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3,4,5-Trimethoxybenzoic acid

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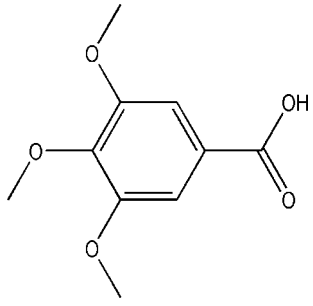
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.039; wR factor = 0.094; data-to-parameter ratio = 8.9.

The asymmetric unit of the title compound, $C_{10}H_{12}O_5$, contains two crystallographically independent molecules. In the crystal structure, intermolecular C—H···O and O—H···O hydrogen bonds link the molecules.

Related literature

For related literature, see: Gopalakrishna & Cartz (1972); Bryan & White (1982*a*,*b*); Frankenbach *et al.* (1991); Khan *et al.* (2006). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{10}H_{12}O_5$
M_r = 212.20
Monoclinic, Pc
a = 7.3384 (3) Å
b = 8.8325 (3) Å
c = 15.7560 (5) Å
β = 96.576 (2)°
V = 1014.53 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 298 (2) K
0.25 × 0.15 × 0.13 mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.935, T_{max} = 0.984
7599 measured reflections
2510 independent reflections
1563 reflections with $I > 2\sigma(I)$
R_{int} = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.094
S = 1.06
2510 reflections
281 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C9—H9C···O7^{i}	0.96	2.49	3.405 (4)	159
C18—H18A···O5^{ii}	0.96	2.51	3.321 (4)	142
C19—H19C···O1^{iii}	0.96	2.50	3.404 (5)	158
O2—H2···O7^{iv}	0.82	1.83	2.641 (3)	172
O6—H6···O1^{v}	0.96 (2)	1.71 (2)	2.656 (3)	170 (5)

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *APEX2*; 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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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2288).

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supplementary materials

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3,4,5-Trimethoxybenzoic acid

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Comment

ortho-Alkoxybenzoic acids are a class of acids which crystallize with different packing modes. The distinctive behaviour of 2-ethoxybenzoic acid which forms monomers is due to the formation of an intramolecular hydrogen bond (Gopalakrishna & Cartz, 1972). 2,3-Dimethoxybenzoic acid forms the normal acid dimer pattern (Bryan & White, 1982*a*). 2,6- Dimethoxybenzoic acid (Bryan & White, 1982*b*) and 2,6-dimethoxy-3-nitrobenzoic acid (Frankenbach *et al.*, 1991) form catemers. The carboxyl group of 2,6-dimethoxybenzoic acid exists in an anti conformation, while the carboxyl group of 2,6-dimethoxy-3-nitrobenzoic acid in a *syn* conformation. We report herein the crystal structure of the title compound, (I).

The asymmetric unit of the title compound, (I), (Fig. 1) contains two crystallographicaly independent molecules, in which the bond lengths and angles are generally within normal ranges (Allen *et al.*, 1987). The C—O bonds of the carboxyl groups (Table 1) are compatible with the corresponding values in similar structure (Khan *et al.*, 2006), and smaller than those usually observed in carboxylic acid [1.365 Å]. The valence angles C3—C2—C7 [121.5 (3)°] and C13—C12—C17 [121.9 (2)°] are larger than the standard value of 120°, due to the presence of methoxy and carboxyl groups.

In the crystal structure, the intermolecular O—H···O hydrogen bonds (Table 2) form catemers, as observed in 2,6-dimethoxybenzoic acid and 2,6-dimethoxy-3 -nitrobenzoic acid, the intermolecular C—H···O and O—H···O hydrogen bonds (Table 2, Fig. 2) link the molecules, in which they seem to be effective in the stabilization of the structure.

Experimental

The title compound was purchased and crystallized from ethyl acetate by slow evaporation.

Refinement

H6 and H7 were located in difference syntheses and refined isotropicaly [O6—H6 = 0.96 (2) Å, U_{iso}(H) = 0.14 (2) Å^2 and C7—H7 = 0.99 (3) Å, U_{iso}(H) = 0.046 (8) Å^2]. The remaining H atoms were positioned geometrically, with O—H = 0.82 Å (for OH) and C—H = 0.93 and 0.96 Å for aromatic and methyl H, respectively, and constrained to ride on their parent atoms, with U_{iso}(H) = xU_{eq}(C,*O*), where x = 1.2 for aromatic H, and x = 1.5 for all other H atoms.

Figures

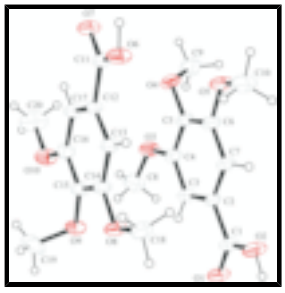

Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

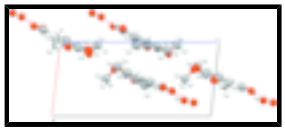

Fig. 2. A partial packing diagram of (I). Hydrogen bonds are shown as dashed lines.

3,4,5-Trimethoxybenzoic acid

Crystal data

$C_{10}H_{12}O_5$	F_{000} = 448
M_r = 212.20	D_x = 1.389 Mg m^{-3}
Monoclinic, *Pc*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: P -2yc	Cell parameters from 1520 reflections
a = 7.3384 (3) Å	θ = 2.8–22.6º
b = 8.8325 (3) Å	μ = 0.11 mm^{-1}
c = 15.7560 (5) Å	*T* = 298 (2) K
β = 96.576 (2)º	Monoclinic, colourless
V = 1014.53 (6) Å^3	0.25 × 0.15 × 0.13 mm
Z = 4	

Data collection

Bruker APEXII area-detector diffractometer	2510 independent reflections
Radiation source: fine-focus sealed tube	1563 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.032
T = 298(2) K	θ_{max} = 28.3º
φ and ω scans	θ_{min} = 2.6º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	*h* = −8→9
T_{min} = 0.935, T_{max} = 0.984	*k* = −11→11
7599 measured reflections	*l* = −21→20

Refinement

Refinement on F^2	H atoms treated by a mixture of independent and constrained refinement

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.039$

$wR(F^2) = 0.094$

$S = 1.06$

2510 reflections

281 parameters

3 restraints

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

$w = 1/[\sigma^2(F_o^2) + (0.0445P)^2]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.18$ e Å^{-3}

$\Delta\rho_{min} = -0.17$ e Å^{-3}

Extinction correction: SHELXL97, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.015 (2)

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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	−0.1652 (4)	0.4366 (4)	−0.11562 (19)	0.0433 (7)
C2	−0.0769 (4)	0.3669 (4)	−0.03518 (17)	0.0395 (7)
C3	−0.0469 (4)	0.2135 (4)	−0.03295 (19)	0.0441 (7)
H3	−0.0773	0.1551	−0.0816	0.053*
C4	0.0301 (4)	0.1455 (4)	0.04333 (18)	0.0443 (8)
C5	0.0762 (4)	0.2341 (4)	0.11517 (18)	0.0445 (7)
C6	0.0479 (4)	0.3899 (4)	0.11177 (18)	0.0468 (8)
C7	−0.0298 (4)	0.4573 (4)	0.03633 (18)	0.0447 (7)
C8	0.0387 (6)	−0.0963 (4)	−0.0221 (2)	0.0709 (11)
H8A	0.0682	−0.1996	−0.0074	0.106*
H8B	0.1169	−0.0610	−0.0627	0.106*
H8C	−0.0870	−0.0898	−0.0465	0.106*
C9	0.0388 (5)	0.0870 (5)	0.2365 (2)	0.0827 (13)
H9A	0.1068	0.0464	0.2871	0.124*
H9B	−0.0155	0.0056	0.2020	0.124*
H9C	−0.0560	0.1526	0.2523	0.124*
C10	0.1072 (6)	0.6268 (4)	0.1798 (2)	0.0699 (10)
H10A	0.1452	0.6680	0.2354	0.105*

H10B	−0.0122	0.6651	0.1592	0.105*
H10C	0.1933	0.6558	0.1412	0.105*
C11	0.6042 (4)	0.3894 (3)	0.17572 (18)	0.0413 (7)
C12	0.5381 (4)	0.3165 (3)	0.09221 (17)	0.0389 (7)
C13	0.4686 (4)	0.4063 (3)	0.02396 (17)	0.0417 (7)
H13	0.4595	0.5106	0.0303	0.050*
C14	0.4126 (4)	0.3378 (3)	−0.05409 (17)	0.0414 (7)
C15	0.4295 (4)	0.1813 (4)	−0.06306 (18)	0.0431 (7)
C16	0.4987 (4)	0.0940 (4)	0.00702 (19)	0.0454 (7)
C17	0.5527 (4)	0.1624 (3)	0.08492 (18)	0.0419 (7)
H17	0.5984	0.1044	0.1318	0.050*
C18	0.3239 (5)	0.5732 (4)	−0.1208 (2)	0.0571 (8)
H18A	0.2743	0.6122	−0.1755	0.086*
H18B	0.4418	0.6179	−0.1043	0.086*
H18C	0.2428	0.5973	−0.0791	0.086*
C19	0.4960 (6)	0.0527 (5)	−0.1884 (2)	0.0837 (12)
H19A	0.4354	0.0096	−0.2400	0.126*
H19B	0.5644	−0.0246	−0.1559	0.126*
H19C	0.5780	0.1312	−0.2024	0.126*
C20	0.5773 (7)	−0.1522 (4)	0.0628 (3)	0.0877 (14)
H20A	0.5782	−0.2558	0.0445	0.132*
H20B	0.4990	−0.1419	0.1072	0.132*
H20C	0.6996	−0.1216	0.0840	0.132*
O1	−0.2149 (3)	0.3553 (3)	−0.17842 (12)	0.0592 (6)
O2	−0.1847 (3)	0.5806 (3)	−0.11614 (14)	0.0617 (6)
H2	−0.2344	0.6076	−0.1630	0.093*
O3	0.0653 (3)	−0.0053 (3)	0.05251 (14)	0.0598 (6)
O4	0.1584 (3)	0.1701 (3)	0.18945 (13)	0.0590 (7)
O5	0.1003 (4)	0.4673 (3)	0.18502 (13)	0.0628 (6)
O6	0.6062 (4)	0.5329 (2)	0.17925 (14)	0.0608 (6)
O7	0.6579 (3)	0.3066 (2)	0.23837 (12)	0.0541 (6)
O8	0.3429 (3)	0.4135 (2)	−0.12612 (13)	0.0558 (6)
O9	0.3628 (3)	0.1150 (3)	−0.13918 (13)	0.0575 (6)
O10	0.5106 (3)	−0.0589 (3)	−0.00757 (14)	0.0615 (6)
H6	0.661 (7)	0.568 (6)	0.234 (2)	0.14 (2)*
H7	−0.064 (4)	0.565 (4)	0.0350 (18)	0.046 (8)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0456 (18)	0.051 (2)	0.0310 (15)	−0.0060 (15)	−0.0047 (12)	0.0086 (13)
C2	0.0339 (16)	0.054 (2)	0.0291 (14)	−0.0009 (13)	−0.0029 (12)	0.0098 (13)
C3	0.0480 (18)	0.051 (2)	0.0318 (15)	−0.0043 (14)	−0.0010 (13)	0.0044 (12)
C4	0.046 (2)	0.0479 (19)	0.0378 (17)	0.0009 (14)	−0.0010 (13)	0.0063 (14)
C5	0.0430 (17)	0.057 (2)	0.0313 (16)	0.0000 (15)	−0.0046 (13)	0.0122 (14)
C6	0.0467 (19)	0.058 (2)	0.0333 (16)	−0.0025 (15)	−0.0047 (14)	0.0053 (13)
C7	0.0487 (17)	0.051 (2)	0.0329 (15)	0.0030 (15)	−0.0043 (12)	0.0086 (13)
C8	0.099 (3)	0.058 (2)	0.055 (2)	0.002 (2)	0.007 (2)	−0.0005 (16)

C9	0.080 (3)	0.116 (4)	0.053 (2)	0.021 (2)	0.0102 (19)	0.042 (2)
C10	0.097 (3)	0.060 (2)	0.0473 (19)	−0.006 (2)	−0.0164 (18)	−0.0026 (16)
C11	0.0448 (17)	0.0470 (19)	0.0298 (14)	−0.0001 (14)	−0.0052 (12)	−0.0052 (13)
C12	0.0369 (17)	0.049 (2)	0.0292 (15)	−0.0046 (13)	−0.0028 (12)	−0.0073 (13)
C13	0.0453 (17)	0.0470 (19)	0.0309 (15)	−0.0012 (14)	−0.0039 (12)	−0.0043 (12)
C14	0.0424 (18)	0.051 (2)	0.0284 (16)	−0.0046 (14)	−0.0050 (13)	−0.0028 (13)
C15	0.0448 (17)	0.0515 (19)	0.0314 (15)	−0.0060 (14)	−0.0030 (13)	−0.0094 (13)
C16	0.0482 (19)	0.0428 (18)	0.0441 (18)	−0.0072 (15)	0.0007 (14)	−0.0076 (14)
C17	0.0492 (19)	0.043 (2)	0.0317 (15)	0.0009 (14)	−0.0010 (13)	0.0005 (12)
C18	0.066 (2)	0.059 (2)	0.0427 (18)	0.0059 (18)	−0.0086 (14)	0.0063 (15)
C19	0.087 (3)	0.114 (3)	0.053 (2)	−0.024 (2)	0.0203 (19)	−0.038 (2)
C20	0.139 (4)	0.045 (2)	0.073 (3)	−0.005 (2)	−0.016 (3)	0.0014 (18)
O1	0.0769 (16)	0.0596 (14)	0.0354 (12)	−0.0041 (12)	−0.0178 (10)	0.0064 (10)
O2	0.0873 (17)	0.0527 (16)	0.0389 (12)	0.0024 (13)	−0.0192 (10)	0.0081 (10)
O3	0.0867 (17)	0.0501 (15)	0.0410 (13)	0.0093 (12)	0.0007 (11)	0.0095 (10)
O4	0.0598 (14)	0.0743 (17)	0.0388 (13)	0.0058 (11)	−0.0125 (10)	0.0168 (11)
O5	0.0889 (17)	0.0606 (15)	0.0329 (12)	−0.0023 (13)	−0.0195 (11)	0.0012 (9)
O6	0.0958 (18)	0.0425 (14)	0.0385 (13)	0.0029 (12)	−0.0162 (11)	−0.0090 (9)
O7	0.0741 (15)	0.0502 (14)	0.0334 (11)	−0.0018 (11)	−0.0132 (10)	−0.0021 (9)
O8	0.0729 (16)	0.0597 (16)	0.0300 (11)	0.0019 (12)	−0.0152 (10)	−0.0018 (9)
O9	0.0653 (15)	0.0680 (15)	0.0359 (12)	−0.0065 (11)	−0.0083 (10)	−0.0180 (10)
O10	0.0888 (18)	0.0434 (13)	0.0489 (13)	−0.0058 (12)	−0.0066 (11)	−0.0093 (10)

Geometric parameters (Å, °)

C1—O1	1.243 (4)	C11—O6	1.269 (3)
C1—O2	1.279 (4)	C11—C12	1.495 (4)
C1—C2	1.489 (4)	C12—C17	1.372 (4)
C2—C3	1.373 (4)	C12—C13	1.386 (4)
C2—C7	1.392 (4)	C13—C14	1.390 (4)
C3—C4	1.403 (4)	C13—H13	0.9300
C3—H3	0.9300	C14—O8	1.365 (3)
C4—O3	1.361 (4)	C14—C15	1.396 (4)
C4—C5	1.386 (4)	C15—O9	1.374 (3)
C5—O4	1.375 (3)	C15—C16	1.394 (4)
C5—C6	1.391 (4)	C16—O10	1.374 (4)
C6—O5	1.359 (4)	C16—C17	1.385 (4)
C6—C7	1.392 (4)	C17—H17	0.9300
C7—H7	0.99 (3)	C18—O8	1.420 (4)
C8—O3	1.418 (4)	C18—H18A	0.9600
C8—H8A	0.9600	C18—H18B	0.9600
C8—H8B	0.9600	C18—H18C	0.9600
C8—H8C	0.9600	C19—O9	1.426 (4)
C9—O4	1.417 (4)	C19—H19A	0.9600
C9—H9A	0.9600	C19—H19B	0.9600
C9—H9B	0.9600	C19—H19C	0.9600
C9—H9C	0.9600	C20—O10	1.422 (5)
C10—O5	1.413 (4)	C20—H20A	0.9600
C10—H10A	0.9600	C20—H20B	0.9600

C10—H10B	0.9600	C20—H20C	0.9600
C10—H10C	0.9600	O2—H2	0.8200
C11—O7	1.255 (3)	O6—H6	0.96 (2)
C1—O2—H2	109.5	H10A—C10—H10B	109.5
C4—O3—C8	117.4 (3)	O5—C10—H10C	109.5
C5—O4—C9	114.9 (2)	H10A—C10—H10C	109.5
C6—O5—C10	117.5 (2)	H10B—C10—H10C	109.5
C11—O6—H6	111 (3)	O7—C11—O6	123.1 (3)
C14—O8—C18	117.9 (2)	O7—C11—C12	118.9 (3)
C15—O9—C19	116.2 (2)	O6—C11—C12	118.0 (3)
C16—O10—C20	117.5 (2)	C17—C12—C13	121.9 (2)
O1—C1—O2	123.1 (3)	C17—C12—C11	118.7 (2)
O1—C1—C2	119.8 (3)	C13—C12—C11	119.4 (3)
O2—C1—C2	117.0 (3)	C12—C13—C14	118.9 (3)
C3—C2—C7	121.4 (2)	C12—C13—H13	120.6
C3—C2—C1	118.9 (3)	C14—C13—H13	120.6
C7—C2—C1	119.7 (3)	O8—C14—C13	124.5 (3)
C2—C3—C4	119.5 (3)	O8—C14—C15	115.4 (2)
C2—C3—H3	120.3	C13—C14—C15	120.0 (2)
C4—C3—H3	120.3	O9—C15—C16	121.1 (3)
O3—C4—C5	116.1 (3)	O9—C15—C14	118.9 (3)
O3—C4—C3	124.2 (3)	C16—C15—C14	119.7 (2)
C5—C4—C3	119.6 (3)	O10—C16—C17	124.1 (3)
O4—C5—C4	120.3 (3)	O10—C16—C15	115.8 (2)
O4—C5—C6	119.2 (3)	C17—C16—C15	120.1 (3)
C4—C5—C6	120.4 (3)	C12—C17—C16	119.4 (3)
O5—C6—C7	123.9 (3)	C12—C17—H17	120.3
O5—C6—C5	116.0 (2)	C16—C17—H17	120.3
C7—C6—C5	120.0 (3)	O8—C18—H18A	109.5
C6—C7—C2	119.0 (3)	O8—C18—H18B	109.5
C6—C7—H7	120.7 (17)	H18A—C18—H18B	109.5
C2—C7—H7	119.9 (17)	O8—C18—H18C	109.5
O3—C8—H8A	109.5	H18A—C18—H18C	109.5
O3—C8—H8B	109.5	H18B—C18—H18C	109.5
H8A—C8—H8B	109.5	O9—C19—H19A	109.5
O3—C8—H8C	109.5	O9—C19—H19B	109.5
H8A—C8—H8C	109.5	H19A—C19—H19B	109.5
H8B—C8—H8C	109.5	O9—C19—H19C	109.5
O4—C9—H9A	109.5	H19A—C19—H19C	109.5
O4—C9—H9B	109.5	H19B—C19—H19C	109.5
H9A—C9—H9B	109.5	O10—C20—H20A	109.5
O4—C9—H9C	109.5	O10—C20—H20B	109.5
H9A—C9—H9C	109.5	H20A—C20—H20B	109.5
H9B—C9—H9C	109.5	O10—C20—H20C	109.5
O5—C10—H10A	109.5	H20A—C20—H20C	109.5
O5—C10—H10B	109.5	H20B—C20—H20C	109.5
O1—C1—C2—C3	2.0 (4)	C12—C13—C14—O8	−179.6 (3)
O2—C1—C2—C3	−177.5 (3)	C12—C13—C14—C15	−1.0 (4)

O1—C1—C2—C7	−176.8 (3)	O8—C14—C15—O9	−5.3 (4)
O2—C1—C2—C7	3.6 (4)	C13—C14—C15—O9	176.0 (3)
C7—C2—C3—C4	1.1 (5)	O8—C14—C15—C16	−179.7 (3)
C1—C2—C3—C4	−177.7 (3)	C13—C14—C15—C16	1.5 (5)
C2—C3—C4—O3	179.9 (3)	O9—C15—C16—O10	5.6 (5)
C2—C3—C4—C5	−0.6 (4)	C14—C15—C16—O10	−180.0 (3)
O3—C4—C5—O4	2.1 (4)	O9—C15—C16—C17	−175.2 (3)
C3—C4—C5—O4	−177.4 (3)	C14—C15—C16—C17	−0.9 (5)
O3—C4—C5—C6	179.1 (3)	C13—C12—C17—C16	0.8 (5)
C3—C4—C5—C6	−0.5 (5)	C11—C12—C17—C16	−177.5 (3)
O4—C5—C6—O5	−2.0 (4)	O10—C16—C17—C12	178.8 (3)
C4—C5—C6—O5	−178.9 (3)	C15—C16—C17—C12	−0.3 (5)
O4—C5—C6—C7	178.0 (3)	C5—C4—O3—C8	−173.1 (3)
C4—C5—C6—C7	1.0 (5)	C3—C4—O3—C8	6.4 (4)
O5—C6—C7—C2	179.5 (3)	C4—C5—O4—C9	−76.3 (4)
C5—C6—C7—C2	−0.5 (5)	C6—C5—O4—C9	106.8 (4)
C3—C2—C7—C6	−0.6 (5)	C7—C6—O5—C10	−12.0 (5)
C1—C2—C7—C6	178.2 (3)	C5—C6—O5—C10	168.0 (3)
O7—C11—C12—C17	−5.4 (4)	C13—C14—O8—C18	−0.9 (4)
O6—C11—C12—C17	173.4 (3)	C15—C14—O8—C18	−179.6 (3)
O7—C11—C12—C13	176.3 (3)	C16—C15—O9—C19	−73.3 (4)
O6—C11—C12—C13	−5.0 (4)	C14—C15—O9—C19	112.3 (4)
C17—C12—C13—C14	−0.2 (4)	C17—C16—O10—C20	2.0 (5)
C11—C12—C13—C14	178.1 (3)	C15—C16—O10—C20	−178.9 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C9—H9C···O7^{i}	0.96	2.49	3.405 (4)	159
C18—H18A···O5^{ii}	0.96	2.51	3.321 (4)	142
C19—H19C···O1^{iii}	0.96	2.50	3.404 (5)	158
O2—H2···O7^{iv}	0.82	1.83	2.641 (3)	172
O6—H6···O1^{v}	0.96 (2)	1.71 (2)	2.656 (3)	170 (5)

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

Fig. 1

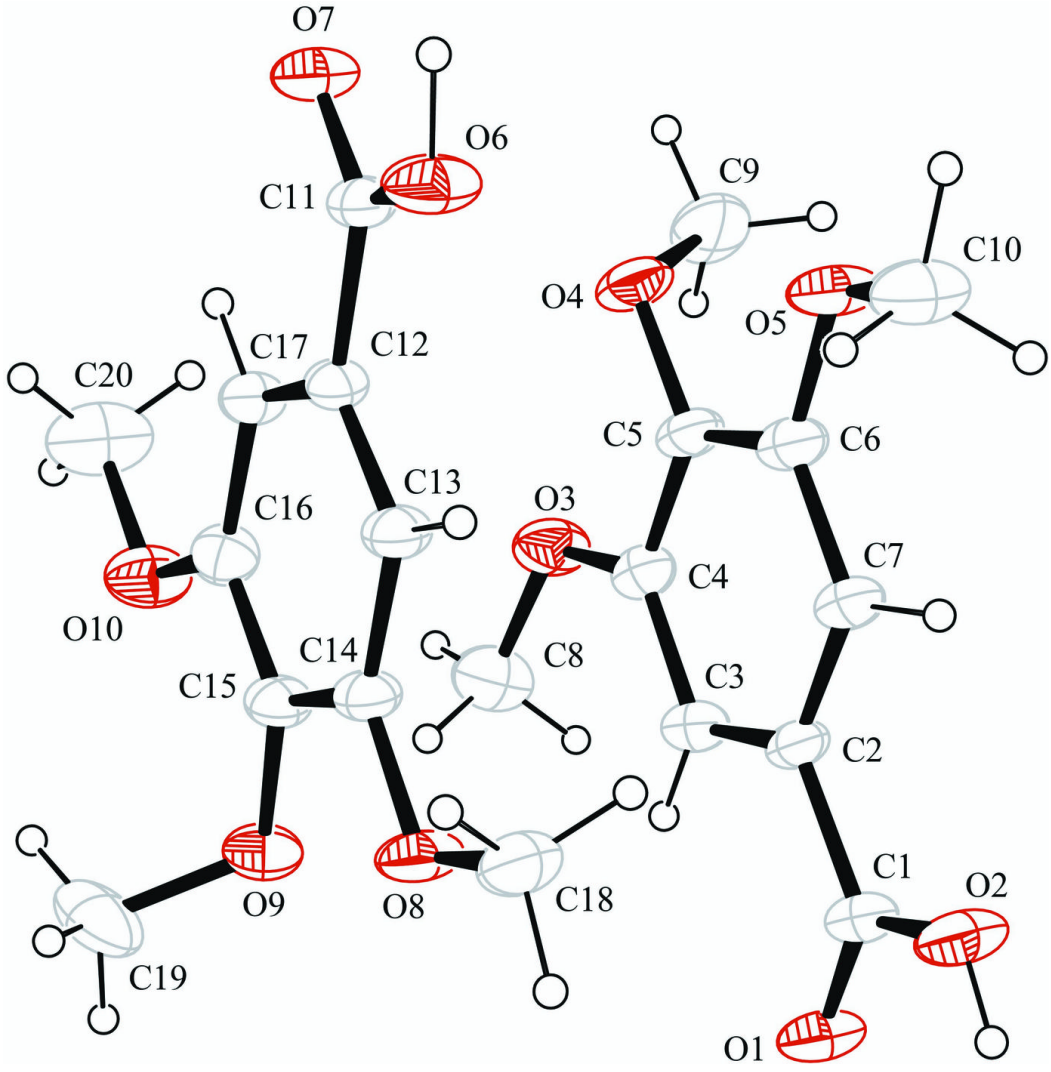
O7
O6
C11
C9
C10
O4
O5
C17
C12
C20
C5
C6
C16
C13
O3
C4
C7
O10
C14
C8
C3
C15
C2
C1
O2
O9
O8
C18
C19
O1

Fig. 2