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Ethyl 2-(4-benzoyl-2,5-dimethylphenoxy)acetate

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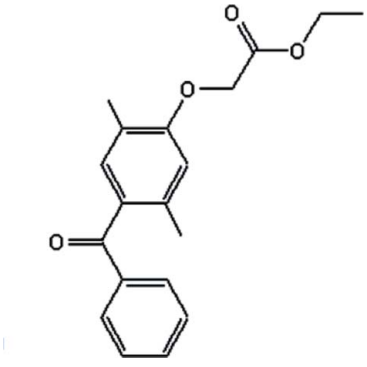
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.003 Å; R factor = 0.057; wR factor = 0.173; data-to-parameter ratio = 16.2.

The title compound, $C_{19}H_{20}O_4$, was synthesized *via* a Fries rearrangement of hydroxy benzophenone. The dihedral angle between the least-squares planes of the two benzene rings is 69.04 (11)°. The molecular structure displays an intramolecular non-classical C—H···O hydrogen bond.

Related literature

hydroxy benzophenones may obtained from natural products, see: Henry *et al.* (1999); Vidya *et al.* (2003); Cuesta-Rubio *et al.* (2002) and by synthetic methods, see: Hsieh *et al.* (2003); Revesz *et al.* (2004); Schlitzer *et al.* (2002). For their biological activity, see: Jiri *et al.* (1991); Palomer *et al.* (2000, 2002); Palaska *et al.* (2002); Khanum *et al.* (2004*a*,*b*). Benzophenone analogues with nitro substituents exhibit significant *in vivo* antitumor activity and they have been reported to show activity as immunomodulators, see: Leonard (1997). Nitro benzophenone derivatives show strong cytotoxic activity while the corresponding aminobenzophenone derivatives show weak activity, see: Kumazawa *et al.* (1997). For the antimicobial activity of benzophenone derivatives, see: Selvi *et al.* (2003).



Experimental

Crystal data

$C_{19}H_{20}O_4$
M_r = 312.35
Triclinic, $P\overline{1}$
a = 8.148 (4) Å
b = 8.635 (4) Å
c = 13.029 (7) Å
α = 84.054 (8)°
β = 81.176 (8)°
γ = 66.559 (7)°
V = 830.2 (7) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 295 K
0.21 × 0.20 × 0.10 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.982, T_{max} = 0.991
8847 measured reflections
3391 independent reflections
2630 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.173
S = 1.05
3391 reflections
209 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.36 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
C15—H15A···O2	0.96	2.28	2.751 (3)	110

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1999); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RK2174).

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S1. Comment

Hydroxy benzophenones are achieved from natural products (Henry *et al.*, 1999; Vidya *et al.*, 2003; Cuesta-Rubio *et al.*, 2002) as well as by synthetic methods (Hsieh *et al.*, 2003; Schlitzer *et al.*, 2002; Revesz *et al.*, 2004). The great importance of these substances is essentially due to the diverse biological and chemical properties they acquire. Benzophenone analogues possess a high analgesic (Jiri *et al.*, 1991) efficacy and also endowed with anti-inflammatory property (Palomer *et al.*, 2000; Palomer *et al.*, 2002; Palaska *et al.*, 2002; Khanum *et al.*, 2004a,b).

Benzophenone analogues with nitro substituent exhibit significant *in vivo* antitumor activity and they have been reported to show activity as immunomodulators (Leonard, 1997). Based on these report, *in vitro* and *in vivo* studies of a series of novel nitro- and amino-substituted benzophenones have been investigated as potential anticancer agents. Nitro benzophenone derivative showed strong cytotoxic activity while the corresponding aminobenzophenone derivatives showed weak activity (Kumazawa *et al.*, 1997). Besides benzophenone derivatives endowed with anti-microbial activity, for instance isoprenylated benzophenone, at its lower concentration of 500 to 1000 p.p.m. inhibits aflatoxin production in *Aspergillus flavus*, relatively greater than inhibition growth of the fungus - Selvi *et al.*, (2003).

The molecular structure of title compound is shown on Fig.1. The dihedral angle between least-squares planes (two phenyl rings) is 69.04 (11)°. The intramolecular non-classical C–H···O hydrogen bond (Table 1) is observed.

S2. Experimental

2,5-Dimethyl phenyl benzoate was synthesized from 2,5-dimethyl phenol and benzoyl chloride in presence of 10% sodium hydroxide. 4-Hydroxy-2,5-dimethyl benzophenone was achieved from 2,5-dimethyl phenyl benzoate by Fries rearrangement.

In a typical procedure, a mixture of 4-hydroxy-2,5-dimethylbenzophenone (4.5 g, 0.02 mol) and ethylchloroacetate (2.4 g, 0.02 mol) in dry acetone (60 ml) and anhydrous potassium carbonate (2.8 g, 0.02 mol) was refluxed for 6 h then cooled and the solvent removed under reduced pressure. The residual mass was triturated with ice water to remove potassium carbonate and extracted with ether (3 × 50ml) and the ether layer was washed with 10% sodium hydroxide solution (3 × 30ml) followed by water (3 × 30ml) and then dried over anhydrous sodium sulfate and evaporated to dryness to get crude solid, which on recrystallization with ethanol gave 4-benzoyl-2,5-dimethyl phenoxy ethyl acetate.

M.p. 329 K; IR (Nujol): 1740 (ester, C═O), 1665 cm^{-1} (C═O). ^{1}H NMR ($CDCl_3$): δ 1.2 (t, J=7 Hz, 3H, CH_3 of ester), 2.2-2.3 (d, 6H, 2*Ar*-CH_3), 4.25 (q, J=6 Hz, 2H, CH_2 of ester), 4.45 (s, 2H, OCH_2), 7.2-7.8 (bm, 7H, *Ar*–H); Anal. Cal. for $C_{19}H_{20}O_4$: C, 72.61%; H, 6.36%. Found: C, 72.29%; H, 6.15%.

S3. Refinement

All H atoms were positioned at calculated positions with C–H = 0.93Å for aromatic H, 0.97Å for methylene H and 0.96Å for methyl H, and refined using a riding model with U_{iso}(H) = 1.5U_{eq}(C) for methyl H and U_{iso}(H) = 1.2U_{eq}(C) for other.

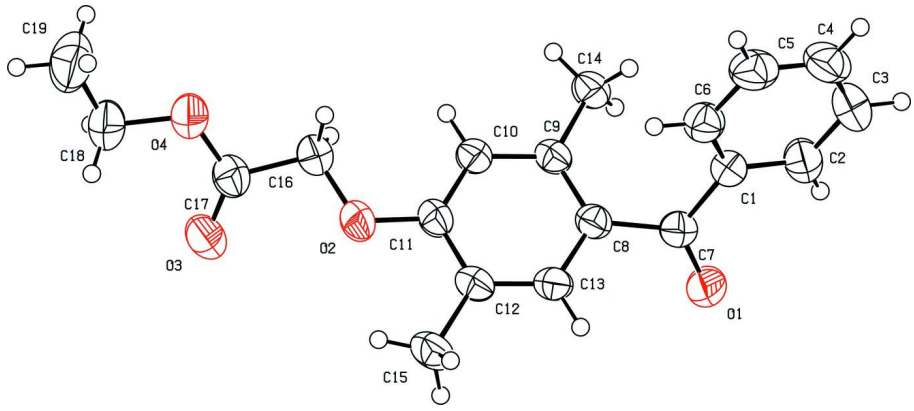

Figure 1

The asymmetric unit of the title compound with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are presented as a small spheres of arbitrary radius.

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Crystal data

$C_{19}H_{20}O_4$
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Triclinic, $P\overline{1}$
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b = 8.635 (4) Å
c = 13.029 (7) Å
α = 84.054 (8)°
β = 81.176 (8)°
γ = 66.559 (7)°
V = 830.2 (7) Å^3

Z = 2
F(000) = 332
D_x = 1.250 Mg m^{-3}
Melting point: 329 K
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3391 reflections
θ = 1.6–26.4°
μ = 0.09 mm^{-1}
T = 295 K
Plate, colourless
0.21 × 0.20 × 0.10 mm

Data collection

Bruker SMART CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.982, T_{max} = 0.991

8847 measured reflections
3391 independent reflections
2630 reflections with $I > 2\sigma(I)$
R_{int} = 0.025
θ_{max} = 26.4°, θ_{min} = 1.6°
h = −10→10
k = −10→10
l = −16→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.173
S = 1.05
3391 reflections

209 parameters
0 restraints
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

$w = 1/[\sigma^2(F_o^2) + (0.0848P)^2 + 0.2822P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.36$ e Å^{-3}
$\Delta\rho_{min} = -0.25$ e Å^{-3}

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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_{iso}*/U_{eq}
O1	0.4354 (3)	0.82563 (19)	0.84149 (12)	0.0691 (5)
O2	0.14909 (19)	1.14174 (17)	0.41431 (11)	0.0546 (4)
O3	0.1127 (2)	1.37122 (19)	0.24885 (14)	0.0715 (5)
O4	0.1339 (2)	1.16785 (19)	0.14867 (12)	0.0662 (5)
C1	0.4303 (3)	0.5733 (2)	0.79154 (15)	0.0462 (5)
C2	0.5409 (3)	0.4695 (3)	0.86317 (18)	0.0642 (6)
H2	0.6073	0.5104	0.8967	0.077*
C3	0.5525 (4)	0.3051 (3)	0.8849 (2)	0.0760 (7)
H3	0.6276	0.2356	0.9324	0.091*
C4	0.4536 (4)	0.2448 (3)	0.8364 (2)	0.0731 (7)
H4	0.4611	0.1347	0.8516	0.088*
C5	0.3435 (4)	0.3461 (3)	0.7654 (2)	0.0667 (6)
H5	0.2761	0.3047	0.7331	0.080*
C6	0.3327 (3)	0.5103 (3)	0.74180 (17)	0.0537 (5)
H6	0.2600	0.5780	0.6927	0.064*
C7	0.4101 (3)	0.7530 (2)	0.77353 (15)	0.0476 (5)
C8	0.3509 (2)	0.8461 (2)	0.67388 (15)	0.0425 (4)
C9	0.4344 (2)	0.7866 (2)	0.57555 (14)	0.0413 (4)
C10	0.3660 (2)	0.8849 (2)	0.48841 (14)	0.0432 (4)
H10	0.4193	0.8466	0.4225	0.052*
C11	0.2199 (2)	1.0389 (2)	0.49763 (15)	0.0437 (4)
C12	0.1369 (2)	1.1014 (2)	0.59520 (16)	0.0449 (4)
C13	0.2055 (3)	1.0032 (2)	0.68133 (15)	0.0457 (4)
H13	0.1531	1.0430	0.7470	0.055*
C14	0.6014 (3)	0.6268 (2)	0.56025 (16)	0.0490 (5)
H14A	0.6369	0.6093	0.4872	0.074*
H14B	0.5765	0.5326	0.5935	0.074*
H14C	0.6970	0.6368	0.5902	0.074*
C15	−0.0212 (3)	1.2694 (2)	0.60437 (19)	0.0596 (6)
H15A	−0.0484	1.3174	0.5362	0.089*

H15B	0.0086	1.3446	0.6403	0.089*
H15C	−0.1241	1.2532	0.6425	0.089*
C16	0.2201 (3)	1.0816 (3)	0.31397 (16)	0.0523 (5)
H16A	0.1847	0.9904	0.3029	0.063*
H16B	0.3507	1.0388	0.3062	0.063*
C17	0.1474 (3)	1.2266 (3)	0.23580 (17)	0.0519 (5)
C18	0.0828 (4)	1.2910 (3)	0.06180 (19)	0.0752 (7)
H18A	0.1834	1.3212	0.0322	0.090*
H18B	−0.0173	1.3927	0.0856	0.090*
C19	0.0308 (5)	1.2153 (4)	−0.0163 (2)	0.0967 (10)
H19A	−0.0037	1.2947	−0.0742	0.145*
H19B	−0.0689	1.1860	0.0136	0.145*
H19C	0.1310	1.1153	−0.0398	0.145*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.1070 (13)	0.0530 (9)	0.0549 (9)	−0.0327 (9)	−0.0290 (9)	−0.0015 (7)
O2	0.0530 (8)	0.0449 (8)	0.0511 (8)	−0.0028 (6)	−0.0123 (6)	0.0043 (6)
O3	0.0911 (12)	0.0458 (9)	0.0748 (11)	−0.0189 (8)	−0.0288 (9)	0.0057 (8)
O4	0.0907 (12)	0.0566 (9)	0.0522 (9)	−0.0281 (8)	−0.0194 (8)	0.0076 (7)
C1	0.0514 (11)	0.0412 (10)	0.0429 (10)	−0.0149 (8)	−0.0053 (8)	−0.0019 (8)
C2	0.0795 (16)	0.0530 (12)	0.0612 (13)	−0.0237 (11)	−0.0233 (12)	0.0062 (10)
C3	0.0950 (19)	0.0504 (13)	0.0734 (16)	−0.0189 (13)	−0.0212 (14)	0.0142 (11)
C4	0.0944 (19)	0.0442 (12)	0.0723 (16)	−0.0254 (12)	0.0105 (14)	−0.0030 (11)
C5	0.0800 (16)	0.0592 (13)	0.0688 (15)	−0.0373 (12)	0.0026 (12)	−0.0127 (11)
C6	0.0568 (12)	0.0522 (11)	0.0534 (12)	−0.0226 (10)	−0.0058 (9)	−0.0036 (9)
C7	0.0524 (11)	0.0426 (10)	0.0468 (11)	−0.0158 (9)	−0.0092 (9)	−0.0043 (8)
C8	0.0451 (10)	0.0354 (9)	0.0472 (10)	−0.0142 (8)	−0.0103 (8)	−0.0026 (7)
C9	0.0379 (9)	0.0346 (9)	0.0494 (10)	−0.0105 (7)	−0.0088 (8)	−0.0029 (7)
C10	0.0412 (10)	0.0391 (9)	0.0437 (10)	−0.0088 (8)	−0.0064 (8)	−0.0038 (8)
C11	0.0412 (9)	0.0384 (9)	0.0489 (11)	−0.0118 (8)	−0.0113 (8)	0.0027 (8)
C12	0.0402 (9)	0.0350 (9)	0.0552 (11)	−0.0092 (8)	−0.0066 (8)	−0.0044 (8)
C13	0.0491 (10)	0.0374 (9)	0.0473 (10)	−0.0132 (8)	−0.0018 (8)	−0.0084 (8)
C14	0.0439 (10)	0.0415 (10)	0.0532 (11)	−0.0060 (8)	−0.0095 (8)	−0.0038 (8)
C15	0.0524 (12)	0.0397 (10)	0.0711 (14)	−0.0017 (9)	−0.0052 (10)	−0.0056 (10)
C16	0.0562 (12)	0.0454 (10)	0.0509 (12)	−0.0142 (9)	−0.0131 (9)	0.0035 (9)
C17	0.0492 (11)	0.0502 (11)	0.0550 (12)	−0.0166 (9)	−0.0143 (9)	0.0045 (9)
C18	0.103 (2)	0.0683 (15)	0.0531 (13)	−0.0326 (15)	−0.0191 (13)	0.0145 (11)
C19	0.130 (3)	0.108 (2)	0.0701 (18)	−0.061 (2)	−0.0400 (18)	0.0194 (16)

Geometric parameters (Å, º)

O1—C7	1.222 (2)	C9—C14	1.508 (2)
O2—C11	1.373 (2)	C10—C11	1.389 (3)
O2—C16	1.408 (3)	C10—H10	0.9300
O3—C17	1.190 (3)	C11—C12	1.397 (3)
O4—C17	1.327 (3)	C12—C13	1.382 (3)

O4—C18	1.459 (3)	C12—C15	1.510 (3)
C1—C6	1.387 (3)	C13—H13	0.9300
C1—C2	1.389 (3)	C14—H14A	0.9600
C1—C7	1.491 (3)	C14—H14B	0.9600
C2—C3	1.387 (3)	C14—H14C	0.9600
C2—H2	0.9300	C15—H15A	0.9600
C3—C4	1.370 (4)	C15—H15B	0.9600
C3—H3	0.9300	C15—H15C	0.9600
C4—C5	1.375 (4)	C16—C17	1.512 (3)
C4—H4	0.9300	C16—H16A	0.9700
C5—C6	1.390 (3)	C16—H16B	0.9700
C5—H5	0.9300	C18—C19	1.461 (4)
C6—H6	0.9300	C18—H18A	0.9700
C7—C8	1.494 (3)	C18—H18B	0.9700
C8—C9	1.400 (3)	C19—H19A	0.9600
C8—C13	1.402 (3)	C19—H19B	0.9600
C9—C10	1.392 (3)	C19—H19C	0.9600

C11—O2—C16	117.92 (15)	C11—C12—C15	120.57 (18)
C17—O4—C18	116.19 (18)	C12—C13—C8	122.77 (18)
C6—C1—C2	119.25 (19)	C12—C13—H13	118.6
C6—C1—C7	120.90 (18)	C8—C13—H13	118.6
C2—C1—C7	119.76 (18)	C9—C14—H14A	109.5
C3—C2—C1	120.2 (2)	C9—C14—H14B	109.5
C3—C2—H2	119.9	H14A—C14—H14B	109.5
C1—C2—H2	119.9	C9—C14—H14C	109.5
C4—C3—C2	120.1 (2)	H14A—C14—H14C	109.5
C4—C3—H3	119.9	H14B—C14—H14C	109.5
C2—C3—H3	119.9	C12—C15—H15A	109.5
C3—C4—C5	120.3 (2)	C12—C15—H15B	109.5
C3—C4—H4	119.8	H15A—C15—H15B	109.5
C5—C4—H4	119.8	C12—C15—H15C	109.5
C4—C5—C6	120.1 (2)	H15A—C15—H15C	109.5
C4—C5—H5	119.9	H15B—C15—H15C	109.5
C6—C5—H5	119.9	O2—C16—C17	108.12 (16)
C1—C6—C5	120.0 (2)	O2—C16—H16A	110.1
C1—C6—H6	120.0	C17—C16—H16A	110.1
C5—C6—H6	120.0	O2—C16—H16B	110.1
O1—C7—C1	120.15 (18)	C17—C16—H16B	110.1
O1—C7—C8	120.08 (17)	H16A—C16—H16B	108.4
C1—C7—C8	119.71 (16)	O3—C17—O4	124.87 (19)
C9—C8—C13	119.31 (17)	O3—C17—C16	125.4 (2)
C9—C8—C7	123.67 (16)	O4—C17—C16	109.72 (18)
C13—C8—C7	117.01 (17)	O4—C18—C19	108.2 (2)
C10—C9—C8	118.21 (16)	O4—C18—H18A	110.1
C10—C9—C14	118.84 (17)	C19—C18—H18A	110.1
C8—C9—C14	122.83 (16)	O4—C18—H18B	110.1
C11—C10—C9	121.49 (17)	C19—C18—H18B	110.1

C11—C10—H10	119.3	H18A—C18—H18B	108.4
C9—C10—H10	119.3	C18—C19—H19A	109.5
O2—C11—C10	123.79 (17)	C18—C19—H19B	109.5
O2—C11—C12	115.21 (16)	H19A—C19—H19B	109.5
C10—C11—C12	120.99 (17)	C18—C19—H19C	109.5
C13—C12—C11	117.21 (16)	H19A—C19—H19C	109.5
C13—C12—C15	122.22 (18)	H19B—C19—H19C	109.5

C6—C1—C2—C3	−0.3 (4)	C8—C9—C10—C11	0.6 (3)
C7—C1—C2—C3	176.3 (2)	C14—C9—C10—C11	−175.62 (17)
C1—C2—C3—C4	−0.6 (4)	C16—O2—C11—C10	4.9 (3)
C2—C3—C4—C5	0.5 (4)	C16—O2—C11—C12	−176.40 (17)
C3—C4—C5—C6	0.4 (4)	C9—C10—C11—O2	179.02 (17)
C2—C1—C6—C5	1.3 (3)	C9—C10—C11—C12	0.4 (3)
C7—C1—C6—C5	−175.3 (2)	O2—C11—C12—C13	−179.07 (16)
C4—C5—C6—C1	−1.3 (3)	C10—C11—C12—C13	−0.4 (3)
C6—C1—C7—O1	151.5 (2)	O2—C11—C12—C15	1.0 (3)
C2—C1—C7—O1	−25.1 (3)	C10—C11—C12—C15	179.66 (18)
C6—C1—C7—C8	−25.8 (3)	C11—C12—C13—C8	−0.7 (3)
C2—C1—C7—C8	157.6 (2)	C15—C12—C13—C8	179.29 (18)
O1—C7—C8—C9	130.0 (2)	C9—C8—C13—C12	1.7 (3)
C1—C7—C8—C9	−52.7 (3)	C7—C8—C13—C12	−179.52 (17)
O1—C7—C8—C13	−48.7 (3)	C11—O2—C16—C17	−169.54 (16)
C1—C7—C8—C13	128.6 (2)	C18—O4—C17—O3	3.8 (3)
C13—C8—C9—C10	−1.6 (3)	C18—O4—C17—C16	−174.0 (2)
C7—C8—C9—C10	179.72 (16)	O2—C16—C17—O3	32.4 (3)
C13—C8—C9—C14	174.45 (17)	O2—C16—C17—O4	−149.82 (18)
C7—C8—C9—C14	−4.3 (3)	C17—O4—C18—C19	−165.9 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C15—H15*A*···O2	0.96	2.28	2.751 (3)	110