longer than the sum of the covalent radii of 2·15 Å (Pauling, 1960), yet distinctly smaller than the sum of the van der Waals radii of 3·7 Å (Pauling, 1960). No structural information for other Sb^{III} complexes with neutral N-donor ligands is available. However, it is noteworthy that in the EDTA complex $HSb(C_{10}H_{12}N_2O_8).2H_2O$ the Sb–N distances [2·31 (1), 2·39 (1) Å] are also rather long (Kita, Uehiro, Iwamoto, Ouchi & Yoshino, 1976).

Intermolecular distances do not indicate interactions exceeding van der Waals forces.

The two least-squares planes defined by the atoms (I): C(n) (n = 1–6) and (II): N(1), N(2), C(m) (m = 7–18) show that the atoms in planes (I) and (II) respectively do not deviate significantly from them. The positions of the atoms Sb(1), O(1) and O(2) lie 0·097 (1), 0·039 (9) and 0·006 (7) Å respectively out of the plane (I), and Sb(1) lies 0·158 (1) Å out of plane (II). The angle between plane (I) and plane (II) is 96·6°.

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Structure of Manganese(II) L-Lactate Dihydrate

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Abstract. $Mn(C_3H_5O_3)_2.2H_2O$, orthorhombic, $P2_12_12_1$, a = 6·117 (2), b = 12·183 (5), c = 14·633 (5) Å, M_r = 269·1, V = 1090·5 Å^3, Z = 4, D_m = 1·64, D_x = 1·64 Mg m^{-3}, μ(Mo $K\alpha$, λ = 0·71069 Å) = 1·29 mm^{-1}, final R = 0·037 and R_w = 0·032 for 1601 non-zero reflexions. The Mn atom is octahedrally coordinated by one carboxylate O atom and one hydroxyl O atom from each lactate ligand and two water O atoms in *cis* positions. In this way neutral molecules $[Mn(CH_3CHOHCOO)_2(H_2O)_2]$ are formed which are held together through hydrogen bonds. Mn–O distances range between 2·146 (3) and 2·185 (2) Å.

Introduction. This investigation was undertaken as part of a study on the stereochemistry of Mn carboxylate salts. Preliminary data of the crystal structures of racemic Zn^{II} and Mn^{II} lactate trihydrates have been reported by Singh, Jain, Sakore & Biswas (1975), who have solved the structure of the Zn salt and have found both salts to be isotypic.

Single crystals of $Mn(C_3H_5O_3)_2.2H_2O$ were prepared by dissolving Mn^{II} carbonate in a commercially available L-lactic acid, and allowing the solution to evaporate. Nearly colorless crystals grew as orthorhombic needles or plates. Weissenberg photographs showed the space group to be $P2_12_12_1$. A

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Table 1. *The final atom coordinates and equivalent isotropic thermal parameters with e.s.d.'s in parentheses*

$B_{eq} = \frac{1}{3}(B_{11} + B_{22} + B_{33})$.

	x	y	z	B_{eq} (Å^2)
Mn	0·20303 (8)	0·14558 (4)	0·14623 (3)	1·85 (2)
O(1)	0·5177 (4)	0·1741 (2)	0·2097 (2)	2·39 (16)
O(2)	0·7116 (5)	0·2880 (2)	0·2964 (2)	2·70 (16)
O(3)	0·2480 (5)	0·3224 (2)	0·1556 (2)	2·98 (19)
O(4)	0·3458 (5)	0·1366 (2)	0·0113 (2)	2·59 (17)
O(5)	0·4401 (6)	0·0332 (3)	−0·1072 (2)	3·69 (21)
O(6)	0·2226 (5)	−0·0286 (2)	0·1116 (2)	2·46 (17)
O(7)	0·0410 (5)	0·1347 (3)	0·2760 (2)	2·75 (19)
O(8)	−0·1157 (5)	0·1678 (3)	0·0829 (2)	2·75 (20)
C(1)	0·5523 (6)	0·2673 (3)	0·2456 (3)	2·08 (22)
C(2)	0·3940 (6)	0·3612 (3)	0·2246 (3)	2·23 (21)
C(3)	0·2707 (8)	0·3969 (4)	0·3090 (4)	3·33 (30)
C(4)	0·3582 (6)	0·0453 (3)	−0·0292 (3)	2·15 (22)
C(5)	0·2657 (7)	−0·0560 (3)	0·0173 (3)	2·53 (25)
C(6)	0·0579 (11)	−0·0950 (6)	−0·0293 (4)	4·91 (45)
H(3)	0·159 (6)	0·371 (3)	0·144 (3)	2·6 (9)
H(6)	0·242 (8)	−0·085 (4)	0·144 (3)	4·9 (12)
H(71)	−0·073 (7)	0·171 (4)	0·283 (3)	3·9 (11)
H(72)	0·028 (9)	0·078 (4)	0·315 (4)	5·9 (14)
H(81)	−0·216 (9)	0·172 (5)	0·107 (4)	6·4 (17)
H(82)	−0·153 (9)	0·232 (5)	0·044 (3)	6·0 (13)
H(2)	0·483 (6)	0·429 (3)	0·199 (3)	2·5 (8)
H(5)	0·387 (7)	−0·116 (4)	0·013 (3)	3·0 (9)
H(31)	0·168 (9)	0·457 (4)	0·296 (4)	6·6 (14)
H(32)	0·371 (9)	0·435 (4)	0·353 (4)	6·2 (13)
H(33)	0·193 (9)	0·335 (5)	0·339 (4)	7·2 (15)
H(61)	−0·016 (10)	−0·168 (5)	−0·002 (4)	7·1 (15)
H(62)	0·090 (8)	−0·116 (4)	−0·093 (4)	5·0 (12)
H(63)	−0·069 (12)	−0·050 (6)	−0·023 (5)	10·0 (25)

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

Mn–O(1)	2·165 (2)	Mn–O(4)	2·162 (2)
Mn–O(3)	2·176 (2)	Mn–O(6)	2·185 (2)
Mn–O(7)	2·146 (3)	Mn–O(8)	2·175 (3)
C(1)–O(1)	1·268 (4)	C(4)–O(4)	1·263 (4)
C(1)–O(2)	1·251 (4)	C(4)–O(5)	1·255 (4)
C(1)–C(2)	1·530 (5)	C(4)–C(5)	1·518 (5)
C(2)–C(3)	1·512 (6)	C(5)–C(6)	1·519 (7)
C(2)–O(3)	1·429 (4)	C(5)–O(6)	1·444 (4)
O(1)–Mn–O(3)	72·6 (1)	O(1)–Mn–O(4)	92·3 (1)
O(1)–Mn–O(6)	102·0 (1)	O(1)–Mn–O(7)	92·3 (1)
O(1)–Mn–O(8)	163·6 (1)	O(3)–Mn–O(4)	93·2 (1)
O(3)–Mn–O(6)	165·7 (1)	O(3)–Mn–O(7)	93·6 (1)
O(3)–Mn–O(8)	90·9 (2)	O(4)–Mn–O(6)	73·5 (1)
O(4)–Mn–O(7)	172·6 (1)	O(4)–Mn–O(8)	88·8 (1)
O(6)–Mn–O(7)	99·8 (1)	O(6)–Mn–O(8)	94·1 (1)
O(7)–Mn–O(8)	88·3 (2)		
Mn–O(1)–C(1)	118·0 (3)	Mn–O(4)–C(4)	119·8 (3)
Mn–O(3)–C(2)	116·8 (3)	Mn–O(6)–C(5)	117·2 (3)
O(1)–C(1)–O(2)	123·8 (4)	O(4)–C(4)–O(5)	123·6 (4)
O(1)–C(1)–C(2)	118·7 (3)	O(4)–C(4)–C(5)	119·0 (3)
O(2)–C(1)–C(2)	117·5 (3)	O(5)–C(4)–C(5)	117·4 (4)
C(1)–C(2)–C(3)	111·5 (3)	C(4)–C(5)–C(6)	111·4 (4)
C(1)–C(2)–O(3)	106·9 (3)	C(4)–C(5)–O(6)	107·9 (3)
C(3)–C(2)–O(3)	111·1 (3)	C(6)–C(5)–O(6)	110·4 (4)

specimen 0·4 × 0·35 × 0·3 mm was cut from a large crystal. Data were collected on a Syntex $P2_1$ diffractometer with monochromatized Mo $K\alpha$ radiation. The intensities were measured by the 2θ–ω scan technique. After each group of 50 reflexions one standard was measured: no significant change in intensity was observed. Of 1877 reflexions accessible below $\theta = 30°$, 1601 with $I > 1{\cdot}96\sigma(I)$ were used for the structure determination. Empirical absorption corrections were made from φ-scan data. All calculations were performed on a NOVA 1200 computer with programs supplied by Syntex (1976). Neutral-atom scattering factors used were those listed in *International Tables for X-ray Crystallography* (1974); both real and imaginary components of the anomalous dispersion were included for Mn and O atoms.

The Mn–Mn vectors were identified in a Patterson function. All other atoms were found from difference syntheses. Full-matrix least-squares refinement with anisotropic (isotropic for H atoms) thermal parameters gave $R = 0{\cdot}037$ and $R_w = 0{\cdot}032$. [The refinement of the parameters for the inverted structure gave $R = 0{\cdot}047$ and $R_w = 0{\cdot}043$.] A final difference synthesis was featureless.

The final atomic coordinates are listed in Table 1, interatomic distances and angles in Table 2.* A view of the crystal structure down **a** and the atom-numbering scheme are shown in Fig. 1.

* Lists of structure factors, anisotropic thermal parameters and least-squares planes have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 36444 (14 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

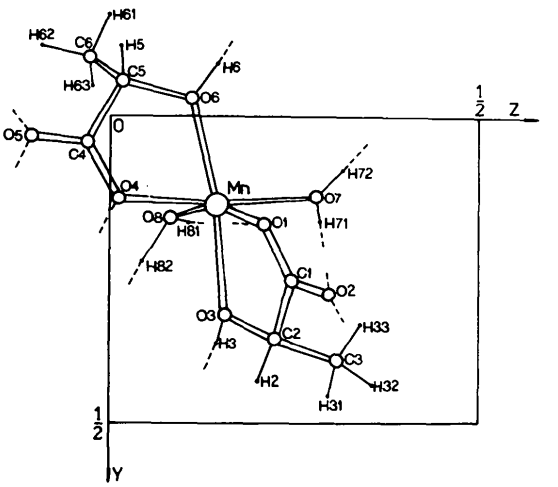

Fig. 1. The crystal structure projected on the (100) plane.

Table 3. *Geometry of the hydrogen bonds*

O–H···O	O···O	O–H	H···O	O–H···O
O(3)–H(3)···O(5^{i})	2·673 (4) Å	0·82 (4) Å	1·86 (4) Å	172 (4)°
O(6)–H(6)···O(2^{ii})	2·640 (3)	0·85 (5)	1·80 (5)	175 (5)
O(7)–H(71)···O(2^{iii})	2·763 (4)	0·83 (5)	1·95 (5)	165 (4)
O(7)–H(72)···O(5^{iv})	2.669 (4)	0·90 (5)	1·78 (5)	169 (5)
O(8)–H(81)···O(1^{iii})	2·912 (4)	0·71 (6)	2·21 (6)	167 (6)
O(8)–H(82)···O(4^{i})	2·762 (4)	0·99 (5)	1·79 (5)	164 (5)

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

Table 4. *Analysis of the configuration of the lactate anions*

(*a*) Distances (Å) from planes through lactate anions (atoms used to define the planes are indicated by an asterisk)

O(1)*	0·001 (3)	O(4)*	0·001 (3)
O(2)*	0·001 (3)	O(5)*	0·002 (4)
C(1)*	−0·007 (4)	C(4)*	−0·007 (4)
C(2)*	0·002 (4)	C(5)*	0·002 (5)
O(3)	0·193 (3)	O(6)	−0·286 (3)
H(3)	0·18 (4)	H(6)	−0·71 (5)

(*b*) Conformational angles (°)

H(3)–O(3)–C(2)–C(1)	178 (3)
H(6)–O(6)–C(5)–C(4)	−148 (4)
O(3)–C(2)–C(1)–O(1)	−7·3 (4)
O(6)–C(5)–C(4)–O(4)	−12·8 (4)
O(3)–C(2)–C(1)–O(2)	171·5 (4)
O(6)–C(5)–C(4)–O(5)	168·4 (4)

Discussion. The Mn atom is octahedrally coordinated by one carboxylate O atom and one hydroxyl O atom from each L-lactate ligand and two water O atoms in *cis* positions. The structure is built up from discrete molecules $[Mn(C_3H_5O_3)_2(H_2O)_2]$ held together through hydrogen bonds. Hydrogen-bond data are given in Table 3.

The molecular structure of the title compound is similar to that of Mn^{II} glycolate dihydrate (Lis, 1980) but different from that of Mn^{II} DL-lactate trihydrate (Singh *et al.*, 1975), where the water molecules are in *trans* positions.

The bond lengths and angles (Table 2) are the normally expected values and comparable with those for Zn DL-lactate trihydrate (Singh *et al.*, 1975). The configuration of the C–C$\begin{smallmatrix}O\\O\end{smallmatrix}$ group of each ligand is planar (Table 4). There is also a tendency for the O(3) or O(6) hydroxy atoms to lie in this plane. Similar trends have been observed in most α-hydroxycarbonyl systems (Newton & Jeffrey, 1977; Lis, 1981).

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Structure of μ-[2,4,6-Tri(2-pyridyl)-1,3,5-triazine]-bis[bis(trifluoroacetato)mercury(II)]

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Abstract. $[Hg_2(CF_3CO_2)_4(C_{18}H_{12}N_6)]$, $C_{26}H_{12}F_{12}Hg_2N_6O_8$, triclinic, $P\bar{1}$, $a = 13{\cdot}47\ (1)$, $b = 15{\cdot}85\ (2)$, $c = 9{\cdot}60\ (1)$ Å, $\alpha = 112{\cdot}4\ (1)$, $\beta = 100{\cdot}0\ (1)$, $\gamma = 110{\cdot}3\ (1)°$, $U = 1663$ Å^3, $D_m = 2{\cdot}360$, $Z = 2$, $D_x = 2{\cdot}328$ Mg m^{-3}, μ(Mo $K\alpha$) $= 8{\cdot}98$ mm^{-1}. $R = 0{\cdot}055$ for 2062 diffractometer-measured intensities. The 2,4,6-tri(2-pyridyl)-1,3,5-triazine molecule acts as a bidentate ligand to Hg(1) [Hg–N 2·17 (2), 2·61 (2) Å] and as a tridentate ligand towards Hg(2) [Hg–N 2·40 (2), 2·44 (2), 2·50 (2) Å]. The trifluoroacetate groups remain covalently attached to Hg [Hg(1)–O 2·13 (2), 2·86 (2), 2·35 (2), 2·63 (2) Å and Hg(2)–O 2·37 (2), 2·63 (2), 2·37 (2), 2·60 (3) Å]. Effectively, Hg(1) is six-coordinated and Hg(2) is seven-coordinated.

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