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Poly[[μ-aqua-tetraaquabis(μ-2-hydroxy-4-oxocyclobut-1-ene-1,3-diolato)-strontium] hemihydrate]

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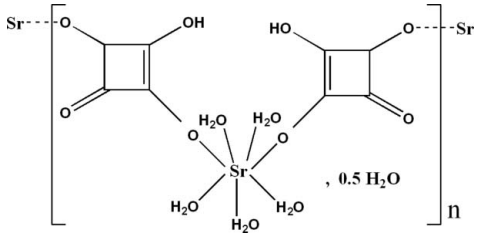
Key indicators: single-crystal X-ray study; T = 150 K; mean σ(C–C) = 0.004 Å; R factor = 0.028; wR factor = 0.068; data-to-parameter ratio = 12.6.

In the title coordination polymer, $\{[Sr(C_4HO_4)_2(H_2O)_5]\cdot 0.5H_2O\}_n$, the Sr^{2+} ion is coordinated by three monodentate hydrogensquarate (hsq) anions and six aqua ligands in a distorted SrO_9 monocapped square-antiprismatic geometry. The hsq anions and water molecules bridge the metal ions into infinite sheets lying parallel to (100). The O atom of the uncoordinated water molecule lies on a crystallographic twofold axis. The packing is stabilized by numerous O—H···O hydrogen bonds.

Related literature

For the isostructural mixed-metal Ba/Sr analogue of the title compound and background references, see: Trifa *et al.* (2011).



Experimental

Crystal data

$[Sr(C_4HO_4)_2(H_2O)_5]\cdot 0.5H_2O$
M_r = 412.81
Monoclinic, $C2/c$
a = 24.885 (3) Å
b = 8.8026 (9) Å
c = 13.8918 (17) Å
β = 119.609 (4)°
V = 2645.7 (5) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 4.15 mm^{-1}
T = 150 K
0.57 × 0.27 × 0.10 mm

Data collection

Bruker APEXII diffractometer
Absorption correction: multi-scan
SADABS (Bruker, 2006)
T_{min} = 0.365, T_{max} = 0.660
9165 measured reflections
3006 independent reflections
2243 reflections with $I > 2\sigma(I)$
R_{int} = 0.037

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.068
S = 1.03
3006 reflections
239 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.51 e Å^{-3}

Table 1
Selected bond lengths (Å).

Sr1—O1	2.691 (2)	Sr1—O6	2.6179 (18)
Sr1—O2	2.642 (2)	Sr1—O12	2.6646 (16)
Sr1—O3	2.690 (2)	Sr1—O14^{i}	2.5906 (16)
Sr1—O4	2.641 (3)	Sr1—O3^{ii}	2.7154 (19)
Sr1—O5	2.572 (2)		

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···O9^{iii}	0.76 (4)	2.27 (4)	2.983 (3)	158 (4)
O1—H1B···O7^{iv}	0.79 (4)	1.99 (4)	2.715 (2)	153 (4)
O1W—H1W···O13^{ii}	0.76 (2)	2.39 (2)	2.801 (2)	115 (2)
O1W—H1W···O8^{v}	0.76 (2)	2.51 (3)	3.118 (2)	138 (3)
O2—H2A···O14^{vi}	0.92 (4)	1.91 (4)	2.794 (3)	161 (4)
O2—H2B···O1W^{vii}	0.70 (4)	2.52 (4)	3.165 (3)	154 (4)
O3—H3A···O13^{ii}	0.93 (4)	1.79 (4)	2.712 (3)	174 (3)
O3—H3B···O4^{viii}	0.76 (4)	2.59 (4)	3.172 (3)	136 (3)
O4—H4A···O7^{ix}	0.78 (4)	2.01 (4)	2.785 (3)	177 (4)
O4—H4B···O1W	0.87 (4)	2.03 (4)	2.871 (3)	163 (3)
O5—H5A···O1^{x}	0.72 (4)	2.09 (4)	2.787 (3)	166 (4)
O5—H5B···O8^{xi}	0.90 (4)	1.82 (4)	2.716 (3)	175 (4)
O9—H9···O12	0.82	1.74	2.548 (3)	169
O11—H11···O6^{vii}	0.82	1.77	2.580 (2)	172

Symmetry codes: (ii) $-x+2, -y+2, -z+1$; (iii) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$; (iv) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$; (v) $x+\frac{1}{2}, -y+\frac{5}{2}, z+\frac{1}{2}$; (vi) $-x+2, -y+1, -z+1$; (vii) $x, y-1, z$; (viii) $-x+2, y, -z+\frac{1}{2}$; (ix) $-x+\frac{3}{2}, -y+\frac{5}{2}, -z$; (x) $x, -y+2, z-\frac{1}{2}$; (xi) $-x+\frac{3}{2}, -y+\frac{3}{2}, -z$.

Data collection: *APEX2* (Bruker, 2006); cell refinement: *SAINT* (Bruker, 2006); data reduction: *SAINT*; program(s) used to solve structure: *SIR2002* (Burla *et al.*, 2003); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg & Berndt, 2001); software used to prepare material for publication: *WinGX* publication routines (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5939).

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