Acta Cryst E
CRYSTALLOGRAPHIC COMMUNICATIONS

ISSN 2056-9890

Crystal structure of *catena*-poly[calcium-di-μ_3-benzoato-κ^6O,O':O-μ_2-(dimethyl sulfoxide)-κ^2O:O]

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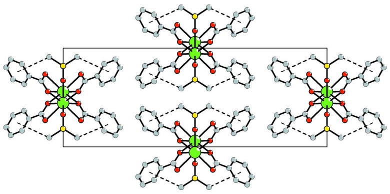
Received 8 May 2015
Accepted 29 June 2015

Edited by G. Smith, Queensland University of Technology, Australia

Keywords: crystal structure; calcium benzoate; coordination polymer; C—H$\cdots\pi$ interactions

CCDC reference: 1409468
Supporting information: this article has supporting information at journals.iucr.org/e



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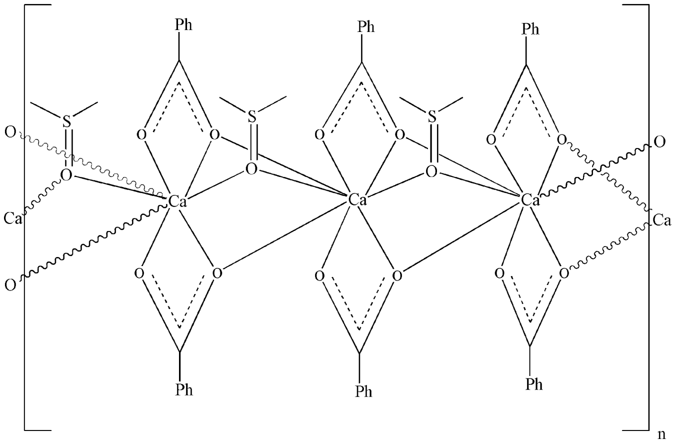
In the title complex, $[Ca(C_7H_5O_2)_2(C_2H_6OS)]_n$, the Ca^{2+} ion (site symmetry *m*..) is surrounded by eight O atoms, six from two bridging–chelating tridentate benzoate carboxyl groups and two from a bridging dimethyl sulfoxide molecule (point group symmetry *m*..), giving an irregular coordination geometry [Ca—O bond length range = 2.345 (2)–2.524 (2) Å]. One-dimensional coordination complex chains extending parallel to *c* are generated in which the triply μ_2-O-bridged Ca^{2+} cations are separated by 3.6401 (5) Å. In the crystal, weak intrachain C—H$\cdots\pi$ hydrogen bonds are present between the methyl H atoms of the dimethyl sulfoxide molecules as donors and the aromatic rings as acceptors [C—H$\cdots$*Cg* = 3.790 (4) Å].

1. Chemical context

Compounds of benzoic acid with calcium are of special interest due to their wide-ranging applications, for example as a preservative in the food industry, in cosmetics and in medicine. In spite of that, the crystal structures of such compounds have been poorly investigated. Searches of the Cambridge Structural Database (CSD; Version 5.35, November 2013 + 2 updates; Groom & Allen, 2014) for simple calcium benzoate complexes revealed only three results: $[Ca(benz)_2(dmf)(H_2O)]_n$ (Yano *et al.*, 2001), $\{[Ca(benz)(H_2O)_3]^+ (benz)^-\}_n$ (Senkovska & Thewalt, 2005) and $[Ca(benz)_2(Hbenz)(H_2O)]_n$ (Azizov *et al.*, 2011) (where benz = benzoate).



Here we report the synthesis of a new calcium benzoate–dimethyl sulfoxide complex, $[Ca(benz)_2(dmso)]_n$, which was obtained as a by-product of an attempted synthesis of an Mn/

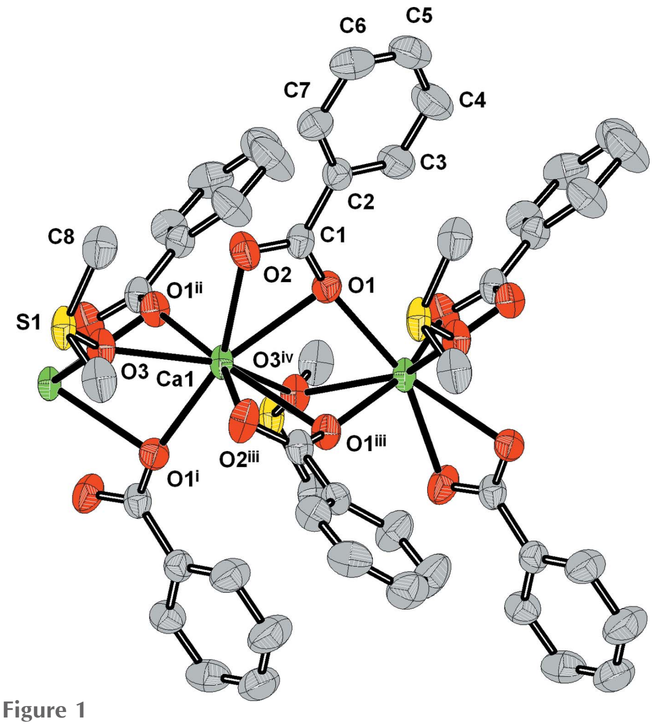


Figure 1
A fragment of the $[Ca(benz)_2(dmso)]_n$ chain with the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms have been omitted for clarity. For symmetry codes, see Table 1.

Cu heterometallic complex (in crystalline form available for X-ray analysis) from the system: Mn–Cu–(bhz–sal)–CaO–KSCN–dmso (in open air), where manganese and copper were used as unactivated metal powders, bhz = benzohydrazide and sal = salicylaldehyde. The investigation of the system was carried out as a part of systematic research on the elaboration the 'direct synthesis' approach to both homo- and hetero-metallic coordination compounds (Babich *et al.*, 1996; Buvaylo *et al.*, 2005; Vassilyeva *et al.*, 1997). It is worth noting that an alternative method of synthesis using a classical reaction between calcium oxide and benzoic acid in dmso, affords the same complex in good yield (up to 90%), but does not give X-ray quality crystals. The crystal structure of the title complex, $[Ca(benz)_2(dmso)]_n$, is reported herein.

2. Structural commentary

The asymmetric unit of $[Ca(benz)_2(dmso)]_n$ comprises one Ca^{2+} cation (site symmetry *m*..), one benzoate ligand and half of a dmso molecule, the other half being generated by mirror symetry. The irregular CaO_8 coordination polyhedron consists of six O atom donors from two *O,O′* chelating-bridging benzoate carboxyl groups with the same coordination modes, $[2.1_11_{12}]$ in the Harris notation (Coxall *et al.*, 2000), and two from μ_2-bridging dmso molecules (Fig. 1). The coordination geometry deviates strongly from ideal, the Ca—O bond lengths varying from 2.345 (2) to 2.524 (2) Å (Table 1) and the O—Ca—O angles from 52.19 (7) to 156.06 (8)°. The bridging Ca1—O1^{i} and Ca1—O1^{ii} (carboxyl) bond lengths are considerably shorter than the chelate ones, as is usually observed in polymeric benzoates. For the title complex, the bond-valence index [BVS (Ca)] (Allmann, 1975) is 2.03.

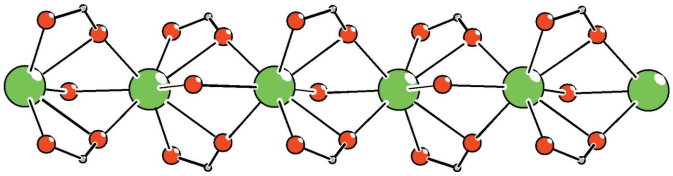


Figure 2
Bridging interactions observed in the title complex polymer which extends along the *c*- axis direction. Phenyl rings and H atoms have been omitted for clarity.

Table 1
Selected bond lengths (Å).

Ca1—O1^{i}	2.345 (2)	Ca1—O3	2.494 (3)
Ca1—O1^{ii}	2.345 (2)	Ca1—O3^{iv}	2.516 (3)
Ca1—O2^{iii}	2.481 (2)	Ca1—O1^{iii}	2.524 (2)
Ca1—O2	2.481 (2)	Ca1—O1	2.524 (2)

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

Table 2
C—H···π interactions (Å, °).

Cg is the centroid of the benzoate ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8*A*···*Cg*	0.96	2.84	3.790 (4)	169

3. Supramolecular features

The triple-O-bridged CaO_8 polyhedra form one-dimensional coordination polymeric chains which extend parallel to the *c*-axis direction (Figs. 2–4). The Ca···Ca^{i} and Ca1···Ca1^{iv} separation in the chain is 3.6401 (5) Å [symmetry code (iv): $-x+1, -y, z-\frac{1}{2}$]. To the best of our knowledge, this is the first Ca carboxylate polymer based on non-centrosymmetric bridges $(\mu\text{-}\eta^2:\eta^1)_2$. For bridging modes in coordination poly-

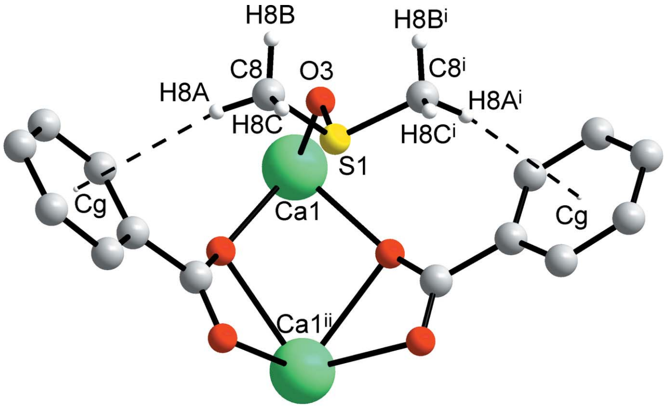


Figure 3
C—H···π hydrogen bonds involving a dmso donor as found in the title complex. For symmetry codes, see Table 1).

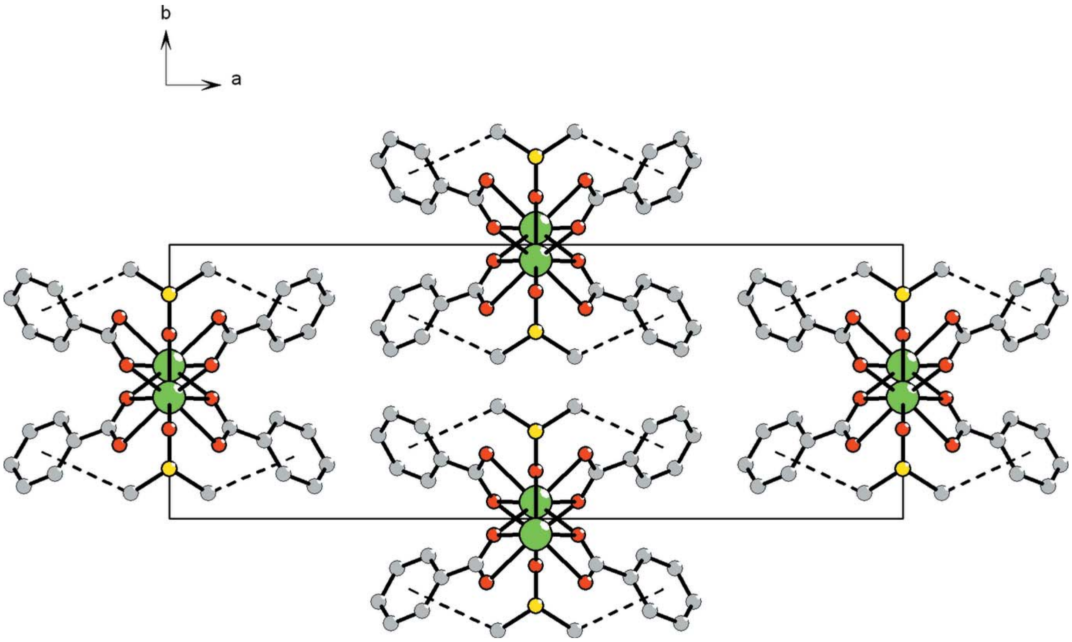


Figure 4
Packing of the molecular chains viewed down the chain direction (the crystallographic *c* axis). C—H$\cdots\pi$ bonds are shown as dashed lines.

meric structures, reference should be made to Deacon *et al.* (2007) and Busskamp *et al.* (2007). The polymer chains in the title compound are additionally stabilized by weak C—H$\cdots\pi$ interactions between the methyl groups of the dmso molecule and the benzoate rings (centroid *Cg*) (Table 2, Figs. 3 and 4).

4. Synthesis and crystallization

Calcium oxide (0.056 g, 1 mmol) and benzoic acid (0.244 g, 2 mmol) were added to 20 ml of dmso and stirred magnetically for *ca* 5 h at 323 K, after which the solution was filtered. The white precipitate which formed after one day was collected and dried in air; yield: 0.4 g (90%). Elemental analysis for $C_{16}H_{16}CaO_5S$ (M_r = 360.43). Calculated: Ca, 11.12%; found: Ca, 11.0%. IR (KBr, cm^{-1}): 1603 (*s*), 1562 (*s*), 1405 (*s*), 1024 (*s*), 721 (*s*). Crystals suitable for X-ray analysis were obtained by slow evaporation at room temperature of a solution which was the product from the reaction between manganese powder (0.05 g, 1 mmol), copper powder (0.06 g, 1 mmol), benzohydrazide (0.409 g, 3 mmol), salicylaldehyde (0.314 ml, 3 mmol), CaO (0.168 g, 3 mmol), KSCN (0.291 g, 3 mmol) and dmso (20 ml). The reaction was carried out at 353 K with magnetic stirring for eight hours, after which undissolved products were filtered off.

5. Refinement details

Crystal data, data collection and structure refinement details are given in Table 3. Hydrogen atoms were placed in calculated positions [C—H$_{\rm aromatic}$ = 0.95; C—H$_{\rm methyl}$ = 0.99 Å] and were allowed to ride in the refinements, with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(aromatic C) or 1.5$U_{\rm eq}$(methyl C). Although not of relevance in this crystal involving achiral molecules, the Flack absolute structure parameter (Flack, 1983) was determined as 0.04 (8) by classical fit to all intensities and 0.07 (3) from 557 selected quotients (Parsons *et al.*, 2013).

Table 3
Experimental details.

Crystal data	
Chemical formula	$[Ca(C_7H_5O_2)_2(C_2H_6OS)]$
M_r	360.43
Crystal system, space group	Orthorhombic, $Cmc2_1$
Temperature (K)	200
a, *b*, *c* (Å)	25.531 (2), 9.5351 (8), 6.9330 (4)
V (Å^3)	1687.7 (2)
Z	4
Radiation type	Mo *Kα*
μ (mm^{-1})	0.52
Crystal size (mm)	0.22 × 0.15 × 0.11
Data collection	
Diffractometer	Rigaku Mercury CCD
Absorption correction	Multi-scan (Blessing, 1995)
$T_{\min}$, $T_{\max}$	0.798, 0.951
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	3704, 1897, 1676
$R_{\rm int}$	0.025
$(\sin \theta/\lambda)_{\max}$ (Å^{-1})	0.683
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.044, 0.103, 1.13
No. of reflections	1897
No. of parameters	109
No. of restraints	1
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\max}$, $\Delta\rho_{\min}$ (e Å^{-3})	0.59, −0.39
Absolute structure	Flack *x* determined using 557 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	0.07 (3)

Computer programs: *CrystalClear* (Rigaku, 1999), *SIR92* (Altomare *et al.*, 1993)., *SHELXL97* (Sheldrick, 2008), *DIAMOND* (Brandenburg & Putz, 2006) and *WinGX* (Farrugia, 2012).

Acknowledgements

This work was partly supported by the State Fund for Fundamental Research of Ukraine (project 54.3/005).

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supporting information

Acta Cryst. (2015). E**71**, 906-909   [https://doi.org/10.1107/S2056989015012487]

Crystal structure of *catena*-poly[calcium-di-μ_3-benzoato-κ^6O,O':O-μ_2-(dimethyl sulfoxide)-κ^2O:O]

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Computing details

Data collection: *CrystalClear* (Rigaku, 1999); cell refinement: *CrystalClear* (Rigaku, 1999); data reduction: *CrystalClear* (Rigaku, 1999); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993).; program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg & Putz, 2006); software used to prepare material for publication: *WinGX* (Farrugia, 2012).

catena-Poly[calcium-di-μ_3-benzoato-κ^6O,O':O-μ_2-(dimethyl sulfoxide)-κ^2O:O]

Crystal data

$[Ca(C_7H_5O_2)_2(C_2H_6OS)]$
$M_r = 360.43$
Orthorhombic, $Cmc2_1$
$a = 25.531$ (2) Å
$b = 9.5351$ (8) Å
$c = 6.9330$ (4) Å
$V = 1687.7$ (2) Å^3
$Z = 4$
$F(000) = 752$

$D_x = 1.418$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71069$ Å
Cell parameters from 1872 reflections
$\theta = 2.3$–$28.7°$
$\mu = 0.52$ mm^{-1}
$T = 200$ K
Block, colorless
0.22 × 0.15 × 0.11 mm

Data collection

Rigaku Mercury CCD (2x2 bin mode) diffractometer
Graphite monochromator
Detector resolution: 14.7059 pixels mm^{-1}
dtprofit.ref scans
Absorption correction: multi-scan (Blessing, 1995)
$T_{min} = 0.798$, $T_{max} = 0.951$

3704 measured reflections
1897 independent reflections
1676 reflections with $I > 2\sigma(I)$
$R_{int} = 0.025$
$\theta_{max} = 29.0°$, $\theta_{min} = 2.3°$
$h = -34 \rightarrow 26$
$k = -12 \rightarrow 6$
$l = -9 \rightarrow 9$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.103$
$S = 1.13$
1897 reflections
109 parameters
1 restraint
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.040P)^2 + 0.7932P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.59$ e Å^{-3}
$\Delta\rho_{min} = -0.39$ e Å^{-3}

Absolute structure: Flack *x* determined using 557 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: 0.07 (3)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	$U_{\rm iso}$*/$U_{\rm eq}$
Ca1	0.5000	0.05825 (7)	0.36175 (11)	0.0325 (2)
O1	0.44205 (8)	0.06089 (19)	0.0668 (3)	0.0388 (5)
O2	0.43213 (9)	0.2334 (2)	0.2748 (4)	0.0509 (6)
O3	0.5000	0.1724 (3)	0.6855 (5)	0.0414 (7)
C1	0.41769 (12)	0.1682 (3)	0.1275 (5)	0.0375 (7)
C2	0.37045 (12)	0.2146 (3)	0.0171 (5)	0.0388 (7)
C3	0.35274 (13)	0.1367 (4)	−0.1381 (7)	0.0589 (10)
H3	0.3695	0.0533	−0.1704	0.071*
C4	0.31036 (16)	0.1818 (5)	−0.2452 (8)	0.0756 (13)
H4	0.2988	0.1289	−0.3495	0.091*
C5	0.28529 (14)	0.3044 (4)	−0.1984 (7)	0.0624 (11)
H5	0.2567	0.3340	−0.2707	0.075*
C6	0.30222 (15)	0.3831 (4)	−0.0461 (7)	0.0584 (11)
H6	0.2855	0.4669	−0.0160	0.070*
C7	0.34453 (12)	0.3375 (3)	0.0639 (6)	0.0464 (8)
H7	0.3555	0.3900	0.1695	0.056*
C8	0.44725 (16)	0.4090 (3)	0.6588 (6)	0.0560 (10)
H8A	0.4146	0.3721	0.7051	0.084*
H8B	0.4493	0.3964	0.5217	0.084*
H8C	0.4494	0.5071	0.6889	0.084*
S1	0.5000	0.31863 (10)	0.77164 (16)	0.0444 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ca1	0.0504 (4)	0.0257 (3)	0.0214 (4)	0.000	0.000	0.0005 (3)
O1	0.0472 (11)	0.0343 (11)	0.0349 (13)	0.0085 (8)	0.0000 (10)	−0.0033 (9)
O2	0.0720 (14)	0.0427 (12)	0.0381 (13)	0.0142 (11)	−0.0139 (13)	−0.0064 (11)
O3	0.069 (2)	0.0218 (12)	0.0333 (17)	0.000	0.000	−0.0020 (12)
C1	0.0515 (17)	0.0302 (14)	0.0307 (17)	0.0017 (13)	0.0019 (13)	0.0022 (12)
C2	0.0421 (15)	0.0389 (16)	0.0353 (17)	0.0002 (13)	0.0011 (13)	0.0042 (14)

C3	0.0556 (18)	0.060 (2)	0.061 (2)	0.0180 (16)	−0.014 (2)	−0.022 (2)
C4	0.067 (2)	0.086 (3)	0.074 (3)	0.020 (2)	−0.031 (2)	−0.022 (3)
C5	0.0483 (19)	0.069 (2)	0.070 (3)	0.0101 (19)	−0.0107 (18)	0.010 (2)
C6	0.0478 (19)	0.045 (2)	0.082 (3)	0.0097 (16)	0.0054 (19)	0.003 (2)
C7	0.0483 (17)	0.0390 (17)	0.052 (2)	0.0063 (14)	0.0025 (16)	−0.0028 (16)
C8	0.083 (3)	0.0357 (15)	0.049 (2)	0.0096 (17)	0.005 (2)	−0.0010 (17)
S1	0.0829 (8)	0.0257 (5)	0.0244 (6)	0.000	0.000	−0.0015 (4)

Geometric parameters (Å, º)

Ca1—O1^{i}	2.345 (2)	C1—C2	1.496 (4)
Ca1—O1^{ii}	2.345 (2)	C2—C3	1.383 (5)
Ca1—O2^{iii}	2.481 (2)	C2—C7	1.384 (4)
Ca1—O2	2.481 (2)	C3—C4	1.381 (5)
Ca1—O3	2.494 (3)	C3—H3	0.9300
Ca1—O3^{iv}	2.516 (3)	C4—C5	1.371 (5)
Ca1—O1^{iii}	2.524 (2)	C4—H4	0.9300
Ca1—O1	2.524 (2)	C5—C6	1.365 (6)
Ca1—C1^{iii}	2.855 (3)	C5—H5	0.9300
Ca1—C1	2.855 (3)	C6—C7	1.392 (5)
Ca1—Ca1^{i}	3.6401 (5)	C6—H6	0.9300
Ca1—Ca1^{iv}	3.6401 (5)	C7—H7	0.9300
O1—C1	1.269 (3)	C8—S1	1.780 (4)
O1—Ca1^{iv}	2.345 (2)	C8—H8A	0.9600
O2—C1	1.251 (4)	C8—H8B	0.9600
O3—S1	1.517 (3)	C8—H8C	0.9600
O3—Ca1^{i}	2.516 (3)	S1—C8^{iii}	1.780 (4)

O1^{i}—Ca1—O1^{ii}	78.22 (11)	C1^{iii}—Ca1—Ca1^{i}	130.82 (7)
O1^{i}—Ca1—O2^{iii}	91.88 (8)	C1—Ca1—Ca1^{i}	130.82 (7)
O1^{ii}—Ca1—O2^{iii}	156.06 (8)	O1^{i}—Ca1—Ca1^{iv}	115.44 (6)
O1^{i}—Ca1—O2	156.06 (8)	O1^{ii}—Ca1—Ca1^{iv}	115.44 (6)
O1^{ii}—Ca1—O2	91.88 (8)	O2^{iii}—Ca1—Ca1^{iv}	88.51 (6)
O2^{iii}—Ca1—O2	88.60 (12)	O2—Ca1—Ca1^{iv}	88.51 (6)
O1^{i}—Ca1—O3	70.48 (7)	O3—Ca1—Ca1^{iv}	171.90 (7)
O1^{ii}—Ca1—O3	70.48 (7)	O3^{iv}—Ca1—Ca1^{iv}	43.17 (8)
O2^{iii}—Ca1—O3	85.70 (8)	O1^{iii}—Ca1—Ca1^{iv}	39.79 (5)
O2—Ca1—O3	85.70 (8)	O1—Ca1—Ca1^{iv}	39.79 (5)
O1^{i}—Ca1—O3^{iv}	82.59 (8)	C1^{iii}—Ca1—Ca1^{iv}	64.56 (7)
O1^{ii}—Ca1—O3^{iv}	82.59 (8)	C1—Ca1—Ca1^{iv}	64.56 (7)
O2^{iii}—Ca1—O3^{iv}	118.06 (7)	Ca1^{i}—Ca1—Ca1^{iv}	144.47 (4)
O2—Ca1—O3^{iv}	118.06 (7)	C1—O1—Ca1^{iv}	154.2 (2)
O3—Ca1—O3^{iv}	144.93 (11)	C1—O1—Ca1	91.54 (19)
O1^{i}—Ca1—O1^{iii}	97.25 (7)	Ca1^{iv}—O1—Ca1	96.69 (7)
O1^{ii}—Ca1—O1^{iii}	149.97 (5)	C1—O2—Ca1	94.01 (18)
O2^{iii}—Ca1—O1^{iii}	52.19 (7)	S1—O3—Ca1	139.05 (18)
O2—Ca1—O1^{iii}	101.88 (8)	S1—O3—Ca1^{i}	127.75 (19)
O3—Ca1—O1^{iii}	136.43 (6)	Ca1—O3—Ca1^{i}	93.19 (9)

O3^{iv}—Ca1—O1^{iii}	67.37 (7)	O2—C1—O1	121.8 (3)
O1^{i}—Ca1—O1	149.97 (5)	O2—C1—C2	120.6 (3)
O1^{ii}—Ca1—O1	97.25 (7)	O1—C1—C2	117.6 (3)
O2^{iii}—Ca1—O1	101.88 (8)	O2—C1—Ca1	60.08 (16)
O2—Ca1—O1	52.19 (7)	O1—C1—Ca1	62.08 (16)
O3—Ca1—O1	136.43 (6)	C2—C1—Ca1	173.4 (2)
O3^{iv}—Ca1—O1	67.37 (7)	C3—C2—C7	118.8 (3)
O1^{iii}—Ca1—O1	71.78 (10)	C3—C2—C1	120.2 (3)
O1^{i}—Ca1—C1^{iii}	93.35 (8)	C7—C2—C1	121.1 (3)
O1^{ii}—Ca1—C1^{iii}	170.72 (8)	C4—C3—C2	120.4 (3)
O2^{iii}—Ca1—C1^{iii}	25.91 (8)	C4—C3—H3	119.8
O2—Ca1—C1^{iii}	97.39 (9)	C2—C3—H3	119.8
O3—Ca1—C1^{iii}	110.58 (8)	C5—C4—C3	120.3 (4)
O3^{iv}—Ca1—C1^{iii}	92.57 (8)	C5—C4—H4	119.9
O1^{iii}—Ca1—C1^{iii}	26.38 (7)	C3—C4—H4	119.9
O1—Ca1—C1^{iii}	88.11 (8)	C6—C5—C4	120.2 (4)
O1^{i}—Ca1—C1	170.72 (8)	C6—C5—H5	119.9
O1^{ii}—Ca1—C1	93.35 (8)	C4—C5—H5	119.9
O2^{iii}—Ca1—C1	97.39 (9)	C5—C6—C7	119.9 (3)
O2—Ca1—C1	25.91 (8)	C5—C6—H6	120.1
O3—Ca1—C1	110.58 (8)	C7—C6—H6	120.1
O3^{iv}—Ca1—C1	92.57 (8)	C2—C7—C6	120.4 (3)
O1^{iii}—Ca1—C1	88.11 (8)	C2—C7—H7	119.8
O1—Ca1—C1	26.38 (7)	C6—C7—H7	119.8
C1^{iii}—Ca1—C1	94.77 (13)	S1—C8—H8A	109.5
O1^{i}—Ca1—Ca1^{i}	43.52 (5)	S1—C8—H8B	109.5
O1^{ii}—Ca1—Ca1^{i}	43.52 (5)	H8A—C8—H8B	109.5
O2^{iii}—Ca1—Ca1^{i}	115.90 (7)	S1—C8—H8C	109.5
O2—Ca1—Ca1^{i}	115.90 (7)	H8A—C8—H8C	109.5
O3—Ca1—Ca1^{i}	43.63 (7)	H8B—C8—H8C	109.5
O3^{iv}—Ca1—Ca1^{i}	101.29 (8)	O3—S1—C8^{iii}	105.78 (14)
O1^{iii}—Ca1—Ca1^{i}	140.76 (5)	O3—S1—C8	105.78 (14)
O1—Ca1—Ca1^{i}	140.76 (5)	C8^{iii}—S1—C8	98.4 (3)

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

Hydrogen-bond geometry (Å, º)

Cg is the centroid of the benzoate ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8*A*···*Cg*	0.96	2.84	3.790 (4)	169