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Glycinemanganese(II) Dichloride Dihydrate [*catena*-Diaquadichloro-μ-glycine-manganese(II)]

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Abstract. $[Mn(C_2H_5NO_2)Cl_2(H_2O)_2]$, $C_2H_9Cl_2MnNO_4$, monoclinic, $P2_1/c$, $a = 8{\cdot}413$ (2), $b = 5{\cdot}613$ (2), $c = 16{\cdot}816$ (6) Å, $\beta = 90{\cdot}20$ (3)°, $M_r = 236{\cdot}95$, $V = 794{\cdot}1$ Å^3, $Z = 4$, $D_m = 1{\cdot}98$, $D_c = 1{\cdot}98$ Mg m^{-3}, μ(Mo $K\alpha$) = 2·37 mm^{-1}, $\lambda = 0{\cdot}71069$ Å. The title compound is polymeric. The glycine molecules link the Mn^{2+} ions by a carboxyl bridge system. The structure was refined to $R = 0{\cdot}051$ for 1431 diffractometer data.

Introduction. Colourless crystals of the title compound were grown from an aqueous solution of glycine and manganese(II) chloride (2:1).

Preliminary Weissenberg photographs indicated a monoclinic lattice with systematic absences $h0l$: $l = 2n + 1$, $0k0$: $k = 2n + 1$, consistent with the space group $P2_1/c$. All measurements for a crystal 0·10 × 0·12 × 0·22 mm were made on a Syntex $P2_1$ computer-controlled four-circle diffractometer equipped with a scintillation counter and graphite monochromator. The cell parameters were determined by least squares from the setting angles of 15 reflections given by the automatic centring program. Intensities of 1756 independent reflections were measured up to $2\theta = 55°$ with the variable θ–2θ scan technique. The scan rate varied from 2·0 to 20·0° min^{-1}, depending on the intensity. 1431 reflections with $I > 1{\cdot}96\sigma(I)$ were used in the analysis. The intensities were corrected for Lorentz and polarization factors, but not for absorption.

The structure was solved by the heavy-atom method. Full-matrix least-squares refinement with isotropic thermal parameters to R_1 $(= \sum ||F_o| - |F_c|| / \sum |F_o|) = 0{\cdot}072$ and anisotropic thermal parameters to $R_1 = 0{\cdot}055$ was performed. Positions of two of the glycine H atoms were calculated, with C—H = 1·0 Å; seven other H atoms were located from difference syntheses. The H atoms were included with individual isotropic thermal parameters, but not refined. Final refinement yielded $R_1 = 0{\cdot}051$ and R_2 $[= \sum w(|F_o| - |F_c|)^2 / \sum w(F_o)^2]^{1/2} = 0{\cdot}052$. The function minimized was $\sum w(F_o - F_c)^2$ with $w = 1/\sigma^2(F)$. Scattering factors for neutral atoms and anomalous scattering factors for Mn and Cl were taken from Cromer & Waber (1974).

All calculations were performed with the Syntex *XTL* structure determination system (Nova 1200 computer and additional external disc memory). The final positional parameters are listed in Table 1.*

* Lists of structure factors and thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 35091 (34 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. *Final positional parameters* ($\times 10^4$) *with e.s.d.'s in parentheses*

The H atom positions ($\times 10^3$) are unrefined.

	x	*y*	*z*
Mn	2107 (1)	519 (2)	1654 (0)
Cl(1)	4590 (2)	−1919 (3)	1208 (1)
Cl(2)	2179 (2)	2863 (3)	406 (1)
O(1)	2437 (5)	−1015 (7)	2849 (2)
O(2)	118 (5)	−2891 (7)	2954 (2)
O(*W*1)	644 (5)	−2563 (7)	1316 (2)
O(*W*2)	3522 (6)	3379 (8)	2175 (2)
N	3473 (6)	−2160 (9)	4292 (3)
C(1)	1441 (7)	−2266 (9)	3219 (3)
C(2)	1873 (7)	−3008 (1	4059 (3)
H(1)	133	−400	117
H(2)	13	−277	181
H(3)	367	500	200
H(4)	439	315	260
H(5)	417	−312	417
H(6)	375	−187	479
H(7)	347	−571	402
H(8)	185	−480	410
H(9)	107	−234	445

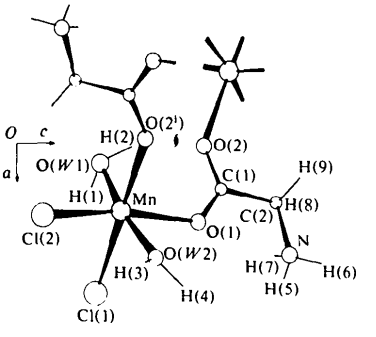

Fig. 1. Projection along *b* of part of a single chain of the polymer.

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Table 2. *Bond lengths* (Å) *and angles* (°) *with e.s.d.'s in parentheses*

For symmetry code see Table 4.

Mn–Cl(1)	2·610 (2)	Mn–O(W2)	2·180 (5)
Mn–Cl(2)	2·477 (2)	C(1)–O(1)	2·160 (7)
Mn–O(1)	2·203 (4)	C(1)–O(2)	1·248 (7)
Mn–O(2^{i})	2·178 (4)	C(1)–C(2)	1·515 (8)
Mn–O(W1)	2·197 (4)	C(2)–N	1·480 (8)
Cl(1)–Mn–Cl(2)	90·76 (6)	O(1)–Mn–O(W2)	81·6 (2)
Cl(1)–Mn–O(1)	87·6 (1)	O(2^{i})–Mn–O(W1)	85·4 (1)
Cl(1)–Mn–O(2^{i})	172·5 (1)	O(2^{i})–Mn–O(W2)	92·6 (2)
Cl(1)–Mn–O(W1)	87·8 (1)	O(W1)–Mn–O(W2)	171·2 (2)
Cl(1)–Mn–O(W2)	93·7 (1)	C(1)–O(1)–Mn	125·9 (3)
Cl(2)–Mn–O(1)	167·6 (1)	C(1)–O(2)–Mn^{vii}	140·7 (4)
Cl(2)–Mn–O(2^{i})	93·6 (1)	O(1)–C(1)–O(2)	125·1 (5)
Cl(2)–Mn–O(W1)	102·4 (1)	O(1)–C(1)–C(2)	117·1 (5)
Cl(2)–Mn–O(W2)	86·2 (1)	O(2)–C(1)–C(2)	117·8 (5)
O(1)–Mn–O(2^{i})	89·4 (1)	C(1)–C(2)–N	112·0 (5)
O(1)–Mn–O(W1)	89·8 (1)		

Table 3. *Least-squares planes*

Values are given in the following order: atoms defining the plane, equation of plane, deviations of atoms from the plane (Å) with e.s.d.'s in parentheses.

Plane (1): O(1), O(2^{i}), Cl(1), Cl(2)

$$-0{\cdot}6048X - 0{\cdot}6873Y - 0{\cdot}4023Z + 2{\cdot}4464 = 0$$

O(1) −0·319 (4), O(2^{i}) 0·318 (4), Cl(1) 0·038 (1), Cl(2) −0·040 (1), Mn 0·061 (1)

Plane (2): O(1), O(2), C(1), C(2)

$$0{\cdot}4174X - 0{\cdot}8341Y - 0{\cdot}3607Z + 0{\cdot}4026 = 0$$

O(1) −0·002 (4), O(2) −0·002 (4), C(1) 0·009 (5), C(2) −0·003 (6), N 0·019 (5), Mn −0·108 (1), Mn^{vii} −0·278 (1)

Plane (3): C(1), C(2), N

$$0{\cdot}4022X - 0{\cdot}8454Y - 0{\cdot}3515Z + 0{\cdot}3477 = 0$$

Dihedral angle (2)–(3) 1·21°

Discussion. As shown in Fig. 1, the Mn atoms situated on both sides of the 2_1 screw axis (Mn–Mn distance = 5·36 Å) are linked by carboxyl bridges of the glycine molecules. Other coordination positions in the Mn octahedron are occupied by the Cl atoms and two water molecules. Mn–O lengths range from 2·178 (4) to 2·203 (4) Å. The valency angles in the octahedron differ from 90° by 12° (maximum). Bond lengths and angles are summarized in Table 2. The best planes are presented in Table 3.

Table 4. *Hydrogen-bond lengths* (Å) *and angles* (°) *with e.s.d.'s in parentheses*

Symmetry code superscript: none x,y,z; (i) $-x, \frac{1}{2}+y, \frac{1}{2}-z$; (ii) $x, -1+y, z$; (iii) $x, 1+y, z$; (iv) $1-x, \frac{1}{2}+y, \frac{1}{2}+z$; (v) $1-x, -\frac{1}{2}+y, \frac{1}{2}-z$; (vi) $x, -\frac{1}{2}-y, \frac{1}{2}+z$; (vii) $-x, -\frac{1}{2}+y, \frac{1}{2}-z$.

D–H···*A*	*D*···*A*	H···*A*	*D*–H···*A*
O(W1)–H(1)···Cl(2^{ii})	3·256 (4)	2·29	156·5
O(W1)–H(2)···O(2)	2·800 (5)	1·92	152·5
O(W2)–H(3)···Cl(1^{iii})	3·228 (5)	2·32	157·3
O(W2)–H(4)···Cl(1^{iv})	3·147 (5)	2·18	156·8
N–H(5)···Cl(1^{v})	3·235 (6)	2·46	159·7
N–H(6)···Cl(1^{vi})	3·384 (5)	2·57	154·3
N–H(7)···Cl(1^{iv})	3·466 (6)	2·65	139·1

The glycine molecules appear in the crystals under investigation as zwitterions. They form *syn*[O(1)–Mn] and *anti*[O(2)–Mn^{vii}] bonds with the Mn atoms. The C–O–Mn angles are 125·9 (3) and 140·7 (4)° respectively.

Hydrogen-bond lengths and angles are summarized in Table 4. Four hydrogen bonds link adjacent polymeric $[Mn(glycine)Cl_2(H_2O)_2]_n$ chains, and others, owing to the spiral structure of chains, are formed between the atoms of the same polymer. The proton acceptor in one of them is O(2). The H(2)–O(2)–C(1) and H(2)–O(2)–Mn angles are 109·8 and 108·9°, respectively.

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Reference

CROMER, D. T. & WABER, J. T. (1974). *International Tables for X-ray Crystallography*, Vol. IV. Birmingham: Kynoch Press.