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catena-Poly[[[diaquacalcium(II)]-di-μ-3-carboxyphenoxyacetato] dihydrate]

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Key indicators

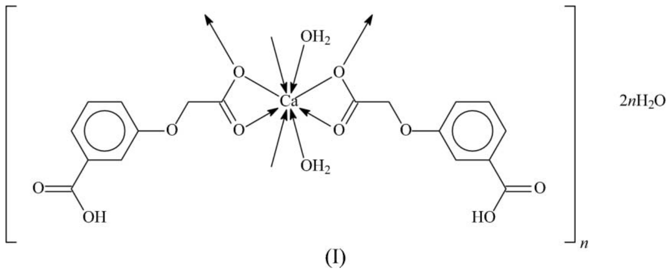
Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.003 Å
H-atom completeness 82%
Disorder in solvent or counterion
R factor = 0.045
wR factor = 0.131
Data-to-parameter ratio = 16.9

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

The Ca atom in the title compound, $\{[Ca(HO_2CC_6H_4OCH_2CO_2)_2(H_2O)_2]\cdot 2H_2O\}_n$, is eight-coordinate. The $HO_2CC_6H_4OCH_2CO_2^-$ monoanion binds in a chelating mode; it also functions as a bridge, linking adjacent Ca atoms into a zigzag chain. Hydrogen bonds link the chains into a three-dimensional network. The Ca atom lies on a special position of site symmetry 2.

Comment

A preceeding study (Gao & Ng, 2006) reports the structure of the cadmium derivative of 3-carboxyphenoxyacetic acid; the acid is doubly deprotonated and the dianion links the water-coordinated Cd atoms into a linear chain.



(I)

With calcium in place of cadmium, a similar synthesis, but employing less than half the stoichiometric quantity of the acid, has ensured that the acid is only mono-deprotonated. The calcium derivative is formally the water-coordinated complex, $(H_2O)_2(HO_2CC_6H_4OCH_2CO_2)_2Ca$, which crystallizes as a dihydrate (Scheme, Fig. 1). The acid H atom is retained by the carboxyl unit that is directly connected to the benzene ring, and the carboxylic acid portion engages in hydrogen-bonding interactions (Table 2), giving rise to a three-dimensional network.

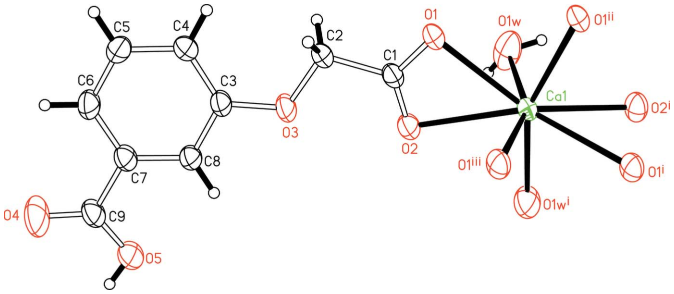


Figure 1
*ORTEP*II plot of a portion of the chain structure of $Ca(C_9H_7O_5)_2(H_2O)_2\cdot 2H_2O$. Displacement ellipsoids are drawn at the 50% probability level, and H atoms are drawn as spheres of arbitrary radii. The disordered uncoordinated water molecule is not shown.

The carboxylate group of the oxyacetate arm binds in a chelating mode; additionally, one of the two O atoms interacts with an adjacent Ca atom. Such a bridging interaction leads to the formation of a zigzag chain that runs along the *c* axis (Fig. 2). The Ca atom is eight-coordinate; however, the geometry cannot be ascribed to a regular polyhedron.

Experimental

Calcium nitrate tetrahydrate (0.78 g, 5 mmol) and 3-carboxyphenoxyacetic acid (0.39 g, 2 mmol) were dissolved in a small volume of hot water. Colorless prisms separated from the solution after several days. C&H analysis. Calc. for $C_{18}H_{22}O_{14}Ca$: C 43.02, H 4.42%. Found: C 43.06, H 4.45%.

Crystal data

$[Ca(C_9H_7O_5)_2(H_2O)_2]\cdot 2H_2O$
$M_r = 502.44$
Monoclinic, $C2/c$
$a = 26.902$ (5) Å
$b = 14.492$ (3) Å
$c = 6.057$ (1) Å
$\beta = 101.28$ (3)°
$V = 2315.6$ (8) Å^3
$Z = 4$
$D_x = 1.441$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 10195 reflections
$\theta = 3.1$–27.4°
$\mu = 0.34$ mm^{-1}
$T = 295$ (2) K
Prism, colorless
0.36 × 0.25 × 0.18 mm

Data collection

Rigaku RAXIS-RAPID IP diffractometer
ω scans
Absorption correction: multi-scan *ABSCOR* (Higashi, 1995)
$T_{min} = 0.691$, $T_{max} = 0.941$
10847 measured reflections
2622 independent reflections
2340 reflections with $I > 2\sigma(I)$
$R_{int} = 0.021$
$\theta_{max} = 27.4°$
$h = -34 \rightarrow 33$
$k = -18 \rightarrow 18$
$l = -7 \rightarrow 7$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.131$
$S = 1.04$
2622 reflections
155 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0777P)^2 + 2.6608P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.42$ e Å^{-3}
$\Delta\rho_{min} = -0.37$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ca1—O1	2.488 (2)	Ca1—O2	2.537 (2)
Ca1—O1^{i}	2.488 (2)	Ca1—O2^{i}	2.537 (2)
Ca1—O1^{ii}	2.386 (1)	Ca1—O1*w*	2.393 (2)
Ca1—O1^{iii}	2.386 (1)	Ca1—O1*w*^{i}	2.393 (2)
O1—Ca1—O1^{i}	146.2 (1)	O1^{ii}—Ca1—O2	126.3 (1)
O1—Ca1—O1^{ii}	74.4 (1)	O1^{ii}—Ca1—O2^{i}	80.9 (1)
O1—Ca1—O1^{iii}	81.6 (1)	O1^{ii}—Ca1—O1*w*	95.9 (1)
O1—Ca1—O2	52.0 (1)	O1^{ii}—Ca1—O1*w*^{i}	155.5 (1)
O1—Ca1—O2^{i}	142.4 (1)	O2—Ca1—O2^{i}	144.7 (1)
O1—Ca1—O1*w*	76.6 (1)	O2—Ca1—O1*w*	77.0 (1)
O1—Ca1—O1*w*^{i}	130.1 (1)	O2—Ca1—O1*w*^{i}	78.2 (1)
O1^{ii}—Ca1—O1^{iii}	88.7 (1)	O1*w*—Ca1—O1*w*^{i}	89.9 (1)

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

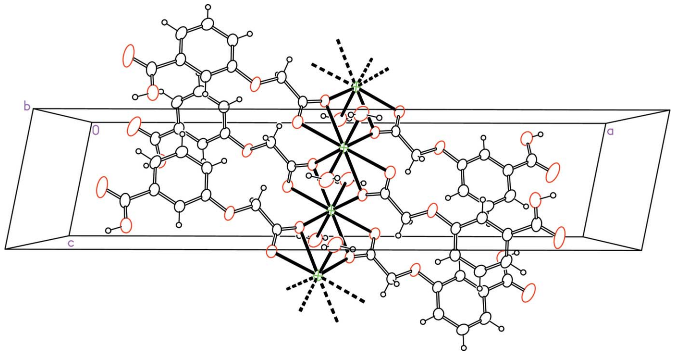


Figure 2
*ORTEP*II plot of the chain motif; the uncoordinated water molecules are not shown.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H5*o*···O2^{iv}	0.85	1.89	2.720 (2)	166
O1*w*—H1*w*1···O2*w*	0.85	2.09	2.925 (8)	168
O1*w*—H1*w*2···O4^{v}	0.85	1.91	2.704 (2)	156

Symmetry codes: (iv) $-x+\frac{1}{2}, -y+\frac{1}{2}, -z+1$; (v) $x+\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$.

The carbon-bound H atoms were positioned geometrically [C–H 0.93 or 0.97 Å] and were included in the refinement in the riding-model approximation, with $U(H) = 1.2U_{eq}(C)$. The H atoms of the coordinated water molecule were similarly treated [O–H 0.85 Å, $U(H) = 1.5U_{eq}(O)$]; these were rotated to fit the electron density.

The uncoordinated water molecule is disordered over two positions and the occupancy refined to 0.67 (1):0.33 (1). The displacement parameters of the two components were set to equal each other; these were restrained to be nearly isotropic. H atoms were not added to the disordered components.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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References

Gao, S. & Ng, S. W. (2006). *Acta Cryst.* E**62**, m179–m180.
Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
Johnson, C. K. (1976). *ORTEP*II. Report ORNL-5138, Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA.
Rigaku (1998). *RAPID-AUTO*. Rigaku Corporation, Tokyo, Japan.
Rigaku/MSC (2002). *CrystalStructure*. Rigaku/MSC Inc., The Woodlands, Texas, USA.
Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.