Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

Di-μ-chloro-bis[bis(ethane-1,2-diamine-κ^2N,N')-manganese(II)] dichloride

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.032
wR factor = 0.086
Data-to-parameter ratio = 13.6

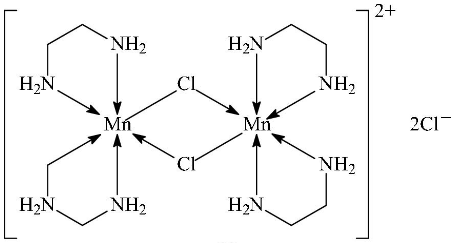
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The dinuclear cation of the title compound, $[Mn_2Cl_2(C_2H_8N_2)_4]Cl_2$, has the Cl atoms bridging the ethane-1,2-diamine-chelated Mn atoms across a centre of inversion. The cations are linked to the chloride anions by hydrogen bonds, forming a three-dimensional network.

Received 29 March 2005
Accepted 31 March 2005
Online 27 April 2005

Comment

In the crystal structure of the title compound, (I) (Fig. 1), the dication lies on an inversion site; the Cl atoms of the dication bridges unsymmetrically the two ethane-1,2-diamine-chelated Mn atoms, which show octahedral coordination. The cations interact with the anions by hydrogen bonds to form a three-dimensional network. Only some of the amino H atoms are engaged in hydrogen bonding (Table 2). The red compound is isostructural with the nickel(II) analogue, whose structure has been described in detail (Bottomley *et al.*, 1978). *N*,*N*,*N*′,*N*′-Tetramethylethane-1,2-diamine forms a colourless 1/1 adduct with manganese dichloride that features two bridging chlorine atoms and the metal atom in an octahedral coordination in the resulting chain motif (Sobota *et al.*, 1996); *N*,*N*,*N*′,*N*′-tetramethylpropane-1,3-diamine also forms a colourless 1/1 adduct but the compound exists instead as a tetrahedral molecule (Handley *et al.*, 2001).



(I)

Experimental

Manganese dichloride tetrahydrate (0.20 g, 0.1 mmol), fumaric acid (0.28 g, 0.2 mmol), ethylenediamine (0.12 g, 0.2 mmol) and acetonitrile (5 ml) were sealed into a 15 ml Teflon-lined, stainless steel bomb. The bomb was heated at 423 K for 96 h. It was then slowly cooled to room temperature to give pale yellow block-shaped crystals in about 35% yield (based on $MnCl_2{\cdot}4H_2O$).

Crystal data

$[Mn_2Cl_2(C_2H_8N_2)_4]Cl_2$
M_r = 492.10
Monoclinic, $P2_1/n$
a = 6.4058 (6) Å
b = 11.284 (1) Å
c = 14.510 (1) Å
β = 93.686 (2)°
V = 1046.7 (2) Å^3
Z = 2

D_x = 1.561 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2596 reflections
θ = 2.3–28.0°
μ = 1.72 mm^{-1}
T = 293 (2) K
Block, pale yellow
0.20 × 0.18 × 0.13 mm

Data collection

Bruker SMART APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{\min} = 0.638$, $T_{\max} = 0.807$
5195 measured reflections
1793 independent reflections
1605 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.021$
$\theta_{\max} = 25.0°$
$h = -5 \rightarrow 7$
$k = -13 \rightarrow 13$
$l = -16 \rightarrow 17$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.032$
$wR(F^2) = 0.086$
$S = 1.06$
1793 reflections
132 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0507P)^2 + 0.3082P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.71$ e Å^{-3}
$\Delta\rho_{\min} = -0.37$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Mn1—N1	2.251 (2)	Mn1—N4	2.259 (2)
Mn1—N2	2.293 (2)	Mn1—Cl1	2.526 (1)
Mn1—N3	2.242 (2)	Mn1—Cl1^{i}	2.622 (1)
N1—Mn1—N2	77.17 (9)	N2—Mn1—Cl1	97.20 (7)
N1—Mn1—N3	96.20 (9)	N2—Mn1—Cl1^{i}	173.46 (7)
N1—Mn1—N4	162.67 (9)	N3—Mn1—N4	78.59 (8)
N1—Mn1—Cl1	92.49 (7)	N3—Mn1—Cl1^{i}	85.35 (6)
N1—Mn1—Cl1^{i}	96.65 (6)	N3—Mn1—Cl1	167.76 (6)
N2—Mn1—N3	93.14 (9)	N4—Mn1—Cl1	95.46 (6)
N2—Mn1—N4	86.56 (9)	N4—Mn1—Cl1^{i}	99.35 (6)

Symmetry code: (i) $1 - x, 1 - y, 1 - z$.

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N1—H1n2$\cdots$Cl1^{ii}	0.85 (1)	2.53 (1)	3.361 (2)	164 (3)
N1—H1n1$\cdots$Cl2	0.86 (1)	2.67 (2)	3.484 (2)	159 (3)
N3—H3n1$\cdots$Cl2^{iii}	0.86 (1)	2.44 (1)	3.288 (2)	172 (3)
N4—H4n1$\cdots$Cl2^{i}	0.86 (1)	2.56 (1)	3.388 (2)	162 (2)

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

The amino H atoms were found in difference Fourier maps, and were refined with a distance restraint of N—H = 0.86 (1) Å. The carbon-bound H atoms were placed at calculated positions (C—H = 0.97 Å) and were included in the refinement in the riding-model approximation, with their displacement parameters set at 1.2 times $U_{\rm eq}$ of the parent atoms.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

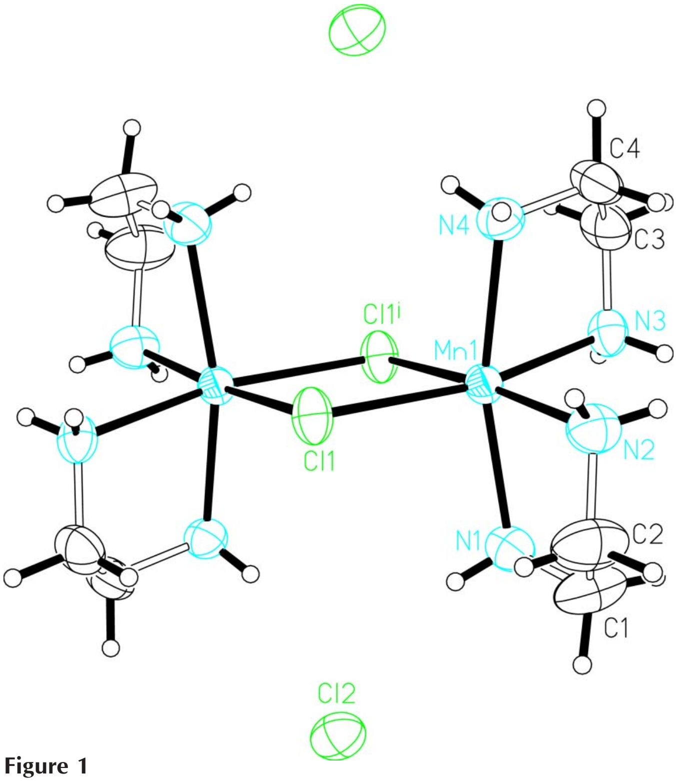


Figure 1
ORTEPII plot (Johnson, 1976) of the formula unit of (I), with displacement ellipsoids drawn at the 50% probability level. H atoms are drawn as spheres of arbitrary radii. [Symmetry code: (i) $1 - x, 1 - y, 1 - z$.]

We thank the National Natural Science Foundation of China, Shanxi Normal University and the University of Malaya for supporting this study.

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