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Polymeric triaquabis(μ_3-3-carboxybenzenesulfonato)barium(II)

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.003 Å
R factor = 0.017
wR factor = 0.046
Data-to-parameter ratio = 14.5

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

The Ba atom in the title polymeric compound, poly[[triaquabarium(II)]-di-μ_3-3-carboxybenzenesulfonato] [$Ba(C_7H_5O_5S)_2(H_2O)_3]_n$, exists in a nine-coordinate tricapped trigonal prismatic geometry; the dianionic units engage in μ_3-bridging, giving a three-dimensional network. The crystal packing network is dominated by hydrogen bonds.

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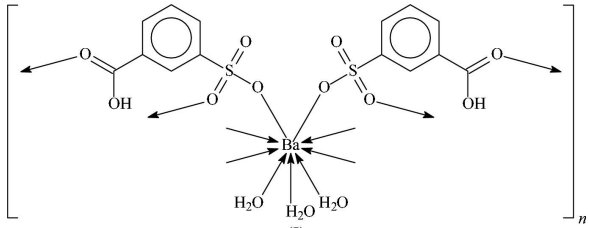
Comment

In the crystal structure of the compound having the empirical formulation $(C_7H_5O_6S)_2(H_2O)_5Ba$, a pair of 3-carboxybenzenesulfonate monoanionic ligands bind through their negatively charged sulfonate groups and the carbonyl O atoms of carboxyl groups to two Ba atoms; the two anions are engaged with adjacent dinuclear entities to form a ladder motif, the μ_3-bridging 3-carboxybenzenesulfonate anions serving as the rungs of the ladder (Ma *et al.*, 2003). That the hydroxyl substituents do not appear to serve any function led to the present study on the barium derivative of 3-carboxybenzenesulfonic acid. The title compound, (I), also has the dianionic units engaged in a similar type of μ_3-bridging (Fig. 1);



(I)

however, the compound instead adopts a three-dimensional network structure although its Ba atom is also nine-coordinate

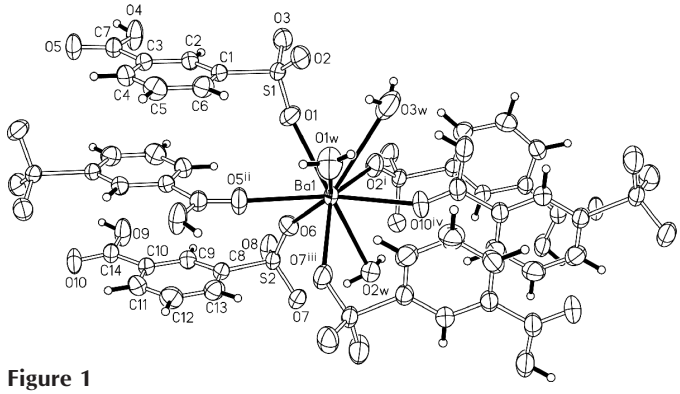


Figure 1
ORTEPII plot (Johnson, 1976) of a fragment of polymeric (I). Displacement ellipsoids are drawn at the 70% probability level and H atoms are drawn as spheres of arbitrary radii. [Symmetry codes: (i) $\frac{3}{2}-x, y-\frac{1}{2}, \frac{3}{2}-z$; (ii) $1-x, 1-y, 1-z$; (iii) $\frac{1}{2}-x, \frac{1}{2}+y, \frac{3}{2}-z$; (iv) $\frac{1}{2}+x, \frac{1}{2}-y, \frac{1}{2}+z$].

(Fig. 2). The crystal packing network is dominated by hydrogen bonds (Table 2).

Experimental

Barium chloride dihydrate (1.22 g, 5 mmol) was added to an aqueous solution of 3-carboxybenzenesulfonic acid (1.01 g, 5 mmol). The mixture was stirred to dissolve the reactants. Colourless crystals were deposited from the filtered solution after several days. Analysis calculated for $C_{14}H_{16}BaO_{13}S_2$: C 28.32, H 2.72%; found: C 28.34, H 2.71%.

Crystal data

$[Ba(C_7H_5O_5S)_2(H_2O)_3]$	D_x = 2.053 Mg m^{-3}
M_r = 593.73	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 17416 reflections
a = 10.259 (2) Å	θ = 3.0–27.5°
b = 8.775 (2) Å	μ = 2.35 mm^{-1}
c = 21.813 (4) Å	T = 295 (2) K
β = 101.93 (3)°	Block, colourless
V = 1921.2 (7) Å^3	0.34 × 0.26 × 0.19 mm
Z = 4	

Data collection

Rigaki R-AXIS RAPID IP diffractometer	4402 independent reflections
ω scans	4132 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)	R_{int} = 0.017
T_{min} = 0.392, T_{max} = 0.636	θ_{max} = 27.5°
18503 measured reflections	$h = -13 \rightarrow 13$
	$k = -11 \rightarrow 11$
	$l = -28 \rightarrow 28$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0311P)^2 + 0.7392P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.017	$(\Delta/\sigma)_{max}$ = 0.001
$wR(F^2)$ = 0.046	$\Delta\rho_{max}$ = 0.52 e Å^{-3}
S = 1.01	$\Delta\rho_{min}$ = −0.30 e Å^{-3}
4402 reflections	
303 parameters	
H atoms treated by a mixture of independent and constrained refinement	

Table 1
Selected geometric parameters (Å, °).

Ba1—O1	2.754 (2)	Ba1—O10^{iv}	2.718 (2)
Ba1—O2^{i}	2.777 (1)	Ba1—O1*w*	2.739 (2)
Ba1—O5^{ii}	2.799 (2)	Ba1—O2*w*	2.969 (2)
Ba1—O6	2.765 (2)	Ba1—O3*w*	3.276 (2)
Ba1—O7^{iii}	2.834 (1)		
O1—Ba1—O10^{iv}	123.24 (5)	O5^{ii}—Ba1—O1*w*	78.13 (4)
O1—Ba1—O2^{i}	77.96 (4)	O5^{ii}—Ba1—O2*w*	117.50 (4)
O1—Ba1—O5^{ii}	69.23 (5)	O5^{ii}—Ba1—O3*w*	118.83 (5)
O1—Ba1—O6	87.20 (4)	O6—Ba1—O7^{iii}	97.81 (5)
O1—Ba1—O7^{iii}	140.91 (4)	O6—Ba1—O10^{iv}	124.72 (4)
O1—Ba1—O1*w*	81.14 (4)	O6—Ba1—O1*w*	150.39 (4)
O1—Ba1—O2*w*	143.70 (4)	O6—Ba1—O2*w*	64.13 (4)
O1—Ba1—O3*w*	63.72 (4)	O6—Ba1—O3*w*	137.69 (5)
O2^{i}—Ba1—O5^{ii}	132.67 (4)	O7^{iii}—Ba1—O10^{iv}	85.26 (5)
O2^{i}—Ba1—O6	72.97 (5)	O7^{iii}—Ba1—O1*w*	75.59 (5)
O2^{i}—Ba1—O7^{iii}	140.60 (4)	O7^{iii}—Ba1—O2*w*	68.90 (4)
O2^{i}—Ba1—O10^{iv}	70.91 (5)	O7^{iii}—Ba1—O3*w*	124.28 (5)
O2^{i}—Ba1—O1*w*	129.84 (5)	O10^{iv}—Ba1—O1*w*	84.00 (5)
O2^{i}—Ba1—O2*w*	72.80 (4)	O10^{iv}—Ba1—O2*w*	66.02 (4)
O2^{i}—Ba1—O3*w*	71.40 (5)	O10^{iv}—Ba1—O3*w*	61.85 (5)
O5^{ii}—Ba1—O6	72.29 (4)	O1*w*—Ba1—O2*w*	134.56 (4)
O5^{ii}—Ba1—O7^{iii}	75.47 (5)	O1*w*—Ba1—O3*w*	58.46 (5)
O5^{ii}—Ba1—O10^{iv}	156.37 (4)	O2*w*—Ba1—O3*w*	123.63 (4)

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

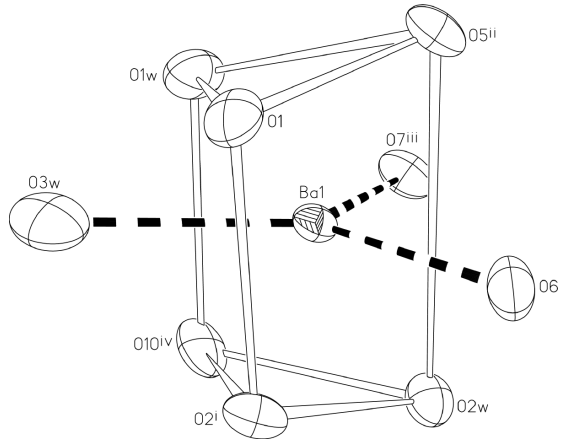


Figure 2
ORTEPII plot (Johnson, 1976) of the tricapped trigonal prismatic coordination geometry of the Ba atom in (I).

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

D—H···A	D—H	H···A	D···A	D—H···A
O4—H4*o*···O2*w*^{v}	0.84 (1)	1.88 (1)	2.697 (2)	163 (3)
O9—H9*o*···O3*w*^{vi}	0.85 (1)	1.78 (1)	2.611 (2)	165 (3)
O1*w*—H1*w*1···O3^{vii}	0.84 (1)	2.08 (1)	2.907 (2)	168 (2)
O1*w*—H1*w*2···O8^{viii}	0.85 (1)	1.95 (1)	2.793 (2)	176 (2)
O2*w*—H2*w*1···O3^{i}	0.86 (1)	2.00 (1)	2.849 (2)	170 (3)
O2*w*—H2*w*2···O7	0.85 (1)	2.03 (1)	2.845 (2)	161 (3)
O3*w*—H3*w*1···O2	0.84 (1)	2.36 (3)	2.949 (2)	127 (3)
O3*w*—H3*w*2···O6^{vii}	0.85 (1)	2.28 (2)	3.036 (2)	148 (3)

Symmetry codes: (i) $\frac{3}{2}-x, y-\frac{1}{2}, \frac{3}{2}-z$; (v) $\frac{1}{2}+x, \frac{1}{2}-y, z-\frac{1}{2}$; (vi) $x-\frac{1}{2}, \frac{1}{2}-y, z-\frac{1}{2}$; (vii) $\frac{3}{2}-x, \frac{1}{2}+y, \frac{3}{2}-z$; (viii) $x, 1+y, z$.

The carboxyl and water H atoms were located in difference Fourier maps, and were refined with distance restraints of O—H = 0.85 (1) Å and H···H = 1.39 (1) Å. The carbon-bound H atoms were positioned geometrically (C—H = 0.93 Å) and were included in the refinement [U_{iso}(H) = 1.2U_{eq}(C)] in the riding-model approximation.

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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