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catena-Poly[[[diaquabarium(II)]-bis[μ-2-(4-carboxyphenoxy)propionato-$\kappa^3O,O':O'$] dihydrate]

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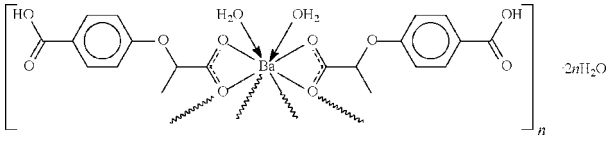
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.003 Å; disorder in solvent or counterion; R factor = 0.022; wR factor = 0.058; data-to-parameter ratio = 16.0.

In the crystal structure of the polymeric title compound, $\{[Ba(C_{10}H_9O_5)_2(H_2O)_2]\cdot 2H_2O\}_n$, the Ba^{II} atom is O,O'-chelated by the carboxylate end of two 2-(4-carboxyphenoxy)propionate monoanions, and is coordinated by two water molecules. It also interacts with the carboxylate O atom of two adjacent monoanions; these bonds give rise to a chain structure along the c axis. Meanwhile, the carboxyl $-CO_2H$ end of the anion interacts with an acceptor site [O···O = 2.608 (2) Å]; this interaction and hydrogen bonding involving the coordinated and lattice water molecules give rise to a three-dimensional network. The eight coordinating O atoms comprise a square-antiprism around the metal atom, which lies on a special position of site symmetry 2.

Related literature

For the strontium derivative of 2-(4-carboxyphenoxy)propionic acid, see: Kong *et al.* (2007).



Experimental

Crystal data

$[Ba(C_{10}H_9O_5)_2(H_2O)_2]\cdot 2H_2O$
M_r = 627.75
Monoclinic, $C2/c$
a = 24.5348 (8) Å
b = 13.2964 (4) Å
c = 7.5147 (2) Å
β = 97.3494 (9)°
V = 2431.34 (13) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.70 mm^{-1}
T = 295 (2) K
0.38 × 0.32 × 0.30 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.471, T_{max} = 0.629
11558 measured reflections
2754 independent reflections
2684 reflections with $I > 2\sigma(I)$
R_{int} = 0.030

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.022
$wR(F^2)$ = 0.058
S = 1.05
2754 reflections
172 parameters
12 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O5—H51···O2^{i}	0.82	1.79	2.608 (2)	174
O1W—H11···O4^{ii}	0.82	2.16	2.979 (3)	176
O1W—H12···O2W'	0.82	2.13	2.875 (7)	152
O2W—H21···O4^{iii}	0.82	2.25	2.900 (6)	137
O2W—H22···O2W^{iv}	0.82	2.32	2.881 (14)	126
O2W—H22···O2W^{v}	0.82	2.32	2.742 (17)	113
O2W—H22···O2W'^{iv}	0.82	1.99	2.746 (9)	152
O2W'—H23···O4^{iii}	0.82	2.25	2.885 (7)	134
O2W'—H24···O2W^{iv}	0.82	2.03	2.746 (9)	145

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

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: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2007).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2487).

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supplementary materials

Acta Cryst. (2007). E**63**, m2850 [**doi:10.1107/S1600536807052178**]

catena-Poly[[[diaquabarium(II)]-bis[μ-2-(4-carboxyphenoxy)propionato-$\kappa^3O,O':O'$] dihydrate]

L.-L. Kong, S. Gao, L.-H. Huo and S. W. Ng

Comment

This report continues a previous study on the main-group metal derivative of 2-[4-carboxylatophenoxy]propionic acid (Kong *et al.*, 2007). In the present barium compound (Fig. 1), the metal shows irregular square-antiprismatic coordination (Fig. 2).

Experimental

To a suspension of barium carbonate (2 mmol) in water was added 2-(4-carboxylatophenoxy)propionic acid (1 mmol). The mixture was heated to dissolve most of the carbonate; the unchanged reagent was removed by filtration. Colourless crystals separated out after a few days. C&H elemental analysis. Calculated for $C_{20}H_{22}O_{14}Ba$: C 38.51, H 3.56%; found: C 38.52, H 3.55%.

Refinement

The lattice water molecule is disordered over two positions; as the occupancy refined to a nearly 50:50 ratio, the occupancy was fixed as 0.5 each. Carbon- and oxygen-bound H atoms were placed in calculated positions [C—H = 0.93–0.97 Å and U_{iso}(H) = 1.2–1.5U_{eq}(C); O–H = 0.82 Å and U_{iso}(H) = 1.5U_{eq}(O)], and were included in the refinement in the riding-model approximation. The final difference Fourier map had large peaks/holes in the vicinity of the barium atom.

Figures

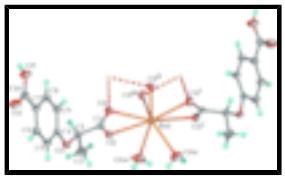

Fig. 1. Part of the polymeric structure of the title compound, showing 50% probability displacement ellipsoids. H atoms are shown as small spheres of arbitrary radii. The disordered lattice water molecule is not shown. Symmetry codes; (i) 1 − *x*, *y*, 1/2 − *z*; (ii) 1 − *x*, 1 − *y*, 1 − *z*; (iii) *x*, 1 − *y*, *z* − 1/2.

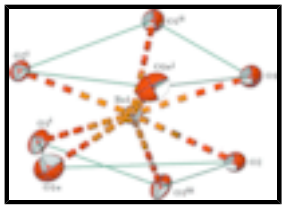

Fig. 2. Square-antiprimastic geometry of Ba.

catena-Poly[[[diaquabarium(II)]-bis[μ-2-(4-carboxyphenoxy)propionato-\ $\kappa^3O,O':O'$] dihydrate]

Crystal data

$[Ba(C_{10}H_9O_5)_2(H_2O)_2]\cdot 2H_2O$ F_{000} = 1256

M_r = 627.75	D_x = 1.715 Mg m^{-3}
Monoclinic, $C2/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 11193 reflections
a = 24.5348 (8) Å	θ = 3.0–27.5º
b = 13.2964 (4) Å	μ = 1.70 mm^{-1}
c = 7.5147 (2) Å	T = 295 (2) K
β = 97.3494 (9)º	Prism, colourless
V = 2431.34 (13) Å^3	0.38 × 0.32 × 0.30 mm
Z = 4	

Data collection

Rigaku R-AXIS RAPID diffractometer	2754 independent reflections
Radiation source: fine-focus sealed tube	2684 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.030
Detector resolution: 10.000 pixels mm^{-1}	θ_{max} = 27.4º
T = 295(2) K	θ_{min} = 3.1º
ω scans	h = −31→31
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	k = −16→17
T_{min} = 0.471, T_{max} = 0.629	l = −8→9
11558 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.022	H-atom parameters constrained
$wR(F^2)$ = 0.058	$w = 1/[\sigma^2(F_o^2) + (0.0386P)^2 + 1.6587P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.05	$(\Delta/\sigma)_{max}$ = 0.001
2754 reflections	$\Delta\rho_{max}$ = 1.34 e Å^{-3}
172 parameters	$\Delta\rho_{min}$ = −0.40 e Å^{-3}
12 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
Ba1	0.5000	0.602876 (9)	0.2500	0.02394 (7)	
O1	0.44439 (6)	0.53508 (11)	0.5434 (2)	0.0362 (3)	
O2	0.39379 (6)	0.62910 (11)	0.34507 (19)	0.0297 (3)	
O3	0.31354 (5)	0.64630 (9)	0.56511 (18)	0.0280 (3)	

O4	0.11457 (8)	0.38322 (13)	0.1840 (3)	0.0499 (5)	
O5	0.17634 (7)	0.26668 (11)	0.2823 (2)	0.0447 (4)	
H51	0.1561	0.2206	0.2426	0.067*	
O1W	0.51164 (8)	0.77491 (13)	0.0446 (3)	0.0548 (4)	
H11	0.5391	0.8060	0.0874	0.082*	
H12	0.4844	0.8107	0.0450	0.082*	
O2W	0.4618 (3)	0.9497 (5)	−0.1321 (11)	0.103 (2)	0.50
H21	0.4457	0.9907	−0.2014	0.155*	0.50
H22	0.4945	0.9641	−0.1136	0.155*	0.50
O2W'	0.4433 (3)	0.9510 (6)	0.0023 (12)	0.112 (2)	0.50
H23	0.4151	0.9849	−0.0095	0.168*	0.50
H24	0.4656	0.9757	0.0807	0.168*	0.50
C1	0.40400 (8)	0.59159 (13)	0.4991 (3)	0.0250 (4)	
C2	0.36759 (8)	0.61791 (14)	0.6437 (3)	0.0267 (4)	
H2	0.3653	0.5601	0.7233	0.032*	
C3	0.39133 (10)	0.70747 (18)	0.7519 (3)	0.0434 (5)	
H3A	0.3697	0.7207	0.8472	0.065*	
H3B	0.3908	0.7653	0.6753	0.065*	
H3C	0.4285	0.6931	0.8017	0.065*	
C4	0.27903 (7)	0.57216 (14)	0.4905 (2)	0.0244 (3)	
C5	0.22872 (9)	0.60562 (12)	0.4031 (3)	0.0305 (4)	
H5	0.2212	0.6741	0.3946	0.037*	
C6	0.19019 (8)	0.53692 (15)	0.3293 (3)	0.0317 (4)	
H6	0.1566	0.5593	0.2713	0.038*	
C7	0.20121 (8)	0.43396 (14)	0.3409 (2)	0.0282 (4)	
C8	0.25192 (9)	0.40175 (13)	0.4258 (3)	0.0301 (4)	
H8	0.2597	0.3333	0.4323	0.036*	
C9	0.29105 (8)	0.46983 (14)	0.5007 (2)	0.0281 (4)	
H9	0.3248	0.4475	0.5570	0.034*	
C10	0.15978 (8)	0.36010 (15)	0.2615 (3)	0.0321 (4)	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ba1	0.02067 (9)	0.02101 (9)	0.02963 (10)	0.000	0.00124 (6)	0.000
O1	0.0281 (7)	0.0376 (8)	0.0434 (8)	0.0131 (6)	0.0060 (6)	0.0122 (6)
O2	0.0259 (7)	0.0305 (6)	0.0323 (7)	0.0063 (5)	0.0022 (5)	0.0042 (6)
O3	0.0206 (6)	0.0219 (6)	0.0408 (7)	0.0004 (5)	0.0012 (5)	−0.0063 (5)
O4	0.0330 (9)	0.0379 (8)	0.0736 (13)	−0.0037 (7)	−0.0131 (8)	−0.0042 (8)
O5	0.0411 (9)	0.0255 (7)	0.0619 (10)	−0.0062 (6)	−0.0150 (7)	−0.0053 (7)
O1W	0.0519 (11)	0.0370 (9)	0.0724 (12)	−0.0018 (7)	−0.0037 (9)	0.0129 (8)
O2W	0.079 (4)	0.069 (3)	0.155 (6)	0.015 (3)	−0.018 (4)	0.018 (4)
O2W'	0.087 (4)	0.094 (4)	0.151 (6)	0.030 (3)	0.003 (4)	0.034 (4)
C1	0.0208 (9)	0.0208 (8)	0.0326 (10)	0.0002 (6)	0.0010 (7)	−0.0004 (6)
C2	0.0223 (9)	0.0269 (8)	0.0304 (9)	−0.0004 (7)	0.0014 (7)	−0.0020 (7)
C3	0.0353 (11)	0.0449 (12)	0.0485 (12)	−0.0050 (9)	−0.0001 (9)	−0.0205 (10)
C4	0.0216 (8)	0.0234 (8)	0.0284 (8)	−0.0011 (7)	0.0039 (6)	−0.0033 (7)
C5	0.0266 (10)	0.0232 (9)	0.0407 (11)	0.0036 (6)	−0.0001 (8)	−0.0022 (7)

C6	0.0248 (9)	0.0296 (9)	0.0390 (10)	0.0025 (7)	−0.0024 (7)	−0.0031 (8)
C7	0.0274 (9)	0.0258 (9)	0.0307 (9)	−0.0035 (7)	0.0012 (7)	−0.0030 (7)
C8	0.0314 (11)	0.0223 (9)	0.0360 (11)	−0.0005 (6)	0.0018 (8)	0.0004 (6)
C9	0.0238 (8)	0.0253 (8)	0.0342 (9)	0.0016 (7)	−0.0003 (7)	−0.0011 (7)
C10	0.0296 (10)	0.0304 (10)	0.0354 (10)	−0.0049 (8)	0.0008 (7)	−0.0034 (8)

Geometric parameters (Å, °)

Ba1—O1	2.882 (1)	O2W'—H23	0.82
Ba1—O1^{i}	2.882 (1)	O2W'—H24	0.82
Ba1—O1^{ii}	2.664 (1)	C1—C2	1.533 (3)
Ba1—O1^{iii}	2.664 (1)	C2—C3	1.515 (3)
Ba1—O2	2.811 (1)	C2—H2	0.98
Ba1—O2^{i}	2.811 (1)	C3—H3A	0.96
Ba1—O1W	2.794 (2)	C3—H3B	0.96
Ba1—O1W^{i}	2.794 (2)	C3—H3C	0.96
O1—C1	1.254 (2)	C4—C5	1.395 (3)
O2—C1	1.256 (3)	C4—C9	1.392 (2)
O3—C4	1.371 (2)	C5—C6	1.379 (3)
O3—C2	1.432 (2)	C5—H5	0.93
O4—C10	1.224 (3)	C6—C7	1.396 (3)
O5—C10	1.310 (3)	C6—H6	0.93
O5—H51	0.82	C7—C8	1.391 (3)
O1W—H11	0.82	C7—C10	1.483 (3)
O1W—H12	0.82	C8—C9	1.386 (3)
O2W—H21	0.82	C8—H8	0.93
O2W—H22	0.82	C9—H9	0.93
O1^{iii}—Ba1—O1^{ii}	92.96 (7)	H23—O2W'—H24	109.5
O1^{iii}—Ba1—O1W^{i}	143.59 (5)	O1—C1—O2	122.68 (18)
O1^{ii}—Ba1—O1W^{i}	108.82 (5)	O1—C1—C2	117.47 (18)
O1^{iii}—Ba1—O1W	108.82 (5)	O2—C1—C2	119.80 (17)
O1^{ii}—Ba1—O1W	143.59 (5)	O3—C2—C3	106.64 (16)
O1W^{i}—Ba1—O1W	70.11 (9)	O3—C2—C1	111.15 (16)
O1^{iii}—Ba1—O2^{i}	111.08 (4)	C3—C2—C1	109.92 (17)
O1^{ii}—Ba1—O2^{i}	79.11 (4)	O3—C2—H2	109.7
O1W^{i}—Ba1—O2^{i}	101.68 (5)	C3—C2—H2	109.7
O1W—Ba1—O2^{i}	66.08 (5)	C1—C2—H2	109.7
O1^{iii}—Ba1—O2	79.11 (4)	C2—C3—H3A	109.5
O1^{ii}—Ba1—O2	111.08 (4)	C2—C3—H3B	109.5
O1W^{i}—Ba1—O2	66.08 (5)	H3A—C3—H3B	109.5
O1W—Ba1—O2	101.68 (5)	C2—C3—H3C	109.5
O2^{i}—Ba1—O2	165.75 (6)	H3A—C3—H3C	109.5
O1^{iii}—Ba1—O1^{i}	66.17 (5)	H3B—C3—H3C	109.5
O1^{ii}—Ba1—O1^{i}	88.46 (3)	O3—C4—C5	115.21 (16)

O1W^{i}—Ba1—O1^{i}	140.39 (5)	O3—C4—C9	124.37 (17)
O1W—Ba1—O1^{i}	75.03 (5)	C5—C4—C9	120.40 (16)
O2^{i}—Ba1—O1^{i}	45.51 (4)	C6—C5—C4	119.87 (16)
O2—Ba1—O1^{i}	141.12 (4)	C6—C5—H5	120.1
O1^{iii}—Ba1—O1	88.46 (3)	C4—C5—H5	120.1
O1^{ii}—Ba1—O1	66.17 (5)	C5—C6—C7	120.46 (18)
O1W^{i}—Ba1—O1	75.03 (5)	C5—C6—H6	119.8
O1W—Ba1—O1	140.39 (5)	C7—C6—H6	119.8
O2^{i}—Ba1—O1	141.12 (4)	C8—C7—C6	119.04 (17)
O2—Ba1—O1	45.51 (4)	C8—C7—C10	120.50 (17)
O1^{i}—Ba1—O1	143.54 (6)	C6—C7—C10	120.45 (18)
C1—O1—Ba1^{ii}	153.58 (13)	C9—C8—C7	121.17 (16)
C1—O1—Ba1	92.59 (12)	C9—C8—H8	119.4
Ba1^{ii}—O1—Ba1	113.83 (5)	C7—C8—H8	119.4
C1—O2—Ba1	95.91 (11)	C8—C9—C4	119.03 (17)
C4—O3—C2	118.03 (14)	C8—C9—H9	120.5
C10—O5—H51	120.0	C4—C9—H9	120.5
Ba1—O1W—H11	109.5	O4—C10—O5	122.92 (19)
Ba1—O1W—H12	109.5	O4—C10—C7	123.91 (19)
H11—O1W—H12	109.5	O5—C10—C7	113.18 (17)
H21—O2W—H22	109.5		
O1^{iii}—Ba1—O1—C1	−86.03 (10)	Ba1—O2—C1—O1	−19.5 (2)
O1^{ii}—Ba1—O1—C1	−179.94 (16)	Ba1—O2—C1—C2	158.09 (14)
O1W^{i}—Ba1—O1—C1	61.17 (12)	C4—O3—C2—C3	−167.01 (16)
O1W—Ba1—O1—C1	32.26 (15)	C4—O3—C2—C1	73.20 (19)
O2^{i}—Ba1—O1—C1	151.29 (11)	O1—C1—C2—O3	−156.65 (17)
O2—Ba1—O1—C1	−9.82 (11)	O2—C1—C2—O3	25.7 (2)
O1^{i}—Ba1—O1—C1	−130.27 (12)	O1—C1—C2—C3	85.5 (2)
O1^{iii}—Ba1—O1—Ba1^{ii}	93.91 (9)	O2—C1—C2—C3	−92.1 (2)
O1^{ii}—Ba1—O1—Ba1^{ii}	0.0	C2—O3—C4—C5	−174.86 (17)
O1W^{i}—Ba1—O1—Ba1^{ii}	−118.89 (7)	C2—O3—C4—C9	6.3 (3)
O1W—Ba1—O1—Ba1^{ii}	−147.80 (7)	O3—C4—C5—C6	−177.60 (18)
O2^{i}—Ba1—O1—Ba1^{ii}	−28.77 (10)	C9—C4—C5—C6	1.3 (3)
O2—Ba1—O1—Ba1^{ii}	170.12 (9)	C4—C5—C6—C7	−0.2 (3)
O1^{i}—Ba1—O1—Ba1^{ii}	49.68 (5)	C5—C6—C7—C8	−1.0 (3)
O1^{iii}—Ba1—O2—C1	108.52 (12)	C5—C6—C7—C10	−180.0 (2)
O1^{ii}—Ba1—O2—C1	19.54 (12)	C6—C7—C8—C9	1.0 (3)
O1W^{i}—Ba1—O2—C1	−82.42 (12)	C10—C7—C8—C9	−179.97 (19)
O1W—Ba1—O2—C1	−144.28 (11)	C7—C8—C9—C4	0.1 (3)
O2^{i}—Ba1—O2—C1	−114.53 (11)	O3—C4—C9—C8	177.54 (18)
O1^{i}—Ba1—O2—C1	135.15 (11)	C5—C4—C9—C8	−1.2 (3)
O1—Ba1—O2—C1	9.85 (10)	C8—C7—C10—O4	−179.5 (2)
Ba1^{ii}—O1—C1—O2	−161.0 (2)	C6—C7—C10—O4	−0.5 (3)

Ba1—O1—C1—O2	18.88 (19)	C8—C7—C10—O5	0.5 (3)
Ba1^{ii}—O1—C1—C2	21.4 (4)	C6—C7—C10—O5	179.5 (2)
Ba1—O1—C1—C2	−158.73 (14)		

Symmetry codes: (i) −*x*+1, *y*, −*z*+1/2; (ii) −*x*+1, −*y*+1, −*z*+1; (iii) *x*, −*y*+1, *z*−1/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H51···O2^{iv}	0.82	1.79	2.608 (2)	174
O1W—H11···O4^{v}	0.82	2.16	2.979 (3)	176
O1W—H12···O2W'	0.82	2.13	2.875 (7)	152
O2W—H21···O4^{vi}	0.82	2.25	2.900 (6)	137
O2W—H22···O2W^{vii}	0.82	2.32	2.881 (14)	126
O2W—H22···O2W^{viii}	0.82	2.32	2.742 (17)	113
O2W—H22···O2W'^{vii}	0.82	1.99	2.746 (9)	152
O2W'—H23···O4^{vi}	0.82	2.25	2.885 (7)	134
O2W'—H24···O2W^{vii}	0.82	2.03	2.746 (9)	145

Symmetry codes: (iv) −*x*+1/2, *y*−1/2, −*z*+1/2; (v) *x*+1/2, *y*+1/2, *z*; (vi) −*x*+1/2, −*y*+3/2, −*z*; (vii) −*x*+1, −*y*+2, −*z*; (viii) −*x*+1, *y*, −*z*−1/2.

Fig. 1

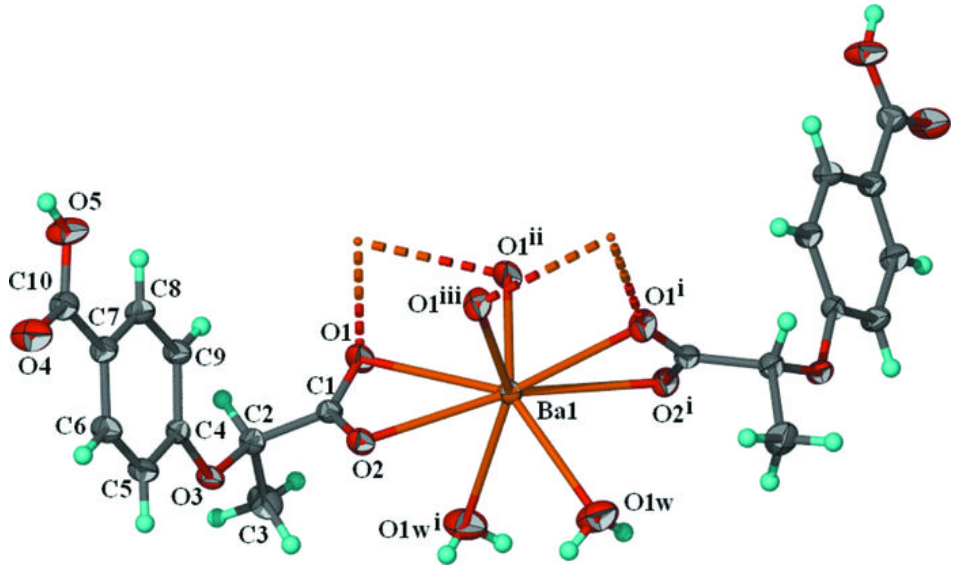
O5
C10
C8
C7
O4
C9
C6
C4
C2
C1
O1
O1ii
O1iii
O1i
Ba1
O2i
O2
C5
O3
C3
O1wi
O1w

Fig. 2