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Heptaaquabis(4-formylbenzoato-κO)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 = 0.018
wR factor = 0.043
Data-to-parameter ratio = 15.5

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

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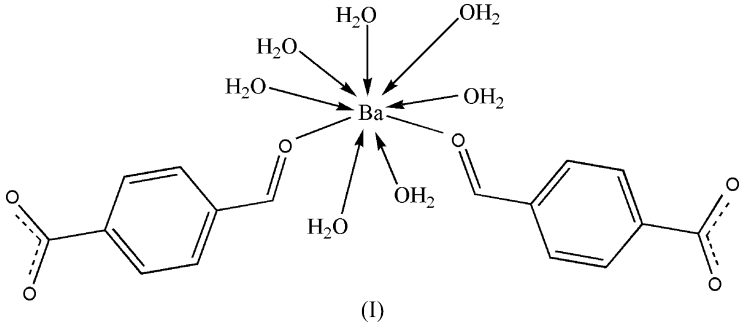
The Ba atom in the title complex, $[Ba(C_8H_5O_3)_2(H_2O)_7]$, is nine-coordinated by two formyl O atoms and seven water molecules. A mirror plane bisects the molecule, with the Ba and three water O atoms lying on the plane. O—H···O hydrogen bonds link molecules into a three-dimensional network.

Comment

4-Formylbenzoic acid, which crystallizes in two forms (Haisa *et al.*, 1976), has been used in the synthesis of metal carboxylates, but only transition metal complexes have been characterized crystallographically (Deng *et al.*, 2006*a*,*b*,*c*,*d*). In this contribution, we describe the characterization of a new alkali earth metal complex, (I), obtained from the reaction of 4-formylbenzoic acid and barium carbonate in an aqueous solution.



(I)

The Ba atom in (I) (Fig. 1) is nine-coordinated by two formyl O atoms and seven water molecules, as highlighted in Fig. 2. The molecule is disposed about a mirror plane, with atoms Ba, O1*w* and O3*w* and the O4*w* water molecule lying on the plane. The carboxylate C—O bond lengths (Table 1) suggest delocalization of π-electron density over the CO_2

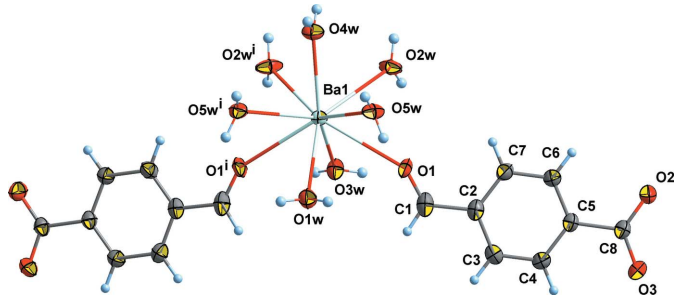


Figure 1
The molecular structure of (I), showing the atom-labeling scheme and displacement ellipsoids drawn at the 30% probability level. [Symmetry code: (i) $x, \frac{3}{2} - y, z$.]

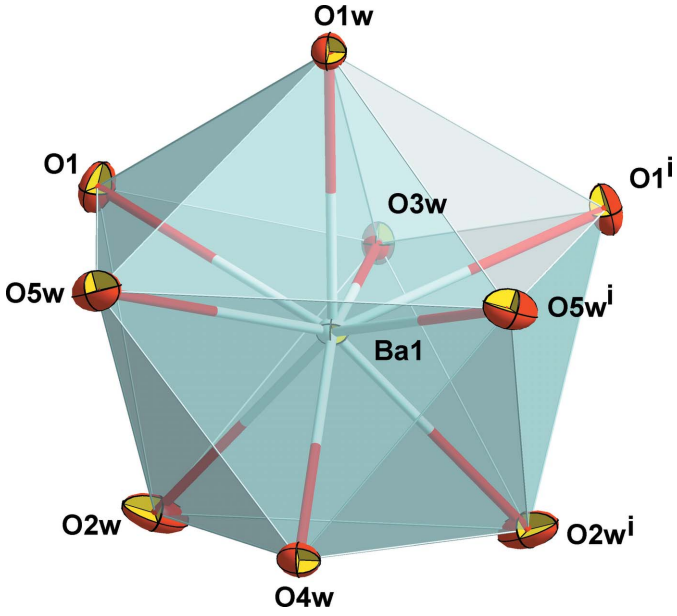


Figure 2
The coordination polyhedron of the Ba atom in (I). [Symmetry code: (i) x, $\frac{3}{2} - y$+, z.]

atoms. The water molecules and the O atoms of uncoordinated carboxylate groups form extensive intermolecular hydrogen bonds (Table 2) which connect the molecules into a three-dimensional supramolecular network. In addition, there are π–π stacking interactions between adjacent aromatic rings of the 4-formylbenzoate ligands, which strengthen the stability of the whole crystal structure; the centroid–centroid distance is 3.709 (3) Å.

Experimental

Barium carbonate (0.099 g, 0.5 mmol) and 4-formylbenzoic acid (0.15 g, 1 mmol) were dissolved in hot water (35 ml). The mixture was stirred for 30 min and then filtered. The final pH value of the mixture was about 5. The solution was allowed to evaporate at room temperature and colorless prismatic crystals of (I) separated after several days. Analysis calculated for $C_{16}H_{24}BaO_{13}$: C 34.21, H 4.31%; found: C 34.19, H 4.34%.

Crystal data

$[Ba(C_8H_5O_3)_2(H_2O)_7]$
M_r = 561.69
Monoclinic, $P2_1/m$
a = 6.4213 (13) Å
b = 23.000 (5) Å
c = 7.4070 (15) Å
β = 96.11 (3)°
V = 1087.7 (4) Å^3
Z = 2
D_x = 1.715 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 1.89 mm^{-1}
T = 295 (2) K
Prism, colorless
0.38 × 0.26 × 0.18 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.557, T_{max} = 0.716
10743 measured reflections
2552 independent reflections
2419 reflections with $I > 2\sigma(I)$
R_{int} = 0.020
θ_{max} = 27.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.018
$wR(F^2)$ = 0.043
S = 1.05
2552 reflections
165 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0229P)^2 + 0.5003P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0028 (5)

Table 1
Selected bond lengths (Å).

Ba1—O1	2.8849 (15)	Ba1—O5*W*	2.8191 (16)
Ba1—O1*W*	2.850 (2)	O1—C1	1.201 (3)
Ba1—O2*W*	2.7804 (17)	O2—C8	1.259 (2)
Ba1—O3*W*	2.844 (2)	O3—C8	1.253 (2)
Ba1—O4*W*	2.664 (2)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O1*W*—H1*W*1···O3^{i}	0.848 (7)	1.984 (5)	2.8192 (17)	168.0 (12)
O2*W*—H2*W*1···O3^{ii}	0.846 (10)	1.996 (12)	2.834 (2)	171 (3)
O2*W*—H2*W*2···O2^{iii}	0.846 (10)	2.048 (11)	2.888 (2)	172 (3)
O3*W*—H3*W*1···O2^{ii}	0.849 (7)	1.916 (8)	2.7631 (18)	175 (2)
O4*W*—H4*W*1···O1*W*^{iv}	0.845 (10)	1.927 (14)	2.755 (3)	166 (3)
O4*W*—H4*W*2···O3*W*^{iv}	0.849 (10)	1.935 (11)	2.783 (3)	176 (3)
O5*W*—H5*W*1···O3^{i}	0.846 (10)	2.085 (15)	2.890 (2)	159 (3)
O5*W*—H5*W*2···O2^{v}	0.841 (10)	2.094 (14)	2.913 (2)	164 (3)

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

Carbon-bound H atoms were included in the riding-model approximation, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C). The H atoms of the water molecules were refined with O—H and H···H distance restraints of 0.85 (1) and 1.39 (1) Å, respectively, and with U_{iso}(H) = 1.5U_{eq}(O).

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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