Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(+)-(1*R*,2*S*,3*R*)-2-[(Benzyloxycarbonyl)-methyl]-3-phenylcyclopropanecarboxylic acid

Thomas D. Avery,[a] Ben W. Greatrex,[a] Dennis K. Taylor[b]* and Edward R. T. Tiekink[c]*

[a]Department of Chemistry, University of Adelaide, 5005 South Australia, Australia, [b]Department of Wine and Horticulture, University of Adelaide, Waite Campus, Glen Osmond, 5064 South Australia, Australia, and [c]Department of Chemistry, University of Texas at San Antonio, One UTSA Circle, San Antonio, TX 78249-0698, USA
Correspondence e-mail: dennis.taylor@adelaide.edu.au, edward.tiekink@utsa.edu

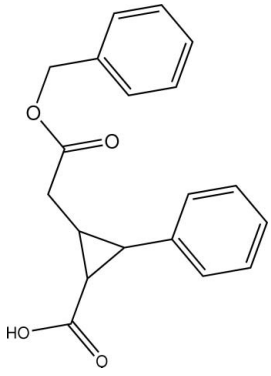
Received 14 June 2007; accepted 25 June 2007

Key indicators: single-crystal X-ray study; T = 223 K; mean σ(C–C) = 0.003 Å; R factor = 0.048; wR factor = 0.149; data-to-parameter ratio = 17.4.

In the title compound, $C_{19}H_{18}O_4$, the carboxyl group lies on the opposite side of the cyclopropane ring to the other substituents. Molecules associate *via* $(\cdots HOC{=}O)_2$ synthons around centres of symmetry and are linked into double layers by cooperative C—H···O contacts.

Related literature

For related literature, see: Avery *et al.* (2000, 2001).



Experimental

Crystal data

$C_{19}H_{18}O_4$
M_r = 310.33
Triclinic, $P\overline{1}$
a = 5.5550 (5) Å
b = 8.9606 (8) Å
c = 16.6586 (16) Å
α = 101.698 (2)°
β = 98.907 (2)°
γ = 92.186 (2)°
V = 800.11 (13) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 223 (2) K
0.39 × 0.09 × 0.08 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: none
5723 measured reflections
3668 independent reflections
2831 reflections with $I > 2\sigma(I)$
R_{int} = 0.015

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.149
S = 1.06
3668 reflections
211 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3O···O4^{i}	0.84	1.78	2.6224 (16)	176
C1—H1···O1^{ii}	0.99	2.36	3.249 (2)	149
C5—H5*B*···O1^{ii}	0.98	2.53	3.219 (2)	127
C7—H7*A*···O3^{iii}	0.98	2.55	3.368 (2)	141

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *SHELXL97*.

The authors are grateful to the Australian Research Council for financial support. We also thank the Faculty of Science, University of Adelaide, for Postgraduate Scholarships to TDA and BWG.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2238).

References

Altomare, A., Cascarano, M., Giacovazzo, C., Guagliardi, A., Burla, M. C., Polidori, G. & Camalli, M. (1994). *J. Appl. Cryst.* **27**, 435.
Avery, T. D., Fallon, G., Greatrex, B. W., Pyke, S. M., Taylor, D. K. & Tiekink, E. R. T. (2001). *J. Org. Chem.* **66**, 7955–7966.
Avery, T. D., Taylor, D. K. & Tiekink, E. R. T. (2000). *J. Org. Chem.* **65**, 5531–5546.
Brandenburg, K. (2006). *DIAMOND*. Release 3.1. Crystal Impact GbR, Bonn, Germany.
Bruker (2000). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Johnson, C. K. (1976). *ORTEPII*. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.

  doi:10.1107/S1600536807030838

supplementary materials

Acta Cryst. (2007). E**63**, o3344 [**doi:10.1107/S1600536807030838**]

(+)-(1*R*,2*S*,3*R*)-2-[(Benzyloxycarbonyl)methyl]-3-phenylcyclopropanecarboxylic acid

T. D. Avery, B. W. Greatrex, D. K. Taylor and E. R. T. Tiekink

Comment

The title compound (I) was synthesized in the course of an investigation of selective deprotections of cyclopropanes generated through the reaction of 1,2-dioxines and stabilized phosphorus ylides (Avery *et al.*, 2000, 2001). The molecular structure (Fig. 1) shows the carboxylic acid functional group at the C1 atom to lie to the opposite side of the cyclopropane ring to the substituents at the C2 and C3 atoms. Centrosymmetrically related molecules are connected by the familiar $\{\cdots HOC{=}O\}_2$ synthon and these are connected into a double layer *via* C—H···O contacts (Table 1). The double layers thus formed stack along the c-direction, being separated by hydrophobic interactions (Fig. 2).

Experimental

To a solution of potassium carbonate (335 mg, 1.31 mmol) in water (10 ml) was added a solution of ±(1*R*,2S,3*R*)-phenyl 2-(2-(benzyloxy)-2-oxoethyl)-3- phenylcyclopropanecarboxylate (950 mg, 2.46 mmol) in acetone (10 ml). The mixture was allowed to stir overnight after which time the acetone was removed *in vacuo* and the aqueous solution acidified (conc. HCl). The solution was then extracted with ethyl acetate (3 *x* 20 ml), dried ($MgSO_4$), filtered and the volatiles removed *in vacuo* to give a crude solid consisting of (I) and phenol. Phenol was removed by sublimation and the crude acid recrystallized (dichloromethane/hexanes) to give (I) (701 mg, 92%) as a colourless solid. *M*.p 409–411 K. Elemental analysis found: C 73.50, H, 5.97%; $C_{19}H_{18}O_4$ requires: C 73.53, H, 5.85%. IR: 2538, 1732, 1682, 1603, 1449, 1240, 1170, 961 cm^{-1}. ^1H NMR ($CDCl_3$, 300 MHz) δ 2.03 (t, J = 3.9 Hz, 1H), 2.15–2.26 (m, 3H), 2.91–3.00 (m, 1H), 5.03–5.12 (m, 2H), 7.15–7.34 (m, 10H), 12.20 (bs, 1H). ^{13}C NMR ($CDCl_3$, 75 MHz) δ 24.5, 24.6, 31.3, 32.7, 66.4, 127.0, 128.2, 128.2, 128.4, 128.5, 128.8, 134.8, 135.6, 171.5, 179.6.

Refinement

All C-bound H atoms were included in the riding-model approximation, with C—H = 0.94 to 0.99 Å, and with U_{iso}(H) = 1.5U_{eq}(methyl-C) or 1.2U_{eq}(remaining-C). The hydroxyl-H atoms were located from a difference map and included so that O—H = 0.84 Å and U_{iso}(H) = 1.5U_{eq}(O).

Figures

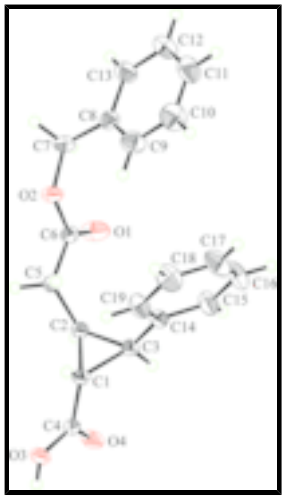


Fig. 1. Molecular structure of (I) showing atom-labelling scheme and displacement ellipsoids at the 50% probability level.

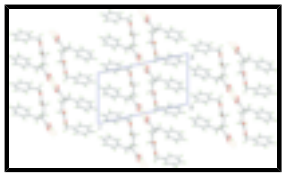


Fig. 2. View of the unit-cell contents of (I) highlighting the stacking of double layers along the c-direction. Hydrogen bonds are shown as orange-dashed lines. Colour code: red (oxygen), grey (carbon) and green (hydrogen).

(+)-(1*R*,2S,3*R*)-2-[(Benzyloxycarbonyl)methyl]-3-phenylcyclopropanecarboxylic acid

Crystal data

$C_{19}H_{18}O_4$	$Z = 2$
$M_r = 310.33$	$F_{000} = 328$
Triclinic, $P\bar{1}$	$D_x = 1.288$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71069$ Å
$a = 5.5550$ (5) Å	Cell parameters from 1829 reflections
$b = 8.9606$ (8) Å	$\theta = 2.5$–29.3º
$c = 16.6586$ (16) Å	$\mu = 0.09$ mm^{-1}
$\alpha = 101.698$ (2)º	$T = 223$ (2) K
$\beta = 98.907$ (2)º	Prism, colourless
$\gamma = 92.186$ (2)º	0.39 × 0.09 × 0.08 mm
$V = 800.11$ (13) Å^3	

Data collection

Bruker SMART CCD area-detector diffractometer	2831 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{int} = 0.015$
Monochromator: graphite	$\theta_{max} = 27.5$º
$T = 223(2)$ K	$\theta_{min} = 1.3$º
ω and φ scans	$h = -6 \rightarrow 7$

Absorption correction: none
5723 measured reflections
3668 independent reflections

$k = -11 \rightarrow 11$
$l = -16 \rightarrow 21$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.149$
$S = 1.06$
3668 reflections
211 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
$w = 1/[\sigma^2(F_o^2) + (0.0829P)^2 + 0.0916P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.28$ e Å^{-3}
$\Delta\rho_{min} = -0.25$ e Å^{-3}
Extinction correction: none

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 $F^2 > 2$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}
O1	0.6349 (2)	0.36870 (14)	0.37643 (10)	0.0613 (4)
O2	0.3799 (2)	0.16367 (12)	0.36059 (7)	0.0399 (3)
O3	−0.1845 (2)	0.82536 (12)	0.46136 (7)	0.0394 (3)
H3O	−0.1801	0.9142	0.4903	0.059*
O4	0.1916 (2)	0.90033 (12)	0.44703 (8)	0.0452 (3)
C1	0.0252 (3)	0.65051 (15)	0.38033 (9)	0.0302 (3)
H1	−0.1308	0.5863	0.3652	0.036*
C2	0.2544 (3)	0.56716 (15)	0.39526 (9)	0.0303 (3)
H2	0.3883	0.6259	0.4373	0.036*
C3	0.1967 (3)	0.62665 (16)	0.31702 (9)	0.0310 (3)
H3	0.2983	0.7201	0.3174	0.037*
C4	0.0177 (3)	0.80346 (16)	0.43215 (9)	0.0304 (3)
C5	0.2214 (3)	0.40048 (16)	0.39673 (10)	0.0329 (3)
H5A	0.1921	0.3908	0.4520	0.040*

H5B	0.0766	0.3547	0.3565	0.040*
C6	0.4366 (3)	0.31359 (16)	0.37669 (9)	0.0311 (3)
C7	0.5724 (3)	0.06418 (18)	0.34375 (11)	0.0406 (4)
H7A	0.5573	−0.0223	0.3709	0.049*
H7B	0.7306	0.1202	0.3678	0.049*
C8	0.5662 (3)	0.00447 (18)	0.25231 (10)	0.0383 (4)
C9	0.3839 (4)	0.0327 (2)	0.19188 (12)	0.0541 (5)
H9	0.2593	0.0952	0.2071	0.065*
C10	0.3848 (4)	−0.0311 (3)	0.10899 (13)	0.0675 (6)
H10	0.2614	−0.0104	0.0682	0.081*
C11	0.5631 (4)	−0.1240 (3)	0.08567 (13)	0.0633 (6)
H11	0.5609	−0.1678	0.0293	0.076*
C12	0.7448 (4)	−0.1528 (3)	0.14513 (14)	0.0658 (6)
H12	0.8676	−0.2164	0.1295	0.079*
C13	0.7477 (4)	−0.0882 (2)	0.22818 (12)	0.0528 (5)
H13	0.8740	−0.1073	0.2686	0.063*
C14	0.1254 (3)	0.52696 (17)	0.23264 (9)	0.0353 (3)
C15	0.2719 (4)	0.5390 (2)	0.17366 (11)	0.0518 (5)
H15	0.4093	0.6094	0.1877	0.062*
C16	0.2179 (4)	0.4483 (3)	0.09420 (12)	0.0691 (6)
H16	0.3182	0.4582	0.0547	0.083*
C17	0.0195 (4)	0.3443 (3)	0.07291 (12)	0.0686 (6)
H17	−0.0164	0.2829	0.0191	0.082*
C18	−0.1257 (4)	0.3304 (3)	0.13032 (13)	0.0642 (6)
H18	−0.2607	0.2582	0.1160	0.077*
C19	−0.0758 (3)	0.4221 (2)	0.20976 (11)	0.0493 (4)
H19	−0.1794	0.4128	0.2483	0.059*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0349 (7)	0.0366 (7)	0.1152 (12)	0.0015 (5)	0.0257 (7)	0.0124 (7)
O2	0.0382 (6)	0.0256 (5)	0.0574 (7)	0.0056 (4)	0.0150 (5)	0.0061 (5)
O3	0.0428 (6)	0.0286 (5)	0.0475 (7)	0.0068 (5)	0.0182 (5)	0.0005 (5)
O4	0.0479 (7)	0.0284 (6)	0.0572 (7)	−0.0027 (5)	0.0216 (5)	−0.0047 (5)
C1	0.0340 (7)	0.0239 (7)	0.0332 (7)	0.0029 (5)	0.0096 (6)	0.0038 (5)
C2	0.0310 (7)	0.0268 (7)	0.0324 (7)	0.0032 (5)	0.0071 (5)	0.0033 (5)
C3	0.0358 (7)	0.0248 (7)	0.0330 (7)	0.0025 (6)	0.0103 (6)	0.0042 (5)
C4	0.0380 (8)	0.0259 (7)	0.0298 (7)	0.0062 (6)	0.0101 (6)	0.0074 (5)
C5	0.0323 (7)	0.0287 (7)	0.0406 (8)	0.0048 (6)	0.0107 (6)	0.0096 (6)
C6	0.0326 (7)	0.0279 (7)	0.0339 (7)	0.0036 (6)	0.0069 (6)	0.0082 (6)
C7	0.0439 (9)	0.0315 (8)	0.0479 (9)	0.0129 (7)	0.0101 (7)	0.0084 (7)
C8	0.0393 (8)	0.0319 (8)	0.0453 (9)	0.0024 (6)	0.0102 (7)	0.0093 (6)
C9	0.0476 (10)	0.0559 (11)	0.0556 (11)	0.0108 (9)	0.0034 (8)	0.0068 (9)
C10	0.0643 (13)	0.0805 (15)	0.0504 (11)	0.0058 (11)	−0.0047 (10)	0.0078 (10)
C11	0.0728 (14)	0.0686 (14)	0.0447 (11)	−0.0010 (11)	0.0141 (10)	0.0006 (9)
C12	0.0713 (14)	0.0698 (14)	0.0608 (12)	0.0204 (11)	0.0308 (11)	0.0066 (10)
C13	0.0532 (11)	0.0608 (12)	0.0489 (10)	0.0212 (9)	0.0154 (8)	0.0132 (9)

C14	0.0412 (8)	0.0342 (8)	0.0311 (7)	0.0082 (6)	0.0088 (6)	0.0052 (6)
C15	0.0569 (11)	0.0581 (11)	0.0412 (9)	0.0003 (9)	0.0191 (8)	0.0048 (8)
C16	0.0796 (15)	0.0891 (16)	0.0400 (10)	0.0082 (13)	0.0283 (10)	0.0025 (10)
C17	0.0748 (14)	0.0848 (16)	0.0350 (10)	0.0105 (12)	0.0057 (9)	−0.0112 (10)
C18	0.0590 (12)	0.0728 (14)	0.0472 (11)	−0.0076 (10)	−0.0005 (9)	−0.0099 (9)
C19	0.0467 (9)	0.0589 (11)	0.0369 (9)	−0.0040 (8)	0.0085 (7)	−0.0018 (8)

Geometric parameters (Å, °)

O1—C6	1.1910 (18)	C8—C9	1.382 (3)
O2—C6	1.3309 (18)	C9—C10	1.384 (3)
O2—C7	1.4424 (18)	C9—H9	0.9400
O3—C4	1.2978 (18)	C10—C11	1.369 (3)
O3—H3O	0.8401	C10—H10	0.9400
O4—C4	1.2338 (18)	C11—C12	1.371 (3)
C1—C4	1.4701 (19)	C11—H11	0.9400
C1—C2	1.514 (2)	C12—C13	1.385 (3)
C1—C3	1.5168 (19)	C12—H12	0.9400
C1—H1	0.9900	C13—H13	0.9400
C2—C3	1.500 (2)	C14—C19	1.386 (2)
C2—C5	1.5035 (19)	C14—C15	1.387 (2)
C2—H2	0.9900	C15—C16	1.387 (3)
C3—C14	1.491 (2)	C15—H15	0.9400
C3—H3	0.9900	C16—C17	1.369 (3)
C5—C6	1.495 (2)	C16—H16	0.9400
C5—H5A	0.9800	C17—C18	1.364 (3)
C5—H5B	0.9800	C17—H17	0.9400
C7—C8	1.503 (2)	C18—C19	1.390 (2)
C7—H7A	0.9800	C18—H18	0.9400
C7—H7B	0.9800	C19—H19	0.9400
C8—C13	1.386 (2)		
C6—O2—C7	117.49 (12)	H7A—C7—H7B	107.8
C4—O3—H3O	110.5	C13—C8—C9	118.80 (17)
C4—C1—C2	117.76 (12)	C13—C8—C7	117.95 (15)
C4—C1—C3	119.46 (12)	C9—C8—C7	123.20 (15)
C2—C1—C3	59.35 (9)	C10—C9—C8	120.03 (18)
C4—C1—H1	116.1	C10—C9—H9	120.0
C2—C1—H1	116.1	C8—C9—H9	120.0
C3—C1—H1	116.1	C11—C10—C9	120.9 (2)
C3—C2—C5	122.65 (12)	C11—C10—H10	119.6
C3—C2—C1	60.43 (9)	C9—C10—H10	119.6
C5—C2—C1	117.10 (12)	C10—C11—C12	119.57 (19)
C3—C2—H2	115.2	C10—C11—H11	120.2
C5—C2—H2	115.2	C12—C11—H11	120.2
C1—C2—H2	115.2	C11—C12—C13	120.13 (19)
C14—C3—C2	123.86 (12)	C11—C12—H12	119.9
C14—C3—C1	122.54 (13)	C13—C12—H12	119.9
C2—C3—C1	60.22 (9)	C8—C13—C12	120.59 (18)
C14—C3—H3	113.4	C8—C13—H13	119.7

C2—C3—H3	113.4	C12—C13—H13	119.7
C1—C3—H3	113.4	C19—C14—C15	118.04 (15)
O4—C4—O3	123.72 (13)	C19—C14—C3	124.23 (14)
O4—C4—C1	122.19 (13)	C15—C14—C3	117.73 (15)
O3—C4—C1	114.08 (13)	C14—C15—C16	120.75 (19)
C6—C5—C2	113.23 (12)	C14—C15—H15	119.6
C6—C5—H5A	108.9	C16—C15—H15	119.6
C2—C5—H5A	108.9	C17—C16—C15	120.40 (19)
C6—C5—H5B	108.9	C17—C16—H16	119.8
C2—C5—H5B	108.9	C15—C16—H16	119.8
H5A—C5—H5B	107.7	C18—C17—C16	119.61 (18)
O1—C6—O2	123.53 (14)	C18—C17—H17	120.2
O1—C6—C5	125.52 (14)	C16—C17—H17	120.2
O2—C6—C5	110.94 (12)	C17—C18—C19	120.6 (2)
O2—C7—C8	112.59 (13)	C17—C18—H18	119.7
O2—C7—H7A	109.1	C19—C18—H18	119.7
C8—C7—H7A	109.1	C14—C19—C18	120.60 (17)
O2—C7—H7B	109.1	C14—C19—H19	119.7
C8—C7—H7B	109.1	C18—C19—H19	119.7
C4—C1—C2—C3	−109.52 (14)	O2—C7—C8—C9	−4.8 (2)
C4—C1—C2—C5	136.49 (13)	C13—C8—C9—C10	0.0 (3)
C3—C1—C2—C5	−113.99 (14)	C7—C8—C9—C10	−177.41 (18)
C5—C2—C3—C14	−6.3 (2)	C8—C9—C10—C11	0.8 (3)
C1—C2—C3—C14	−111.25 (16)	C9—C10—C11—C12	−0.8 (4)
C5—C2—C3—C1	104.97 (15)	C10—C11—C12—C13	0.0 (4)
C4—C1—C3—C14	−139.96 (14)	C9—C8—C13—C12	−0.8 (3)
C2—C1—C3—C14	113.35 (15)	C7—C8—C13—C12	176.76 (18)
C4—C1—C3—C2	106.68 (15)	C11—C12—C13—C8	0.8 (3)
C2—C1—C4—O4	44.4 (2)	C2—C3—C14—C19	58.9 (2)
C3—C1—C4—O4	−24.3 (2)	C1—C3—C14—C19	−14.8 (2)
C2—C1—C4—O3	−134.54 (13)	C2—C3—C14—C15	−120.33 (17)
C3—C1—C4—O3	156.83 (13)	C1—C3—C14—C15	166.00 (15)
C3—C2—C5—C6	85.53 (17)	C19—C14—C15—C16	−0.1 (3)
C1—C2—C5—C6	156.23 (12)	C3—C14—C15—C16	179.20 (18)
C7—O2—C6—O1	1.3 (2)	C14—C15—C16—C17	−0.5 (4)
C7—O2—C6—C5	−177.29 (13)	C15—C16—C17—C18	0.1 (4)
C2—C5—C6—O1	15.3 (2)	C16—C17—C18—C19	0.8 (4)
C2—C5—C6—O2	−166.14 (12)	C15—C14—C19—C18	1.0 (3)
C6—O2—C7—C8	−98.97 (16)	C3—C14—C19—C18	−178.22 (18)
O2—C7—C8—C13	177.73 (15)	C17—C18—C19—C14	−1.4 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3O···O4^{i}	0.84	1.78	2.6224 (16)	176
C1—H1···O1^{ii}	0.99	2.36	3.249 (2)	149
C5—H5B···O1^{ii}	0.98	2.53	3.219 (2)	127
C7—H7A···O3^{iii}	0.98	2.55	3.368 (2)	141

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

Fig. 1

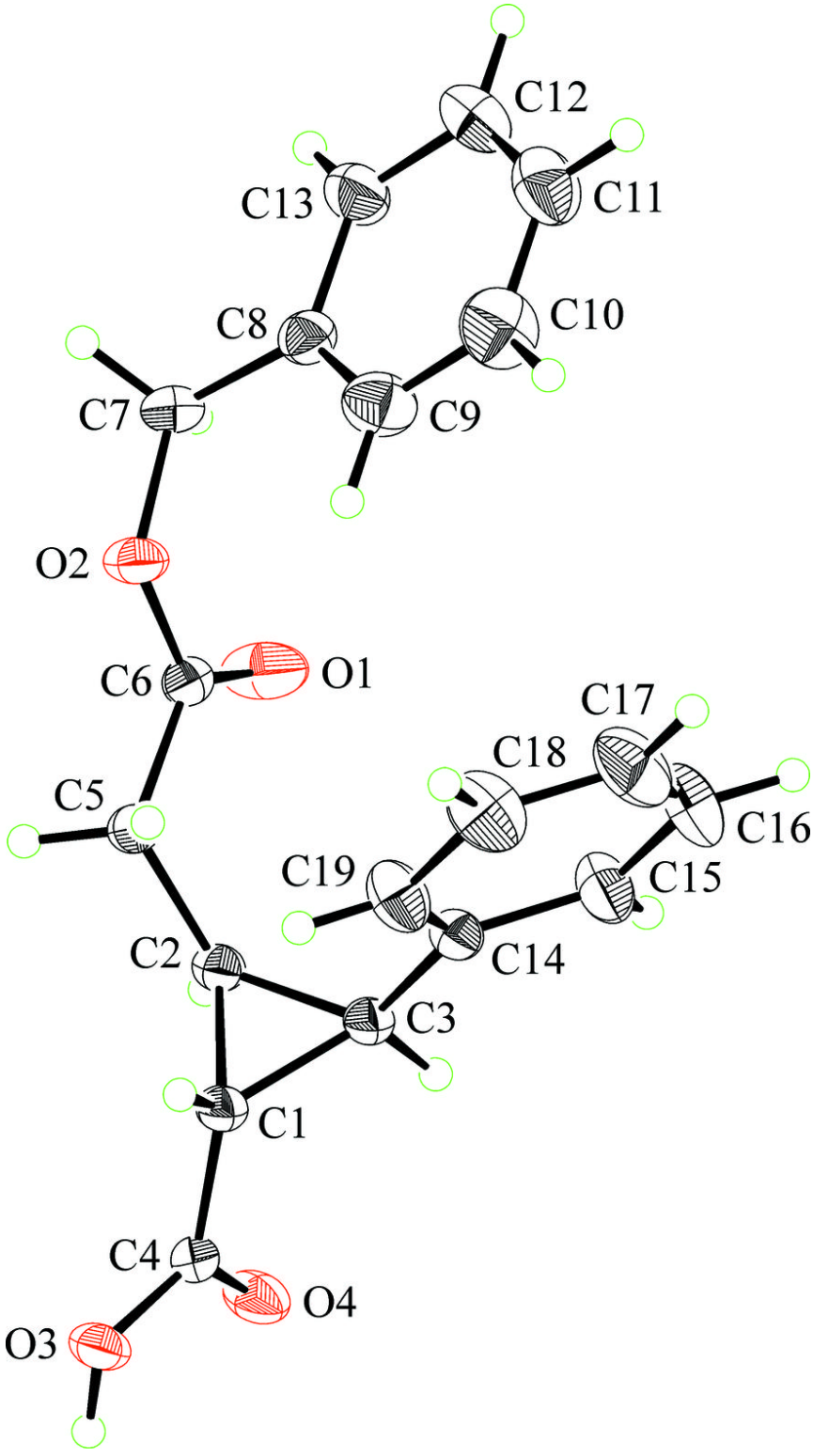


Fig. 2