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5,5-Dimethyl-3,4-di-*p*-tolylcyclopent-2-enone

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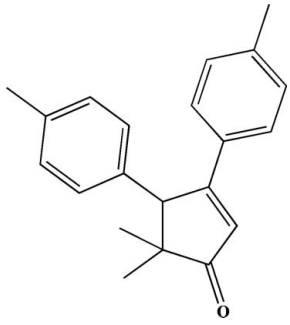
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.033; wR factor = 0.086; data-to-parameter ratio = 11.7.

In the title compound, $C_{21}H_{22}O$, the five-membered non-aromatic cyclopentenone ring is approximately planar and the two *p*-tolyl rings form dihedral angles of 28.6 (2) and 66.9 (1)° with this plane. Intermolecular C—H···O and C—H···π interactions are observed. The C—H···π distance (measured to the centroid of the benzene ring) is 2.86 Å and the C—H···π angle is 123°.

Related literature

For related literature, see: Akella & Vince (1996); Heller & Vincent (1999); Kyoshi *et al.* (1994); Roberts *et al.* (1999); Sanatoro & Roberts (1999); Shiosaki *et al.* (1993).



Experimental

Crystal data

$C_{21}H_{22}O$
M_r = 290.39
Monoclinic, *Cc*
a = 14.8886 (8) Å
b = 13.8910 (8) Å
c = 10.3902 (6) Å
β = 130.426 (5)°
V = 1635.8 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 100 (2) K
0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.979, T_{max} = 0.989
10447 measured reflections
2365 independent reflections
2318 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.087
S = 1.01
2365 reflections
203 parameters
2 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

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

Cg is the centroid of the C6–C11 ring.

D—H···A	D—H	H···A	D···A	D—H···A
C12—H12*B*···O1^{i}	0.98	2.48	3.429 (3)	164
C17—H17···*Cg*^{ii}	0.95	2.86	3.477 (2)	123

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2001); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

Financial assistance from the Teacher Training University is acknowledged.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BI2205).

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supplementary materials

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5,5-Dimethyl-3,4-di-*p*-tolylcyclopent-2-enone

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Comment

Cyclopentenones are of interest for their anti-viral (Sanatoro & Roberts, 1999; Roberts *et al.*, 1999; Akella & Vince 1996), anti-tumor and anti-diabetes (Akella & Vince, 1996; Shiosaki *et al.*,1993), pesticide and bactericide (Kyoshi *et al.*, 1994) properties. They are also used in labeling materials for commercial goods (Heller & Vincent, 1999) on account of their photochemical properties. The structure determination of title compound was undertaken as part of our studies on cyclopentenone derivatives.

The title compound consists of two aromatic phenyl rings and a central non aromatic cyclopentenone ring. The five-membered ring C1–C5 is almost planar and has internal angles ranging from 103.58 (10) to 112.52 (11)°. The distortion from a regular five-membered homocyclic ring is due to different hybridization of the ring atoms and different substituents bonded to them. The bond distances range from 1.3500 (17) to 1.5640 (17) Å. Two sp^3 carbon atoms of this ring, C4 and C5, have distorted tetrahedral geometries, with angles ranging from 104.62 (10) to 115.49 (10)° for C4 and 103.58 (10) to 115.12 (11) for C5. The phenyl ring bonded to C3 is rotated from the plane of the cylopentenone ring with a dihedral angle of 28.6 (2)° (Figure 1). The other phenyl ring makes an angle of 66.9 (1)° with the cyclopentenone ring.

Intermolecular C—H···O interactions exist between H12B and O1 (Figure 2 and Table 1), and C—H···π interactions are formed between C17 and the phenyl ring C6–C11 (Figure 3).

Experimental

The title compound was synthesized in three steps:

a) To a solution of NaOH (1 g, 25 mmol) in methanol (10 ml) was added 4,4-dimethylbenzil (1 g, 4.2 mmol) and isopropylmethylketone (2 ml, 18.6 mmol). The mixture was refluxed for 1.5 h then water (20 ml) was added. The resulting precipitate was filtered and dried *in vacuo* to give 4-hydroxy-5,5-dimethyl-3,4-di-*p*-tolyl-cyclopent-2-enone (0.85 g, 2.9 mmol) in 85% yield; m.p. 419–421 K.

b) To a solution of 4-hydroxy-5,5-dimethyl-3,4-di-*p*-tolyl-cyclopent-2-enone (1 g, 3.3 mmol) in MeOH (30 ml) was added a solution of $NaBH_4$ (1 g, 26.4 mmol) in water (0.2 ml). The mixture was stirred for 3 h at room temperature, then diethylether (30 ml) was added. The ether solution was washed three times with water (30 ml) and dried over Na_2SO_4, then the solvent was evaporated to give 2,2-dimethyl-1,5-di-*p*-tolyl-cylopent-4-ene-1,3-diol (0.80 g, 2.6 mmol) in 80% yield.

c) To a stirred solution of 2,2-dimethyl-1,5-di-*p*-tolyl-cylopent-4-ene-1,3-diol (1 g, 3.2 mmol) in EtOH (20 ml), was added HCl (5 ml). The mixture was refluxed for 3 h, then diethylether (30 ml) was added. The ether solution was washed with water (30 ml) and dried over Na_2SO_4, then the solvent was evaporated to give 5,5-dimethyl-3,4-di-*p*-tolyl-cyclopent-2-enone (0.65 g, 2.2 mmol) in 65% yield; m.p. 375–377 K.

Refinement

H atoms were placed in calculated positions and refined as riding with C—H = 0.95–1.00 Å and with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(C). The methyl groups were allowed to rotate about their local threefold axes. In the absence of significant anomalous scattering effects, Friedel pairs have been merged as equivalent data.

Figures

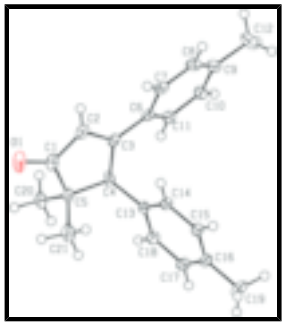

Fig. 1. The molecular structure of the title compound with displacement ellipsoids drawn at the 50% probability level for non-H atoms.

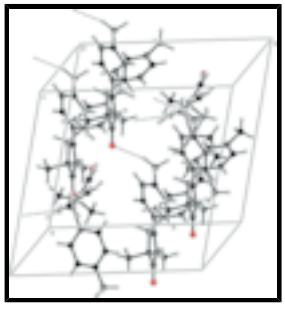

Fig. 2. The unit-cell contents of the title compound. C—H···O interactions are shown as dashed lines.

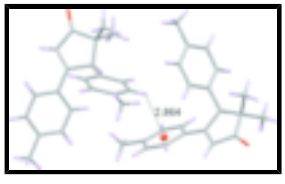

Fig. 3. C—H···π interaction between C17 and the aromatic ring C6–C11. The C—H···π distance (measured to the centroid of the phenyl ring) is 2.86 Å and the C—H···π angle is 123°.

5,5-Dimethyl-3,4-di-*p*-tolylcyclopent-2-enone

Crystal data

$C_{21}H_{22}O$	F_{000} = 624
M_r = 290.39	D_x = 1.179 Mg m^{-3}
Monoclinic, *Cc*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: C -2yc	Cell parameters from 6448 reflections
a = 14.8886 (8) Å	θ = 2.3–30.1°
b = 13.8910 (8) Å	μ = 0.07 mm^{-1}
c = 10.3902 (6) Å	*T* = 100 (2) K
β = 130.426 (5)°	Prism, colourless

V = 1635.8 (2) Å^3
Z = 4

0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Monochromator: graphite
T = 100(2) K
φ and ω scans
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)
T_{min} = 0.979, T_{max} = 0.989
10447 measured reflections

2365 independent reflections
2318 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 30.1°
θ_{min} = 2.3°
h = −20→20
k = −19→19
l = −14→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.087
S = 1.01
2365 reflections
203 parameters
2 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
$w = 1/[\sigma^2(F_o^2) + (0.068P)^2 + 0.2P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}
Extinction correction: none

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.

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 $F^2 > 2\text{sigma}(F^2)$ 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}
O1	0.29633 (12)	0.50200 (8)	0.22848 (18)	0.0343 (3)

C1	0.27003 (12)	0.42152 (10)	0.16715 (19)	0.0227 (3)
C2	0.25295 (12)	0.39032 (9)	0.01826 (18)	0.0212 (2)
H2A	0.2673	0.4290	−0.0422	0.025*
C3	0.21383 (10)	0.29855 (9)	−0.02097 (15)	0.0161 (2)
C4	0.20845 (10)	0.25363 (8)	0.10639 (15)	0.0149 (2)
H4A	0.1242	0.2374	0.0467	0.018*
C5	0.24629 (11)	0.33618 (9)	0.23522 (16)	0.0183 (2)
C6	0.17742 (11)	0.24495 (9)	−0.16999 (15)	0.0160 (2)
C7	0.22584 (12)	0.26583 (9)	−0.24578 (16)	0.0193 (2)
H7A	0.2835	0.3151	−0.2002	0.023*
C8	0.18999 (13)	0.21489 (11)	−0.38715 (17)	0.0220 (3)
H8A	0.2249	0.2289	−0.4357	0.026*
C9	0.10359 (12)	0.14339 (10)	−0.45960 (16)	0.0213 (2)
C10	0.05415 (12)	0.12320 (10)	−0.38551 (16)	0.0200 (2)
H10A	−0.0057	0.0756	−0.4341	0.024*
C11	0.09185 (11)	0.17215 (9)	−0.24115 (16)	0.0178 (2)
H11A	0.0592	0.1561	−0.1900	0.021*
C12	0.06775 (16)	0.08719 (14)	−0.6102 (2)	0.0316 (3)
H12A	0.0531	0.1316	−0.6953	0.047*
H12B	−0.0043	0.0508	−0.6586	0.047*
H12C	0.1311	0.0425	−0.5749	0.047*
C13	0.28004 (10)	0.16155 (8)	0.18249 (14)	0.0144 (2)
C14	0.37655 (10)	0.14336 (9)	0.19216 (15)	0.0158 (2)
H14A	0.3982	0.1893	0.1488	0.019*
C15	0.44137 (10)	0.05868 (9)	0.26474 (15)	0.0171 (2)
H15A	0.5054	0.0469	0.2674	0.021*
C16	0.41375 (11)	−0.00923 (9)	0.33366 (16)	0.0180 (2)
C17	0.31813 (12)	0.00912 (10)	0.32504 (16)	0.0200 (2)
H17A	0.2981	−0.0358	0.3719	0.024*
C18	0.25136 (11)	0.09263 (9)	0.24840 (16)	0.0184 (2)
H18A	0.1850	0.1028	0.2409	0.022*
C19	0.48622 (13)	−0.09959 (11)	0.4148 (2)	0.0274 (3)
H19A	0.4690	−0.1299	0.4819	0.041*
H19B	0.5703	−0.0833	0.4884	0.041*
H19C	0.4665	−0.1443	0.3267	0.041*
C20	0.14578 (12)	0.36188 (10)	0.23427 (18)	0.0230 (3)
H20A	0.1690	0.4173	0.3085	0.034*
H20B	0.1292	0.3068	0.2749	0.034*
H20C	0.0749	0.3780	0.1189	0.034*
C21	0.35969 (13)	0.31701 (12)	0.41703 (19)	0.0299 (3)
H21A	0.3807	0.3746	0.4860	0.045*
H21B	0.4239	0.3013	0.4171	0.045*
H21C	0.3470	0.2629	0.4641	0.045*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0359 (6)	0.0203 (5)	0.0508 (7)	−0.0077 (4)	0.0300 (6)	−0.0128 (5)

C1	0.0175 (5)	0.0175 (5)	0.0314 (6)	−0.0010 (4)	0.0152 (5)	−0.0035 (5)
C2	0.0192 (6)	0.0153 (5)	0.0287 (6)	0.0007 (4)	0.0154 (5)	0.0013 (5)
C3	0.0135 (5)	0.0145 (5)	0.0190 (5)	0.0027 (4)	0.0100 (5)	0.0025 (4)
C4	0.0139 (5)	0.0130 (5)	0.0171 (5)	0.0015 (4)	0.0098 (4)	−0.0007 (4)
C5	0.0154 (5)	0.0165 (5)	0.0195 (5)	0.0009 (4)	0.0097 (5)	−0.0042 (4)
C6	0.0152 (5)	0.0157 (5)	0.0172 (5)	0.0037 (4)	0.0106 (5)	0.0046 (4)
C7	0.0177 (5)	0.0196 (5)	0.0204 (6)	0.0016 (4)	0.0123 (5)	0.0060 (4)
C8	0.0224 (6)	0.0273 (6)	0.0202 (6)	0.0022 (5)	0.0156 (5)	0.0060 (5)
C9	0.0194 (6)	0.0276 (6)	0.0168 (5)	0.0024 (5)	0.0117 (5)	0.0021 (5)
C10	0.0190 (6)	0.0229 (6)	0.0193 (5)	−0.0007 (5)	0.0130 (5)	−0.0004 (5)
C11	0.0174 (5)	0.0188 (5)	0.0194 (5)	0.0005 (4)	0.0129 (5)	0.0010 (4)
C12	0.0326 (7)	0.0450 (9)	0.0234 (6)	−0.0059 (7)	0.0209 (6)	−0.0072 (6)
C13	0.0136 (5)	0.0137 (5)	0.0151 (5)	0.0003 (4)	0.0090 (4)	−0.0002 (4)
C14	0.0147 (5)	0.0154 (5)	0.0184 (5)	0.0013 (4)	0.0112 (4)	0.0019 (4)
C15	0.0145 (5)	0.0167 (5)	0.0200 (5)	0.0018 (4)	0.0112 (5)	0.0011 (4)
C16	0.0164 (5)	0.0150 (5)	0.0174 (5)	0.0011 (4)	0.0087 (4)	0.0011 (4)
C17	0.0216 (6)	0.0186 (5)	0.0216 (6)	−0.0002 (4)	0.0148 (5)	0.0035 (4)
C18	0.0183 (5)	0.0198 (6)	0.0218 (6)	0.0012 (4)	0.0151 (5)	0.0018 (4)
C19	0.0234 (7)	0.0192 (6)	0.0338 (7)	0.0066 (5)	0.0159 (6)	0.0097 (5)
C20	0.0232 (6)	0.0230 (6)	0.0275 (6)	0.0023 (5)	0.0185 (6)	−0.0040 (5)
C21	0.0208 (6)	0.0284 (7)	0.0220 (6)	0.0032 (5)	0.0057 (5)	−0.0078 (5)

Geometric parameters (Å, °)

O1—C1	1.2189 (17)	C12—H12A	0.980
C1—C2	1.461 (2)	C12—H12B	0.980
C1—C5	1.5344 (19)	C12—H12C	0.980
C2—C3	1.3500 (17)	C13—C18	1.3954 (16)
C2—H2A	0.950	C13—C14	1.3970 (16)
C3—C6	1.4687 (17)	C14—C15	1.3927 (16)
C3—C4	1.5113 (17)	C14—H14A	0.950
C4—C13	1.5179 (16)	C15—C16	1.3978 (17)
C4—C5	1.5640 (17)	C15—H15A	0.950
C4—H4A	1.000	C16—C17	1.3908 (18)
C5—C20	1.5322 (18)	C16—C19	1.5067 (18)
C5—C21	1.5342 (19)	C17—C18	1.3933 (17)
C6—C7	1.4001 (17)	C17—H17A	0.950
C6—C11	1.4037 (17)	C18—H18A	0.950
C7—C8	1.388 (2)	C19—H19A	0.980
C7—H7A	0.950	C19—H19B	0.980
C8—C9	1.397 (2)	C19—H19C	0.980
C8—H8A	0.950	C20—H20A	0.980
C9—C10	1.3957 (18)	C20—H20B	0.980
C9—C12	1.503 (2)	C20—H20C	0.980
C10—C11	1.3912 (18)	C21—H21A	0.980
C10—H10A	0.950	C21—H21B	0.980
C11—H11A	0.950	C21—H21C	0.980
O1—C1—C2	127.00 (14)	H12A—C12—H12B	109.5
O1—C1—C5	124.03 (14)	C9—C12—H12C	109.5

C2—C1—C5	108.96 (11)	H12A—C12—H12C	109.5
C3—C2—C1	110.15 (12)	H12B—C12—H12C	109.5
C3—C2—H2A	124.9	C18—C13—C14	117.93 (11)
C1—C2—H2A	124.9	C18—C13—C4	119.93 (11)
C2—C3—C6	126.09 (12)	C14—C13—C4	122.13 (11)
C2—C3—C4	112.52 (11)	C15—C14—C13	120.73 (11)
C6—C3—C4	121.38 (10)	C15—C14—H14A	119.6
C3—C4—C13	112.71 (10)	C13—C14—H14A	119.6
C3—C4—C5	104.62 (10)	C14—C15—C16	121.11 (11)
C13—C4—C5	115.49 (10)	C14—C15—H15A	119.4
C3—C4—H4A	107.9	C16—C15—H15A	119.4
C13—C4—H4A	107.9	C17—C16—C15	118.17 (11)
C5—C4—H4A	107.9	C17—C16—C19	121.37 (12)
C20—C5—C21	109.80 (12)	C15—C16—C19	120.45 (12)
C20—C5—C1	109.45 (10)	C16—C17—C18	120.70 (11)
C21—C5—C1	107.65 (12)	C16—C17—H17A	119.6
C20—C5—C4	110.92 (10)	C18—C17—H17A	119.6
C21—C5—C4	115.12 (11)	C17—C18—C13	121.32 (11)
C1—C5—C4	103.58 (10)	C17—C18—H18A	119.3
C7—C6—C11	118.39 (11)	C13—C18—H18A	119.3
C7—C6—C3	121.01 (12)	C16—C19—H19A	109.5
C11—C6—C3	120.60 (11)	C16—C19—H19B	109.5
C8—C7—C6	120.31 (12)	H19A—C19—H19B	109.5
C8—C7—H7A	119.8	C16—C19—H19C	109.5
C6—C7—H7A	119.8	H19A—C19—H19C	109.5
C7—C8—C9	121.37 (12)	H19B—C19—H19C	109.5
C7—C8—H8A	119.3	C5—C20—H20A	109.5
C9—C8—H8A	119.3	C5—C20—H20B	109.5
C10—C9—C8	118.44 (13)	H20A—C20—H20B	109.5
C10—C9—C12	120.77 (13)	C5—C20—H20C	109.5
C8—C9—C12	120.75 (13)	H20A—C20—H20C	109.5
C11—C10—C9	120.54 (12)	H20B—C20—H20C	109.5
C11—C10—H10A	119.7	C5—C21—H21A	109.5
C9—C10—H10A	119.7	C5—C21—H21B	109.5
C10—C11—C6	120.92 (12)	H21A—C21—H21B	109.5
C10—C11—H11A	119.5	C5—C21—H21C	109.5
C6—C11—H11A	119.5	H21A—C21—H21C	109.5
C9—C12—H12A	109.5	H21B—C21—H21C	109.5
C9—C12—H12B	109.5		

O1—C1—C2—C3	−174.33 (14)	C11—C6—C7—C8	−0.41 (18)
C5—C1—C2—C3	4.22 (15)	C3—C6—C7—C8	−179.62 (12)
C1—C2—C3—C6	174.66 (12)	C6—C7—C8—C9	1.4 (2)
C1—C2—C3—C4	−4.37 (15)	C7—C8—C9—C10	−0.6 (2)
C2—C3—C4—C13	−123.54 (11)	C7—C8—C9—C12	−178.52 (14)
C6—C3—C4—C13	57.38 (14)	C8—C9—C10—C11	−1.1 (2)
C2—C3—C4—C5	2.71 (14)	C12—C9—C10—C11	176.80 (13)
C6—C3—C4—C5	−176.37 (10)	C9—C10—C11—C6	2.1 (2)
O1—C1—C5—C20	57.90 (18)	C7—C6—C11—C10	−1.31 (18)
C2—C1—C5—C20	−120.70 (11)	C3—C6—C11—C10	177.91 (12)

O1—C1—C5—C21	−61.39 (17)	C3—C4—C13—C18	−155.44 (11)
C2—C1—C5—C21	120.00 (12)	C5—C4—C13—C18	84.38 (14)
O1—C1—C5—C4	176.25 (14)	C3—C4—C13—C14	25.73 (15)
C2—C1—C5—C4	−2.35 (13)	C5—C4—C13—C14	−94.45 (14)
C3—C4—C5—C20	117.27 (11)	C18—C13—C14—C15	0.32 (17)
C13—C4—C5—C20	−118.23 (12)	C4—C13—C14—C15	179.17 (11)
C3—C4—C5—C21	−117.30 (13)	C13—C14—C15—C16	−1.64 (18)
C13—C4—C5—C21	7.20 (17)	C14—C15—C16—C17	1.20 (18)
C3—C4—C5—C1	−0.06 (12)	C14—C15—C16—C19	−178.81 (12)
C13—C4—C5—C1	124.44 (11)	C15—C16—C17—C18	0.54 (19)
C2—C3—C6—C7	28.61 (19)	C19—C16—C17—C18	−179.46 (13)
C4—C3—C6—C7	−152.43 (12)	C16—C17—C18—C13	−1.87 (19)
C2—C3—C6—C11	−150.58 (13)	C14—C13—C18—C17	1.42 (18)
C4—C3—C6—C11	28.37 (17)	C4—C13—C18—C17	−177.46 (11)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C12—H12B···O1^{i}	0.98	2.48	3.429 (3)	164
C17—H17···Cg^{ii}	0.95	2.86	3.477 (2)	123

Symmetry codes: (i) *x*−1/2, *y*−1/2, *z*−1; (ii) *x*, −*y*, *z*+1/2.

Fig. 1

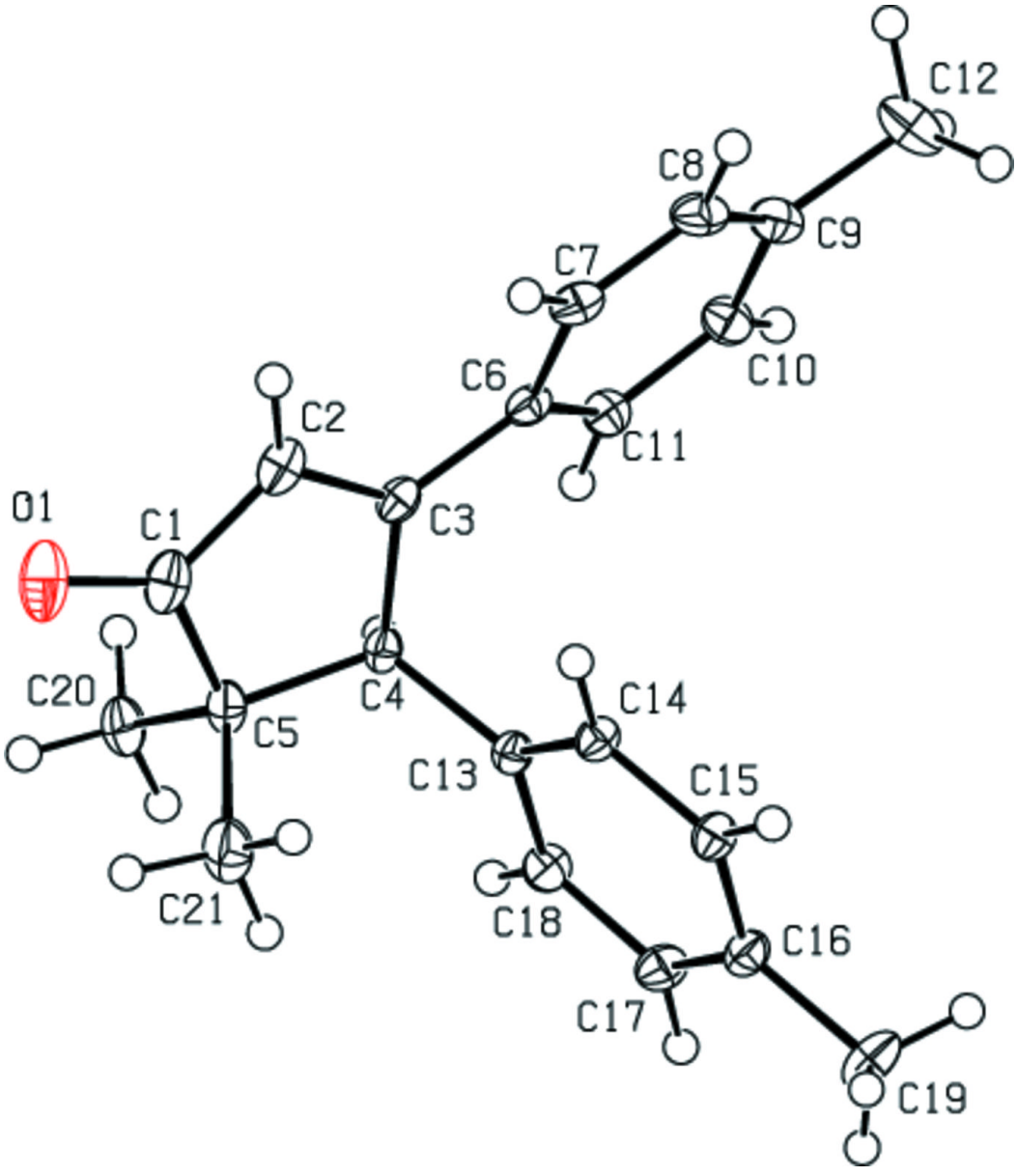
C12
C8
C9
C7
C10
C6
C2
C11
O1
C1
C3
C20
C4
C14
C5
C13
C15
C21
C18
C16
C17
C19

Fig. 2

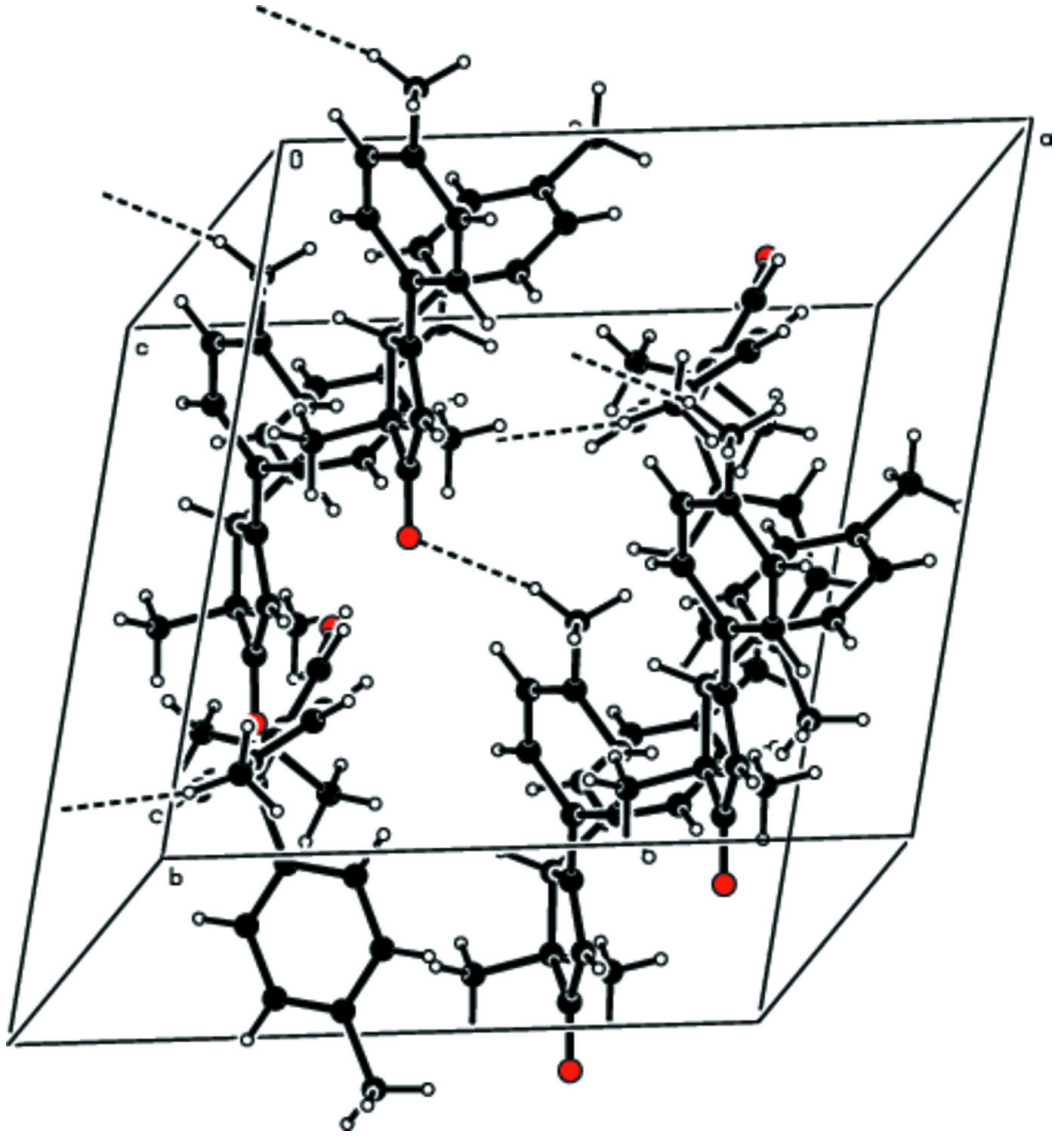

Fig. 3