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4-(4-Methoxybenzoyl)-5-(4-methoxyphenyl)-2,3-dihydro-2,3-furandione

Tuncer Hökelek,[a] Emin Sarıpınar,[b] Ismail Yıldırım,[b] Mehmet Akkurt[c]* and Yunus Akçamur[b]

[a]Department of Physics, Hacettepe University, 06532 Beytepe, Ankara, Turkey, [b]Department of Chemistry, Faculty of Arts and Sciences, University of Erciyes, 38039 Kayseri, Turkey, and [c]Department of Physics, Faculty of Arts and Sciences, University of Erciyes, 38039 Kayseri, Turkey

Correspondence e-mail: akkurt@erciyes.edu.tr

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.045
wR factor = 0.116
Data-to-parameter ratio = 10.2

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

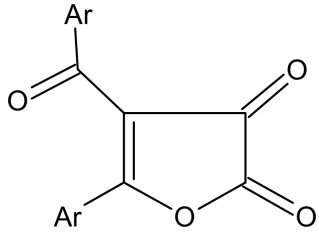
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The title compound, $C_{19}H_{14}O_6$, is a derivative of 2,3-dioxo-2,3-dihydrofuran. The furan ring is essentially planar and the phenyl rings in the methoxyphenyl and methoxybenzoyl groups are not parallel to each other. The furan and phenyl rings are not coplanar. In the crystal, there are two weak C—H···O-type intermolecular interactions.

Comment

Recently, reactions of cyclic oxalyl compounds have been reported to give substituted heterocyclic compounds (Kollenz, Kappe & el Nabey, 1991). The reactions of substituted 2,3-furandiones with various dienophiles (Akçamur & Kollenz, 1987; Kollenz *et al.*, 1984; Kollenz, Sterk & Hutter, 1991) or nucleophiles (Akçamur *et al.*, 1997) in different solvents and at various temperatures have also been studied. A convenient method for the synthesis, together with mechanisms of reactions and calculations on the interaction of 2,3-dioxo-2,3-dihydrofurans with several semicarbazones, ureas and their thio-analogues have been reported recently (Altural *et al.*, 1989; Yıldırım *et al.*, 1995).



Ar : p-CH_3O-C_6H_4-

(I)

Thermal decomposition of 2,3-dioxo-2,3-dihydrofurans leads to the formation of reactive α-oxoketene (acylketene) intermediates (Kollenz *et al.*, 1972; Ziegler *et al.*, 1977). α-Oxoketenes are highly reactive molecules which can be trapped by nucleophiles to give β-ketocarboxylic acid derivatives (Yıldırım & Ílhan, 1997) or alternatively undergo cycloaddition reactions (Sarıpınar *et al.*, 2001; Kollenz *et al.*, 1977; Ziegler *et al.*, 1977).

Fig. 1 shows the title compound, (I), with the atomic numbering. The bond lengths and angles are in accordance with other reported values. The furan ring is almost planar [C1—C2—C3—C4 = −3.3 (3)°], due to strong overlap of the *p*-orbitals.

An examination of the deviations from the least-squares planes through the individual rings shows that rings *A* (O1/

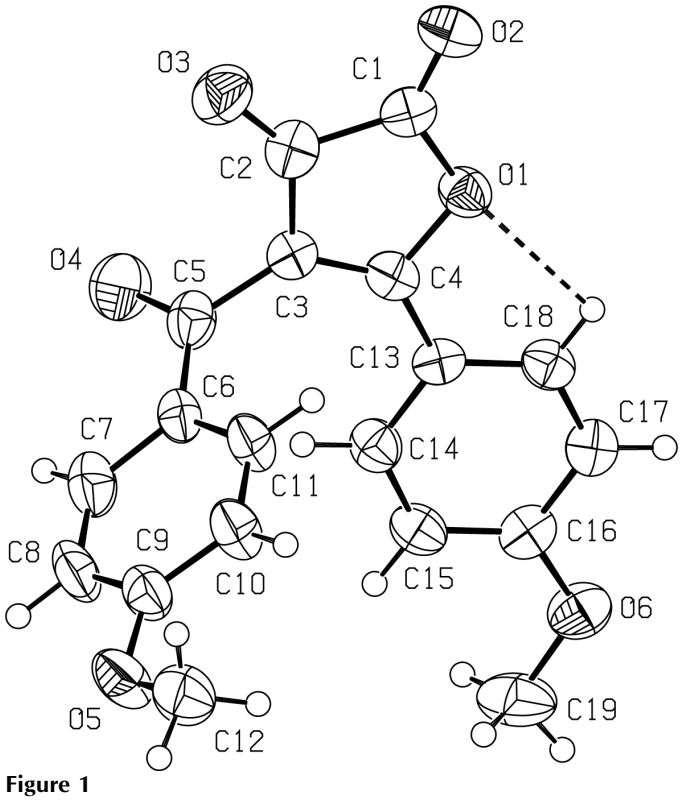


Figure 1
An *ORTEP*II (Johnson, 1976) drawing of the title molecule with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

C1–C4), *B* (C6–C11) and *C* (C13–C18) are nearly planar with maximum deviations for atoms C2 [−0.019 (4) Å], C9 [−0.021 (4) Å] and C16 [−0.019 (3) Å]. The phenyl rings in the 4-methoxybenzoyl and 4-methoxyphenyl groups are not parallel to each other, the angle between these rings being 79.9 (1)°. The dihedral angles between the phenyl rings and the furan ring are *A/B* = 77.5 (1)° and *A/C* = 6.3 (1)°.

The coplanarity of methoxy carbon with the phenyl rings [0.280 (4) Å for C12 and 0.063 (4) Å for C19] results in a close approach between C9 and C10 [1.379 (4) Å] and between C15 and C16 [1.384 (4) Å] and this causes widening of C10—C9—O5 [124.5 (3)°] and C15—C16—O6 [124.8 (3)°] and narrowing of C8—C9—O5 [115.8 (3)°] and C17—C16—O6 [115.8 (3)°] from 120°. Atoms O2 and O3 are nearly coplanar with the furan ring [O1—C1—C2—O3 = −177.9 (3)°, O2—C1—C2—C3 = −177.2 (4)°].

A quantum-chemical calculation using the *AM*1 technique showed that the charges on atoms C1 and C2 are 0.334 and 0.187 e$^-$, respectively, whereas the charges on atoms C3 and C4 are −0.360 and 0.230 e$^-$, respectively. Atoms O2 and O3 have charges of −0.210 and −0.203 e$^-$, respectively (Yılmaz, 2000).

The molecules in the crystal structure are bonded by van der Waals interactions. As can be seen from the packing diagram (Fig. 2), there are two intermolecular hydrogen bonds involving O3 atoms [(C12)H12*C*···O3(1+*x*, *y*, *z*) = 2.494 Å and (C19)H19*A*···O3(1+*x*, −1+*y*, *z*) = 2.577 Å] and one intramolecular hydrogen bond [(C18)H18···O1 = 2.395 Å].

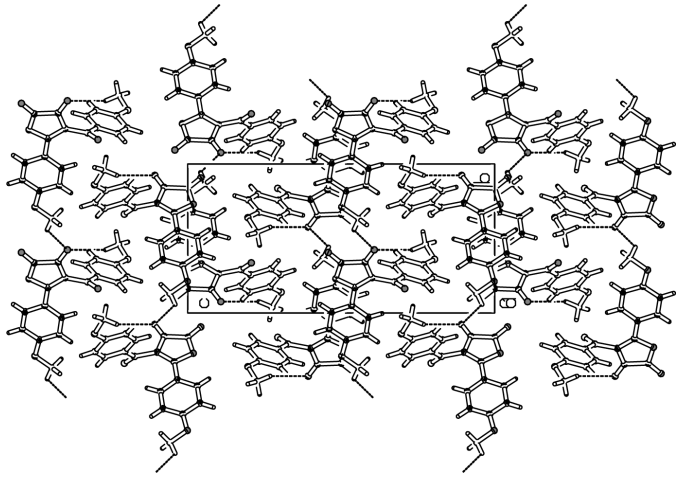


Figure 2
Packing diagram for the title compound. Hydrogen bonds are shown as dotted lines.

Experimental

3.0 g (10.6 mmol) of *p,p′*-dimethoxydibenzoylmethane was dissolved in 100 ml of dry diethyl ether, 1 ml (11.7 mmol) of oxalyl chloride was added and the mixture kept at room temperature for 48 h. The liquid phase was pipetted from the yellow crystals. It was washed several times with dry diethylether; yield 2.4 g (67%), m.p. 428 K. Solvents were dried by refluxing with the appropriate drying agent and distilled before use. Melting points were determined on an Electrothermal 9200 apparatus and uncorrected. Elemental analysis was performed with a Carlo Erba Elemental Analyzer, 1108. IR spectra were recorded on a Shimadzu 435-V-04 apparatus, using potassium bromide tablets. The ^{1}H and ^{13}C NMR spectra were obtained on a Gemini–Varian 200 instrument. The chemical shifts are reported in p.p.m. from tetramethylsilane and given in δ units. IR (KBr): ν = 1810 cm^{-1} (C_2═O); 1720 (C_3═O); 1645 (Ar–C═O); 1600 (C═C). ^{1}H-NMR ($CDCl_3$): δ = 3.87 p.p.m. (3H, CH_3O); 3.88 (3H, CH_3O); 6.92 (2H, Ar–H); 6.94 (2H, Ar–H); 6.97 (2Ar–H); 7.90 (2H, Ar–H); ^{13}C NMR ($CDCl_3$): δ = 187.81 p.p.m. (C_6); 176.46 (C_3); 175.84 (C_5); 154.53 (C_2); 118.2 (C_4); 166.62–114.74 (aromatic C); 56.35 (CH_3O); 56.11 (CH_3O). Found: C 67.62; H 4.13%; calculated for $C_{19}H_{14}O_6$: C 67.45; H 4.17%.

Crystal data

$C_{19}H_{14}O_6$
M_r = 338.3
Monoclinic, $P2_1/n$
a = 8.3574 (10) Å
b = 9.5422 (10) Å
c = 19.775 (2) Å
β = 96.197 (8)°
V = 1567.8 (3) Å^3
Z = 4
D_x = 1.433 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 10–18°
μ = 0.11 mm^{-1}
T = 293 (2) K
Rod-shaped, colorless
0.30 × 0.25 × 0.20 mm

Data collection

Enraf–Nonius Turbo–CAD-4 diffractometer
Non-profiled $\omega/2\theta$ scans
Absorption correction: ψ scan (*MolEN*; Fair, 1990)
T_{min} = 0.968, T_{max} = 0.979
2479 measured reflections
2395 independent reflections
1188 reflections with $I > 2\sigma(I)$
R_{int} = 0.019
θ_{max} = 24.2°
$h = -9 \rightarrow 9$
$k = -11 \rightarrow 11$
$l = -22 \rightarrow 22$
3 standard reflections
frequency: 120 min
intensity decay: none

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.045$	$w = 1/[\sigma^2(F_o^2) + (0.0507P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.116$	$(\Delta/\sigma)_{max} = 0.001$
$S = 0.98$	$\Delta\rho_{max} = 0.15$ e Å^{-3}
2300 reflections	$\Delta\rho_{min} = -0.22$ e Å^{-3}
226 parameters	

Table 1
Selected geometric parameters (Å, °).

O1—C1	1.381 (4)	O6—C19	1.436 (4)
O1—C4	1.414 (4)	C1—C2	1.528 (5)
O2—C1	1.191 (4)	C3—C2	1.436 (5)
O4—C5	1.215 (4)	C3—C5	1.501 (5)
O5—C9	1.362 (4)	C4—C3	1.353 (4)
O5—C12	1.425 (4)	C4—C13	1.435 (4)
O6—C16	1.355 (4)	C6—C5	1.462 (5)
C1—O1—C4	107.4 (3)	C3—C4—C13	133.9 (3)
C9—O5—C12	117.4 (3)	O1—C4—C13	113.4 (3)
C16—O6—C19	117.5 (3)	O4—C5—C6	122.4 (3)
O2—C1—C2	130.7 (3)	O4—C5—C3	117.9 (3)
O1—C1—C2	107.1 (3)	C6—C5—C3	119.6 (3)
O3—C2—C3	132.6 (3)	C7—C6—C5	120.4 (3)
C3—C2—C1	104.8 (3)	O5—C9—C10	124.5 (3)
C4—C3—C2	108.0 (3)	O6—C16—C15	124.8 (3)
C4—C3—C5	130.3 (3)	O6—C16—C17	115.4 (3)
C3—C4—O1	112.6 (3)	C15—C16—C17	119.7 (3)
C2—C3—C5—O4	64.2 (4)	C12—O5—C9—C8	−171.6 (3)
C11—C6—C5—O4	−167.1 (3)	C19—O6—C16—C15	−2.2 (5)
C11—C6—C5—C3	8.6 (5)	C19—O6—C16—C17	180.0 (3)
C12—O5—C9—C10	9.3 (5)		

H atoms were placed geometrically and refined using the usual riding model.

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD*4 (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *SHELXL*97.

The authors wish to acknowledge the purchase of the CAD-4 diffractometer under grant DPT/TBAG1 of the Scientific and Technical Research Council of Turkey. This project was financially supported by the Research Center of Erciyes University.

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Tuncer Hökelek, Emin Sarıpınar, İsmail Yıldırım, Mehmet Akkurt and Yunus Akçamur

S1. Comment

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Fig. 1 shows the title compound, (I), with the atomic numbering. The bond lengths and angles are in accordance with other reported values. The furan ring is almostly planar [C1—C2—C3—C4 = -3.3 (3)°], due to strong overlap of the *p*-orbitals.

An examination of the deviations from the least-squares planes through the individual rings shows that rings A(O1/C1–C4), B(C6–C11) and C(C13–C18) are nearly planar with maximum deviations for atoms C2 [-0.019 (4) Å], C9 [-0.021 (4) Å] and C16 [-0.019 (3) Å]. The phenyl rings in the 4-methoxybenzoyl and 4-methoxyphenyl groups are not parallel to each other, the angle between these rings being 79.9 (1)°. The dihedral angles between the phenyl rings and the furan ring are A/B = 77.5 (1)° and A/C = 6.3 (1)°.

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S2. Experimental

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S3. Refinement

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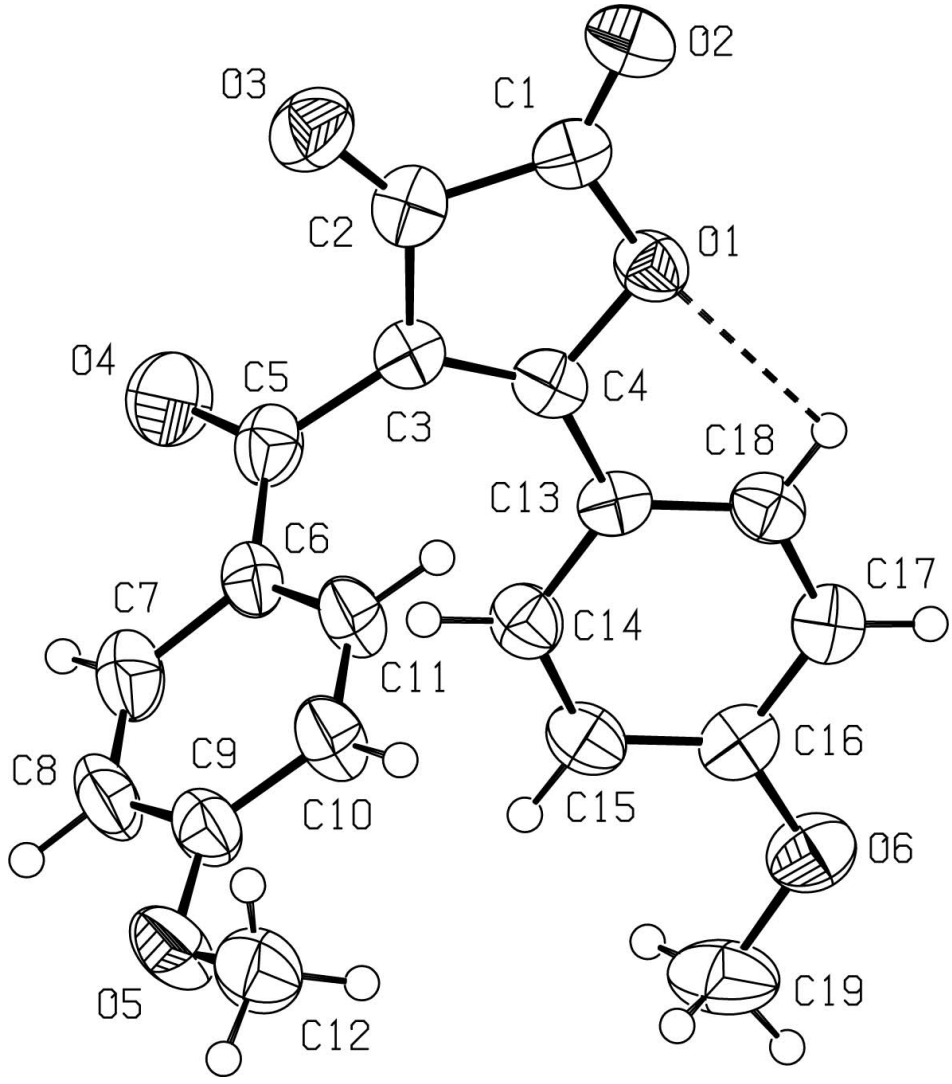


Figure 1

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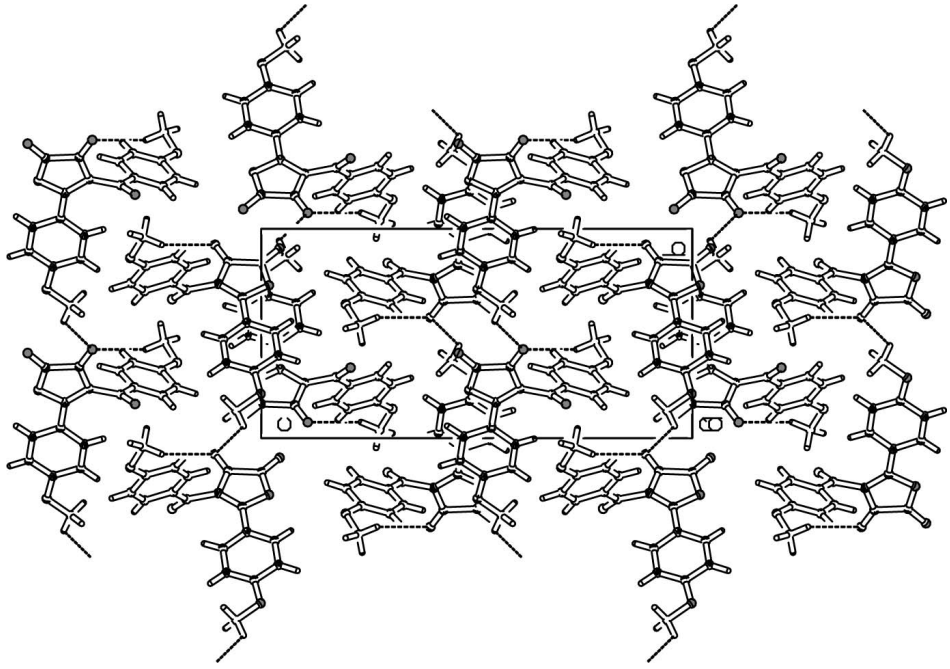


Figure 2

Packing diagram for the title compound. Hydrogen bonds are shown as dotted lines.

(I)

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V = 1567.8 (3) Å^3
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R_{int} = 0.019
θ_{max} = 24.2°, θ_{min} = 2.4°
$h = -9 \rightarrow 9$
$k = -11 \rightarrow 11$
$l = -22 \rightarrow 22$
3 standard reflections every 120 min
intensity decay: none

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.116

S = 0.98
2300 reflections
226 parameters
0 restraints

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0507P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.15$ e Å^{-3}
$\Delta\rho_{min} = -0.22$ e Å^{-3}

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O6	0.5005 (3)	0.2114 (2)	1.00187 (13)	0.0570 (7)
C19	0.5758 (5)	0.1314 (4)	1.0580 (2)	0.0733 (13)
H19A	0.6388	0.0576	1.0412	0.11*
H19B	0.4946	0.0916	1.083	0.11*
H19C	0.6444	0.1914	1.0874	0.11*
O1	0.0380 (3)	0.7298 (2)	0.98265 (11)	0.0437 (6)
O2	−0.1373 (3)	0.9064 (2)	0.95772 (12)	0.0523 (7)
O5	0.7175 (3)	0.8604 (3)	1.30417 (11)	0.0635 (8)
C16	0.4062 (4)	0.3205 (4)	1.01637 (18)	0.0427 (9)
O3	−0.1266 (3)	0.9238 (3)	1.10754 (12)	0.0622 (7)
C4	0.1114 (4)	0.6713 (3)	1.04403 (17)	0.0393 (9)
C13	0.2095 (4)	0.5512 (3)	1.03394 (17)	0.0377 (8)
C1	−0.0614 (4)	0.8368 (4)	0.99964 (18)	0.0417 (9)
C6	0.2749 (4)	0.7437 (3)	1.20470 (16)	0.0404 (9)
C3	0.0671 (4)	0.7371 (3)	1.09969 (17)	0.0389 (9)
C18	0.2406 (4)	0.5086 (3)	0.96916 (17)	0.0415 (9)
H18	0.1958	0.5584	0.9313	0.05*
C15	0.3731 (4)	0.3577 (4)	1.08106 (18)	0.0466 (9)
H15	0.4156	0.306	1.1186	0.056*
C17	0.3358 (4)	0.3950 (4)	0.96036 (18)	0.0449 (9)
H17	0.3535	0.3673	0.9167	0.054*
C14	0.2769 (4)	0.4716 (3)	1.08922 (17)	0.0443 (9)
H14	0.2559	0.4967	1.1328	0.053*
C10	0.5311 (4)	0.8602 (4)	1.20126 (16)	0.0522 (10)
H10	0.6004	0.9118	1.1772	0.063*
C11	0.3825 (4)	0.8196 (4)	1.17067 (16)	0.0481 (10)
H11	0.3533	0.844	1.1255	0.058*
O4	0.0099 (3)	0.6634 (3)	1.20688 (13)	0.0735 (9)
C5	0.1131 (5)	0.7083 (3)	1.17384 (17)	0.0466 (10)
C2	−0.0492 (4)	0.8425 (4)	1.07723 (18)	0.0456 (9)
C9	0.5758 (4)	0.8234 (4)	1.26806 (17)	0.0487 (10)
C8	0.4738 (5)	0.7415 (4)	1.30239 (17)	0.0576 (11)
H8	0.5059	0.7127	1.3467	0.069*
C7	0.3262 (5)	0.7030 (4)	1.27137 (17)	0.0555 (10)
H7	0.2587	0.6486	1.2951	0.067*
C12	0.8156 (5)	0.9598 (4)	1.27410 (19)	0.0679 (12)

H12A	0.9117	0.9767	1.3042	0.102*
H12B	0.7573	1.046	1.2662	0.102*
H12C	0.844	0.9237	1.2317	0.102*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O6	0.0611 (16)	0.0399 (15)	0.0703 (17)	0.0112 (14)	0.0088 (14)	−0.0005 (13)
C19	0.069 (3)	0.054 (3)	0.093 (3)	0.019 (2)	−0.014 (2)	0.001 (2)
O1	0.0492 (16)	0.0385 (14)	0.0422 (14)	0.0032 (12)	−0.0003 (12)	0.0006 (11)
O2	0.0505 (17)	0.0456 (16)	0.0578 (16)	−0.0004 (13)	−0.0072 (13)	0.0074 (14)
O5	0.0648 (19)	0.078 (2)	0.0438 (15)	−0.0049 (16)	−0.0133 (14)	0.0031 (14)
C16	0.043 (2)	0.029 (2)	0.058 (3)	−0.0048 (19)	0.0098 (19)	−0.0016 (19)
O3	0.0638 (18)	0.0582 (17)	0.0661 (18)	0.0129 (15)	0.0143 (14)	−0.0044 (14)
C4	0.038 (2)	0.036 (2)	0.044 (2)	−0.0069 (19)	0.0000 (18)	0.0050 (19)
C13	0.034 (2)	0.032 (2)	0.047 (2)	−0.0006 (18)	0.0039 (17)	0.0014 (18)
C1	0.037 (2)	0.035 (2)	0.053 (2)	−0.0046 (19)	0.0046 (19)	0.000 (2)
C6	0.050 (2)	0.040 (2)	0.031 (2)	0.0002 (19)	0.0060 (18)	−0.0019 (17)
C3	0.039 (2)	0.035 (2)	0.043 (2)	−0.0013 (17)	0.0051 (17)	0.0001 (18)
C18	0.044 (2)	0.037 (2)	0.044 (2)	−0.0024 (18)	0.0020 (18)	0.0069 (17)
C15	0.052 (2)	0.039 (2)	0.047 (2)	0.001 (2)	−0.0020 (19)	0.0080 (18)
C17	0.049 (2)	0.040 (2)	0.047 (2)	−0.0061 (19)	0.0087 (19)	−0.0005 (19)
C14	0.049 (2)	0.041 (2)	0.042 (2)	−0.002 (2)	0.0010 (18)	−0.0046 (18)
C10	0.058 (3)	0.060 (3)	0.037 (2)	−0.013 (2)	−0.0001 (19)	0.0059 (19)
C11	0.056 (3)	0.056 (2)	0.032 (2)	−0.007 (2)	0.0009 (19)	0.0061 (18)
O4	0.063 (2)	0.093 (2)	0.0685 (18)	−0.0066 (17)	0.0221 (15)	0.0247 (16)
C5	0.058 (3)	0.040 (2)	0.044 (2)	0.002 (2)	0.015 (2)	0.0023 (18)
C2	0.053 (3)	0.034 (2)	0.051 (2)	−0.005 (2)	0.010 (2)	−0.0031 (19)
C9	0.056 (3)	0.053 (2)	0.035 (2)	0.001 (2)	−0.002 (2)	−0.003 (2)
C8	0.075 (3)	0.069 (3)	0.028 (2)	0.004 (2)	−0.001 (2)	0.009 (2)
C7	0.072 (3)	0.057 (2)	0.040 (2)	−0.001 (2)	0.014 (2)	0.006 (2)
C12	0.055 (3)	0.088 (3)	0.058 (3)	−0.008 (3)	−0.005 (2)	−0.008 (2)

Geometric parameters (Å, º)

C19—H19A	0.96	C6—C11	1.384 (4)
C19—H19B	0.96	C6—C7	1.397 (4)
C19—H19C	0.96	C6—C5	1.462 (5)
O1—C1	1.381 (4)	C18—C17	1.367 (4)
O1—C4	1.414 (4)	C18—H18	0.93
O2—C1	1.191 (4)	C15—C14	1.372 (4)
O4—C5	1.215 (4)	C15—H15	0.93
O5—C9	1.362 (4)	C17—H17	0.93
O5—C12	1.425 (4)	C14—H14	0.93
O6—C16	1.355 (4)	C10—C11	1.377 (4)
O6—C19	1.436 (4)	C10—C9	1.379 (4)
C16—C15	1.384 (4)	C10—H10	0.93
C16—C17	1.392 (4)	C11—H11	0.93

O3—C2	1.210 (4)	C9—C8	1.387 (5)
C1—C2	1.528 (5)	C8—C7	1.368 (5)
C3—C2	1.436 (5)	C8—H8	0.93
C3—C5	1.501 (5)	C7—H7	0.93
C4—C3	1.353 (4)	C12—H12A	0.96
C4—C13	1.435 (4)	C12—H12B	0.96
C13—C18	1.395 (4)	C12—H12C	0.96
C13—C14	1.399 (4)		

O6—C19—H19A	109.5	C17—C18—C13	121.1 (3)
O6—C19—H19B	109.5	C17—C18—H18	119.4
H19A—C19—H19B	109.5	C13—C18—H18	119.4
O6—C19—H19C	109.5	C14—C15—C16	119.3 (3)
H19A—C19—H19C	109.5	C14—C15—H15	120.3
H19B—C19—H19C	109.5	C16—C15—H15	120.3
C1—O1—C4	107.4 (3)	C18—C17—C16	120.4 (3)
C9—O5—C12	117.4 (3)	C18—C17—H17	119.8
C16—O6—C19	117.5 (3)	C16—C17—H17	119.8
O2—C1—C2	130.7 (3)	C15—C14—C13	122.0 (3)
O1—C1—C2	107.1 (3)	C15—C14—H14	119
O3—C2—C3	132.6 (3)	C13—C14—H14	119
C3—C2—C1	104.8 (3)	C11—C10—C9	119.2 (3)
C4—C3—C2	108.0 (3)	C11—C10—H10	120.4
C4—C3—C5	130.3 (3)	C9—C10—H10	120.4
C3—C4—O1	112.6 (3)	C10—C11—C6	122.4 (3)
C3—C4—C13	133.9 (3)	C10—C11—H11	118.8
O1—C4—C13	113.4 (3)	C6—C11—H11	118.8
O4—C5—C6	122.4 (3)	O3—C2—C1	122.6 (3)
O4—C5—C3	117.9 (3)	O5—C9—C8	115.8 (3)
C6—C5—C3	119.6 (3)	C10—C9—C8	119.7 (4)
C7—C6—C5	120.4 (3)	C7—C8—C9	120.3 (3)
O5—C9—C10	124.5 (3)	C7—C8—H8	119.9
O6—C16—C15	124.8 (3)	C9—C8—H8	119.9
O6—C16—C17	115.4 (3)	C8—C7—C6	121.3 (3)
C15—C16—C17	119.7 (3)	C8—C7—H7	119.4
C18—C13—C14	117.4 (3)	C6—C7—H7	119.4
C18—C13—C4	121.7 (3)	O5—C12—H12A	109.5
C14—C13—C4	120.9 (3)	O5—C12—H12B	109.5
O2—C1—O1	122.2 (3)	H12A—C12—H12B	109.5
C11—C6—C7	117.0 (3)	O5—C12—H12C	109.5
C11—C6—C5	122.6 (3)	H12A—C12—H12C	109.5
C2—C3—C5	121.6 (3)	H12B—C12—H12C	109.5

C1—O1—C4—C3	−1.3 (3)	C11—C6—C5—O4	−167.1 (3)
C1—O1—C4—C13	175.6 (2)	C7—C6—C5—O4	11.9 (5)
C3—C4—C13—C18	−177.5 (3)	C11—C6—C5—C3	8.6 (5)
O1—C4—C13—C18	6.5 (4)	C7—C6—C5—C3	−172.5 (3)
C3—C4—C13—C14	3.0 (6)	C4—C3—C5—O4	−111.2 (4)

O1—C4—C13—C14	−173.1 (3)	C4—C3—C5—C6	73.0 (5)
C4—O1—C1—O2	178.9 (3)	C2—C3—C5—C6	−111.7 (4)
C4—O1—C1—C2	−0.8 (3)	C4—C3—C2—O3	177.2 (4)
C2—C3—C5—O4	64.2 (4)	C5—C3—C2—O3	0.9 (6)
O1—C4—C3—C2	3.0 (4)	C4—C3—C2—C1	−3.3 (3)
C13—C4—C3—C2	−173.1 (3)	C5—C3—C2—C1	−179.5 (3)
O1—C4—C3—C5	178.8 (3)	O2—C1—C2—O3	2.4 (6)
C13—C4—C3—C5	2.7 (6)	O1—C1—C2—O3	−177.9 (3)
C14—C13—C18—C17	−1.2 (5)	O2—C1—C2—C3	−177.2 (4)
C4—C13—C18—C17	179.2 (3)	O1—C1—C2—C3	2.5 (3)
O6—C16—C15—C14	179.3 (3)	C12—O5—C9—C10	9.3 (5)
C17—C16—C15—C14	−2.9 (5)	C12—O5—C9—C8	−171.6 (3)
C13—C18—C17—C16	−1.1 (5)	C11—C10—C9—O5	−178.3 (3)
O6—C16—C17—C18	−178.9 (3)	C11—C10—C9—C8	2.7 (5)
C15—C16—C17—C18	3.2 (5)	O5—C9—C8—C7	177.7 (3)
C16—C15—C14—C13	0.6 (5)	C10—C9—C8—C7	−3.2 (5)
C18—C13—C14—C15	1.5 (5)	C9—C8—C7—C6	0.5 (6)
C4—C13—C14—C15	−179.0 (3)	C11—C6—C7—C8	2.6 (5)
C9—C10—C11—C6	0.5 (5)	C5—C6—C7—C8	−176.4 (3)
C7—C6—C11—C10	−3.1 (5)	C19—O6—C16—C15	−2.2 (5)
C5—C6—C11—C10	175.9 (3)	C19—O6—C16—C17	180.0 (3)