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catena-Poly[[strontium(II)-di-μ-aqua-di-μ-9-hydroxyfluorene-9-carboxylato] monohydrate]

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Key indicators

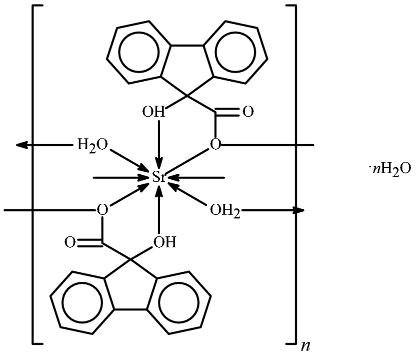
Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.006 Å
Disorder in solvent or counterion
R factor = 0.047
wR factor = 0.115
Data-to-parameter ratio = 19.2

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

The Sr^{II} atom in the title compound, $\{[Sr(C_{14}H_9O_3)(H_2O)_2]\cdot H_2O\}n$, is chelated by the carboxyl and hydroxyl O atoms of two anions, and is coordinated by two water molecules that function in a bridging mode. The eight-coordinate configuration arises from additional interaction with the carboxyl O atoms which are already involved in chelation in adjacent molecules. The geometry is intermediate between dodecahedral and square antiprismatic in the linear chain structure.

Comment

The 9-hydroxyfluorene-9-carboxylate monoanion has been documented to chelate in a small number of metal complexes (Gao *et al.*, 2004; Huo *et al.*, 2004). This feature is also observed in the title strontium derivative, (I), which crystallizes as a diaqua complex with an uncoordinated water molecule (Fig. 1).



(I)

The Sr atom exists in an eight-coordinate environment, but the geometry is intermediate between dodecahedral and square antiprismatic (Fig. 2). The high coordination number arises from the bridging nature of the two water molecules, and also from bridging by carboxyl O atoms, which are themselves already bonded to a metal atom. Adjacent molecules are linked by hydrogen bonds (Table 2) into linear chains.

Experimental

To a solution of strontium carbonate (0.15 g, 1 mmol) in methanol (20 ml) was added 9-hydroxyfluorene-9-carboxylic acid (0.44 g, 2 mmol) in methanol. Aqueous sodium hydroxide was added so that the mixed solvent had a pH of about 6. The mixture was filtered and colourless single crystals of (I) were isolated after several days. CH analysis, calculated for $C_{28}H_{24}O_9Sr$: C 56.80, H 4.09%; found C 56.76, H 4.11%.

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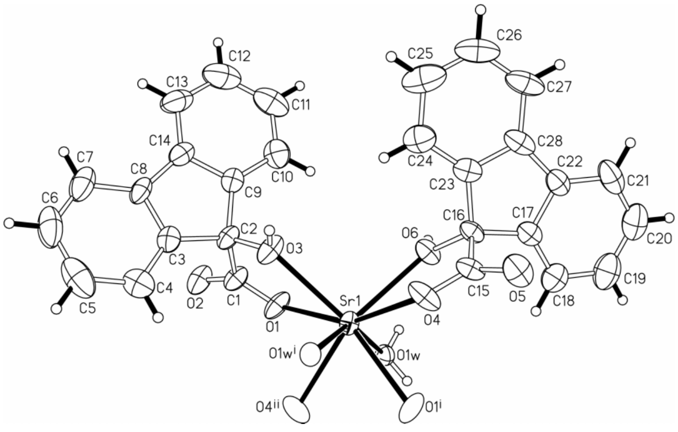

Figure 1
Plot illustrating the eight-coordinate geometry of the Sr atom in (I). Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as spheres of arbitrary radii. [Symmetry codes (i): $1 - x$, $\frac{1}{2} + y$, $1 - z$; (ii) $1 - x$, $y - \frac{1}{2}$, $1 - z$.]

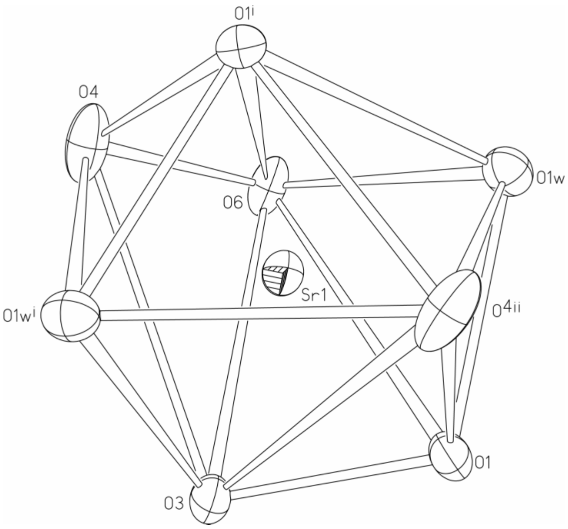

Figure 2
The coordination geometry illustrated as a dodecahedron. (Symmetry codes as given in Fig. 1.)

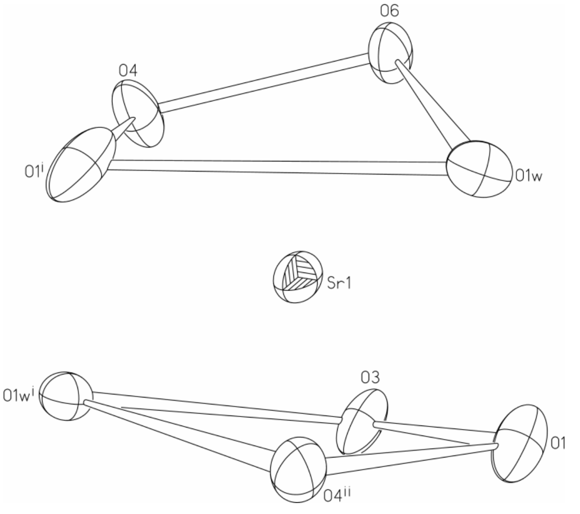

Figure 3
The coordination geometry illustrated as a square antiprism. (Symmetry codes as given in Fig. 1.)

Crystal data

$[Sr(C_{14}H_9O_3)(H_2O)_2]\cdot H_2O$
$M_r = 592.09$
Monoclinic, $P2_1$
$a = 12.727$ (3) Å
$b = 7.231$ (1) Å
$c = 14.947$ (3) Å
$\beta = 108.79$ (3)°
$V = 1302.2$ (4) Å^3
$Z = 2$

$D_x = 1.510$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 11 087 reflections
$\theta = 3.3$–27.4°
$\mu = 2.12$ mm^{-1}
$T = 295$ (2) K
Block, colourless
0.37 × 0.25 × 0.18 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan, (*ABSCOR*; Higashi, 1995)
$T_{\min} = 0.544$, $T_{\max} = 0.701$
11 926 measured reflections

5722 independent reflections
4864 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.037$
$\theta_{\max} = 27.5°$
$h = -16 \rightarrow 16$
$k = -9 \rightarrow 9$
$l = -17 \rightarrow 19$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.115$
$S = 1.05$
5722 reflections
298 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0611P)^2 + 0.6925P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.98$ e Å^{-3}
$\Delta\rho_{\min} = -0.48$ e Å^{-3}
Absolute structure: Flack (1983), with 3266 Friedel pairs
Flack parameter: 0.007 (9)

Table 1
Selected geometric parameters (Å, °).

Sr1—O1	2.553 (3)	Sr1—O4^{ii}	2.573 (3)
Sr1—O1^{i}	2.562 (3)	Sr1—O6	2.600 (3)
Sr1—O3	2.561 (3)	Sr1—O1*w*	2.575 (3)
Sr1—O4	2.551 (3)	Sr1—O1*w*^{i}	2.589 (3)
O1—Sr1—O1^{i}	139.0 (1)	O3—Sr1—O4^{ii}	103.9 (1)
O1—Sr1—O3	60.1 (1)	O3—Sr1—O6	96.8 (1)
O1—Sr1—O4	156.2 (1)	O3—Sr1—O1*w*	127.9 (1)
O1—Sr1—O4^{ii}	64.4 (1)	O3—Sr1—O1*w*^{i}	77.4 (1)
O1—Sr1—O6	105.1 (1)	O4—Sr1—O4^{ii}	138.5 (1)
O1—Sr1—O1*w*	71.5 (1)	O4—Sr1—O6	60.1 (1)
O1—Sr1—O1*w*^{i}	116.3 (1)	O4—Sr1—O1*w*	118.2 (1)
O1^{i}—Sr1—O3	148.3 (1)	O4—Sr1—O1*w*^{i}	68.8 (1)
O1^{i}—Sr1—O4	64.6 (1)	O4^{ii}—Sr1—O6	145.8 (1)
O1^{i}—Sr1—O4^{ii}	76.9 (1)	O4^{ii}—Sr1—O1*w*	68.7 (1)
O1^{i}—Sr1—O6	99.2 (1)	O4^{ii}—Sr1—O1*w*^{i}	85.1 (1)
O1^{i}—Sr1—O1*w*	82.5 (1)	O6—Sr1—O1*w*	77.1 (1)
O1^{i}—Sr1—O1*w*^{i}	71.1 (1)	O6—Sr1—O1*w*^{i}	126.4 (1)
O3—Sr1—O4	101.2 (1)	O1*w*—Sr1—O1*w*^{i}	146.5 (1)

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

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3*o*···O2*w*	0.85	1.83	2.672 (6)	170
O6—H6*o*···O3*w*	0.85	1.85	2.66 (1)	158
O1*w*—H1*w*1···O2^{i}	0.85	1.94	2.697 (5)	147
O1*w*—H1*w*2···O5^{iii}	0.85	1.96	2.691 (5)	143
O2*w*—H2*w*2···O2^{iv}	0.85	1.93	2.716 (7)	154
O3*w*—H3*w*1···O5^{iii}	0.86	1.93	2.76 (1)	159
O3*w*′—H3*w*3···O5^{iii}	0.87	1.70	2.55 (1)	164

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

The benzene rings were refined as rigid hexagons with sides of 1.39 Å. The water H atoms were placed in chemically sensible positions but were not refined. The hydroxyl OH groups were placed in calculated positions assuming sp^2 hybridization (O—H = 0.85 Å); for these O-bound H atoms, U_{iso}(H) was set equal to 1.2U_{eq} of the parent atom. The O3*W* water molecule is disordered over two positions and, as the disorder refined to nearly 50:50, the occupancies were set to 0.5. The displacement parameters of the two components were made equal to each other and were restrained to be approximately isotropic. The C-bound H atoms were placed in calculated positions (C—H = 0.93 Å) and were included in the refinement in the riding-model approximation, with displacement parameters set to 1.2 times U_{eq} of the parent atoms.

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

Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.

Gao, S., Liu, J.-W., Huo, L.-H. & Zhao, H. (2004). *Acta Cryst.* E**60**, m1725–m1727.

Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.

Huo, L.-H., Gao, S., Zhao, H. & Ng, S. W. (2004). *Acta Cryst.* E**60**, m1747–m1749.

Johnson, C. K. (1976). *ORTEPII*. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.

Rigaku (1998). *RAPID-AUTO*. Rigaku Corporation, Tokyo, Japan.

Rigaku/MSC (2002). *CrystalStructure*. Rigaku/MSC Inc., 9009 New Trails Drive, The Woodlands, TX 77381-5209, USA.

Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.