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Crystal structure of (1*S*,2*R*)-6,6-dimethyl-4,8-dioxo-2-phenylspiro[2.5]octane-1-carbaldehyde

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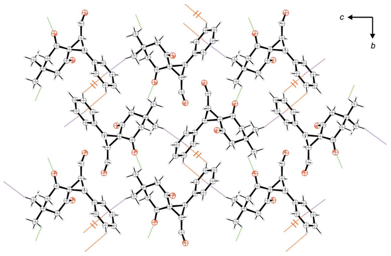
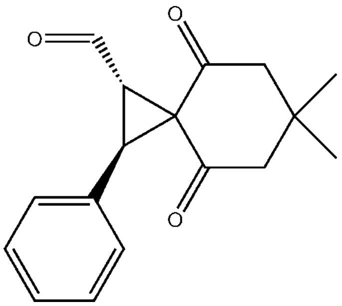
In the title compound, $C_{17}H_{18}O_3$, the two non-spiro C atoms of the cyclopropane ring bear a formyl and a phenyl substituent which are *trans*-oriented. In the crystal, molecules are linked by weak C—H···O and C—H···π contacts resulting in a three-dimensional supramolecular structure.



1. Chemical context

Apart from synthetic transformations, cyclopropane derivatives have attracted interest because of their biological and pharmaceutical applications (Wessjohann *et al.*, 2003). They are present in numerous natural products and have been used extensively as reactive intermediates for the formation of complex structures (Reissig & Zimmer, 2003; Thibodeaux *et al.*, 2012). During our studies on the reactivities of iodonium ylides, we have developed a new method for the synthesis of substituted spiro-cyclopropanes by the organocatalytic reaction of α,β-unsaturated aldehydes with iodonium ylides. The title compound was obtained by the reaction of the cinnamaldehyde-derived iminium ion derived from MacMillan first generation catalyst and the dimedone-derived phenyliodonium ylide.



2. Structural commentary

The molecular structure of the title compound is depicted in Fig. 1. The central cyclopropane ring shares the spiro atom C4 with a cyclohexane ring system while atoms C2 and C3 bear a formyl and a phenyl substituent, respectively. The latter two substituents are *trans*-oriented regarding the plane of the cyclopropane ring. The angles in the three-membered ring range from 58.80 (13)° (C2—C4—C3) to 61.67 (13)° (C3—C2—C4) being close to the ideal value of 60° for such a ring. The six-membered ring containing the spiro atom C4 and ring

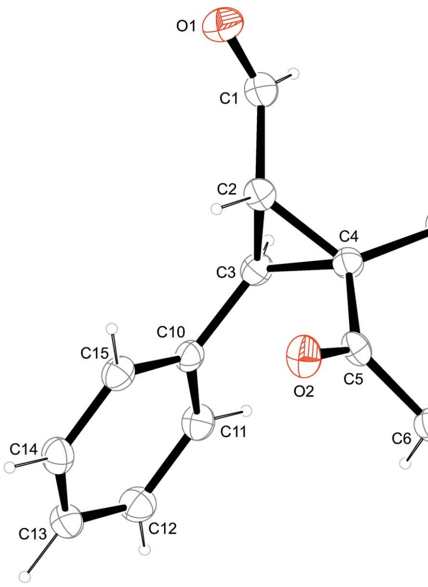


Figure 1
A view of the molecular structure of the title compound, showing the atom labelling. Displacement ellipsoids are drawn at the 50% probability level.

atoms C5–C9 adopts a chair conformation with a puckering amplitude Q of 0.491 (2) Å and θ = 16.8 (2)°, which indicates a slight deviation from an ideal chair conformation with θ = 0°. The plane of the central cyclopropane ring forms dihedral angles of 66.89 (16) and 89.33 (16)°, respectively, with the plane of the phenyl ring and the mean plane of the cyclohexane ring [maximum deviation from this plane is 0.272 (2) Å for atom C7]. The latter two planes form a dihedral angle of 64.15 (10)°. The plane of the formyl group, consisting of atoms C1, H1 and O1, is almost normal to the cyclopropane ring with a dihedral angle of 81.3 (3)°.

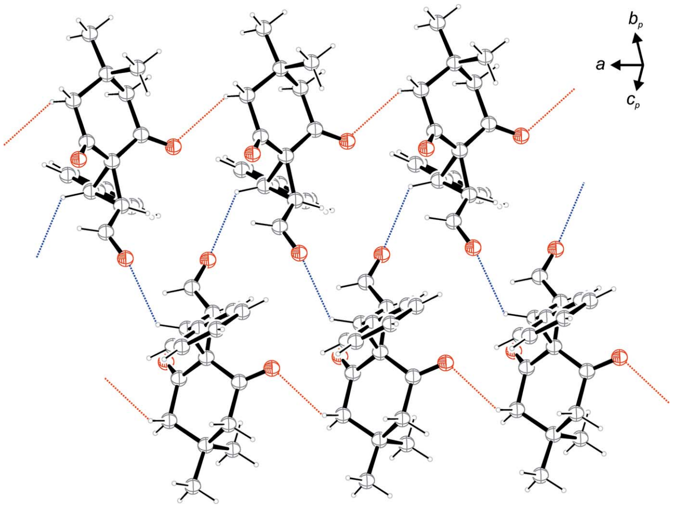


Figure 2
A view of the double strands along [100] formed by two different weak C—H···O contacts (red and blue dashed lines; see Table 1 for details).

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

Cg is the centroid of the C10–C15 phenyl ring.

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···O1^{i}	1.00	2.50	3.159 (3)	123
C8—H8B···O2^{ii}	0.99	2.58	3.365 (2)	137
C16—H16C···O3^{iii}	0.98	2.55	3.271 (3)	131
C12—H12···Cg^{iv}	0.95	2.97	3.688 (2)	133
C17—H17B···Cg^{v}	0.98	2.97	3.916 (2)	163

Symmetry codes: (i) $x-\frac{1}{2}, -y-\frac{1}{2}, -z$; (ii) $x-1, y, z$; (iii) $-x, y+\frac{1}{2}, -z+\frac{1}{2}$; (iv) $x-\frac{1}{2}, -y+\frac{1}{2}, -z$; (v) $-x+\frac{1}{2}, -y, z+\frac{1}{2}$.

3. Supramolecular features

The crystal packing of the title compound shows weak C—H···O and C—H···π interactions (Table 1 and Figs. 2 and 3). Two of the three different C—H···O contacts lead to the formation of double strands along [100]; Fig. 2. Single strands are formed by C8—H8B···O2 contacts (red dotted lines) which are further linked to double strands along the 2_1-screw axes along [100] by C3—H3···O1 contacts (blue dotted lines). The remaining C—H···O as well as the C—H···π interactions are displayed in Fig. 3, which shows details of the crystal packing viewed along [100]. Strands along [010] are established by C16—H16B···O3 contacts (green dotted lines). These strands are linked by two different C—H···π contacts (Table 1), both of which have one of the two sides of the phenyl ring (C10–C15) as π-acceptor (*Cg* is the centroid of this ring). Along [100] the strands are linked by C12—H12···Cg^{iv} contacts (orange dotted lines) while along [001] the links are established by C17—H17B···Cg^{v} interactions (violet dotted lines) enclosing angles between the C—H bond and the plane of the π-system of *ca* 39° and 75° respectively. As a result of these interactions, a three-dimensional supramolecular structure is formed.

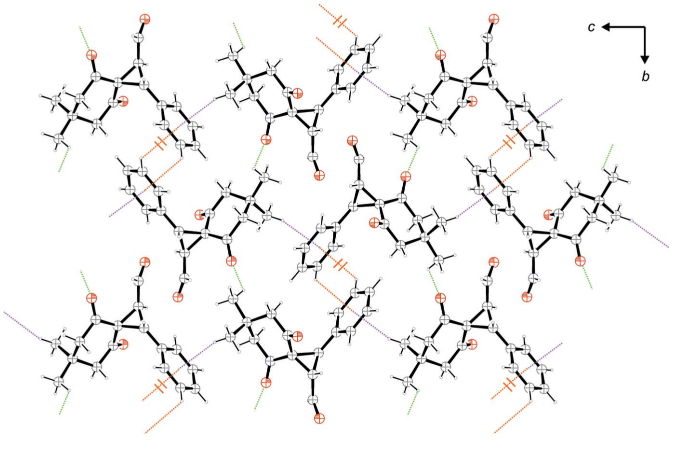


Figure 3
The packing established by weak C—H···O contacts (green dotted lines) C—H···π contacts (violet and orange dotted lines) viewed along [100]; see Table 1 for details. Slashed dotted lines indicate bonds to a symmetry-related molecule.

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Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{17}H_{18}O_3$
M_r	270.31
Crystal system, space group	Orthorhombic, $P2_12_12_1$
Temperature (K)	173
a, *b*, *c* (Å)	5.8831 (1), 12.9095 (4), 18.5655 (5)
V (Å^3)	1410.01 (6)
Z	4
Radiation type	Mo *Kα*
μ (mm^{-1})	0.09
Crystal size (mm)	0.24 × 0.08 × 0.04
Data collection	
Diffractometer	Nonius KappaCCD
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	11599, 3227, 2714
$R_{\rm int}$	0.042
$(\sin \theta/\lambda)_{\rm max}$ (Å^{-1})	0.650
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.037, 0.085, 1.05
No. of reflections	3227
No. of parameters	183
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\rm max}$, $\Delta\rho_{\rm min}$ (e Å^{-3})	0.15, −0.17
Absolute structure	Refined as a perfect inversion twin
Absolute structure parameter	0.5

Computer programs: *COLLECT* (Hooft, 2004), *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997), *SIR97* (Altomare *et al.*, 1999), *SHELXL2014* (Sheldrick, 2015), *ORTEPIII* (Burnett & Johnson, 1996) and *PLATON* (Spek, 2009).

4. Database survey

Structures of spiro[2.5]octane and 4-oxo-spiro[2.5]octane derivatives are numerous; however, there are merely two different structures featuring the 6,6-dimethyl-4,8-dioxo-spiro[2.5]octane moiety as is found in the title compound, namely 6,6-dimethyl-4,8-dioxo-1,1,2,2-tetracyano-spiro(2,5)-octane 1,4-dioxane solvate (NOSMIR; Kayukova *et al.*, 1998) and *trans*-1,2-bis(methoxycarbonyl)-6,6-dimethylspiro(2.5)-octane-4,8-dione (GUHCUI; Maghsoodlou *et al.*, 2009). Two more structures feature the 4,8-dioxo-spiro[2.5]octane building unit, namely. trispiro(2.1.2.1.2.1)dodecane-4,8,12-trione (DAZVEF; Hoffmann *et al.*,1985) and (2*R**)-1,1-di chloro-6,6-dimethyl-2-[(1′*S**)-1′-nitroethyl]spiro[2.5]octane-4,8-dione (YILXIC; Barkov *et al.*, 2013). In NOSMIR, each of the two non-spiro-cyclopropane C atoms bears two cyano groups while in GUHCUI each of the C atoms bears a hydrogen atom and a methoxylcarbonyl group. The latter substituents are, as in the title compound, *trans*-oriented with respect to the plane of the cyclopropane ring.

5. Synthesis and crystallization

A 10 ml round-bottomed flask equipped with a magnetic stirring bar was charged with a solution of the (*S*,*E*)-5-benzyl-2,2,3-trimethyl-4-oxo-1-[(*E*)-3-phenylallylidene]-imidazolidin-1-ium hexafluorophosphate (239 mg, 0.5 mmol, 1eq) and phenyliodonium-4,4-dimethylcyclohexane-2,6-dione (171 mg, 0.5 mmol, 1eq) in acetonitrile (5 ml). After 24 h stirring at ambient temperature, water (10 ml) was added. The aqueous phase was extracted with CH_2Cl_2 (15 ml). The organic layers were combined, washed with brine, and dried over $MgSO_4$. After evaporation of the solvent under vacuum, the crude product was purified by column chromatography (*n*-pentane/Et2O: 7/3 and 6/4) to give the title compound (98 mg, 0.362 mmol, 72%) as colourless crystals (m.p. 397–399 K).

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. C-bound H atoms were positioned geometrically (C—H = 0.95–1.00 Å) and treated as riding on their parent atoms with $U_{\rm iso}$(H) = 1.5$U_{\rm eq}$(C-methyl) and 1.2$U_{\rm eq}$(C) for other H atoms. The methyl groups were allowed to rotate along the C—C bonds to best fit the experimental electron density. As a result of the absence of anomalous scatterers and high angle data, the Flack test results can be considered meaningless. The synthesis resulted in a racemic mixture, hence the structure was refined as an inversion twin.

Acknowledgements

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Saloua Chelli, Konstantin Troshin, Sami Lakhdar, Herbert Mayr and Peter Mayer

Computing details

Data collection: *COLLECT* (Hooft, 2004); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996); software used to prepare material for publication: *PLATON* (Spek, 2009).

(1*S*,2*R*)-6,6-Dimethyl-4,8-dioxo-2-phenylspiro[2.5]octane-1-carbaldehyde

Crystal data

$C_{17}H_{18}O_3$
$M_r = 270.31$
Orthorhombic, $P2_12_12_1$
$a = 5.8831\ (1)$ Å
$b = 12.9095\ (4)$ Å
$c = 18.5655\ (5)$ Å
$V = 1410.01\ (6)$ Å^3
$Z = 4$
$F(000) = 576$
$D_x = 1.273$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5895 reflections
$\theta = 3.1\text{–}27.5°$
$\mu = 0.09$ mm^{-1}
$T = 173$ K
Rod, colourless
0.24 × 0.08 × 0.04 mm

Data collection

Nonius KappaCCD diffractometer
Radiation source: FR591 rotating anode generator
Detector resolution: 9 pixels mm^{-1}
CCD; rotation images; thick slices scans
11599 measured reflections
3227 independent reflections
2714 reflections with $I > 2\sigma(I)$
$R_{\text{int}} = 0.042$
$\theta_{\text{max}} = 27.5°$, $\theta_{\text{min}} = 3.2°$
$h = -7 \rightarrow 7$
$k = -16 \rightarrow 16$
$l = -24 \rightarrow 23$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.085$
$S = 1.05$
3227 reflections
183 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.038P)^2 + 0.2287P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\text{max}} < 0.001$
$\Delta\rho_{\text{max}} = 0.15$ e Å^{-3}
$\Delta\rho_{\text{min}} = -0.17$ e Å^{-3}
Absolute structure: Refined as a perfect inversion twin
Absolute structure parameter: 0.5

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}
O1	0.4197 (3)	−0.32107 (11)	0.04731 (9)	0.0342 (4)
O2	0.7409 (2)	0.01619 (12)	0.11016 (8)	0.0263 (3)
O3	0.1647 (3)	−0.17348 (13)	0.20019 (9)	0.0393 (4)
C1	0.3171 (4)	−0.24439 (16)	0.06610 (11)	0.0266 (5)
H1	0.1638	−0.2515	0.0814	0.032*
C2	0.4217 (4)	−0.13971 (16)	0.06618 (11)	0.0219 (4)
H2	0.5742	−0.1348	0.0426	0.026*
C3	0.2601 (3)	−0.05158 (15)	0.05003 (11)	0.0200 (4)
H3	0.0965	−0.0725	0.0501	0.024*
C4	0.3761 (3)	−0.06024 (15)	0.12514 (10)	0.0193 (4)
C5	0.5547 (3)	0.02063 (16)	0.13825 (10)	0.0201 (4)
C6	0.4809 (4)	0.10926 (16)	0.18537 (11)	0.0229 (5)
H6A	0.3774	0.1545	0.1575	0.027*
H6B	0.6162	0.1508	0.1985	0.027*
C7	0.3597 (3)	0.07468 (16)	0.25467 (11)	0.0221 (4)
C8	0.1576 (3)	0.00558 (16)	0.23406 (11)	0.0243 (5)
H8A	0.0845	−0.0204	0.2786	0.029*
H8B	0.0443	0.0478	0.2077	0.029*
C9	0.2249 (4)	−0.08522 (17)	0.18801 (11)	0.0236 (5)
C10	0.3127 (3)	0.03408 (15)	−0.00113 (10)	0.0186 (4)
C11	0.1524 (3)	0.11331 (15)	−0.00784 (11)	0.0223 (4)
H11	0.0168	0.1111	0.0199	0.027*
C12	0.1900 (4)	0.19527 (16)	−0.05476 (12)	0.0256 (5)
H12	0.0811	0.2493	−0.0586	0.031*
C13	0.3866 (4)	0.19845 (16)	−0.09613 (12)	0.0248 (5)
H13	0.4114	0.2541	−0.1287	0.030*
C14	0.5461 (4)	0.12027 (16)	−0.08971 (11)	0.0241 (5)
H14	0.6812	0.1227	−0.1177	0.029*
C15	0.5103 (3)	0.03793 (15)	−0.04251 (11)	0.0219 (4)
H15	0.6205	−0.0156	−0.0385	0.026*
C16	0.2732 (4)	0.17058 (18)	0.29458 (13)	0.0330 (5)
H16A	0.4007	0.2175	0.3041	0.049*
H16B	0.2039	0.1495	0.3403	0.049*
H16C	0.1598	0.2061	0.2649	0.049*
C17	0.5246 (4)	0.01436 (18)	0.30256 (12)	0.0283 (5)
H17A	0.5775	−0.0474	0.2769	0.042*
H17B	0.4470	−0.0065	0.3470	0.042*
H17C	0.6550	0.0583	0.3145	0.042*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0489 (10)	0.0214 (8)	0.0324 (9)	0.0031 (7)	−0.0002 (8)	−0.0022 (7)
O2	0.0174 (7)	0.0365 (9)	0.0249 (8)	−0.0033 (6)	0.0021 (6)	−0.0018 (7)
O3	0.0496 (10)	0.0335 (9)	0.0349 (9)	−0.0186 (8)	0.0107 (8)	0.0005 (7)
C1	0.0348 (12)	0.0242 (11)	0.0208 (11)	−0.0024 (9)	−0.0013 (9)	0.0010 (8)
C2	0.0242 (10)	0.0217 (10)	0.0199 (10)	0.0005 (8)	0.0005 (8)	0.0011 (8)
C3	0.0190 (10)	0.0206 (10)	0.0204 (10)	−0.0011 (8)	−0.0013 (8)	−0.0026 (8)
C4	0.0195 (10)	0.0193 (10)	0.0192 (10)	−0.0014 (8)	−0.0004 (8)	0.0001 (8)
C5	0.0199 (10)	0.0243 (10)	0.0160 (9)	−0.0008 (8)	−0.0016 (8)	0.0049 (8)
C6	0.0222 (10)	0.0229 (10)	0.0236 (11)	−0.0030 (8)	−0.0003 (9)	0.0008 (8)
C7	0.0204 (10)	0.0259 (11)	0.0200 (10)	0.0022 (8)	0.0008 (8)	−0.0018 (8)
C8	0.0197 (10)	0.0320 (11)	0.0213 (11)	−0.0009 (9)	0.0026 (8)	0.0009 (9)
C9	0.0193 (10)	0.0301 (11)	0.0214 (10)	−0.0062 (9)	−0.0006 (8)	0.0014 (8)
C10	0.0202 (10)	0.0197 (9)	0.0160 (9)	−0.0008 (8)	−0.0019 (8)	−0.0023 (8)
C11	0.0203 (10)	0.0253 (10)	0.0214 (11)	0.0017 (8)	0.0001 (8)	−0.0012 (8)
C12	0.0277 (11)	0.0232 (10)	0.0259 (11)	0.0037 (9)	−0.0028 (9)	0.0007 (9)
C13	0.0303 (12)	0.0235 (11)	0.0207 (11)	−0.0019 (9)	−0.0016 (9)	0.0019 (8)
C14	0.0228 (11)	0.0280 (11)	0.0215 (11)	−0.0013 (9)	0.0033 (9)	−0.0004 (9)
C15	0.0213 (10)	0.0223 (10)	0.0220 (11)	0.0028 (8)	−0.0014 (8)	−0.0026 (8)
C16	0.0344 (12)	0.0332 (12)	0.0314 (12)	0.0079 (10)	0.0025 (11)	−0.0077 (10)
C17	0.0290 (11)	0.0332 (12)	0.0226 (11)	0.0050 (10)	−0.0017 (9)	−0.0020 (9)

Geometric parameters (Å, º)

O1—C1	1.211 (3)	C8—C9	1.504 (3)
O2—C5	1.214 (2)	C8—H8A	0.9900
O3—C9	1.214 (3)	C8—H8B	0.9900
C1—C2	1.485 (3)	C10—C15	1.394 (3)
C1—H1	0.9500	C10—C11	1.396 (3)
C2—C3	1.513 (3)	C11—C12	1.388 (3)
C2—C4	1.524 (3)	C11—H11	0.9500
C2—H2	1.0000	C12—C13	1.389 (3)
C3—C10	1.490 (3)	C12—H12	0.9500
C3—C4	1.557 (3)	C13—C14	1.383 (3)
C3—H3	1.0000	C13—H13	0.9500
C4—C5	1.501 (3)	C14—C15	1.394 (3)
C4—C9	1.503 (3)	C14—H14	0.9500
C5—C6	1.504 (3)	C15—H15	0.9500
C6—C7	1.537 (3)	C16—H16A	0.9800
C6—H6A	0.9900	C16—H16B	0.9800
C6—H6B	0.9900	C16—H16C	0.9800
C7—C17	1.529 (3)	C17—H17A	0.9800
C7—C16	1.530 (3)	C17—H17B	0.9800
C7—C8	1.535 (3)	C17—H17C	0.9800
O1—C1—C2	122.5 (2)	C7—C8—H8A	109.0

O1—C1—H1	118.7	C9—C8—H8B	109.0
C2—C1—H1	118.7	C7—C8—H8B	109.0
C1—C2—C3	115.08 (18)	H8A—C8—H8B	107.8
C1—C2—C4	122.71 (18)	O3—C9—C4	121.2 (2)
C3—C2—C4	61.67 (13)	O3—C9—C8	123.29 (19)
C1—C2—H2	115.4	C4—C9—C8	115.47 (18)
C3—C2—H2	115.4	C15—C10—C11	119.18 (18)
C4—C2—H2	115.4	C15—C10—C3	123.40 (17)
C10—C3—C2	123.65 (17)	C11—C10—C3	117.42 (17)
C10—C3—C4	122.23 (16)	C12—C11—C10	120.45 (19)
C2—C3—C4	59.53 (12)	C12—C11—H11	119.8
C10—C3—H3	113.7	C10—C11—H11	119.8
C2—C3—H3	113.7	C11—C12—C13	120.14 (19)
C4—C3—H3	113.7	C11—C12—H12	119.9
C5—C4—C9	115.97 (17)	C13—C12—H12	119.9
C5—C4—C2	117.47 (17)	C14—C13—C12	119.72 (19)
C9—C4—C2	121.17 (17)	C14—C13—H13	120.1
C5—C4—C3	113.71 (16)	C12—C13—H13	120.1
C9—C4—C3	116.85 (16)	C13—C14—C15	120.53 (19)
C2—C4—C3	58.80 (13)	C13—C14—H14	119.7
O2—C5—C4	121.93 (19)	C15—C14—H14	119.7
O2—C5—C6	123.10 (19)	C14—C15—C10	119.97 (19)
C4—C5—C6	114.90 (16)	C14—C15—H15	120.0
C5—C6—C7	113.56 (16)	C10—C15—H15	120.0
C5—C6—H6A	108.9	C7—C16—H16A	109.5
C7—C6—H6A	108.9	C7—C16—H16B	109.5
C5—C6—H6B	108.9	H16A—C16—H16B	109.5
C7—C6—H6B	108.9	C7—C16—H16C	109.5
H6A—C6—H6B	107.7	H16A—C16—H16C	109.5
C17—C7—C16	109.97 (18)	H16B—C16—H16C	109.5
C17—C7—C8	109.90 (17)	C7—C17—H17A	109.5
C16—C7—C8	109.49 (17)	C7—C17—H17B	109.5
C17—C7—C6	109.89 (17)	H17A—C17—H17B	109.5
C16—C7—C6	108.94 (17)	C7—C17—H17C	109.5
C8—C7—C6	108.63 (16)	H17A—C17—H17C	109.5
C9—C8—C7	113.02 (16)	H17B—C17—H17C	109.5
C9—C8—H8A	109.0		

O1—C1—C2—C3	147.4 (2)	C5—C6—C7—C8	−55.6 (2)
O1—C1—C2—C4	−141.4 (2)	C17—C7—C8—C9	−64.9 (2)
C1—C2—C3—C10	−134.23 (19)	C16—C7—C8—C9	174.16 (17)
C4—C2—C3—C10	110.6 (2)	C6—C7—C8—C9	55.3 (2)
C1—C2—C3—C4	115.2 (2)	C5—C4—C9—O3	−141.2 (2)
C1—C2—C4—C5	154.52 (19)	C2—C4—C9—O3	12.2 (3)
C3—C2—C4—C5	−102.42 (19)	C3—C4—C9—O3	80.3 (3)
C1—C2—C4—C9	1.5 (3)	C5—C4—C9—C8	38.1 (2)
C3—C2—C4—C9	104.5 (2)	C2—C4—C9—C8	−168.43 (18)
C1—C2—C4—C3	−103.1 (2)	C3—C4—C9—C8	−100.3 (2)

C10—C3—C4—C5	−4.1 (2)	C7—C8—C9—O3	131.5 (2)
C2—C3—C4—C5	108.85 (19)	C7—C8—C9—C4	−47.8 (2)
C10—C3—C4—C9	135.3 (2)	C2—C3—C10—C15	4.1 (3)
C2—C3—C4—C9	−111.8 (2)	C4—C3—C10—C15	76.7 (2)
C10—C3—C4—C2	−112.9 (2)	C2—C3—C10—C11	−176.62 (18)
C9—C4—C5—O2	145.1 (2)	C4—C3—C10—C11	−104.1 (2)
C2—C4—C5—O2	−9.3 (3)	C15—C10—C11—C12	−0.4 (3)
C3—C4—C5—O2	−75.2 (2)	C3—C10—C11—C12	−179.71 (18)
C9—C4—C5—C6	−37.9 (2)	C10—C11—C12—C13	0.8 (3)
C2—C4—C5—C6	167.68 (17)	C11—C12—C13—C14	−0.8 (3)
C3—C4—C5—C6	101.85 (19)	C12—C13—C14—C15	0.5 (3)
O2—C5—C6—C7	−135.3 (2)	C13—C14—C15—C10	−0.2 (3)
C4—C5—C6—C7	47.7 (2)	C11—C10—C15—C14	0.1 (3)
C5—C6—C7—C17	64.7 (2)	C3—C10—C15—C14	179.37 (18)
C5—C6—C7—C16	−174.76 (18)		

Hydrogen-bond geometry (Å, º)

Cg is the centroid of the C10–C15 phenyl ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···O1^{i}	1.00	2.50	3.159 (3)	123
C8—H8*B*···O2^{ii}	0.99	2.58	3.365 (2)	137
C16—H16*C*···O3^{iii}	0.98	2.55	3.271 (3)	131
C12—H12···*Cg*^{iv}	0.95	2.97	3.688 (2)	133
C17—H17*B*···*Cg*^{v}	0.98	2.97	3.916 (2)	163

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