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ISSN 2414-3146

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

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Received 30 November 2016
Accepted 3 December 2016

Edited by W. T. A. Harrison, University of Aberdeen, Scotland

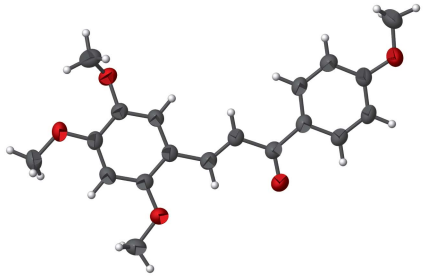
Keywords: crystal structure; chalcone; weak C—H···O hydrogen bonds.

CCDC reference: 1520740

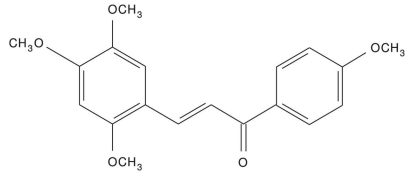
Structural data: full structural data are available from iucrdata.iucr.org

In the title chalcone derivative, $C_{19}H_{20}O_5$, the dihedral angle between the planes of the benzene rings is 3.97 (8)°. In the monosubstituted ring, the methoxy C atom is almost coplanar with the ring [deviation = 0.016 (3) Å]. In the trisubstituted ring, the C atoms of the *ortho*, *meta* and *para* methoxy sustituents deviate by −0.030 (2), 1.127 (2) and −0.052 (2) Å, respectively. In the crystal, molecules are linked by weak C—H···O hydrogen bonds, forming *C*(9) chains propagating along [010].

3D view



Chemical scheme



Structure description

As part of our ongoing work on chalcone derivatives (Naveen *et al.*, 2016), we herein report the synthesis and crystal structure of the title compound.

The *ORTEP* of the molecule is shown in Fig. 1. The central part of the molecule is nearly planar: the dihedral angle between the benzene ring bridged by the olefinic double bond is 3.97 (8)°. The methoxy groups at C6, C4 and C16 are almost coplanar with the C1–C6 and C13–C18 benzene rings whereas the methoxy group at C3 lies outside the plane of the C1–C6 benzene ring, as indicated by the C7—O1—C3—C4 torsion angle of 78.1 (2)°. In the crystal, the molecules are linked *via* weak C—H···O hydrogen bonds (Table 1), forming chains propagating along [010] (Fig. 2).

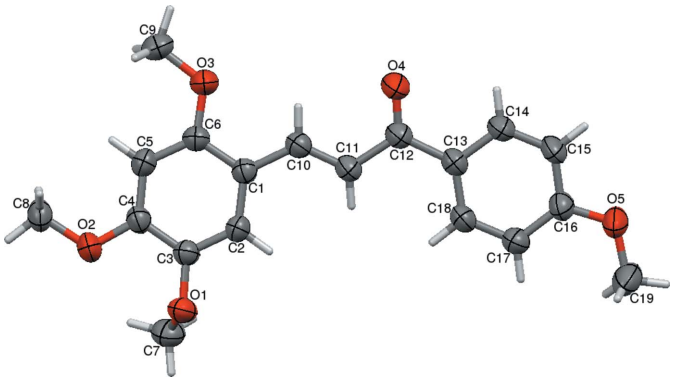


Figure 1
The molecular structure of the title compound, with displacement ellipsoids for non-H atoms drawn at the 50% probability level.

Synthesis and crystallization

A mixture of 2,4,5-trimethoxybenzaldehyde (5 mmol), 1-(4-methoxyphenyl)ethanone (5 mmol) and sodium hydroxide (5 mmol) in 95% ethyl alcohol (25 ml) was stirred at room temperature for 3 h. The progress of the reaction was monitored by TLC. After completion of the reaction, the mixture was poured into ice-cold water and kept in the refrigerator overnight. The solid that formed was filtered, and washed with cold hydrochloric acid (5%). Yellow prisms were obtained from methanol solution by slow solvent evaporation. Yield 91%, m.p. 104–105°C.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

The authors are grateful to the Institution of Excellence, Vijnana Bhavana, University of Mysore, India, for providing the single-crystal X-ray diffractometer facility.

References

Bruker (2013). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.

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

D—H···A	D—H	H···A	D···A	D—H···A
C19—H19C···O4^{i}	0.96	2.48	3.293 (3)	143

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{19}H_{20}O_5$
M_r	328.35
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	296
a, b, c (Å)	8.4043 (5), 8.5518 (5), 12.9352 (7)
α, β, γ (°)	75.400 (2), 88.427 (2), 68.014 (2)
V (Å^3)	831.91 (8)
Z	2
Radiation type	Cu $K\alpha$
μ (mm^{-1})	0.78
Crystal size (mm)	0.29 × 0.26 × 0.22
Data collection	
Diffractometer	Bruker X8 Proteum
Absorption correction	Multi-scan (*SADABS*; Bruker, 2013)
T_{min}, T_{max}	0.806, 0.847
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	7500, 2684, 2528
R_{int}	0.038
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.584
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.052, 0.172, 1.07
No. of reflections	2684
No. of parameters	221
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.18, −0.16

Computer programs: *APEX2* and *SAINT* (Bruker, 2013), *SHELXS97* and *SHELXL97* (Sheldrick, 2008) and *Mercury* (Macrae *et al.*, 2008).

Macrae, C. F., Bruno, I. J., Chisholm, J. A., Edgington, P. R., McCabe, P., Pidcock, E., Rodriguez-Monge, L., Taylor, R., van de Streek, J. & Wood, P. A. (2008). *J. Appl. Cryst.* **41**, 466–470.
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Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

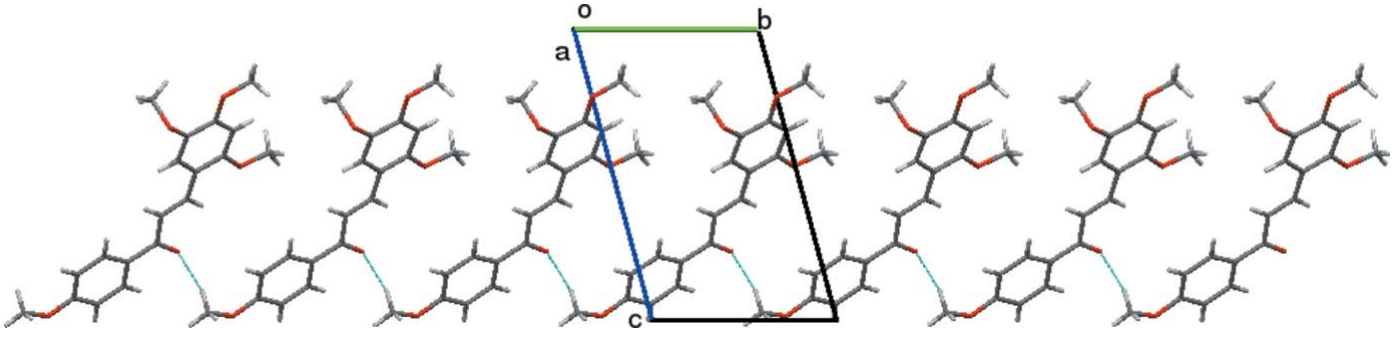

Figure 2
The packing of the molecules, viewed along the [100] direction. The dashed lines represent hydrogen bonds.

full crystallographic data

IUCrData (2016). **1**, x161935 [https://doi.org/10.1107/S2414314616019350]

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

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

Crystal data

$C_{19}H_{20}O_5$
M_r = 328.35
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 8.4043 (5) Å
b = 8.5518 (5) Å
c = 12.9352 (7) Å
α = 75.400 (2)°
β = 88.427 (2)°
γ = 68.014 (2)°
V = 831.91 (8) Å^3
Z = 2
$F(000)$ = 348
D_x = 1.311 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 2528 reflections
θ = 5.7–64.2°
μ = 0.78 mm^{-1}
T = 296 K
Prism, yellow
0.29 × 0.26 × 0.22 mm

Data collection

Bruker X8 Proteum diffractometer
Radiation source: Bruker MicroStar microfocus rotating anode
Helios multilayer optics monochromator
Detector resolution: 18.4 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2013)
T_{min} = 0.806, T_{max} = 0.847
7500 measured reflections
2684 independent reflections
2528 reflections with $I > 2\sigma(I)$
R_{int} = 0.038
θ_{max} = 64.2°, θ_{min} = 5.7°
h = −9→9
k = −9→9
l = −15→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.172
S = 1.07
2684 reflections
221 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.1152P)^2 + 0.1101P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

Special details

Geometry. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted R-factors wR and all goodnesses 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 observed criterion of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating -R-factor-obs 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	−0.08544 (15)	0.66789 (16)	0.33941 (9)	0.0568 (4)
O2	−0.14008 (16)	1.00180 (16)	0.23295 (10)	0.0602 (4)
O3	0.30064 (17)	0.99036 (16)	0.47183 (10)	0.0619 (4)
O4	0.57780 (19)	0.52820 (17)	0.76489 (11)	0.0733 (5)
O5	0.7804 (2)	−0.26807 (16)	0.98697 (11)	0.0752 (5)
C1	0.23192 (19)	0.7438 (2)	0.48953 (12)	0.0424 (5)
C2	0.1357 (2)	0.6634 (2)	0.45203 (12)	0.0448 (5)
C3	0.0145 (2)	0.7502 (2)	0.36718 (12)	0.0458 (5)
C4	−0.0154 (2)	0.9247 (2)	0.31510 (12)	0.0463 (5)
C5	0.0797 (2)	1.0066 (2)	0.34882 (12)	0.0475 (5)
C6	0.20205 (19)	0.9174 (2)	0.43478 (12)	0.0441 (5)
C7	−0.0424 (3)	0.6121 (3)	0.24368 (16)	0.0684 (7)
C8	−0.1753 (2)	1.1788 (2)	0.17818 (14)	0.0592 (5)
C9	0.2730 (2)	1.1681 (2)	0.42455 (16)	0.0605 (6)
C10	0.3533 (2)	0.6570 (2)	0.58348 (12)	0.0461 (5)
C11	0.4058 (2)	0.4919 (2)	0.64046 (12)	0.0479 (5)
C12	0.5255 (2)	0.4286 (2)	0.73643 (13)	0.0486 (5)
C13	0.58235 (19)	0.2432 (2)	0.79999 (12)	0.0449 (5)
C14	0.7088 (2)	0.1848 (2)	0.88415 (13)	0.0527 (5)
C15	0.7692 (2)	0.0159 (2)	0.94495 (14)	0.0575 (6)
C16	0.7061 (2)	−0.1025 (2)	0.92435 (12)	0.0516 (5)
C17	0.5784 (2)	−0.0474 (2)	0.84262 (13)	0.0522 (6)
C18	0.5185 (2)	0.1237 (2)	0.78175 (13)	0.0496 (5)
C19	0.7183 (4)	−0.3948 (3)	0.9746 (2)	0.0885 (9)
H2	0.15480	0.54760	0.48580	0.0540*
H5	0.06150	1.12180	0.31380	0.0570*
H7A	−0.07100	0.71240	0.18330	0.1030*
H7B	−0.10590	0.54270	0.23520	0.1030*
H7C	0.07870	0.54360	0.24820	0.1030*
H8A	−0.20830	1.24950	0.22810	0.0890*
H8B	−0.26730	1.21820	0.12380	0.0890*
H8C	−0.07420	1.18830	0.14560	0.0890*
H9A	0.29970	1.18270	0.35100	0.0910*
H9B	0.34580	1.20220	0.46240	0.0910*
H9C	0.15480	1.23980	0.42830	0.0910*

H10	0.40020	0.72630	0.60660	0.0550*
H11	0.36660	0.41540	0.61960	0.0580*
H14	0.75260	0.26260	0.89890	0.0630*
H15	0.85320	−0.02000	1.00060	0.0690*
H17	0.53350	−0.12510	0.82900	0.0630*
H18	0.43300	0.16000	0.72700	0.0600*
H19A	0.60300	−0.36600	0.99660	0.1330*
H19B	0.79080	−0.50750	1.01810	0.1330*
H19C	0.71880	−0.39730	0.90080	0.1330*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0634 (8)	0.0655 (8)	0.0504 (7)	−0.0392 (6)	−0.0064 (5)	−0.0066 (5)
O2	0.0617 (8)	0.0535 (7)	0.0564 (7)	−0.0224 (6)	−0.0212 (5)	0.0045 (5)
O3	0.0686 (8)	0.0508 (7)	0.0689 (8)	−0.0324 (6)	−0.0183 (6)	−0.0028 (6)
O4	0.0887 (10)	0.0541 (8)	0.0762 (9)	−0.0311 (7)	−0.0355 (7)	−0.0048 (6)
O5	0.1034 (11)	0.0482 (7)	0.0655 (8)	−0.0280 (7)	−0.0345 (7)	0.0026 (6)
C1	0.0417 (8)	0.0441 (8)	0.0406 (8)	−0.0176 (6)	0.0007 (6)	−0.0074 (6)
C2	0.0485 (9)	0.0418 (8)	0.0424 (8)	−0.0196 (7)	−0.0011 (6)	−0.0036 (6)
C3	0.0480 (8)	0.0505 (9)	0.0422 (8)	−0.0253 (7)	−0.0006 (6)	−0.0073 (6)
C4	0.0445 (8)	0.0490 (9)	0.0412 (8)	−0.0174 (7)	−0.0035 (6)	−0.0046 (6)
C5	0.0514 (9)	0.0397 (8)	0.0469 (9)	−0.0175 (7)	−0.0014 (7)	−0.0028 (6)
C6	0.0435 (8)	0.0448 (8)	0.0468 (8)	−0.0204 (6)	0.0011 (6)	−0.0108 (6)
C7	0.0832 (13)	0.0698 (12)	0.0652 (11)	−0.0409 (10)	−0.0045 (9)	−0.0204 (9)
C8	0.0616 (10)	0.0489 (9)	0.0525 (9)	−0.0116 (8)	−0.0111 (7)	−0.0013 (7)
C9	0.0685 (11)	0.0506 (10)	0.0702 (11)	−0.0325 (8)	0.0001 (8)	−0.0135 (8)
C10	0.0446 (8)	0.0499 (9)	0.0450 (8)	−0.0205 (7)	−0.0018 (6)	−0.0101 (7)
C11	0.0505 (9)	0.0476 (9)	0.0448 (8)	−0.0185 (7)	−0.0068 (6)	−0.0096 (7)
C12	0.0488 (9)	0.0488 (9)	0.0484 (9)	−0.0188 (7)	−0.0055 (7)	−0.0119 (7)
C13	0.0418 (8)	0.0498 (9)	0.0413 (8)	−0.0155 (7)	−0.0029 (6)	−0.0109 (7)
C14	0.0577 (10)	0.0512 (9)	0.0508 (9)	−0.0228 (8)	−0.0114 (7)	−0.0114 (7)
C15	0.0632 (11)	0.0549 (10)	0.0501 (9)	−0.0203 (8)	−0.0210 (7)	−0.0069 (7)
C16	0.0601 (10)	0.0478 (9)	0.0421 (8)	−0.0181 (7)	−0.0066 (7)	−0.0062 (6)
C17	0.0568 (10)	0.0545 (10)	0.0492 (9)	−0.0272 (8)	−0.0053 (7)	−0.0101 (7)
C18	0.0471 (9)	0.0542 (9)	0.0458 (8)	−0.0202 (7)	−0.0094 (6)	−0.0071 (7)
C19	0.129 (2)	0.0526 (11)	0.0811 (14)	−0.0407 (12)	−0.0277 (13)	0.0008 (10)

Geometric parameters (Å, º)

O1—C3	1.384 (2)	C16—C17	1.387 (2)
O1—C7	1.427 (2)	C17—C18	1.380 (2)
O2—C4	1.361 (2)	C2—H2	0.9300
O2—C8	1.420 (2)	C5—H5	0.9300
O3—C6	1.366 (2)	C7—H7A	0.9600
O3—C9	1.419 (2)	C7—H7B	0.9600
O4—C12	1.225 (2)	C7—H7C	0.9600
O5—C16	1.356 (2)	C8—H8A	0.9600

O5—C19	1.410 (3)	C8—H8B	0.9600
C1—C2	1.403 (2)	C8—H8C	0.9600
C1—C6	1.403 (2)	C9—H9A	0.9600
C1—C10	1.454 (2)	C9—H9B	0.9600
C2—C3	1.370 (2)	C9—H9C	0.9600
C3—C4	1.402 (2)	C10—H10	0.9300
C4—C5	1.383 (2)	C11—H11	0.9300
C5—C6	1.387 (2)	C14—H14	0.9300
C10—C11	1.326 (2)	C15—H15	0.9300
C11—C12	1.473 (2)	C17—H17	0.9300
C12—C13	1.488 (2)	C18—H18	0.9300
C13—C14	1.399 (2)	C19—H19A	0.9600
C13—C18	1.388 (2)	C19—H19B	0.9600
C14—C15	1.365 (2)	C19—H19C	0.9600
C15—C16	1.387 (2)		

C3—O1—C7	114.51 (15)	O1—C7—H7A	109.00
C4—O2—C8	117.75 (14)	O1—C7—H7B	109.00
C6—O3—C9	119.38 (14)	O1—C7—H7C	109.00
C16—O5—C19	118.90 (17)	H7A—C7—H7B	110.00
C2—C1—C6	117.17 (14)	H7A—C7—H7C	109.00
C2—C1—C10	122.71 (15)	H7B—C7—H7C	109.00
C6—C1—C10	120.08 (15)	O2—C8—H8A	109.00
C1—C2—C3	122.07 (15)	O2—C8—H8B	109.00
O1—C3—C2	119.19 (14)	O2—C8—H8C	109.00
O1—C3—C4	120.94 (15)	H8A—C8—H8B	109.00
C2—C3—C4	119.69 (16)	H8A—C8—H8C	110.00
O2—C4—C3	115.81 (15)	H8B—C8—H8C	109.00
O2—C4—C5	124.56 (15)	O3—C9—H9A	110.00
C3—C4—C5	119.63 (15)	O3—C9—H9B	109.00
C4—C5—C6	120.15 (15)	O3—C9—H9C	110.00
O3—C6—C1	115.64 (14)	H9A—C9—H9B	109.00
O3—C6—C5	123.09 (15)	H9A—C9—H9C	109.00
C1—C6—C5	121.27 (15)	H9B—C9—H9C	109.00
C1—C10—C11	128.37 (16)	C1—C10—H10	116.00
C10—C11—C12	120.64 (15)	C11—C10—H10	116.00
O4—C12—C11	120.34 (15)	C10—C11—H11	120.00
O4—C12—C13	119.65 (15)	C12—C11—H11	120.00
C11—C12—C13	120.01 (15)	C13—C14—H14	119.00
C12—C13—C14	117.90 (15)	C15—C14—H14	119.00
C12—C13—C18	124.59 (15)	C14—C15—H15	120.00
C14—C13—C18	117.51 (15)	C16—C15—H15	120.00
C13—C14—C15	121.25 (16)	C16—C17—H17	120.00
C14—C15—C16	120.45 (16)	C18—C17—H17	120.00
O5—C16—C15	115.28 (15)	C13—C18—H18	119.00
O5—C16—C17	125.16 (16)	C17—C18—H18	119.00
C15—C16—C17	119.54 (15)	O5—C19—H19A	109.00
C16—C17—C18	119.41 (16)	O5—C19—H19B	109.00

C13—C18—C17	121.83 (16)	O5—C19—H19C	109.00
C1—C2—H2	119.00	H19A—C19—H19B	109.00
C3—C2—H2	119.00	H19A—C19—H19C	110.00
C4—C5—H5	120.00	H19B—C19—H19C	109.00
C6—C5—H5	120.00		

C7—O1—C3—C2	−106.74 (18)	O2—C4—C5—C6	178.85 (16)
C7—O1—C3—C4	78.1 (2)	C3—C4—C5—C6	−1.0 (2)
C8—O2—C4—C3	179.72 (14)	C4—C5—C6—O3	179.76 (15)
C8—O2—C4—C5	−0.2 (2)	C4—C5—C6—C1	−0.2 (2)
C9—O3—C6—C1	−176.91 (15)	C1—C10—C11—C12	−177.62 (16)
C9—O3—C6—C5	3.1 (2)	C10—C11—C12—O4	0.1 (3)
C19—O5—C16—C15	177.11 (19)	C10—C11—C12—C13	179.59 (16)
C19—O5—C16—C17	−4.3 (3)	O4—C12—C13—C14	−6.7 (2)
C6—C1—C2—C3	−1.4 (2)	O4—C12—C13—C18	173.22 (17)
C10—C1—C2—C3	176.10 (16)	C11—C12—C13—C14	173.85 (15)
C2—C1—C6—O3	−178.56 (14)	C11—C12—C13—C18	−6.2 (3)
C2—C1—C6—C5	1.4 (2)	C12—C13—C14—C15	−179.02 (16)
C10—C1—C6—O3	3.8 (2)	C18—C13—C14—C15	1.1 (3)
C10—C1—C6—C5	−176.17 (15)	C12—C13—C18—C17	179.03 (16)
C2—C1—C10—C11	7.4 (3)	C14—C13—C18—C17	−1.1 (3)
C6—C1—C10—C11	−175.12 (17)	C13—C14—C15—C16	0.1 (3)
C1—C2—C3—O1	−174.99 (15)	C14—C15—C16—O5	177.44 (16)
C1—C2—C3—C4	0.2 (3)	C14—C15—C16—C17	−1.2 (3)
O1—C3—C4—O2	−3.7 (2)	O5—C16—C17—C18	−177.30 (16)
O1—C3—C4—C5	176.17 (15)	C15—C16—C17—C18	1.2 (3)
C2—C3—C4—O2	−178.85 (15)	C16—C17—C18—C13	−0.1 (3)
C2—C3—C4—C5	1.0 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C19—H19*C*···O4^{i}	0.96	2.48	3.293 (3)	143

Symmetry code: (i) *x*, *y*−1, *z*.