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Key indicators

Single-crystal X-ray study
 $T = 296$ K
Mean $\sigma(\text{C}-\text{C}) = 0.005$ Å
 R factor = 0.024
 wR factor = 0.061
Data-to-parameter ratio = 14.5For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.*catena*-Poly[[diaquabarium(II)]-di- μ -2-formylbenzoato]

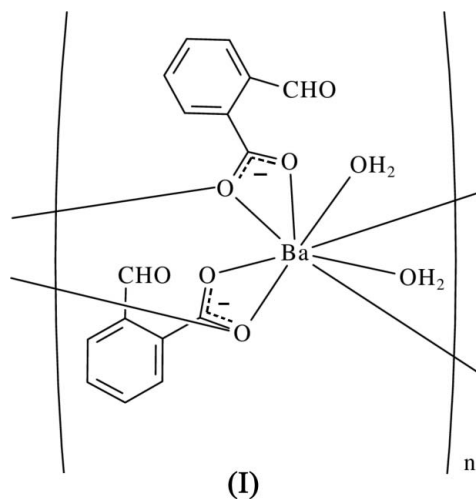
In the title compound, $[\text{Ba}(\text{C}_8\text{H}_5\text{O}_3)_2(\text{H}_2\text{O})_2]_n$, the Ba^{II} atom (site symmetry 2) is eight-coordinated by two bidentate 2-formylbenzoate ligands, two monodentate formylbenzoate ligands and two terminal water molecules. The bridging ligands result in a one-dimensional coordination polymer. A network of $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds links the polymeric chains.

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Comment

The title compound, (I), is a new coordination polymer containing barium cations, 2-formylbenzoate anions and water molecules. The coordination environment around the central barium ion is shown in Fig. 1. The Ba atom lies on a twofold rotation axis and is eight-coordinated by two bidentate carboxylate groups, two monodentate carboxylate O atoms and two water molecules (Table 1). The formyl group O atom does not coordinate to barium. The bond angles around the Ba atom are in the range $45.59(6)$ – $165.77(7)^\circ$. The crystal-packing diagram of this complex reveals a one-dimensional coordination polymer, propagating along $[001]$, as shown in Fig. 2. The carboxylate O1 atom bridges two adjacent Ba atoms, with a Ba–O1–Ba angle of $105.55(7)^\circ$. The Ba \cdots Ba separation in the chain of $4.4336(3)$ Å is comparable to values reported for barium–2,2'-dithiodibenzoate (Murugavel *et al.*, 2001), barium-2-aminobenzoate (Murugavel *et al.*, 2000) and *catena*-poly[tetraaquabis(thiosalicylate)barium(II)] (Lee *et al.*, 2003).



The coordinated water molecule makes two interchain $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds (Table 2). One of the acceptor O atoms is part of the formyl group, the other is part of a carboxylate group.

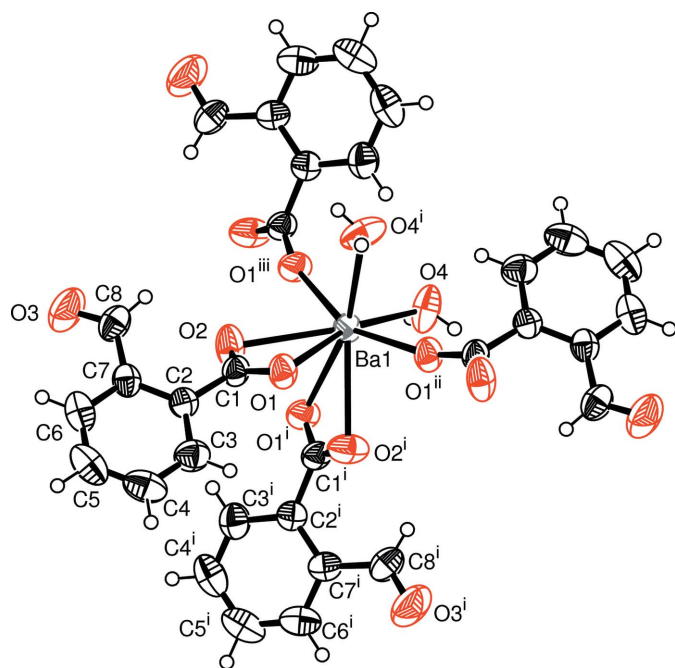


Figure 1
Fragment of (I), showing the environment of the Ba cation (50% displacement ellipsoids; arbitrary spheres for the H atoms). [Symmetry codes: (i) $1 - x, y, \frac{3}{2} - z$; (ii) $x, 1 - y, \frac{1}{2} + z$; (iii) $1 - x, 1 - y, 1 - z$.]

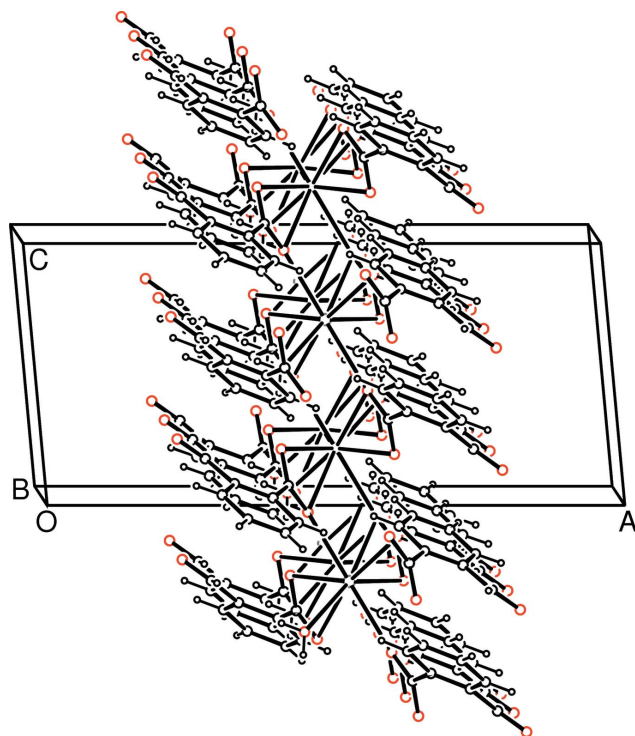


Figure 2
The extended polymeric chains in (I), propagating along [001].

Experimental

BaCO₃ (0.985 g, 5 mmol) was added slowly to an ethanol–water (1:1 v/v) solution (10 ml) of 2-formylbenzoic acid (1.50 g, 10 mmol) with continuous stirring. The reaction mixture was heated in a water bath

for 0.5 h. Colorless crystals of (I) suitable for X-ray analysis were obtained after a week at room temperature (yield 80%; decomposition point > 523 K).

Crystal data

[Ba(C₈H₅O₃)₂(H₂O)₂]
M_r = 471.61
 Monoclinic, *C2/c*
a = 18.4346 (12) Å
b = 11.6009 (7) Å
c = 8.3914 (5) Å
 β = 95.364 (5)°
V = 1786.71 (19) Å³
Z = 4

D_x = 1.753 Mg m⁻³
 Mo *K*α radiation
 Cell parameters from 12690 reflections
 θ = 2.1–28.0°
 μ = 2.26 mm⁻¹
T = 296 (2) K
 Prism, colorless
 0.32 × 0.25 × 0.19 mm

Data collection

Stoe IPDS-2 diffractometer
 ω scans
 Absorption correction: integration
 (*X-RED32*; Stoe & Cie, 2002)
T_{min} = 0.548, *T_{max}* = 0.704
 12690 measured reflections
 1768 independent reflections

1703 reflections with $I > 2\sigma(I)$
R_{int} = 0.086
 θ_{\max} = 26.0°
h = -22 → 22
k = -14 → 14
l = -10 → 10

Refinement

Refinement on *F*²
 $R[F^2 > 2\sigma(F^2)] = 0.024$
 $wR(F^2) = 0.061$
S = 1.03
 1768 reflections
 122 parameters
 H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0326P)^2 + 2.7955P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.85 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.72 \text{ e \AA}^{-3}$

Table 1

Selected bond lengths (Å).

| | | | |
|---------------------|-------------|--------|-----------|
| Ba1–O1 ⁱ | 2.6599 (19) | Ba1–O2 | 2.757 (2) |
| Ba1–O4 | 2.714 (3) | Ba1–O1 | 2.905 (2) |

Symmetry code: (i) $-x + 1, -y + 1, -z + 1$.

Table 2

Hydrogen-bond geometry (Å, °).

| <i>D</i> –H··· <i>A</i> | <i>D</i> –H | H··· <i>A</i> | <i>D</i> ··· <i>A</i> | <i>D</i> –H··· <i>A</i> |
|----------------------------|-------------|---------------|-----------------------|-------------------------|
| O4–H4A···O3 ⁱⁱⁱ | 0.791 (17) | 1.963 (18) | 2.754 (3) | 178 (4) |
| O4–H4B···O2 ⁱⁱⁱ | 0.810 (18) | 1.971 (18) | 2.779 (4) | 175 (3) |

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

All H atoms except those bonded to water O atoms were placed in calculated positions and refined as riding, with C–H = 0.93 Å and *U_{iso}*(H) = 1.2*U_{eq}*(carrier). The H atoms of the aqua ligands were located in a difference map and refined with distance restraints of O–H = 0.82 (2) Å and H···H = 1.30 (2) Å.

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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