This crystal belongs to the orthorhombic system with space group $P2_12_12_1$.

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Magnesium Galactarate Dihydrate

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Abstract. $Mg^{2+}.C_6H_8O_8^{2-}.2H_2O$, $M_r = 268{\cdot}46$, monoclinic, Cc, $a = 7{\cdot}605$ (1), $b = 8{\cdot}785$ (2), $c = 16{\cdot}404$ (2) Å, $\beta = 92{\cdot}56$ (1)°, $V = 1094{\cdot}9$ Å^3, $Z = 8$, $D_x = 1{\cdot}63$ g cm^{-3}, λ(Cu $K\alpha$) = 1·5418 Å, $\mu = 6{\cdot}17$ cm^{-1}, $F(000) = 276$, $T = 293$ K, $R = 0{\cdot}052$ for 862 observed reflections and 105 parameters refined. The galactarate ion is centrosymmetrical and the Mg^{2+} ion is six-coordinated (octahedral). Mg—O distances are in the range 2·003 (3) to 2·117 (2) Å.

Experimental. The sample was prepared from $MgCl_2$ and disodium galactarate and crystallized from water. Crystal tabular, 0·15 × 0·06 × 0·09 mm, Enraf–Nonius CAD-4F diffractometer, Ni-filtered Cu $K\alpha$; cell parameters from 22 θ measurements in the range $22 < \theta < 40°$; reflections measured for half the sphere of reflection to $2\theta = 140°$ for ranges of h, k and l of −9 to 9, 0 to 10 and −20 to 20 respectively; 1535 reflections measured plus 628 with $[F < 3\sigma(F)]$; intensity of 223 reflection measured 54 times: average count of 777·4 with a standard deviation (of the distribution) = 10·7 (1·4%) and no significant trend: no absorption correction; data merged using *SHELX*76 (Sheldrick, 1976) to give 862 unique reflections with $R_{int} = 0{\cdot}05$; h, k, l range −9 to 9, 0 to 10 and 0 to 20; one reflection with a high F_c/F_o ratio (002), possibly due to extinction, removed; structure solved by direct methods with *SHELXS*86 (Sheldrick, 1985), non-H atoms refined by least squares (F magnitudes) with anisotropic thermal parameters; all six H atoms found from difference Fourier syntheses, refined with isotropic thermal parameters; $R = 0{\cdot}052$, $wR = 0{\cdot}06$; for final cycle maximum shift/e.s.d. = 0·245, average = 0·040; $w = [\sigma^2(F) + 0{\cdot}005349F^2]^{-1}$; 105 parameters;

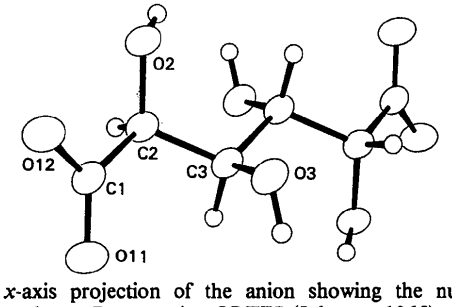

Fig. 1. x-axis projection of the anion showing the numbering scheme. Drawn using *ORTEP* (Johnson, 1965).

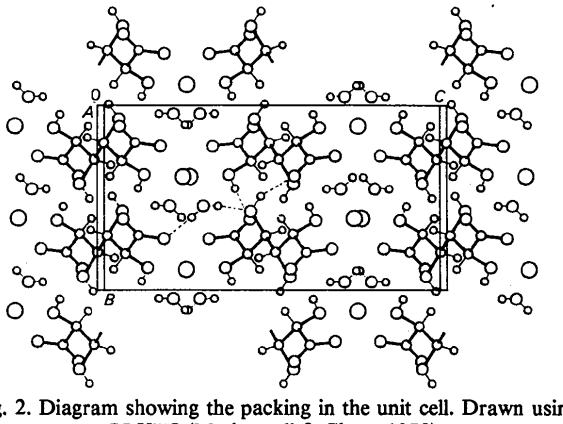

Fig. 2. Diagram showing the packing in the unit cell. Drawn using *PLUTO* (Motherwell & Clegg, 1978).

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Table 1. *Atom positions* ($\times 10^4$) *and equivalent isotropic thermal parameters* ($Å^2 \times 10^4$)

$$U_{eq} = \frac{1}{3}\sum_i\sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	U_{eq}
Mg	0	3878 (2)	2500	268
C1	−995 (4)	2044 (3)	3886 (2)	286
C2	456 (4)	3034 (3)	4294 (2)	265
C3	1674 (4)	2056 (3)	4844 (2)	254
O11	−1824 (3)	1157 (2)	4316 (2)	378
O12	−1280 (3)	2230 (3)	3130 (1)	370
O2	1346 (3)	3769 (2)	3656 (1)	300
O3	2222 (3)	742 (2)	4421 (1)	314
O10	−1707 (4)	5458 (4)	2853 (2)	550

difference Fourier synthesis showed a maximum value of 0·25 and a minimum value of −0·371 e $Å^{-3}$; atom scattering factors from *International Tables for X-ray Crystallography* (1974).

Fig. 1 shows the anion and numbering scheme and Fig. 2 the packing of the molecules in the unit cell. Table 1* lists atom parameters; Table 2 gives bond distances and angles. Each Mg^{2+} ion bridges two galactarate ions and the coordination of the Mg^{2+} ion is octahedral as is normally found (Brown, 1988).

Related literature. The galactarate ion has been studied as the Ca^{2+} and Ba^{2+} salts (Sheldrick, Mackie & Akrigg, 1989), while the coordination of Ca^{2+} with the glucarate ion has been established (Burden, Mackie & Sheldrick, 1985; Taga & Osaki, 1976) where the Ca–O distances agree with values given by Dheu-Andries & Perez (1983).

* Lists of structure factors, anisotropic thermal parameters and H-atom coordinates have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51803 (8 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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

C1–O11	1·242 (4)	C2–C3	1·529 (4)
C1–O12	1·260 (4)	C3–O3	1·419 (3)
C1–C2	1·535 (4)	C3–C3′	1·547 (5)
C2–O2	1·425 (3)		
O11–C1–O12	124·9 (3)	O2–C2–C3	113·1 (2)
O11–C1–C2	118·8 (3)	C2–C3–O3	110·6 (2)
O12–C1–C2	116·3 (2)	C2–C3–C3′	101·3 (3)
C1–C2–O2	107·0 (2)	O3–C3–C3′	99·3 (3)
C1–C2–C3	110·1 (2)		
Magnesium coordination			
Mg–O12 (O12′)	2·050 (2)	Mg–O2(O2′)	2·117 (2)
Mg–O10 (O10′)	2·003 (3)		
O2–Mg–O12	74·8 (1)	O12–Mg–O12′	90·1 (1)
O10–Mg–O12	90·9 (1)	O10–Mg–O10′	92·3 (2)
O10–Mg–O2	93·8 (1)		

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Structure of the Sodium Salt of a Thiazolopyrimidine, a Guanine Analog

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Abstract. Sodium pentahydrate salt of 2,5-diamino-[1,3]thiazolo[4,5-*d*]pyrimidin-7(6*H*)-one, $[C_5H_4N_5OS]^-.[Na(H_2O)_5]^+$, $M_r = 295{\cdot}25$, triclinic, $P\bar{1}$, $a = 6{\cdot}9985$ (9), $b = 8{\cdot}8182$ (15), $c = 10{\cdot}868$ (2) Å, $\alpha = 111{\cdot}83$ (3), $\beta = 99{\cdot}83$ (2), $\gamma = 94{\cdot}18$ (2)°, $V = 606{\cdot}6$ (2) $Å^3$, $Z = 2$, $D_x = 1{\cdot}616$ g cm^{-3}, λ(Cu $K\alpha$) = 1·54178 Å, $\mu = 30{\cdot}009$ cm^{-1}, $F(000) = 308$, $T = 295$ K, $R = 0{\cdot}0358$ for 2411 reflections ($F \geq 4\sigma_F$). The thiazole and pyrimidinone rings are planar [r.m.s. deviation: 0·0059 (6) and 0·0095 (6) Å, respectively]; the dihedral angle between these planes is 1·13 (5)°. The C–S bond lengths are nearly equivalent

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