Extinction coefficient: 0.0316 (9)
101 parameters	Absolute structure: Flack (1983),
H-atom parameters constrained	1155 Friedel pairs
<i>w</i> = 1/[$\sigma^2(F_o^2) + (0.0206P)^2$]	Flack parameter: 0.11 (2)
where <i>P</i> = (<i>F</i> _o ² + 2 <i>F</i> _c ²)/3	

Table 1

Selected geometric parameters (Å, °).

Mn1—O1	2.2055 (16)	Mn1—Cl1	2.5331 (10)
Mn1—O2	2.2080 (17)	Mn1—Cl3 ⁱ	2.5530 (15)
Mn1—Cl2	2.4932 (11)	Mn1—Cl3	2.5668 (15)
O1—Mn1—O2	88.05 (6)	Cl2—Mn1—Cl3 ⁱ	92.82 (4)
O1—Mn1—Cl2	179.33 (6)	Cl1—Mn1—Cl3 ⁱ	91.57 (3)
O2—Mn1—Cl2	91.38 (6)	O1—Mn1—Cl3	87.55 (6)
O1—Mn1—Cl1	88.44 (6)	O2—Mn1—Cl3	85.07 (6)
O2—Mn1—Cl1	176.48 (5)	Cl2—Mn1—Cl3	92.74 (4)
Cl2—Mn1—Cl1	92.14 (4)	Cl1—Mn1—Cl3	94.99 (4)
O1—Mn1—Cl3 ⁱ	86.83 (6)	Cl3 ⁱ —Mn1—Cl3	171.238 (11)
O2—Mn1—Cl3 ⁱ	88.03 (6)	Mn1 ⁱⁱ —Cl3—Mn1	126.60 (4)

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

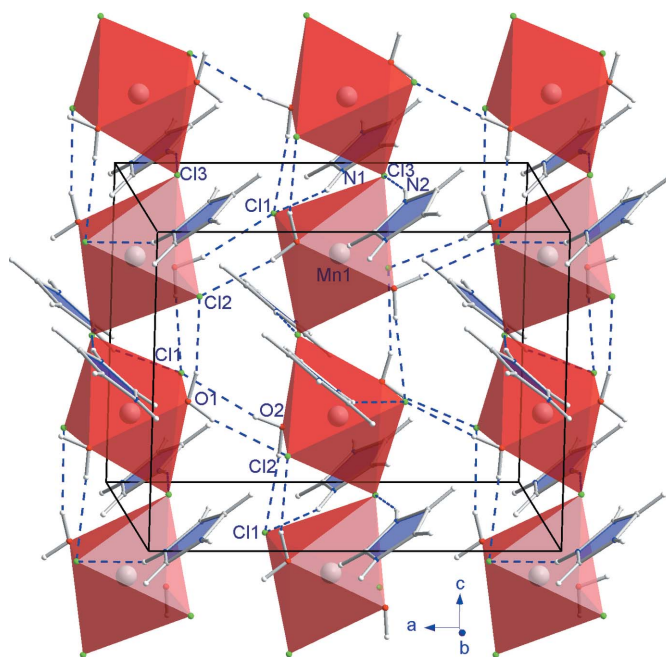


Figure 2

The packing in (I), viewed approximately along the *b* axis. Hydrogen bonds are indicated by dashed lines.

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—H1W...Cl2 ⁱⁱⁱ	0.84	2.35	3.176 (2)	168
O1—H2W...Cl2 ⁱⁱ	0.84	2.38	3.170 (3)	158
O2—H3W...Cl1 ⁱ	0.82	2.36	3.182 (3)	172
O2—H4W...Cl1 ^{iv}	0.84	2.42	3.206 (2)	156
N1—H1...Cl1 ^v	0.86	2.37	3.190 (2)	158
N2—H2...Cl3 ^{vi}	0.86	2.53	3.358 (3)	162

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

The imidazole H atoms were constrained to an ideal geometry, with C—H = 0.94 Å and N—H = 0.86 Å. Aqua atoms H1W, H2W, H3W and H4W were located in a difference electron-density map and refined as riding, with O—H = 0.82–0.84 Å. All H atoms were refined with isotropic displacement parameters of *U*_{iso}(H) = 1.2*U*_{eq}(C,N,O).

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINTE* (Bruker, 1998); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg & Berndt, 1999); software used to prepare material for publication: *SHELXTL*.

This work was supported financially by the Natural Science Foundation of China (NSFC No. 50572078 and No. 20571059), the Opening Foundation of Wuhan University of Technology, and the Opening Foundation of the Key Laboratory of Nonferrous Materials and New Processing Technology, Ministry of Education of China.

References

- Brandenburg, K. & Berndt, M. (1999). *DIAMOND*. Release 2.1e. Crystal Impact GbR, Bonn, Germany.
- Bruker (1998). *SMART* (Version 5.622), *SAINTE* (Version 5.00). Bruker AXS Inc., Madison, Wisconsin, USA.
- Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
- Flack, H. D. (1983). *Acta Cryst.* **A39**, 876–881.
- Garrett, T. P. J., Guss, J. M. & Freeman, H. C. (1983a). *Acta Cryst.* **C39**, 1027–1031.
- Garrett, T. P. J., Guss, J. M. & Freeman, H. C. (1983b). *Acta Cryst.* **C39**, 1031–1034.
- Jensen, S. J. (1967). *Acta Chem. Scand.* **21**, 889–898.
- Jensen, S. J., Andersen, P. & Rasmussen, S. E. (1962). *Acta Chem. Scand.* **16**, 1890–1896.
- Li, B.-L., Zhu, X., Zhou, J.-H. & Zhang, Y. (2004). *Acta Cryst.* **C60**, m373–m374.
- Sheldrick, G. M. (1997). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
- Sheldrick, G. M. (2002). *SADABS*. Version 2.02. University of Göttingen, Germany.