

A schematic drawing of the crystal packing is shown in Fig. 3. The molecules are tied together chiefly by electrostatic, van der Waals and, possibly, very weak hydrogen-bonding forces. No π - π interactions occur between two phenyl rings, adjacent along **a**, because the angle between their least-squares planes is 80° . Omitting the O atoms of the toroidal region, no short van der Waals contacts are present. The structure consists of screw-related layers normal to **b**, two adjacent layers being shifted about $c/5$ and $c/3$ with respect to the PPC and ClO_4^- ions. The molecular packing is very similar in FMP, where the two distinct layers are composed of asymmetric units at (x, y, z) and $(x, \frac{1}{2} - y, \frac{1}{2} + z)$ for the first and at $(\bar{x}, \bar{y}, \bar{z})$ and $(\bar{x}, \frac{1}{2} + y, \frac{1}{2} - z)$ for the second. The approximate halving of **c** in SMP corresponds to the loss of the glide plane present in FMP, so that the glide symmetry is replaced by a translation.

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The Crystal Structure of Calcium 2-Keto-D-gluconate Trihydrate (Calcium D-arabino-Hexulosonate Trihydrate)

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The crystal structure of calcium 2-keto-D-gluconate (calcium D-arabino-hexulosonate) trihydrate, $\text{Ca}(\text{C}_6\text{H}_9\text{O}_7)_2 \cdot 3\text{H}_2\text{O}$, has been determined by the heavy-atom method and refined by full-matrix least-squares calculations to $R=0.094$ for 2235 visually estimated intensities. The crystals are orthorhombic, $P2_12_12_1$, with $a=10.438$ (5), $b=18.368$ (9), $c=9.545$ (4) Å, $Z=4$. Two independent pyran-type rings have formed through lactolization of the ketone groups at C(2) and C(2'). One ring oxygen together with hydroxyl and carboxyl substituents and water of crystallization, provide ninefold coordination for the calcium ions. One 2-ketogluconate ion lies between calcium positions forming chains along the 2_1 axis parallel to **c** through bidentate and tridentate chelate ligands to alternate calcium atoms. An independent 2-ketogluconate ion completes the unusual nine-coordination to calcium through tridentate ligands. The Ca-O distances vary from 2.33 to 2.73 Å with an average value of 2.53 Å.

Introduction

Sequestration of calcium from rocks and soil by 2-ketogluconic acid

(COOH.CO.HOCH.HCOH.HCOH.CH₂OH) is ascribed to the formation of chelate bonds between the metallic and organic ions.

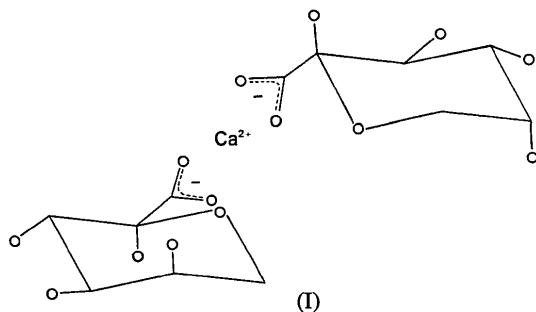
The effectiveness of 2-ketogluconic acid as a seques-

tering agent for calcium under laboratory conditions was established by Prescott, Shaw, Biletto & Cragwall (1953) and Mehlretter, Alexander & Rist (1953). Its industrial manufacture by fermentation of solutions containing calcium and glucose is described by Stubbs, Lockwood, Roe, Tobenkin & Ward (1940). The formation of 2-ketogluconic acid under culture conditions has been demonstrated by Duff, Webley & Scott (1963) by bacterial action of *Pseudomonas fluorescens* and a number of unnamed organisms which were isolated by Louw & Webley (1959) from the roots of oat-plants. These bacteria were found to be capable of solubilizing phosphatic mineral fertilisers.

Duff *et al.* (1963) showed that the presence of bacterially produced 2-ketogluconic acid leads to an increase in the concentration of phosphate dissolved in soil, either by direct attack of otherwise insoluble calcium phosphates or by increasing the soluble silicate to an extent where reaction with insoluble phosphate can occur. Calcium from dicalcium phosphate, natural and synthetic hydroxy- and fluorapatites, calcium silicate, wollastonite, and augite, for example, was found to be dissolved by 2-ketogluconic acid and by the bacteria producing it. Magnesium, iron or aluminum have been solubilized from other minerals.

The formation of chelate ring systems in calcium 5-ketogluconate has been established from a determination of its crystal structure by Balchin & Carlisle (1965). Both 5-ketogluconic acid and 2-ketogluconic acids are oxidation products of gluconic acid, the structure of which was determined by Littleton (1953).

In the ion of 2-ketogluconic acid two sites are available for lactol ring closure. These are provided by the OH groups on C(5) and C(6). Both result in a tetrahedral OH group at C(2), but the first leads to the formation of a furan-type lactone from the straight chain configuration, whereas the second results in the formation of a pyran-type lactone. The structure described below shows the pyran-type lactone to be appropriate to crystalline calcium 2-ketogluconate trihydrate and to be consistent with molecular formula (I). The numbering scheme for atoms in one asymmetric unit is given in Fig. 1.



Experimental

A sample of calcium 2-ketogluconate was supplied by the late Dr R. B. Duff of the Macaulay Institute of

Soil Research, Aberdeen. Dendritic needle clusters were obtained by precipitation from aqueous solution at 20°C by slow addition of ethanol. Preliminary X-ray examination established the space group $P2_12_12_1$. The crystal density was measured by flotation in a mixture of carbon tetrachloride and ethyl iodide. Crystal data are given in Table 1.

Table 1. *Crystal data for calcium 2-ketogluconate trihydrate*

$\text{Ca}(\text{C}_6\text{H}_9\text{O}_7)_2 \cdot 3\text{H}_2\text{O}$, F.W. 480.4	
Crystal system	Orthorhombic
Space group	$P2_12_12_1$
Form/habit	Dendritic needles {110}
Optics	Optically negative $\alpha \parallel b$, $\beta \parallel a$, $\gamma \parallel c$. Optic axial plane $\perp a$. $2v \approx 30^\circ$.
a	10.438 (5) Å
b	18.368 (9)
c	9.545 (4)
V_c	1830.02 (2) Å ³
Z	4
D_m	1.737 (3) g cm ⁻³
D_c	1.743 (1)
$F(000)$	1008
$\mu(\text{Cu } K\alpha)$	39.11 cm ⁻¹
$\lambda(\text{Cu } K\alpha)$	1.5418 Å
Crystal sizes:	a -axis mounting: 1.00 × 0.45 × 0.25 mm b -axis mounting: 1.00 × 1.00 × 1.60 mm c -axis mounting: 0.52 × 0.30 × 1.12 mm

Intensities were estimated visually from multiple-film equi-inclination Weissenberg photographs taken about a ($h=0$ to 7), b ($k=0$ only) and c ($l=0$ to 6) respectively, corrected for L_p factors and merged to form a unique set of 2235 intensities (Balchin, 1967),

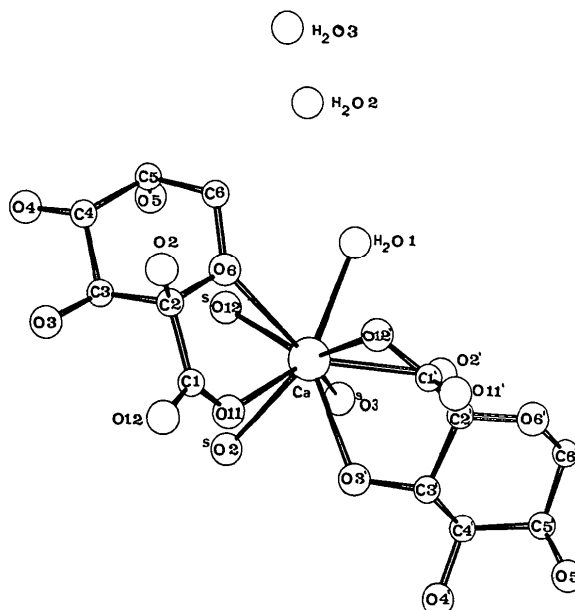


Fig. 1. The asymmetric unit of calcium 2-ketogluconate trihydrate showing numbering scheme for atoms. Three symmetry-related O atoms (labelled s) generated by the 2_1 axis parallel to c are also shown to complete the Ca coordination.

including 233 unobserved. Comparison of symmetrically related intensities indicated that random errors of visual estimates of intensity were less than 9.5%. No absorption corrections were applied ($\mu r = 0.98$ to 3.91). Cell dimensions were measured from rotation photographs and have since been refined from diffractometer measurements to the values given in Table 1.

Structure determination and refinement

Coordinates for the Ca atoms were derived from a sharpened Patterson synthesis, giving (0.250, 0.119, 0.225). The structure determination was carried out by application of the heavy-atom and successive Fourier methods using weighted coefficients (Sim, 1959). Possible atomic positions were assigned from stereochemical considerations. With estimated isotropic temperature factors, R fell to 0.34 for the 30 non-hydrogen atoms, including the three water molecules, at the completion of Fourier refinement.

Full-matrix least-squares refinement was effected with a modified version of Cruickshank & Smith's program, minimizing

$$\sum_{hkl} w(|F_o| - G|F_c|)^2,$$

where $w = (60.0 + |F_o| + 0.3|F_c|)^{-2}$ and G is an overall scale factor. Following isotropic refinement, aniso-

tropic refinement converged with $R = 0.097$. A difference map then revealed 18 of the 24 H atoms in stereochemically feasible positions. The H atoms were assigned isotropic temperature factors equal to those of the atoms bonded to them for subsequent structure factor calculations. After two further cycles of least-squares calculations for the non-H atomic parameters, refinement was terminated with $R = 0.094$ and weighted $R' = 0.127$. The atomic scattering factors used were those in *International Tables for X-ray Crystallography* (1962).*

Description of the structure

Fractional coordinates and thermal vibration parameters are listed in Table 2. Table 3 gives bond lengths and angles. Fig. 2(a) is a stereo pair of the calcium coordination, and Fig. 2(b) shows in stereo the configuration of atoms around two Ca atoms related by the 2_1 axis parallel to c .

Each Ca^{2+} ion lies between two 2-ketogluconate ions and is coordinated by nine O atoms (three in carboxyl groups, one pyranose O, one in H_2O and four

* A list of structure factors has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 31327 (12 pp., 1 microfiche). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

Table 2. Refined positional and anisotropic thermal parameters for non-hydrogen atoms ($\times 10^4$) with e.s.d.'s in parentheses

Anisotropic thermal parameter is of the form $\exp[-2\pi^2(h^2a^{*2}U_{11} + k^2b^{*2}U_{22} + l^2c^{*2}U_{33} + 2klb^*c^*U_{23} + 2lhc^*a^*U_{31} + 2hka^*b^*U_{12})]$.

	x	y	z	U_{11}	U_{22}	U_{33}	$2U_{32}$	$2U_{31}$	$2U_{21}$
Ca	-0.2552 (2)	0.1186 (1)	0.2260 (2)	163 (7)	150 (7)	148 (7)	-18 (11)	-22 (13)	-21 (12)
O(11)	-0.1616 (6)	0.0353 (4)	0.3805 (7)	271 (31)	323 (32)	302 (33)	224 (57)	26 (60)	21 (55)
O(12)	-0.1517 (6)	-0.0296 (3)	0.5788 (7)	271 (30)	297 (30)	294 (32)	169 (55)	-144 (6)	-158 (53)
O(2)	-0.4059 (6)	-0.0315 (3)	0.5962 (6)	320 (32)	291 (30)	165 (27)	-71 (49)	120 (54)	12 (54)
O(3)	-0.3142 (6)	-0.1515 (3)	0.4812 (7)	308 (32)	321 (26)	249 (29)	23 (49)	-44 (55)	179 (51)
O(4)	-0.5232 (7)	-0.1782 (4)	0.2817 (4)	371 (36)	383 (34)	422 (38)	-194 (67)	-61 (74)	-406 (63)
O(5)	-0.5479 (8)	-0.0496 (5)	0.1477 (8)	503 (45)	656 (50)	303 (36)	357 (72)	-304 (74)	654 (82)
O(6)	-0.4112 (6)	0.0308 (3)	0.3817 (7)	186 (26)	261 (29)	300 (31)	114 (54)	-107 (54)	-54 (48)
C(1)	-0.2117 (8)	-0.0029 (4)	0.4728 (9)	230 (43)	193 (35)	177 (36)	-156 (61)	-65 (54)	74 (63)
C(2)	-0.3508 (8)	-0.0247 (4)	0.4621 (8)	131 (34)	223 (36)	124 (32)	48 (58)	31 (61)	-32 (61)
C(3)	-0.3676 (9)	-0.0977 (4)	0.3912 (10)	310 (44)	205 (37)	217 (39)	14 (66)	51 (76)	36 (67)
C(4)	-0.5094 (9)	-0.1154 (5)	0.3646 (10)	258 (41)	342 (42)	300 (44)	-132 (82)	118 (78)	-168 (78)
C(5)	-0.5787 (10)	-0.0497 (6)	0.2947 (11)	265 (44)	516 (58)	334 (49)	340 (96)	-308 (88)	-113 (87)
C(6)	-0.5466 (10)	0.0205 (6)	0.3682 (12)	322 (49)	435 (53)	387 (55)	278 (95)	-54 (93)	-21 (88)
O(11')	-0.1962 (9)	0.2663 (5)	0.5826 (7)	630 (50)	590 (44)	147 (28)	-87 (63)	148 (69)	-480 (84)
O(12')	-0.2976 (7)	0.1880 (3)	0.4433 (7)	308 (32)	328 (31)	315 (33)	-81 (55)	266 (62)	-287 (55)
O(2')	-0.2305 (6)	0.2574 (3)	0.2139 (7)	244 (29)	278 (28)	250 (28)	19 (49)	-32 (54)	-16 (48)
O(3')	-0.0430 (6)	0.1662 (3)	0.2815 (8)	244 (28)	185 (25)	401 (35)	73 (53)	36 (61)	-75 (45)
O(4')	0.1738 (6)	0.2553 (3)	0.1836 (6)	241 (28)	270 (28)	197 (27)	81 (48)	-29 (51)	-21 (48)
O(5')	0.1262 (6)	0.3887 (3)	0.3246 (7)	313 (31)	370 (27)	240 (29)	-77	-52 (54)	-69 (52)
O(6')	-0.1527 (6)	0.3508 (3)	0.3584 (7)	300 (30)	235 (27)	292 (31)	-8 (51)	132 (59)	-57 (50)
C(1')	-0.2232 (8)	0.2407 (5)	0.4655 (9)	159 (39)	261 (39)	257 (41)	-76 (68)	159 (68)	-9 (61)
C(2')	-0.1592 (8)	0.2759 (5)	0.3374 (10)	223 (38)	270 (39)	237 (39)	-122 (70)	-147 (78)	-90 (69)
C(3')	-0.0262 (9)	0.2419 (4)	0.3155 (10)	292 (40)	164 (43)	293 (42)	48 (66)	23 (60)	56 (65)
C(4')	0.0457 (7)	0.2812 (4)	0.1994 (8)	162 (35)	235 (36)	192 (35)	-34 (58)	-62 (62)	-47 (57)
C(5')	0.0384 (9)	0.3642 (4)	0.2208 (10)	303 (43)	210 (36)	231 (38)	-15 (66)	13 (77)	90 (66)
C(6')	-0.0922 (9)	0.3883 (4)	0.2429 (11)	342 (45)	145 (33)	463 (57)	31 (77)	-163 (92)	82 (68)
H ₂ O(1)	-0.4672 (8)	0.1667 (4)	0.1621 (10)	466 (42)	271 (31)	632 (50)	-133 (68)	-388 (90)	-41 (64)
H ₂ O(2)	-0.7239 (9)	0.1158 (5)	0.1009 (10)	633 (56)	699 (56)	572 (52)	-129 (98)	-269 (101)	400 (102)
H ₂ O(3)	-0.8403 (8)	0.0945 (5)	0.3973 (10)	439 (42)	566 (45)	315 (82)	-139 (85)	522 (42)	120 (78)

in hydroxyl groups). Ca–O distances vary from 2.339 to 2.732 Å with an average value of 2.504 Å (*cf.* the values of 2.39 to 2.46 Å found in the eightfold coordination of Ca by O in calcium 5-ketogluconate). The two 2-ketogluconate ions in the molecule show differing linkages to the Ca atoms. Of the nine O atoms coordinating Ca, two – a glycosidic O and a carboxyl O – form a bidentate linkage from the Ca to a 2-ketogluconate ion which lies approximately equidistant from two Ca atoms (those related by the 2_1 axis parallel to *c*). The same 2-ketogluconate ion then forms a tridentate linkage through other side groups, carboxyl O and two OH groups, to the adjacent Ca atom. A chain of molecules is thus formed which zig-zags along the 2_1 axis [Fig. 2(*b*)]. The other 2-ketogluconate ion is then bonded to this chain through tridentate linkages *via* carboxyl oxygen and two OH groups to the calcium atoms. Fig. 3 shows the chelate ring system and Fig. 4 the crystal packing.

Table 3. Bond lengths and angles

(a) Bond lengths (Å) for the non-hydrogen atoms. Standard deviations are given in parentheses.

Ca–H ₂ O(1)	2.459 (8)	Ca–O(6)	2.732 (6)
Ca–O(11)	2.339 (7)	Ca–O(12')	2.475 (7)
Ca– ^s O(12)	2.365 (6)	Ca–O(2')	2.566 (6)
Ca– ^s O(2)	2.631 (7)	Ca–O(3')	2.440 (6)
Ca– ^s O(3)	2.519 (7)		
C(1)–O(11)	1.241 (10)	C(1')–O(11')	1.244 (11)
C(1)–O(12)	1.287 (10)	C(1')–O(12')	1.259 (10)
C(1)–C(2)	1.510 (12)	C(1')–C(2')	1.536 (12)
C(2)–C(3)	1.511 (11)	C(2)–C(3')	1.536 (12)
C(3)–C(4)	1.536 (12)	C(3')–C(4')	1.521 (11)
C(4)–C(5)	1.558 (14)	C(4')–C(5')	1.538 (11)
C(5)–C(6)	1.505 (16)	C(5')–C(6')	1.449 (13)
C(6)–O(6)	1.431 (12)	C(6')–O(6')	1.444 (12)
O(6)–C(2)	1.423 (10)	O(6')–C(2')	1.392 (10)
C(2)–O(2)	1.409 (9)	C(2')–O(2')	1.434 (10)
C(3)–O(3)	1.423 (10)	C(3')–O(3')	1.438 (9)
C(4)–O(4)	1.406 (11)	C(4')–O(4')	1.427 (9)
C(5)–O(5)	1.440 (13)	C(5')–O(5')	1.423 (11)

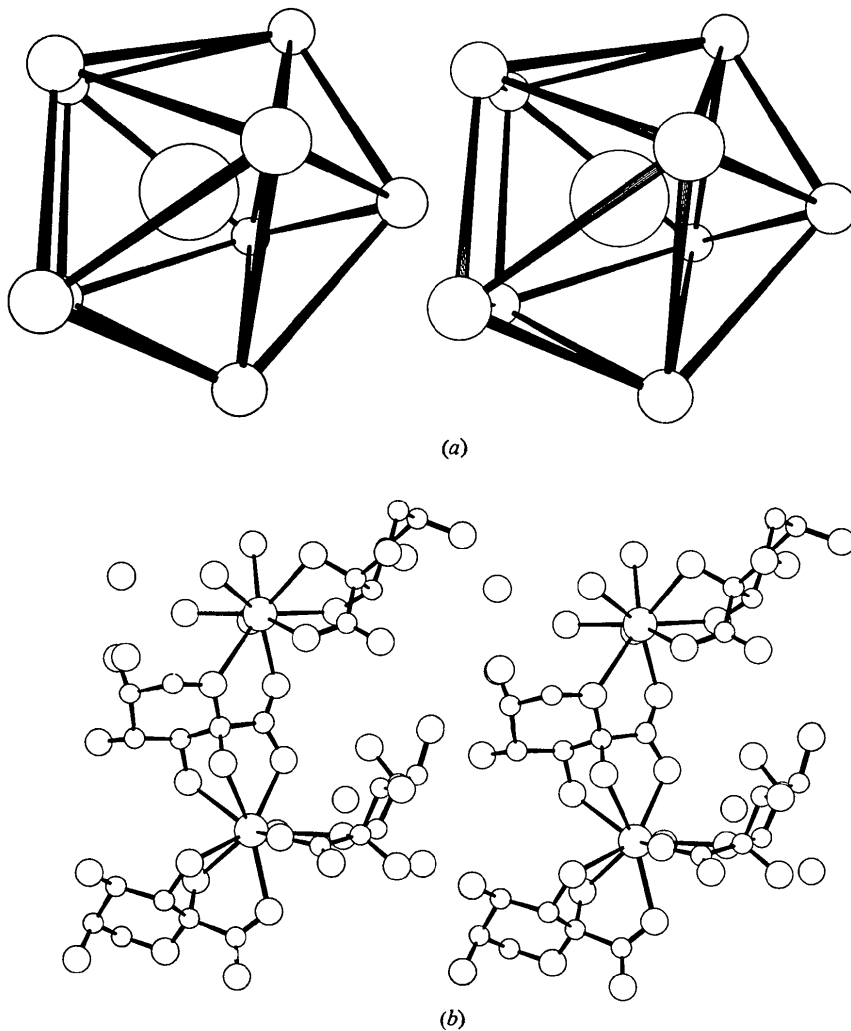


Fig. 2. (a) Stereo pair showing Ca coordination. (b) Stereo pair showing chains of molecules along the 2_1 axis parallel to *c*.

Table 3 (cont.)

(b) Bond angles ($^{\circ}$) for the non-hydrogen atoms. Standard deviations are given in parentheses.

O(11)—C(1)—O(12)	124.63 (82)	O(11')—C(1')—O(12')	125.54 (83)
O(11)—C(1)—C(2)	120.49 (74)	O(11')—C(1')—C(2')	117.26 (72)
O(12)—C(1)—C(2)	114.80 (75)	O(12')—C(1')—C(2')	117.20 (74)
C(1)—C(2)—O(2)	110.77 (65)	C(1')—C(2')—O(2')	109.23 (65)
C(3)—C(2)—O(2)	106.33 (64)	C(3')—C(2')—O(2')	105.11 (68)
O(6)—C(2)—O(2)	111.80 (66)	C(6)—C(2')—O(2')	112.16 (72)
C(1)—C(2)—C(3)	112.20 (66)	C(1')—C(2')—C(3')	109.29 (71)
C(1)—C(2)—O(6)	105.82 (62)	C(1')—C(2')—O(6')	108.79 (71)
C(3)—C(2)—O(6)	110.02 (64)	C(3')—C(2')—O(6')	112.17 (69)
C(2)—C(3)—C(4)	111.96 (70)	C(2')—C(3')—C(4')	110.61 (67)
C(2)—C(3)—O(3)	107.47 (69)	C(2')—C(3')—O(3')	108.29 (68)
C(4)—C(3)—O(3)	109.29 (73)	C(4')—C(3')—O(3')	110.79 (70)
C(3)—C(4)—C(5)	110.78 (75)	C(3')—C(4')—C(5')	110.45 (66)
C(3)—C(4)—O(4)	111.46 (74)	C(3')—C(4')—O(4')	112.38 (64)
C(5)—C(4)—O(4)	110.30 (81)	C(5')—C(4')—O(4')	113.03 (65)
C(4)—C(5)—C(6)	111.11 (79)	C(4')—C(5')—C(6')	111.63 (72)
C(4)—C(5)—O(5)	108.32 (93)	C(4')—C(5')—O(5')	111.97 (69)
C(6)—C(5)—O(5)	113.79 (87)	C(6')—C(5')—O(5')	114.03 (75)
C(5)—C(6)—O(6)	112.02 (88)	C(5')—C(6')—O(6')	112.15 (74)
C(6)—O(6)—C(2)	113.09 (68)	C(6')—O(6')—C(2')	112.49 (69)

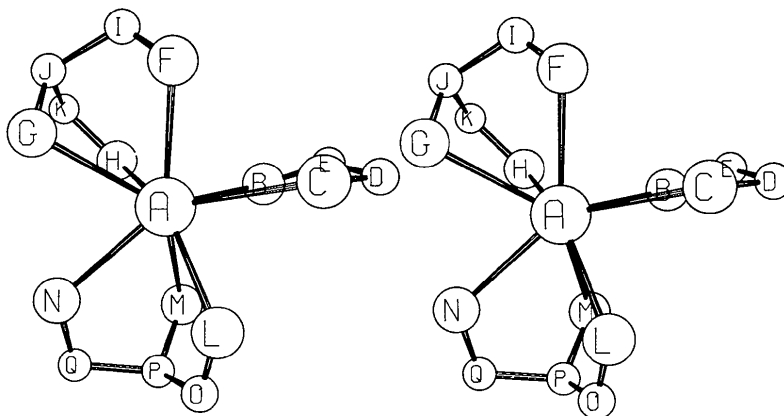


Fig. 3. Stereo pair showing chelate ring system in calcium 2-ketogluconate trihydrate. Key: A = Ca, B = O(11), C = O(6), D = C(2), E = C(1), F = O(12'), G = O(2'), H = O(3'), I = C(1'), J = C(2'), K = C(3'), L = s O(12), M = s O(2), N = s O(3), O = s C(1), P = s C(2), Q = s C(3) (atoms labelled s are generated by operation of the 2_1 screw axis parallel to c on the parent atoms).

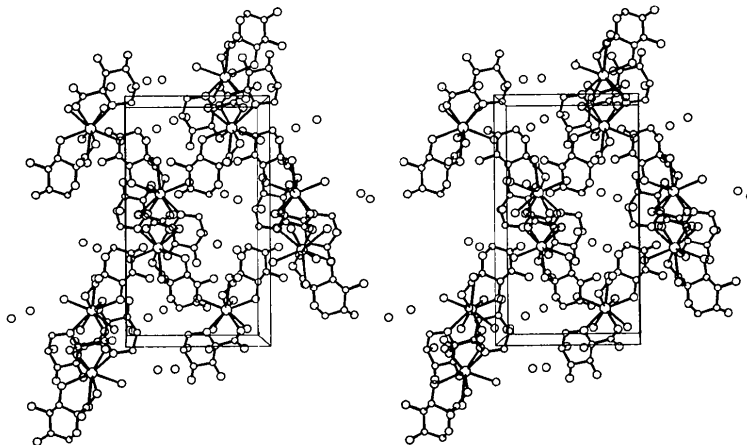


Fig. 4. Calcium 2-ketogluconate trihydrate. Stereo pair showing crystal packing.

Table 4. *Torsion angles* (°)

The sign of the angle $A-B-C-D$ is positive when a clockwise rotation about $B-C$ is required to bring $A-B-C$ into coincidence with $B-C-D$, viewed along $B-C$.

Pyranose ring 1					Pyranose ring 2				
A	B	C	D		A	B	C	D	
C(2)	C(3)	C(4)	C(5)	48.57	C(2')	C(3')	C(4')	C(5')	47.88
C(3)	C(4)	C(5)	C(6)	-46.33	C(3')	C(4')	C(5')	C(6')	-50.57
C(4)	C(5)	C(6)	O(6)	52.13	C(4')	C(5')	C(6')	O(6')	55.58
C(5)	C(6)	O(6)	C(2)	-61.25	C(5')	C(6')	O(6')	C(2')	-60.61
C(6)	O(6)	C(2)	C(3)	61.99	C(6')	O(6')	C(2')	C(3')	58.30
O(6)	C(2)	C(3)	C(4)	-55.59	O(6')	C(2')	C(3')	C(4')	-52.94

Both carboxylate groups are planar, the C-C bonds ranging from 1.510 to 1.536 Å, their average length being 1.523 Å. The lengths of the partial double bonds C...O range from 1.241 to 1.287 Å (average 1.258 Å) with bond angles O...C...O 124.63° and 125.54°. These values are all close to those found in calcium 5-ketogluconate and in other organic sugar acids.

Lactolization of the carbon chain at the keto oxygen has produced two independent six-membered pyranose rings per asymmetric unit. Both are in the normal C1 chair conformation (Kim & Jeffrey, 1967). With the exception of C(5')-C(6') the C-C bond lengths lie within the range 1.505 to 1.558 Å, with an average length of 1.529 Å. C(5')-C(6')=1.449 (13) Å, is significantly shorter. The ring C-O bonds vary in length between 1.392 and 1.444 Å, none being significantly different from the mean value of 1.423 Å. C-OH bond lengths range from 1.406 to 1.440, mean 1.423 Å.

The valency angles involving only C range from 110.02 to 112.17° (mean 111.39°) inside the rings, and external to the rings from 105.11 to 114.03° (mean 110.12°). At the ring oxygens the valency angles are 113.09 and 112.49°, somewhat greater than the mean internal valence angle, a common feature in pyranose rings. The range of values of torsion angles in the pyranose rings (Table 4), 46.33-61.99°, and 47.88-60.61°, as compared with 55.8-61.7° for a hypothetical ideal unstrained 'trans' ring (Kim & Jeffrey, 1967), indicates strain possibly due to crystal packing forces.

There are two tridentate rings and one bidentate ring chelating Ca and probably containing coordinate bonds (Fig. 3). The bidentate ring is approximately planar, unlike the tridentate rings.

An extensive network of hydrogen bonds holds the crystal structure together. Hydrogen-bond distances are given in Table 5. The crystal packing is shown in Fig. 4.

Table 5. *Hydrogen-bond distances and angles*

Symmetry code		Superscript			
(i)	$-x, \frac{1}{2}-y, \frac{1}{2}-z$	(ii)	$\frac{1}{2}+x, \frac{1}{2}-y, 1-z$		
(iii)	$1-x, \frac{1}{2}+y, \frac{1}{2}-z$	(iv)	$1+x, y, z$		
(v)	$\frac{1}{2}+x, \frac{1}{2}-y, z$				
D	H	A	$D \cdots A$ (Å)	$\angle D-H \cdots A$ (°)	
O(2)	H(2)	O(5') ⁱ	2.749 (8)	125.02 (40)	
O(5')	H(51')	O(12') ⁱⁱ	2.744 (9)	146.07 (38)	
O(3)	H(31)	O(4')	2.749 (8)	164.01 (37)	
O(4')	H(41')	O(11') ⁱⁱ	2.642 (9)	161.42 (45)	
O(2')	H(2')	O(4) ⁱⁱⁱ	2.830 (9)	145.34 (42)	
O(3')	H(31')	H ₂ O(3) ^{iv}	2.727 (10)	170.91 (42)	
H ₂ O(1)	-	O(4) ⁱⁱⁱ	2.902 (10)	-	
H ₂ O(1)	-	H ₂ O(2)	2.898 (12)	-	
H ₂ O(2)	-	O(4) ⁱⁱⁱ	2.884 (11)	-	
H ₂ O(2)	-	H ₂ O(3)	3.104 (14)	-	
H ₂ O(3)	-	O(11') ⁱⁱ	2.974 (12)	-	
H ₂ O(3)	-	O(5) ^v	2.783 (11)	-	

Computing was undertaken on the University of London CDC6600 computer using the Birkbeck College Crystallographic Program Library.

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