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Crystal structure of poly[(μ_2 -aqua-tetraaqua-(μ_3 -glutarato- $\kappa_4 O, O': O': O''$)-(μ_5 -glutarato- $\kappa_6 O: O, O': O': O'': O'''$))distrontium(II)], $C_{10}H_{22}O_{13}Sr_2$

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Abstract

$C_{10}H_{22}O_{13}Sr_2$, monoclinic, $P2_1/c$ (no. 14), $a = 13.9371(13)$ Å, $b = 14.3873(14)$ Å, $c = 9.1536(8)$ Å, $\beta = 104.958(4)^\circ$, $V = 1773.3(3)$ Å³, $Z = 4$, $R_{gt}(F) = 0.0294$, $wR_{ref}(F^2) = 0.0785$, $T = 273(2)$ K.

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Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	$0.13 \times 0.10 \times 0.06$ mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ :	6.08 mm^{-1}
Diffractometer, scan mode:	Bruker APEX-II,
$\theta_{\max}$, completeness:	27.5° , 99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	23,735, 4032, 0.069
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 3720
$N(\text{param})_{\text{refined}}$:	226
Programs:	Bruker [1], SHELX [2], WinGX/ORTEP [3], Diamond [4]

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Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material

Block colourless single crystals of the title compound were obtained by a hydrothermal reaction of an equimolar ratio (0.5 mmol) of strontium chloride and glutaric acid (2 mmol) of imidazole and 6 ml of water in a 23 ml Teflon-lined acid digestion bomb (Parr), which was heated for three days at 180°C under autogeneous pressure and then cooled down to room temperature. The product obtained were collected by filtration, thoroughly washed with distilled water and ethanol, and finally dried at room temperature.

Experimental details

The H atoms of water molecules were refined freely. All other hydrogen atoms bonded to C atoms were placed in idealized positions using the standard riding models of the SHELX System (with $C-H = 0.97$ Å) [2].

Comment

The synthesis of coordination polymers requires polyfunctional organic ligands (linkers), which bind metal atoms

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	x	y	z	<i>U</i> _{iso} */ <i>U</i> _{eq}
C1	0.51616 (17)	0.19246 (16)	0.6658 (3)	0.0159 (4)
C2	0.42909 (17)	0.19170 (18)	0.5253 (3)	0.0180 (5)
H2A	0.4198	0.2538	0.4829	0.022*
H2B	0.3692	0.1746	0.554	0.022*
C3	0.44446 (19)	0.1242 (2)	0.4047 (3)	0.0230 (5)
H3A	0.5052	0.1399	0.3773	0.028*
H3B	0.4513	0.0615	0.4452	0.028*
C4	0.35708 (18)	0.12804 (19)	0.2644 (3)	0.0202 (5)
H4A	0.2962	0.1163	0.2941	0.024*
H4B	0.3528	0.1902	0.222	0.024*
C5	0.36496 (17)	0.05896 (16)	0.1441 (3)	0.0159 (5)
C6	−0.06624 (18)	−0.12153 (17)	0.1609 (3)	0.0176 (5)
C7	−0.16274 (18)	−0.1385 (2)	0.2035 (3)	0.0243 (5)
H7A	−0.2056	−0.1761	0.1253	0.029*
H7B	−0.1956	−0.0793	0.2057	0.029*
C8	−0.1512 (2)	−0.18666 (19)	0.3554 (3)	0.0245 (5)
H8A	−0.2165	−0.1937	0.373	0.029*
H8B	−0.1248	−0.2485	0.3492	0.029*
C9	−0.0848 (2)	−0.1375 (2)	0.4901 (3)	0.0317 (7)
H9A	−0.0297	−0.1101	0.4586	0.038*
H9B	−0.0573	−0.1837	0.5665	0.038*
C10	−0.13254 (18)	−0.06194 (18)	0.5629 (3)	0.0195 (5)
O1	0.59173 (13)	0.23877 (13)	0.6605 (2)	0.0235 (4)
O2	0.50993 (14)	0.14622 (14)	0.7787 (2)	0.0277 (4)
O1W	0.05383 (13)	−0.16005 (13)	−0.1429 (2)	0.0240 (4)
H11W	0.0156	−0.1311	−0.1881	0.036*
H12W	0.0372	−0.2114	−0.1714	0.036*
O3	0.29968 (13)	−0.00266 (13)	0.1063 (2)	0.0242 (4)
O2W	0.37484 (15)	0.00523 (16)	−0.2703 (2)	0.0382 (5)
H21W	0.3267	0.0183	−0.3427	0.057*
H22W	0.4119	0.049	−0.2576	0.057*
O4	0.43685 (13)	0.06463 (13)	0.0838 (2)	0.0215 (4)
O3W	0.21968 (14)	−0.11833 (16)	−0.2416 (2)	0.0348 (5)
H31W	0.206	−0.0829	−0.2932	0.052*
H32W	0.1653	−0.1289	−0.2213	0.052*
O5	−0.06442 (14)	−0.05736 (14)	0.0690 (2)	0.0259 (4)
O4W	0.26228 (13)	−0.20336 (12)	0.0631 (2)	0.0222 (4)
H41W	0.2893	−0.2233	0.1305	0.033*
H42W	0.2454	−0.2437	0.0114	0.033*
O6	0.00898 (13)	−0.17032 (13)	0.2169 (2)	0.0250 (4)
O5W	0.23792 (14)	−0.13547 (14)	0.3716 (2)	0.0288 (4)
H51W	0.2915	−0.1455	0.3775	0.043*
H52W	0.2364	−0.0931	0.419	0.043*
O7	−0.19957 (15)	−0.01268 (15)	0.4795 (2)	0.0331 (5)
O8	−0.10218 (15)	−0.05047 (14)	0.7027 (2)	0.0282 (4)
Sr1	0.13186 (2)	−0.07267 (2)	0.10847 (2)	0.01443 (8)
Sr2	0.39088 (2)	−0.10281 (2)	−0.05032 (2)	0.01555 (8)

together to form structures of different dimensionalities. Rational design and synthesis of metal-organic coordination polymers has become one of the most active areas of chemical research and materials science [5]. The anions of polycarboxylic acids, and dicarboxylic acid in particular, are used quite often as linkers [6–10]. Over the past decades

glutaric acid which is an aliphatic dicarboxylic acid was used to obtain coordination polymers [11–13]. It is not only balancing the charge of the metal organic hybrid species, but it also plays a crucial role in deriving structural diversity.

The asymmetric unit of the title compound contains two Sr²⁺ ions, two glutarate ligands and five H₂O molecules, connected together to form a three-dimensional framework. Each Sr polyhedron shares two edges through either two O5 atoms, two O4 atoms or O3 and O4W atoms to form zig-zag chains running along the *a* axis with Sr1 ... Sr1, Sr2 ... Sr2 and Sr1 ... Sr2 distances of 4.2494(3), 4.1719(3) and 4.2475(3) Å, respectively. The connexion between adjacent chains is ensured by the organic ligands. The coordination geometry of each Sr²⁺ ion can be described as a dodecahedral fashion comprised of five O atoms from glutarate anions involved in a mono- and bidentate mode, and water molecules.

In the Sr1 bisdisphenoid, the standard mean deviation from planarity of the first face [O3, O6, O8^{II}, O4W] is 0.1147 Å (for symmetry operation (II) $-x, -y, 1-z$). Also, the distances from the central Sr1 atom to the centre of each face differ from each other [0.6547 Å against 1.8548 Å for the second plane [O5, O5^I, O1W] (for symmetry operation (I) $-x, -y, -z$)]. The Sr1–O distances fall in the range 2.4966(1) – 2.7205(1) Å (av. = 2.61 Å), in good accordance with the value calculated with the bond valence program VALENCE [14] for an eightfold-coordinated Sr²⁺ cation, i.e., 2.62 Å. Then, the sum of the bond valences around the strontium atom, i.e., 2.1 v.u. must be compared with the +2 oxidation state of Sr. In the Sr2 bisdisphenoid, the standard mean deviation from planarity of the first face [O1^{III}, O2^{IV}, O3, O3W] is 0.039 Å (for symmetry operation (III) $1-x, -1/2+y, 1/2-z$ and (IV) $1-x, -y, 1-z$). Also, the distances from the central Sr2 atom to the centre of each face differ from each other (0.7669 Å against 1.8571 Å for the second plane [O4, O4^V, O2W] [for symmetry operation (V) $1-x, -y, -z$]). The Sr–O distances fall in the range 2.5078(1) – 2.7100(1) Å (av. = 2.60 Å), in good accordance with the value calculated with the bond valence program VALENCE [14] for eightfold-coordinated Sr²⁺ cation, i.e., 2.62 Å. Then, the sum of the bond valences around the strontium atom, i.e., 2.2 v.u. must be compared with the +2 oxidation state of Sr.

There are two crystallographically distinct glutarate ligands, which exhibit two different conformations, namely anti-anti and gauche-gauche. One adopts anti-anti conformation, illustrated by the C1–C2–C3–C4 [178.205(5)°] and C2–C3–C4–C5 [176.774(5)°] torsion angles, the other adopt gauche-gauche conformation demonstrated by the C6–C7–C8–C9 [57.498 (8)°] and C7–C8–C9–C10 [84.859(7)°] torsion angles, respectively. The first carboxylate group binds five metal cations through bidentate and

monodentate chelation, the three $C_{sp^3}-C_{sp^3}-C_{sp^3}$ angles of the glutarate anion C1–C2–C3, C2–C3–C4 and C3–C4–C5 are 112.664(5), 110.804(5) and 113.460(5)°. While the second carboxylate group binds three metal cations through bidentate and monodentate chelation, the three $C_{sp^3}-C_{sp^3}-C_{sp^3}$ angles of the glutarate anion C6–C7–C8, C7–C8–C9 and C8–C9–C10 are 114.597(5), 115.425(5) and 116.646(5)°. But they are considerably greater than the tetrahedral angle 109°.

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