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2-Benzoyloxy-5-methylbenzophenone

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
Disorder in main residue
R factor = 0.032
wR factor = 0.088
Data-to-parameter ratio = 10.3

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

In the crystal structure of the title compound, $C_{21}H_{16}O_3$, the molecules are connected into centrosymmetric dimers by weak C—H···O intermolecular hydrogen bonds. The crystal packing is stabilized by C—H···π and π–π stacking interactions.

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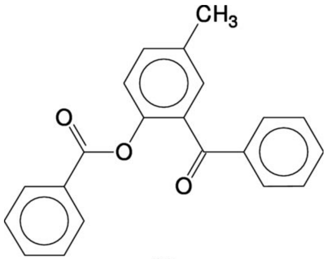
Comment

Benzophenone and related analogues have been reported to act as anti-allergic, anti-inflammatory, anti-asthmatic and anti-anaphylactic agents (Evans *et al.*, 1987). Benzophenone derivatives are widely used in sunscreen lotions for UVA protection (Deleu *et al.*, 1992). In view of the above importance and to understand the conformation of the benzophenone moiety, the crystal structure determination of the title compound, (I), was carried out.



(I)

A view of (I), showing the atom-numbering scheme, is given in Fig. 1 and selected geometric parameters are given in Table 1. The benzoyl and benzoate phenyl rings form dihedral angles with the central benzene ring of 68.93 (5) and 54.88 (5)°, respectively. The dihedral angle formed by the planes of the benzoyl phenyl ring and the carbonyl moiety C7═O3 is 22.22 (9)°. The conformation of the attachment of benzoyl and benzoate phenyls to the central benzene ring can also be characterized by the torsion angles C3—C2—C7—C11 and C2—C1—O1—C9 of 53.02 (15) and 57.13 (15)°, respectively. The orientation of the benzoyl phenyl ring is described by the torsion angle C2—C7—C11—C16 of −159.32 (12)°. The observed conformation differs significantly from that seen in the earlier reported similar structure of 2-benzoyl-l-naphthyl benzoate (Chinnakali *et al.*, 1999), where the corresponding torsion angles are −39.1 (3), 96.2 (2) and 155.7 (2)°, respectively. This can be explained by different intermolecular interactions in both structures.

In the crystal structure of (I), the molecules are linked by weak C—H···O intermolecular hydrogen bonds about a centre of inversion, forming dimeric entities. The separation of

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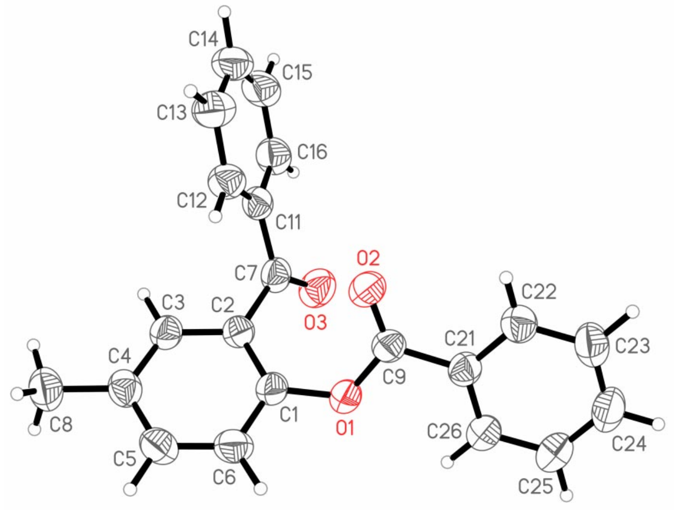

Figure 1
A view of the title molecule with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. Only one orientation of the disordered H atoms of the methyl group is shown.

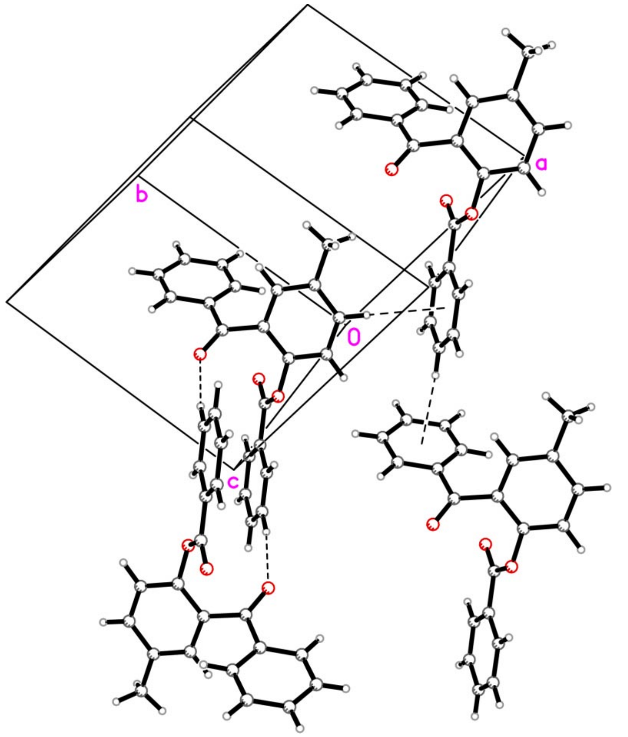

Figure 2
Part of the molecular packing of (I), showing intermolecular C—H$\cdots$O and C—H$\cdots\pi$ interactions as dashed lines. Only one orientation of the disordered H atoms of the methyl group is shown.

3.6780 (9) Å between the C11–C16 phenyl rings related by an inversion centre indicates the existence of π–π stacking interactions between adjacent molecules. The perpendicular distance between the rings is *ca* 3.50 Å. Weak intermolecular C—H$\cdots\pi$ interactions complete the packing in the third dimension (Table 2 and Fig. 2).

Experimental

Equimolar quantities of 2-hydroxy-5-methylbenzophenone and benzoyl chloride were mixed in a conical flask. To this solution, 10% NaOH was added and the resulting mixture stirred in an ice bath for 0.5 h. The separated white solid was filtered off, washed with water, dried and recrystallized from ethanol to give colourless crystals (90% yield).

Crystal data

$C_{21}H_{16}O_3$
M_r = 316.34
Triclinic, $P\overline{1}$
a = 9.2068 (5) Å
b = 9.7961 (5) Å
c = 10.1375 (6) Å
α = 94.732 (4)°
β = 112.570 (5)°
γ = 102.194 (4)°
V = 811.57 (9) Å^3

Z = 2
D_x = 1.294 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 5424 reflections
θ = 2.2–30.6°
μ = 0.09 mm^{-1}
T = 293 K
Prism, colourless
0.60 × 0.52 × 0.13 mm

Data collection

Kuma KM4 CCD diffractometer
ω scans
9605 measured reflections
2842 independent reflections
2563 reflections with $I > 2\sigma(I)$

$R_{\rm int}$ = 0.036
$\theta_{\rm max}$ = 25.0°
$h = -10 \rightarrow 10$
$k = -11 \rightarrow 11$
$l = -12 \rightarrow 12$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.088
S = 1.05
2842 reflections
277 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0405P)^2 + 0.1213P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max}$ = 0.12 e Å^{-3}
$\Delta\rho_{\rm min}$ = −0.12 e Å^{-3}
Extinction correction: *SHELXTL*/*PC*
Extinction coefficient: 0.025 (4)

Table 1
Selected geometric parameters (Å, °).

O1—C1	1.3997 (14)	O2—C9	1.1965 (13)
O1—C9	1.3566 (15)	O3—C7	1.2151 (14)
C1—O1—C9	120.30 (8)	O3—C7—C11	121.20 (11)
O1—C1—C2	123.70 (10)	O1—C9—O2	123.23 (10)
O1—C1—C6	115.21 (10)	O1—C9—C21	111.13 (9)
O3—C7—C2	120.33 (10)	O2—C9—C21	125.64 (10)
C9—O1—C1—C2	57.12 (15)	C3—C2—C7—C11	53.02 (14)
C2—C7—C11—C16	−159.32 (11)		

Table 2
Hydrogen-bonding geometry (Å, °).

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C5—H5$\cdots Cg1^{\rm i}$	0.979 (15)	2.782 (17)	3.5966 (16)	141.2 (11)
C24—H24$\cdots Cg2^{\rm ii}$	0.958 (17)	2.774 (19)	3.6848 (17)	158.7 (13)
C25—H25$\cdots$O3$^{\rm iii}$	0.972 (17)	2.483 (17)	3.4487 (17)	172.4 (13)

Symmetry codes: (i) $1 + x, y, z$; (ii) $x - 1, y - 1, z$; (iii) $-x, -y, 2 - z$. $Cg1$ and $Cg2$ are the centroids of the rings C21–26 and C11–C16, respectively.

All H atoms were initially located in a difference Fourier map, including those of the methyl group, which were found to be disordered over two positions with equal occupancy factors. Methyl H atoms were placed in calculated positions (C—H = 0.99 Å) and refined using a riding model. The remaining H-atom positions and isotropic displacement parameters of all H atoms were refined freely.

Data collection: *CrysAlisCCD* (Oxford Diffraction, 2004); cell refinement: *CrysAlisRED* (Oxford Diffraction, 2004); data reduction: *CrysAlisRED*; program(s) used to solve structure: *SHELXTL*/*PC* (Sheldrick, 1990); program(s) used to refine structure: *SHELXTL*/*PC*; molecular graphics: *SHELXTL*/*PC*; software used to prepare material for publication: *PLATON* (Spek, 2003).

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