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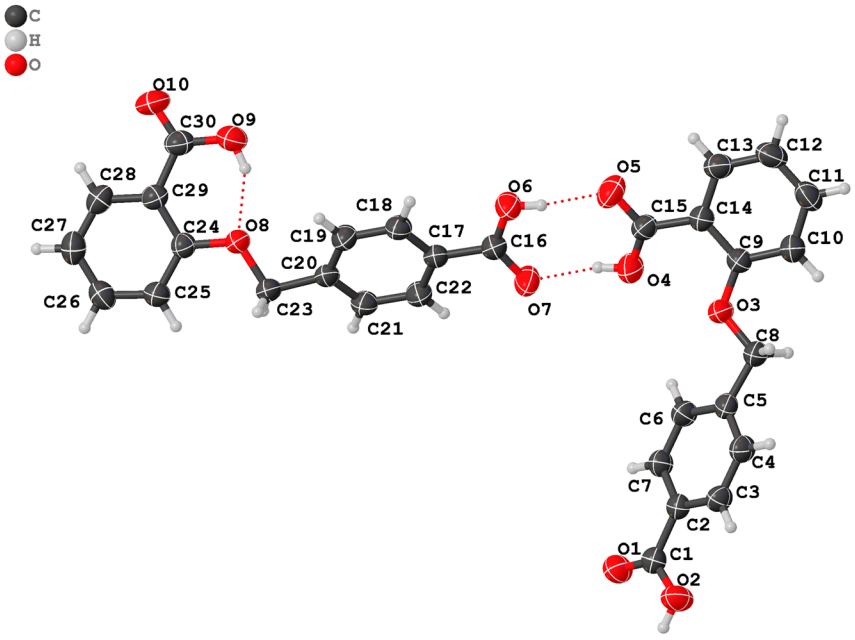
The crystal structure of 2-(2′-carboxybenzyl) benzoic acid, $C_{15}H_{12}O_5$



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Abstract

$C_{15}H_{12}O_5$, monoclinic, $P2_1/c$ (no. 14), a = 16.1399(4) Å, b = 19.2950(5) Å, c = 8.2567(2) Å, β = 97.078(1)°, V = 2551.70(11) Å^3, Z = 8, $R_{gt}(F)$ = 0.0440, $wR_{ref}(F^2)$ = 0.1326, T = 299.15 K.

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A part of the molecular structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Table 1: Data collection and handling.

Crystal:	Colourless needle
Size:	0.20 × 0.18 × 0.15 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ:	0.11 mm^{-1}
Diffractometer, scan mode:	XtaLAB AFC12 (RINC),
θ_{max}, completeness:	28.3°, >99 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	62952, 6299, 0.077
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 4393
$N(param)_{refined}$:	373
Programs:	Bruker,[1] Olex2,[2] SHELX,[3] Diamond[4]

1 Source of materials

0.2722 g 2-(2′–Carboxybenzyl)benzoic acid (1.0 mmol), 0.080 g NaOH (2.0 mmol), and 0.3110 g calcium perchlorate tetrahydrate (1.0 mmol) solids were dissolved into the 16 ml ethanol-water solution (v:v = 1:1) with stirring. The above mixture was stirred at 75 °C for 6 h and cooled to room temperature. It was then filtered and the filtrate was left still for 30 days. The clear light colourless crystals were received.

2 Experimental details

The hydrogen atoms were positioned geometrically (C–H = 0.93–0.97 Å, O–H = 0.82 Å). Their U_{iso} values were set to 1.2 U_{eq} or 1.5 U_{eq} of the parent atoms.

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

Atom	x	y	z	U_{iso}*/U_{eq}
O1	0.13444 (7)	0.03007 (6)	0.24866 (16)	0.0640 (3)
O2	0.21994 (7)	−0.05553 (6)	0.33994 (17)	0.0675 (3)
H2	0.176708	−0.072383	0.365318	0.101*
O3	0.48132 (7)	0.19619 (5)	−0.00492 (16)	0.0606 (3)
O4	0.40405 (7)	0.31753 (6)	−0.00362 (19)	0.0715 (4)
H4	0.371890	0.345503	0.029831	0.107*
O5	0.49253 (8)	0.40326 (6)	0.06636 (17)	0.0688 (3)
C1	0.20332 (9)	0.00508 (8)	0.26788 (18)	0.0475 (3)
C2	0.27806 (9)	0.03739 (7)	0.21094 (17)	0.0435 (3)
C3	0.35631 (9)	0.00677 (8)	0.23988 (19)	0.0494 (3)
H3	0.363442	−0.033834	0.300678	0.059*
C4	0.42334 (9)	0.03664 (7)	0.1784 (2)	0.0505 (4)
H4A	0.475625	0.015944	0.198869	0.061*
C5	0.41451 (9)	0.09669 (7)	0.08703 (18)	0.0447 (3)
C6	0.33671 (9)	0.12837 (8)	0.06145 (19)	0.0506 (4)
H6A	0.330121	0.169647	0.003114	0.061*
C7	0.26915 (9)	0.09869 (8)	0.12245 (19)	0.0489 (3)
H7	0.217140	0.119982	0.104094	0.059*
C8	0.48834 (10)	0.12376 (8)	0.0135 (2)	0.0511 (4)
H8A	0.5412 (12)	0.1122 (10)	0.086 (2)	0.072 (5)*
H8B	0.4913 (12)	0.1022 (10)	−0.099 (2)	0.075 (5)*
C9	0.54668 (9)	0.23079 (7)	−0.05642 (18)	0.0457 (3)
C10	0.61349 (10)	0.19746 (8)	−0.11460 (19)	0.0530 (4)
H10	0.613420	0.149445	−0.124354	0.064*
C11	0.67974 (10)	0.23527 (9)	−0.1578 (2)	0.0590 (4)
H11	0.723740	0.212634	−0.198263	0.071*
C12	0.68138 (10)	0.30619 (9)	−0.1417 (2)	0.0633 (4)
H12	0.727019	0.331355	−0.168003	0.076*
C13	0.61487 (10)	0.33976 (8)	−0.0863 (2)	0.0553 (4)
H13	0.616050	0.387751	−0.075967	0.066*
C14	0.54609 (9)	0.30325 (7)	−0.04565 (17)	0.0450 (3)
C15	0.47616 (9)	0.34273 (7)	0.01016 (19)	0.0477 (3)
O6	0.37366 (7)	0.47515 (6)	0.17952 (16)	0.0602 (3)
H6	0.404622	0.449041	0.136667	0.090*
O7	0.28228 (7)	0.39205 (6)	0.09876 (16)	0.0668 (3)
O8	0.05612 (6)	0.66799 (5)	0.45496 (14)	0.0519 (3)
O9	0.13388 (8)	0.77558 (6)	0.36813 (17)	0.0695 (4)
H9	0.123099	0.734608	0.381641	0.104*
O10	0.08518 (9)	0.87704 (6)	0.42411 (19)	0.0811 (4)
C16	0.30109 (9)	0.44970 (8)	0.16670 (18)	0.0471 (3)
C17	0.23496 (9)	0.48914 (7)	0.23577 (17)	0.0427 (3)
C18	0.25562 (9)	0.54383 (7)	0.34110 (19)	0.0474 (3)
H18	0.311155	0.557011	0.365936	0.057*
C19	0.19402 (9)	0.57895 (8)	0.40954 (19)	0.0491 (3)
H19	0.208411	0.615310	0.481460	0.059*
C20	0.11092 (9)	0.56045 (7)	0.37193 (18)	0.0439 (3)
C21	0.09008 (9)	0.50709 (8)	0.2630 (2)	0.0507 (4)
H21	0.034324	0.495416	0.233880	0.061*
C22	0.15208 (9)	0.47093 (8)	0.1970 (2)	0.0509 (4)
H22	0.137828	0.434179	0.126107	0.061*
C23	0.04364 (9)	0.59434 (7)	0.4545 (2)	0.0496 (4)
H23A	−0.010727	0.583105	0.396816	0.059*
H23B	0.045760	0.577504	0.565664	0.059*
C24	−0.00196 (8)	0.70938 (7)	0.51506 (17)	0.0425 (3)
C25	−0.06977 (9)	0.68312 (8)	0.58304 (19)	0.0499 (3)
H25	−0.076993	0.635472	0.590875	0.060*
C26	−0.12652 (10)	0.72791 (9)	0.6390 (2)	0.0562 (4)
H26	−0.172226	0.710154	0.683734	0.067*
C27	−0.11623 (11)	0.79877 (9)	0.6295 (2)	0.0598 (4)
H27	−0.155055	0.828708	0.666215	0.072*
C28	−0.04808 (10)	0.82451 (8)	0.56523 (19)	0.0534 (4)
H28	−0.040503	0.872235	0.561449	0.064*
C29	0.00982 (9)	0.78126 (7)	0.50573 (17)	0.0444 (3)
C30	0.07875 (10)	0.81482 (8)	0.4315 (2)	0.0532 (4)

3 Comment

Carboxylate compounds and their metal complexes have exhibited novel structure[5,6] and excellent performance in many ways such as vitro antitumor activity,[7,8] electrochemical property,[9] antileishmanial, DNA binding, antioxidant, cytotoxicity, antifungal and antibacterial property,[10] and catalysis.[11] Our research group has also synthesized some carboxylic acid metal complexes, which also showed excellent properties in antitumor, catalysis, fluorescence and other aspects.[12–15] To further investigate the structure and properties of carboxylate metal complexes, in this work, we prepared to synthesize a calcium complex using 2-(2′-carboxybenzyl)benzoic acid, NaOH and calcium perchlorate tetrahydrate. Unfortunately, calcium ions do not take part in coordination, only obtaining the single crystal of 2-(2′-carboxybenzyl)benzoic acid. The molecular structure of the title compound is shown in Figure. The title compound crystallizes in a monoclinic with space group $P12_1/c1$ (no. 14). The molecules are linked together by pairs of intermolecular hydrogen bonds (O6–H6···O5 and O4–H4···O7) to form the dimers. In the title compound, the bond lengths of C1–O1 and C30–O10 are 1.2043(18) and 1.2071(19) Å, respectively, which are in agreement with the value of C=O (1.233 Å). However, the bond lengths of C15–O4, C15–O5, C16–O6 and C16–O7 are 1.2534(18), 1.2723(18), 1.2624(17) and 1.2659(18) Å, respectively, which may be due to the double hydrogen bonds in the dimer. The dihedral angles of ring 1 (C2–C3–C4–C5–C6–C7–C2) and ring 2 (C9–C10–C11–C12–C13–C14–C9), ring 3 (C17–C18–C19–C20–C21–C22–C17) and ring 4 (C24–C25–C26–C27–C28–C29–C24) are 38.43 and 46.01°, showing that two 2-(2′-carboxybenzyl)benzoic acid molecules in dimer are not coplanar. The dimers form a one-dimensional zigzag chain-like structure through single O–H···O hydrogen bond.

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Conflict of interest: The authors declare no conflicts of interest regarding this article.

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