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Poly[[hexaacetatodiethanoltrimagnesium(II)] diethanol solvate], a polymeric acetate-bridged magnesium chain structure

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Key indicators

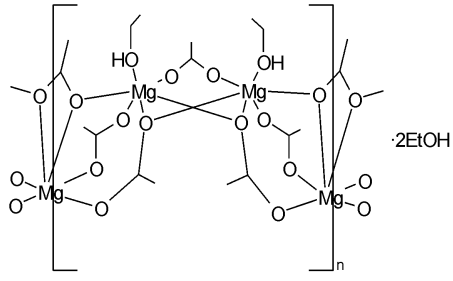
Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.005 Å
Disorder in main residue
R factor = 0.036
wR factor = 0.092
Data-to-parameter ratio = 12.0

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

The title compound, $[Mg_3(C_2H_3O_2)_6(C_2H_6O)_2]\cdot 2C_2H_6O$, contains infinite chains of magnesium ions bridged by acetate ligands in three different coordination modes. There are two independent Mg^{II} ions in the asymmetric unit, and one lies on a twofold axis. The coordination geometry around each Mg ion is distorted octahedral.

Comment

The structure of the title compound, (I), consists of chains of distorted octahedral magnesium ions bridged by acetate ligands. Fig. 1 shows the repeat unit. Mg1, C1, C2, C7 and C8 lie on a twofold axis along *b*. Three distinct acetate coordination modes are observed. The C3- and C7-acetate groups are bidentate bridges, whereas the C1-acetate group chelates to Mg1, with each of the O atoms also bound to Mg2. The C5-acetate groups are tridentate bridges rather than chelating to Mg2; the Mg2—O4 distance is 3.3126 (19) Å.



(I)

Ethanol is coordinated to Mg2, making the coordination sphere up to six O atoms. The coordinated ethanol H atom forms a hydrogen bond to the uncoordinated ethanol molecule, the H atom of this molecule is then hydrogen bonded to

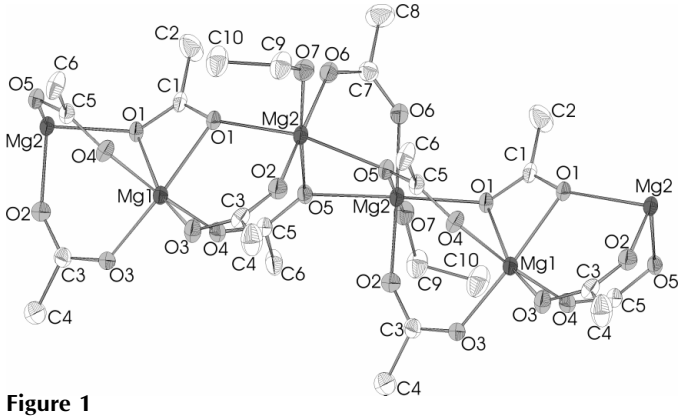


Figure 1
View of the repeat unit of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms have been omitted for clarity.

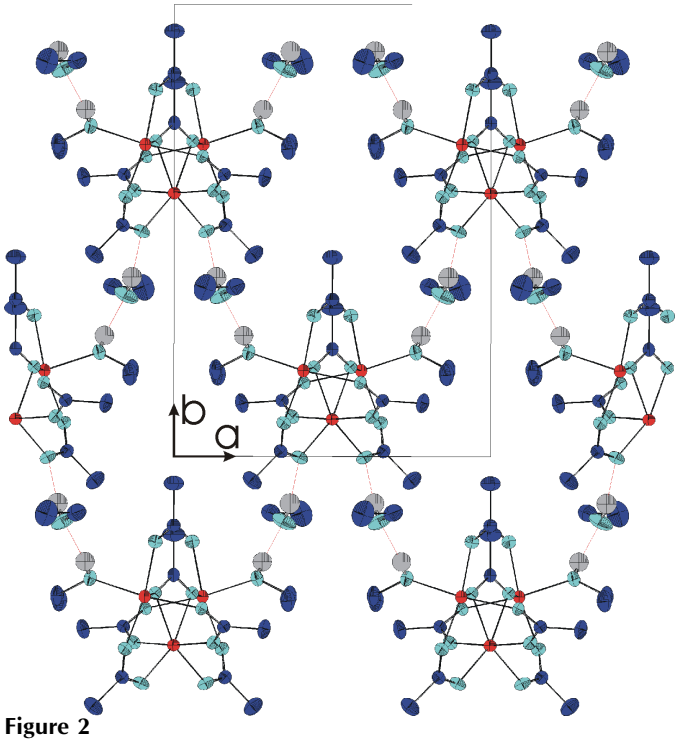


Figure 2
The packing of the chains in (I), viewed along the *c* axis. Displacement ellipsoids are drawn at the 50% probability level. C-bound H atoms have been omitted for clarity. Mg atoms are red, C blue, O light-blue and H grey. Hydrogen bonds are shown as thin red lines.

an O atom (O3) of one of the bidentate bridging acetate ligands (Table 2). Fig. 2 shows the crystal packing with the hydrogen bonds in red.

Previous structural studies of anhydrous and hydrated magnesium acetate are limited to measurement of unit cells, none of which are similar (Walter-Levy & Soleilhavoup, 1954; Walter-Levy *et al.*, 1959).

Experimental

Magnesium powder (0.04 mol) was suspended in dry ethanol under nitrogen. Glacial acetic acid (2 ml) was added and the mixture stirred until the magnesium dissolved. Colourless blocks formed on leaving the solution under nitrogen for 2 d.

Crystal data

$[Mg_3(C_2H_3O_2)_6(C_2H_6O)_2]\cdot 2C_2H_6O$
M_r = 611.47
Monoclinic, *C*2
a = 13.3931 (8) Å
b = 16.2214 (12) Å
c = 8.3414 (6) Å
β = 122.013 (3)°
V = 1536.62 (18) Å^3
Z = 2
D_x = 1.322 Mg m^{-3}
Mo *K*α radiation
Cell parameters from 4981 reflections
θ = 3.2–27.5°
μ = 0.17 mm^{-1}
T = 150 (2) K
Block, colourless
0.2 × 0.1 × 0.1 mm

Data collection

Nonius KappaCCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
T_{min} = 0.941, T_{max} = 0.962
4981 measured reflections
2628 independent reflections
2434 reflections with $I > 2\sigma(I)$
R_{int} = 0.026
θ_{max} = 27.5°
h = −17 → 17
k = −20 → 16
l = −10 → 10

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.092
S = 1.08
2628 reflections
219 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.034P)^2 + 1.1389P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.53 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}
Absolute structure: Flack (1983), 799 Friedel pairs
Flack parameter = −0.6 (3)

Table 1
Selected geometric parameters (Å, °).

O6—Mg2	2.034 (2)	Mg2—O7	2.075 (2)
Mg1—O3^{i}	2.016 (2)	Mg2—O1	2.1056 (17)
Mg1—O4^{i}	2.0503 (16)	Mg2—O5^{i}	2.1173 (17)
Mg1—O1^{i}	2.165 (2)	Mg2—O5^{ii}	2.1614 (18)
Mg1···Mg2^{i}	3.5679 (10)	Mg2···Mg2^{iii}	3.2278 (15)
Mg2—O2	2.024 (2)		
C5—O4—Mg1	145.63 (17)	O3^{i}—Mg1—O1	160.89 (8)
C5—O5—Mg2^{i}	126.50 (15)	O1^{i}—Mg1—O1	60.45 (9)
C5—O5—Mg2^{iv}	133.18 (15)	O2—Mg2—O6	170.09 (8)
Mg2^{i}—O5—Mg2^{iv}	97.94 (7)	O7—Mg2—O5^{i}	172.58 (9)
C7—O6—Mg2	131.5 (2)	O1—Mg2—O5^{ii}	166.41 (7)
C3—O3—Mg1	124.72 (18)	Mg2^{iii}···Mg2···Mg1	116.32 (3)
O1—C1—O1^{i}	118.4 (3)	C1—O1—Mg2	142.51 (16)
O6—C7—O6^{iii}	124.9 (4)	C1—O1—Mg1	90.60 (18)
O4—C5—O5	124.0 (2)	Mg2—O1—Mg1	113.31 (8)
O2—C3—C4	118.7 (2)	C3—O2—Mg2	149.32 (17)
O4^{i}—Mg1—O4	174.41 (13)	C9—O7—Mg2	133.2 (2)
O3^{i}—Mg1—O1^{i}	103.18 (7)		

Symmetry codes: (i) $2-x, y, 1-z$; (ii) $x, y, 1+z$; (iii) $2-x, y, 2-z$; (iv) $x, y, z-1$.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O8—H8O···O3^{i}	0.83 (4)	1.92 (4)	2.751 (3)	172 (4)
O7—H7O···O8	0.75 (4)	1.89 (4)	2.628 (3)	167 (4)

Symmetry codes: (i) $\frac{3}{2}-x, \frac{1}{2}+y, 1-z$.

The H atoms were initially located in difference maps. The H atoms of the C2- and C8-methyl groups are disordered and have 0.5 occupancy, reflecting the siting of these C atoms on the twofold axis. The positional parameters of the H atoms bonded to atoms C2, C8 and C10–C12 were idealized and refined riding on their parent atoms, with C—H distances in the range 0.95–1.00 Å and U_{iso}(H) = 1.5U_{eq}(C). The H atoms bonded to C4, C6 and C9 were refined isotropically, the range of C—H distances being 0.86 (7)–1.11 (4) Å. The hydroxy H atoms were also located and freely refined. In the absence of significant anomalous scattering effects, the Flack (1983) parameter refinement is essentially meaningless.

Data collection: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT* (Hooft, 1998); cell refinement: *DENZO* and *COLLECT*; data reduction: *DENZO*, *COLLECT* and *maXus* (Mackay *et al.*, 1998); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *CAMERON* (Watkin *et al.*, 1993) and *ATOMS* (Dowty, 1999); software used to prepare material for publication: *WinGX* (Farrugia, 1998).

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