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Hexaimidazolium tetrachloromanganate(II) hexachloromanganate(II)

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The title compound, $(C_3H_5N_2)_6[MnCl_4][MnCl_6]$, is composed of discrete imidazolium cations, and $[MnCl_4]^{2-}$ and $[MnCl_6]^{4-}$ anions. Both Mn atoms lie in positions of site symmetry $\bar{4}$. A three-dimensional network is formed *via* N—H···Cl hydrogen bonds.

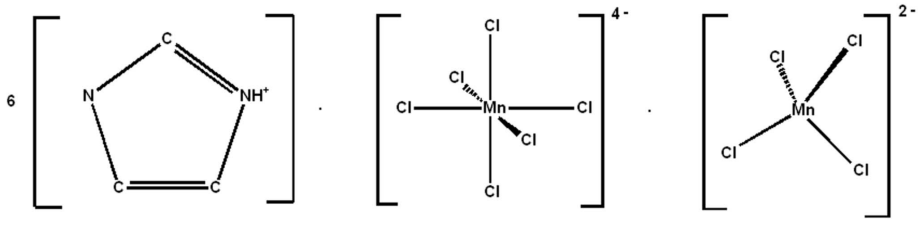
Key indicators

Single-crystal X-ray study
T = 223 K
Mean σ(C–C) = 0.005 Å
Disorder in main residue
R factor = 0.036
wR factor = 0.095
Data-to-parameter ratio = 23.5

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

Comment

Some manganese(II) chloride complexes containing imidazole have been investigated, such as $[Mn(Im)_6]Cl_2{\cdot}4(H_2O)$ (Im is imidazole) and $[Mn(Im)_4(H_2O)_2]Cl_2$ (Garrett *et al.*, 1983). We present here the crystal structure of the title compound, (I).



(I)

In compound (I), atom Mn1 is tetrahedrally coordinated by four Cl atoms, with an Mn1—Cl1 distance of 2.3578 (8) Å. Atom Mn2 is octahedrally coordinated by six Cl atoms, with bond distances of 2.5441 (7) and 2.5994 (10) Å for Mn2—Cl2 and Mn2—Cl3, respectively. Both Mn atoms lie in positions of site symmetry $\bar{4}$.

In comparable compounds, the Mn—Cl distance is 2.343 Å for the four-coordinate Mn atom of Cs_3MnCl_5 (Goodyear & Kennedy, 1976) and 2.5249 (3) Å for the six-coordinate Mn atom of NH_4MnCl_3 (Tornero *et al.*, 1978).

The $[MnCl_4]^{2-}$ and $[MnCl_6]^{4-}$ anions of (I) are bridged by imidazolium cations through N—H···Cl hydrogen bonds, forming one-dimensional chains along the c axis. The $[MnCl_6]^{4-}$ anions are also bridged *via* N—H···Cl hydrogen bonds.

Experimental

The title complex crystallized from a solution of $MnCl_2{\cdot}4H_2O$ (10 mmol) and imidazole (30 mmol) in HCl (2 N, 30 ml) upon slow evaporation. Large light-yellow octahedral crystals of (I) were obtained after several days.

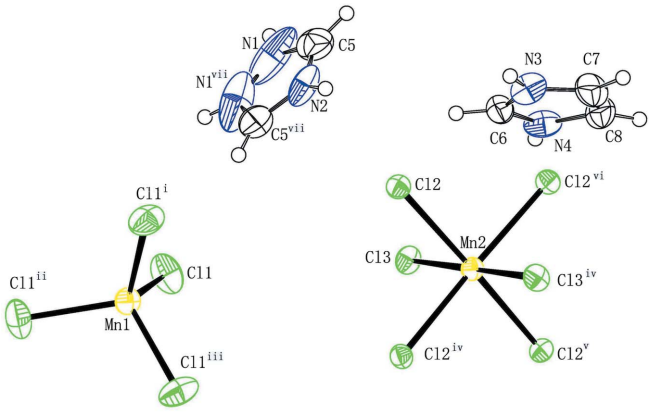


Figure 1
A drawing of (I). Displacement ellipsoids are shown at the 50% probability level. [Symmetry codes: (i) $\frac{5}{4}-y,\frac{1}{4}+x,\frac{1}{4}-z$; (ii) $1-x,\frac{3}{2}-y,z$; (iii) $-\frac{1}{4}+y,\frac{5}{4}-x,\frac{1}{4}-z$; (iv) $\frac{1}{4}-y,\frac{1}{4}+x,\frac{1}{4}-z$; (v) $-x,\frac{1}{2}-y,z$; (vi) $-\frac{1}{4}+y,\frac{1}{4}-x,\frac{1}{4}-z$; (vii) $1-x,\frac{1}{2}-y,z$.]

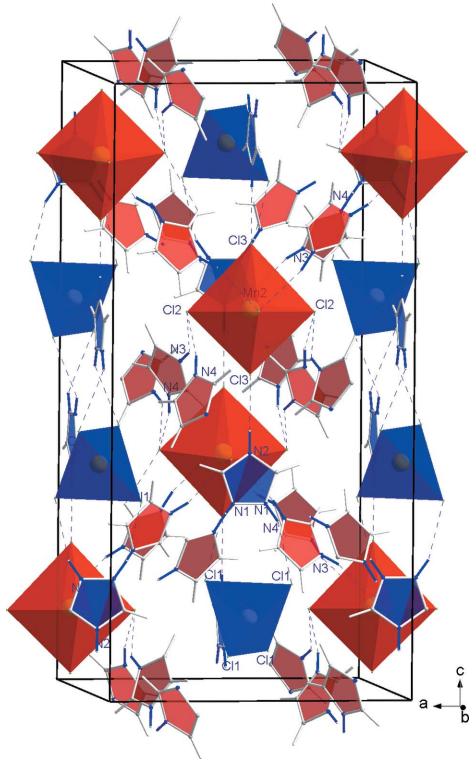


Figure 2
The crystal structure of (I). $[MnCl_4]^{2-}$ anions are indicated by blue tetrahedra and $[MnCl_6]^{4-}$ anions are indicated by red octahedra. Imidazolium-1 and imidazolium-2 are indicated as blue and red pentagons, respectively. N—H···Cl hydrogen bonds are indicated by dashed lines.

Crystal data

$(C_3H_5N_2)_6[MnCl_6][MnCl_4]$
M_r = 878.92
Tetragonal, $I4_1/a$
a = 12.1117 (19) Å
c = 24.475 (6) Å
V = 3590.3 (11) Å^3
Z = 4
D_x = 1.626 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 24947 reflections
θ = 1.9–28.4°
μ = 1.48 mm^{-1}
T = 223 (2) K
Prism, light yellow
0.24 × 0.20 × 0.18 mm

Data collection

Bruker APEX CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
T_{min} = 0.71, T_{max} = 0.77
24947 measured reflections
2253 independent reflections
1690 reflections with $I > 2\sigma(I)$
R_{int} = 0.069
θ_{max} = 28.4°
$h = -16 \rightarrow 16$
$k = -16 \rightarrow 16$
$l = -32 \rightarrow 32$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.095
S = 1.09
2253 reflections
96 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0321P)^2 + 6.1483P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Mn1—Cl1	2.3578 (8)	Mn2—Cl2^{v}	2.5441 (7)
Mn1—Cl1^{i}	2.3578 (8)	Mn2—Cl2^{vi}	2.5441 (7)
Mn1—Cl1^{ii}	2.3578 (8)	Mn2—Cl2	2.5441 (7)
Mn1—Cl1^{iii}	2.3578 (8)	Mn2—Cl3^{v}	2.5994 (10)
Mn2—Cl2^{iv}	2.5441 (7)	Mn2—Cl3	2.5994 (10)
Cl1—Mn1—Cl1^{i}	106.18 (4)	Cl2^{v}—Mn2—Cl3	92.175 (13)
Cl1—Mn1—Cl1^{iii}	111.14 (2)	Cl2—Mn2—Cl3	87.825 (13)
Cl2^{v}—Mn2—Cl2	90.083 (1)	Cl3^{v}—Mn2—Cl3	180.0
Cl2^{vi}—Mn2—Cl2	175.65 (3)		

Symmetry codes: (i) $-x+1,-y+\frac{3}{2},z$; (ii) $-y+\frac{5}{4},x+\frac{1}{4},-z+\frac{1}{4}$; (iii) $y-\frac{1}{4},-x+\frac{5}{4},-z+\frac{1}{4}$; (iv) $-y+\frac{7}{4},x-\frac{1}{4},-z+\frac{7}{4}$; (v) $y+\frac{1}{4},-x+\frac{7}{4},-z+\frac{7}{4}$; (vi) $-x+2,-y+\frac{3}{2},z$.

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···Cl1^{vii}	0.87	2.66	3.419 (4)	146
N2—H2···Cl3^{viii}	0.87	2.24	3.106 (4)	180
N3—H3···Cl2^{ix}	0.87	2.42	3.196 (3)	149
N4—H4···Cl2^{x}	0.87	2.35	3.194 (3)	163

Symmetry codes: (vii) $y+\frac{1}{4},-x+\frac{5}{4},z+\frac{1}{4}$; (viii) $x,y,z-1$; (ix) $-x+1,-y+2,-z+1$; (x) $-x+1,-y+\frac{3}{2},z-1$.

Imidazolium H atoms were constrained to an ideal geometry, with C—H = 0.94 Å and N—H = 0.87 Å. All H atoms were refined with isotropic displacement parameters of U_{iso}(H) = 1.2U_{eq}(C,N). One imidazolium cation is disordered on a twofold rotation axis. As a result of this, one C and one N atom (C1 and N1) were refined sharing the same position and the same anisotropic displacement parameters.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT*; data reduction: *SAINT*; 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*.

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