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(*E*)-1-(4-Methoxyphenyl)-3-(3,4,5-trimethoxyphenyl)prop-2-en-1-one

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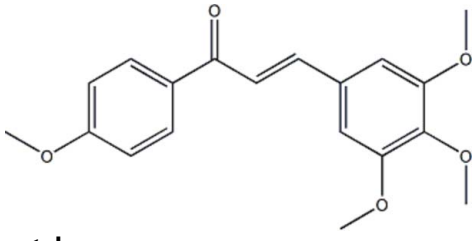
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.056; wR factor = 0.174; data-to-parameter ratio = 16.8.

The title compound, $C_{19}H_{20}O_5$, was synthesized by reaction of 4-methoxyacetophenone and 3,4,5-trimethoxy-benzaldehyde. The aromatic rings form a dihedral angle of 36.39 (7)°. Two intramolecular C—H···O hydrogen bonds occur. The crystal packing features weak C—H···O interactions.

Related literature

For background to chalcones and the biological activity and derivatives, see: Dhar (1981); Dimmock *et al.* (1999). For their applications as organic non-linear optical materials, see: Sarojini *et al.* (2006) and for their choleretic and hepatoprotective activity, see: Ni *et al.* (2004). For the synthesis of chalcones, see: Patil *et al.* (2009). For the potential use of these compounds or chalcone-rich plant extracts as drugs or food preservatives, see: Di Carlo *et al.* (1999). For related structures, see: Sathiya Moorthi *et al.* (2005); Cai *et al.* (2011); Vijay Kumar *et al.* (2011); Bibila Mayaya Bisseyou *et al.* (2007). The title compound wss prepared by an aldol Claisen–Schmidt condensation reaction, see: Bandgar *et al.* (2009, 2010); Hathaway (1987).



Experimental

Crystal data

$C_{19}H_{20}O_5$
M_r = 328.35
Monoclinic, $P2_1/c$
a = 7.5770 (1) Å
b = 16.2530 (3) Å
c = 14.0850 (3) Å
β = 107.528 (1)°
V = 1654.02 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 293 K
0.2 × 0.1 × 0.1 mm

Data collection

Nonius KappaCCD diffractometer
27371 measured reflections
3733 independent reflections
2907 reflections with $I > 2\sigma(I)$
R_{int} = 0.130

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.174
S = 1.02
3733 reflections
222 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C9—H9···O2	0.93	2.51	3.415 (2)	165
C16—H16A···O2	0.96	2.55	3.484 (2)	165
C18—H18C···O1^{i}	0.96	2.53	3.332 (2)	142

Symmetry code: (i) $x, y, z-1$.

Data collection: *COLLECT* (Hooft, 1998); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* (Otwinowski & Minor, 1997) and *SCALEPACK*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); 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: ZJ2014).

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(*E*)-1-(4-Methoxyphenyl)-3-(3,4,5-trimethoxyphenyl)prop-2-en-1-one

P. S. Carvalho-Jr, L. O. Sallum, A. F. Cidade, G. L. B. Aquino and H. B. Napolitano

S1. Comment

Chalcones are a medicinally important class of compounds and are known for possessing various biological activities such as antibacterial, antiviral, anthelmintic, amoebicidal, antiulcer, insecticidal, antiprotozoal, anticancer, cytotoxic, immunosuppressive activities and other bioactivities (Dhar, 1981; Dimmock *et al.*, 1999). Recently, some chalcones were approved for therapeutical use, such as methoxychalcone (*E*)-3-(4-methoxyphenyl)-1-(2,4-methoxyphenyl)prop-2-en-1-one, marketed in France and Italy, with choleretic and hepatoprotective activities (Ni *et al.*, 2004). Moreover, a literature survey showed dimethoxy and trimethoxychalcone derivatives as effective anti-inflammatory agents (Bandgar *et al.*, 2010).

The (*E*)-3-(3,4,5-trimethoxyphenyl)-1-(4-methoxyphenyl)prop-2-en-1-one is a methoxychalcone which the structure shows two aromatic rings linked by prop-2-en-1-one group. The refined molecular structure is shown in Fig. 1. Due to p-π conjugation, the C_{sp^2}—O bonds [O2—C7 = 1.2249 (2) Å] are significantly shorter than the C_{sp^3}—O bonds [O1—C19 = 1.4240 (2) Å; O3—C18 = 1.415 (2) Å; O4—C17 = 1.413 (2) Å and O5—C16 = 1.4294 (2) Å]. The methoxy substituted groups around the benzene rings are almost planar and the dihedral angles C5—C6—C7—C8, C6—C7—C8—C9, C7—C8—C9—C10 and C8—C9—C10—C11 are -23.0 (2)°, 169.3 (2)°, 177.7 (2)° and -4.4 (2)°, respectively, indicating the molecule has a non-planar conformation.

The crystal structure is stabilized by C—H···O contacts (Table 1). There is intermolecular hydrogen bonding involving C9 acting as H-bond donor, via H9, to O2 in the adjacent molecules at -x+1, -y+1, -z resulting in a dimer.

S2. Experimental

The title compound, $C_{19}H_{20}O_5$, has been prepared by the aldol Claisen-Schmidt condensation (Hathaway, 1987; Bandgar *et al.*, 2009) by the reaction of a mixture of 4-methoxy-acetophenone (0,3 mg; 2 mmol) and 3,4,5-trimethoxy-benzaldehyde (0,39 mg; 2 mmol) and NaOH (50% p/v) at 257 K for 24 h. The light yellow solid (m.p. 404.25 - 405.65 K) thus obtained was filtered, washed with water and dried. Crystals of suitable quality for single crystal X-ray diffraction were grown in methanol.

S3. Refinement

The space group $P2_1/c$ was uniquely assigned from the systematic absences. All the H-atoms were placed in calculated positions and treated as riding atoms [C_{aro}—H = 0.93 Å and Csp^3—H = 0.96 Å), with a displacement parameter U_{iso} set equal to 1.2 times U_{eq} that of the parent atom, and C_{sp^3} and aromatic H.

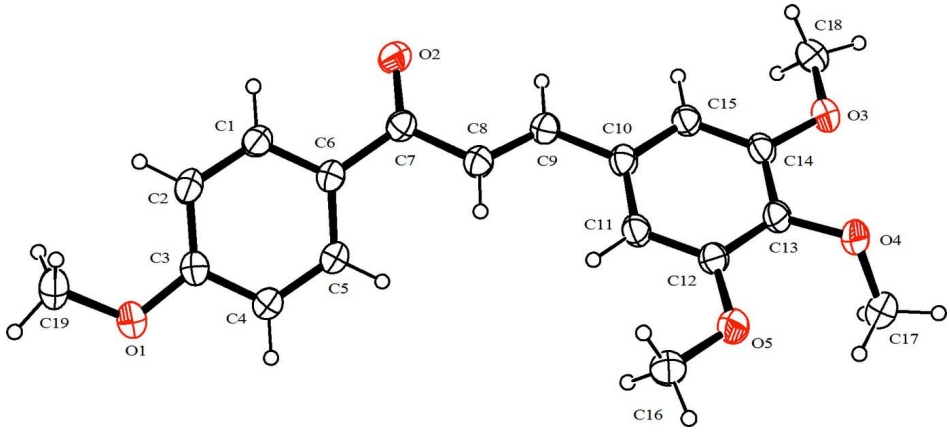

Figure 1

Molecular structre showing 30% probability displacement ellipsoids.

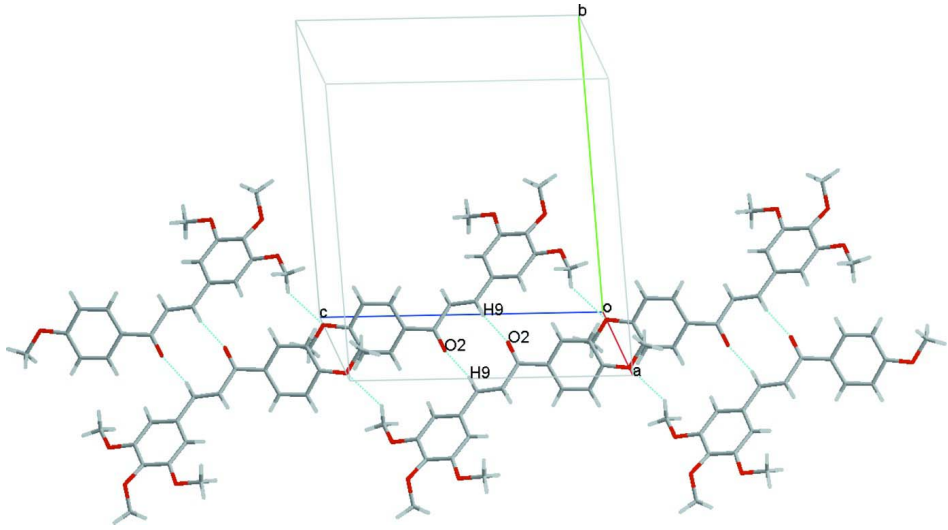

Figure 2

The packing viewed along c axis with C—H···O interactions, indicating the dimer

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Crystal data

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$M_r = 328.35$
Monoclinic, $P2_1/c$
$a = 7.5770\ (1)$ Å
$b = 16.2530\ (3)$ Å
$c = 14.0850\ (3)$ Å
$\beta = 107.528\ (1)°$
$V = 1654.02\ (5)$ Å^3
$Z = 4$

$F(000) = 696$
$D_x = 1.319$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 14574 reflections
$\theta = 2.6–27.5°$
$\mu = 0.10$ mm^{-1}
$T = 293$ K
Prism, pale yellow
0.2 × 0.1 × 0.1 mm

Data collection

Nonius KappaCCD diffractometer
Graphite monochromator
Detector resolution: 9 pixels mm^{-1}
CCD scans
27371 measured reflections
3733 independent reflections

2907 reflections with $I > 2\sigma(I)$
$R_{int} = 0.130$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.8°$
$h = -9 \rightarrow 8$
$k = -20 \rightarrow 21$
$l = -18 \rightarrow 17$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.056$
$wR(F^2) = 0.174$
$S = 1.02$
3733 reflections
222 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
$w = 1/[\sigma^2(F_o^2) + (0.115P)^2 + 0.1311P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.27$ e Å^{-3}
$\Delta\rho_{min} = -0.27$ e Å^{-3}
Extinction correction: *SHELXL*
Extinction coefficient: 0.085 (10)

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 $F^2 > 2\sigma(F^2)$ 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}
C6	0.28843 (19)	0.01968 (8)	0.72913 (10)	0.0440 (3)
C3	0.2444 (2)	0.01579 (9)	0.91868 (10)	0.0478 (4)
O5	−0.33915 (16)	0.26263 (7)	0.32667 (8)	0.0592 (3)
C7	0.3073 (2)	0.01831 (8)	0.62695 (11)	0.0465 (3)
O1	0.21258 (17)	0.01994 (7)	1.00875 (8)	0.0613 (3)
O3	0.06505 (17)	0.22341 (7)	0.13696 (8)	0.0594 (3)
C13	−0.1306 (2)	0.24141 (9)	0.23514 (10)	0.0496 (4)
O2	0.41266 (17)	−0.03016 (7)	0.60508 (9)	0.0623 (3)
C14	0.0304 (2)	0.20629 (8)	0.22489 (9)	0.0472 (3)
C11	−0.0614 (2)	0.18197 (9)	0.39957 (10)	0.0478 (3)
H11	−0.0896	0.1757	0.459	0.057*
C1	0.3390 (2)	−0.04924 (8)	0.78977 (11)	0.0475 (3)
H1	0.3901	−0.0943	0.7669	0.057*
C9	0.21256 (19)	0.09013 (9)	0.46478 (10)	0.0464 (3)
H9	0.3105	0.0638	0.4504	0.056*

C15	0.1421 (2)	0.15689 (9)	0.29994 (10)	0.0471 (3)
H15	0.2474	0.1324	0.2917	0.057*
C10	0.09579 (19)	0.14423 (8)	0.38773 (9)	0.0451 (3)
C5	0.2205 (2)	0.08797 (9)	0.76692 (11)	0.0501 (4)
H5	0.1881	0.1351	0.728	0.06*
O4	−0.24822 (19)	0.28028 (7)	0.15454 (8)	0.0700 (4)
C12	−0.1763 (2)	0.22889 (9)	0.32326 (10)	0.0475 (4)
C4	0.2007 (2)	0.08672 (9)	0.86115 (11)	0.0528 (4)
H4	0.1583	0.1332	0.8861	0.063*
C2	0.3152 (2)	−0.05237 (9)	0.88338 (10)	0.0502 (4)
H2	0.3463	−0.0996	0.9221	0.06*
C8	0.1902 (2)	0.07561 (9)	0.55307 (10)	0.0503 (4)
H8	0.0955	0.103	0.5694	0.06*
C17	−0.2865 (3)	0.36460 (11)	0.16310 (12)	0.0693 (5)
H17A	−0.3621	0.3708	0.2064	0.104*
H17B	−0.3508	0.3863	0.0985	0.104*
H17C	−0.1724	0.394	0.1902	0.104*
C16	−0.3984 (2)	0.24404 (11)	0.41148 (12)	0.0602 (4)
H16A	−0.4186	0.1859	0.4141	0.09*
H16B	−0.5116	0.2728	0.4064	0.09*
H16C	−0.3049	0.261	0.4709	0.09*
C18	0.2381 (3)	0.19903 (12)	0.12726 (13)	0.0702 (5)
H18A	0.3358	0.22	0.1825	0.105*
H18B	0.2513	0.2205	0.0663	0.105*
H18C	0.2446	0.1401	0.1265	0.105*
C19	0.2388 (3)	−0.05277 (12)	1.06778 (12)	0.0666 (5)
H19A	0.1621	−0.096	1.0306	0.1*
H19B	0.2058	−0.0421	1.1273	0.1*
H19C	0.3663	−0.0692	1.0852	0.1*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C6	0.0425 (7)	0.0436 (7)	0.0430 (7)	−0.0002 (5)	0.0086 (5)	0.0042 (5)
C3	0.0491 (8)	0.0517 (8)	0.0401 (7)	−0.0033 (6)	0.0098 (6)	0.0043 (5)
O5	0.0536 (7)	0.0738 (7)	0.0466 (6)	0.0147 (5)	0.0095 (5)	0.0039 (5)
C7	0.0463 (7)	0.0433 (7)	0.0502 (8)	0.0004 (6)	0.0150 (6)	0.0046 (5)
O1	0.0772 (8)	0.0628 (7)	0.0459 (6)	0.0058 (5)	0.0215 (5)	0.0096 (4)
O3	0.0722 (8)	0.0672 (7)	0.0393 (5)	0.0078 (5)	0.0175 (5)	0.0058 (4)
C13	0.0562 (9)	0.0490 (7)	0.0348 (7)	0.0022 (6)	0.0006 (6)	−0.0041 (5)
O2	0.0736 (8)	0.0566 (6)	0.0648 (7)	0.0189 (5)	0.0331 (6)	0.0119 (5)
C14	0.0581 (8)	0.0468 (7)	0.0336 (6)	−0.0044 (6)	0.0090 (6)	−0.0039 (5)
C11	0.0491 (8)	0.0547 (8)	0.0367 (6)	0.0003 (6)	0.0087 (5)	−0.0003 (5)
C1	0.0497 (8)	0.0413 (7)	0.0470 (7)	0.0024 (6)	0.0078 (6)	0.0017 (5)
C9	0.0444 (7)	0.0478 (7)	0.0452 (7)	0.0016 (5)	0.0109 (6)	0.0023 (5)
C15	0.0495 (7)	0.0492 (7)	0.0409 (7)	−0.0006 (6)	0.0112 (6)	−0.0008 (5)
C10	0.0459 (7)	0.0467 (7)	0.0382 (6)	−0.0028 (6)	0.0057 (5)	−0.0002 (5)
C5	0.0577 (8)	0.0432 (7)	0.0489 (7)	0.0076 (6)	0.0152 (6)	0.0092 (6)

O4	0.0862 (9)	0.0722 (8)	0.0379 (6)	0.0246 (6)	−0.0021 (5)	−0.0010 (5)
C12	0.0463 (8)	0.0503 (8)	0.0407 (7)	0.0023 (6)	0.0050 (6)	−0.0043 (5)
C4	0.0623 (9)	0.0463 (7)	0.0494 (8)	0.0075 (6)	0.0163 (7)	0.0041 (6)
C2	0.0556 (8)	0.0428 (7)	0.0462 (7)	0.0006 (6)	0.0062 (6)	0.0096 (5)
C8	0.0484 (8)	0.0562 (8)	0.0453 (7)	0.0087 (6)	0.0125 (6)	0.0053 (6)
C17	0.0765 (11)	0.0667 (10)	0.0584 (9)	0.0204 (9)	0.0110 (8)	0.0105 (8)
C16	0.0577 (9)	0.0657 (10)	0.0594 (9)	0.0082 (7)	0.0210 (8)	0.0027 (7)
C18	0.0911 (13)	0.0769 (11)	0.0506 (9)	0.0143 (9)	0.0333 (9)	0.0034 (7)
C19	0.0736 (11)	0.0730 (11)	0.0529 (9)	0.0016 (8)	0.0188 (8)	0.0205 (7)

Geometric parameters (Å, º)

C6—C1	1.3906 (19)	C9—C10	1.4682 (19)
C6—C5	1.395 (2)	C9—H9	0.93
C6—C7	1.4889 (19)	C15—C10	1.3986 (19)
C3—O1	1.3626 (17)	C15—H15	0.93
C3—C2	1.387 (2)	C5—C4	1.380 (2)
C3—C4	1.3906 (19)	C5—H5	0.93
O5—C12	1.3645 (18)	O4—C17	1.413 (2)
O5—C16	1.4294 (19)	C4—H4	0.93
C7—O2	1.2249 (18)	C2—H2	0.93
C7—C8	1.4771 (19)	C8—H8	0.93
O1—C19	1.4240 (19)	C17—H17A	0.96
O3—C14	1.3699 (16)	C17—H17B	0.96
O3—C18	1.415 (2)	C17—H17C	0.96
C13—O4	1.3685 (17)	C16—H16A	0.96
C13—C14	1.393 (2)	C16—H16B	0.96
C13—C12	1.400 (2)	C16—H16C	0.96
C14—C15	1.393 (2)	C18—H18A	0.96
C11—C12	1.390 (2)	C18—H18B	0.96
C11—C10	1.394 (2)	C18—H18C	0.96
C11—H11	0.93	C19—H19A	0.96
C1—C2	1.384 (2)	C19—H19B	0.96
C1—H1	0.93	C19—H19C	0.96
C9—C8	1.326 (2)		

C1—C6—C5	118.15 (13)	O5—C12—C11	123.77 (13)
C1—C6—C7	119.52 (12)	O5—C12—C13	116.13 (12)
C5—C6—C7	122.33 (12)	C11—C12—C13	120.06 (13)
O1—C3—C2	124.72 (12)	C5—C4—C3	119.79 (13)
O1—C3—C4	115.06 (13)	C5—C4—H4	120.1
C2—C3—C4	120.22 (13)	C3—C4—H4	120.1
C12—O5—C16	117.36 (12)	C1—C2—C3	119.18 (12)
O2—C7—C8	121.82 (14)	C1—C2—H2	120.4
O2—C7—C6	120.82 (12)	C3—C2—H2	120.4
C8—C7—C6	117.33 (12)	C9—C8—C7	123.60 (13)
C3—O1—C19	118.02 (13)	C9—C8—H8	118.2
C14—O3—C18	117.77 (12)	C7—C8—H8	118.2

O4—C13—C14	118.37 (13)	O4—C17—H17A	109.5
O4—C13—C12	121.95 (14)	O4—C17—H17B	109.5
C14—C13—C12	119.36 (12)	H17A—C17—H17B	109.5
O3—C14—C15	124.40 (13)	O4—C17—H17C	109.5
O3—C14—C13	115.01 (12)	H17A—C17—H17C	109.5
C15—C14—C13	120.59 (13)	H17B—C17—H17C	109.5
C12—C11—C10	120.51 (12)	O5—C16—H16A	109.5
C12—C11—H11	119.7	O5—C16—H16B	109.5
C10—C11—H11	119.7	H16A—C16—H16B	109.5
C2—C1—C6	121.57 (13)	O5—C16—H16C	109.5
C2—C1—H1	119.2	H16A—C16—H16C	109.5
C6—C1—H1	119.2	H16B—C16—H16C	109.5
C8—C9—C10	125.52 (13)	O3—C18—H18A	109.5
C8—C9—H9	117.2	O3—C18—H18B	109.5
C10—C9—H9	117.2	H18A—C18—H18B	109.5
C14—C15—C10	119.90 (13)	O3—C18—H18C	109.5
C14—C15—H15	120	H18A—C18—H18C	109.5
C10—C15—H15	120	H18B—C18—H18C	109.5
C11—C10—C15	119.49 (12)	O1—C19—H19A	109.5
C11—C10—C9	121.44 (12)	O1—C19—H19B	109.5
C15—C10—C9	119.06 (13)	H19A—C19—H19B	109.5
C4—C5—C6	120.99 (12)	O1—C19—H19C	109.5
C4—C5—H5	119.5	H19A—C19—H19C	109.5
C6—C5—H5	119.5	H19B—C19—H19C	109.5
C13—O4—C17	118.42 (12)		

C1—C6—C7—O2	−21.4 (2)	C1—C6—C5—C4	−1.2 (2)
C5—C6—C7—O2	158.90 (15)	C7—C6—C5—C4	178.5 (2)
C1—C6—C7—C8	156.7 (2)	C14—C13—O4—C17	−120.1 (2)
C5—C6—C7—C8	−23.0 (2)	C12—C13—O4—C17	66.4 (2)
C2—C3—O1—C19	−5.5 (2)	C16—O5—C12—C11	−3.9 (2)
C4—C3—O1—C19	174.5 (2)	C16—O5—C12—C13	173.9 (2)
C18—O3—C14—C15	−9.2 (2)	C10—C11—C12—O5	175.0 (2)
C18—O3—C14—C13	171.6 (2)	C10—C11—C12—C13	−2.6 (2)
O4—C13—C14—O3	7.7 (2)	O4—C13—C12—O5	−4.4 (2)
C12—C13—C14—O3	−178.7 (2)	C14—C13—C12—O5	−177.7 (2)
O4—C13—C14—C15	−171.4 (2)	O4—C13—C12—C11	173.5 (2)
C12—C13—C14—C15	2.1 (2)	C14—C13—C12—C11	0.1 (2)
C5—C6—C1—C2	3.0 (2)	C6—C5—C4—C3	−1.7 (2)
C7—C6—C1—C2	−176.6 (2)	O1—C3—C4—C5	−177.3 (2)
O3—C14—C15—C10	179.0 (2)	C2—C3—C4—C5	2.8 (2)
C13—C14—C15—C10	−1.9 (2)	C6—C1—C2—C3	−2.0 (2)
C12—C11—C10—C15	2.9 (2)	O1—C3—C2—C1	179.1 (2)
C12—C11—C10—C9	−176.0 (2)	C4—C3—C2—C1	−1.0 (2)
C14—C15—C10—C11	−0.6 (2)	C10—C9—C8—C7	177.7 (2)
C14—C15—C10—C9	178.3 (2)	O2—C7—C8—C9	−12.8 (2)
C8—C9—C10—C11	−4.4 (2)	C6—C7—C8—C9	169.1 (2)
C8—C9—C10—C15	176.7 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C9—H9···O2	0.93	2.51	3.415 (2)	165
C16—H16*A*···O2	0.96	2.55	3.484 (2)	165
C18—H18*C*···O1^{i}	0.96	2.53	3.332 (2)	142

Symmetry code: (i) *x*, *y*, *z*−1.