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[2-(4-Methylbenzoyl)phenyl](4-methylphenyl)methanone

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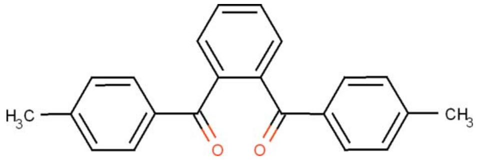
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.002 Å; R factor = 0.050; wR factor = 0.154; data-to-parameter ratio = 19.4.

The asymmetric unit of the title compound, $C_{22}H_{18}O_2$, contains one half-molecule, the complete molecule being generated by the operation of a crystallographic twofold rotation axis. The carbonyl group and the two C atoms attached to it forms interplanar angles of 23.67 (7)° with the methyl-substituted phenyl ring and 50.74 (8)° with the central ring. In the crystal, molecules are linked into infinite chains along the *b*-axis direction by intermolecular C—H···O interactions, generating $R_2^2(10)$ graph-set motifs.

Related literature

For the uses and biological importance of diketones, see: Bennett *et al.* (1999); Sato *et al.* (2008). For related structures, see: Muto *et al.* (2010); Khan *et al.* (2009); For asymmetry parameters, see: Nardelli (1983); Macrae *et al.* (2008). For graph-set notation: Bernstein *et al.* (1995).



Experimental

Crystal data

$C_{22}H_{18}O_2$
M_r = 314.36
Monoclinic, $C2/c$
a = 20.7432 (13) Å
b = 7.7564 (4) Å
c = 11.3946 (6) Å
β = 114.314 (5)°
V = 1670.70 (17) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 295 K
0.30 × 0.25 × 0.20 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.977, T_{max} = 0.984
17689 measured reflections
2133 independent reflections
1729 reflections with $I > 2\sigma(I)$
R_{int} = 0.076

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.154
S = 1.03
2133 reflections
110 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1···O1^{i}	0.93	2.62	3.4305 (17)	145

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2009).

PN and KS thank Dr Babu Varghese, SAIF, IIT, Chennai, India, for the data collection and Dr V. Murugan, Head of the Department of Physics, RKM Vivekananda College, for providing facilities in the department for carrying out this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RK2284).

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supplementary materials

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[2-(4-Methylbenzoyl)phenyl](4-methylphenyl)methanone

P. Narayanan, **K. Sethusankar**, **M. Nandakumar** and **A. K. Mohanakrishnan**

Comment

Diketones are popular in organic synthesis, for their applications in biology and medicine. They are known to exhibit anti-oxidants, antitumour and antibacterial activities (Bennett *et al.*, 1999). They are also key intermediates in the preparation of various heterocyclic compounds (Sato *et al.*, 2008).

The title compound $C_{22}H_{18}O_2$, contains one half molecule in the asymmetric unit, the complete molecule being generated by twofold rotation, with direction [0 1 0], having symmetry code: (i) $-x+1$, y, $-z+3/2$. X-ray analysis confirms the molecular structure and atom connectivity of the compound as illustrated in (Fig. 1). The carbonyl group (C3/C4/C5/O1) forms an interplanar angle of 23.67 (7)° with the phenyl ring (C5/C6/C7/C8/C9/C10). The deviation of atom O1 from the phenyl ring (C5/C6/C7/C8/C9/C10) is -0.4719 (19)Å (Nardelli, 1983). The title compound exhibits structural similarities with the already reported related structures (Muto *et al.*, 2010; Khan *et al.*, 2009).

The central phenyl ring ($C1/C2/C3/C1^i/C2^i/C3^i$) forms dihedral angles of 67.14 (17)° and 50.74 (8)° with the phenyl ring (C5/C6/C7/C8/C9/C10) and the mean plane of the carbonyl group (C3/C4/C5/O1), respectively. The dihedral angle between the phenyl rings (C5/C6/C7/C8/C9/C10) and ($C5^i/C6^i/C7^i/C8^i/C9^i/C10^i$) is 82.83 (2)° (Macrae *et al.*, 2008), and thus they are almost orthogonal to each other.

The crystal packing is stabilized by C—H···O intermolecular interactions. The molecules are linked into infinite chains along the *b* axis *via* C1—H1···$O1^{ii}$ hydrogen bonds, generating the $R^2_2(10)$ graphset motifs (Bernstein *et al.*, 1995). The symmetry code: (ii) x, $-1+y$, z (look Table 1). The packing view of the compound is shown in (Fig. 2).

Experimental

To a stirred suspension of benzo[*c*]furan, 1,3-bis(4-methylphenyl)-4,7-dihydro-2-benzofuran (3 g, 9.554 mmol) in dry *THF* (20 ml), lead tetra acetate (4.23 g, 9.5 mmol) was added and refluxed at 343 K for half an hour. The reaction mixture was then poured into water (200 ml) and extracted with ethyl acetate (2 x 20 ml), washed with brine solution and dried (Na_2SO_4). The removal of solvent *in vacuo* followed by crystallization from methanol afforded the title compound, (4-methylphenyl){2-[(4-methylphenyl)carbonyl]phenyl}methanone as a colourless solid.

Refinement

The hydrogen atoms were placed in calculated positions with C—H = 0.93–0.96Å and refined in the riding model with fixed isotropic displacement parameters: $U_{iso}(H) = 1.5U_{eq}(C)$ for methyl atoms and $U_{iso}(H) = 1.2U_{eq}(C)$ for the aryl atoms.

Figures

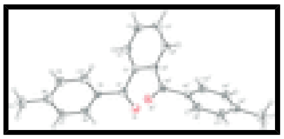

Fig. 1. The molecular structure of the title compound with the atom numbering scheme. Displacement ellipsoids are shown at 30% probability level. The H atoms are presented as a small spheres of arbitrary radius. Related atoms have symmetry code: (i) -*x*+1, *y*, -*z*+3/2.

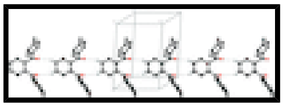

Fig. 2. The crystal packing of the title compound, viewed down *c* axis, showing molecules linked along *b* axis. Intermolecular hydrogen bonds are shown in as dashed lines.

[2-(4-Methylbenzoyl)phenyl](4-methylphenyl)methanone

Crystal data

$C_{22}H_{18}O_2$
$M_r = 314.36$
Monoclinic, $C2/c$
Hall symbol: -C 2yc
$a = 20.7432$ (13) Å
$b = 7.7564$ (4) Å
$c = 11.3946$ (6) Å
$\beta = 114.314$ (5)°
$V = 1670.70$ (17) Å^3
$Z = 4$

$F(000) = 664$
$D_x = 1.250$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2133 reflections
$\theta = 2.2–28.6°$
$\mu = 0.08$ mm^{-1}
$T = 295$ K
Block, colourless
0.30 × 0.25 × 0.20 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
graphite
ω–scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.977$, $T_{\max} = 0.984$
17689 measured reflections

2133 independent reflections
1729 reflections with $I > 2\sigma(I)$
$R_{\text{int}} = 0.076$
$\theta_{\max} = 28.6°$, $\theta_{\min} = 2.2°$
$h = -27 \rightarrow 27$
$k = -10 \rightarrow 10$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.050$
$wR(F^2) = 0.154$
$S = 1.03$

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
$w = 1/[\sigma^2(F_o^2) + (0.0914P)^2 + 0.4904P]$
where $P = (F_o^2 + 2F_c^2)/3$

2133 reflections	$(\Delta/\sigma)_{\max} = 0.005$
110 parameters	$\Delta\rho_{\max} = 0.30$ e Å^{-3}
0 restraints	$\Delta\rho_{\min} = -0.28$ e Å^{-3}

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 $F^2 > \sigma(F^2)$ 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*	$U_{\rm iso}$*/$U_{\rm eq}$
C1	0.47990 (8)	−0.45596 (18)	0.68469 (16)	0.0577 (4)
H1	0.4669	−0.5598	0.6403	0.069*
C2	0.45881 (7)	−0.30216 (17)	0.61934 (13)	0.0493 (3)
H2	0.4310	−0.3030	0.5312	0.059*
C3	0.47868 (6)	−0.14603 (15)	0.68400 (11)	0.0375 (3)
C4	0.46029 (6)	0.01963 (15)	0.61000 (11)	0.0380 (3)
C5	0.38557 (6)	0.05007 (15)	0.52013 (11)	0.0384 (3)
C6	0.37060 (7)	0.16656 (18)	0.41976 (13)	0.0478 (3)
H6	0.4074	0.2221	0.4083	0.057*
C7	0.30152 (8)	0.2002 (2)	0.33701 (13)	0.0535 (4)
H7	0.2924	0.2766	0.2691	0.064*
C8	0.24545 (7)	0.12297 (18)	0.35264 (13)	0.0508 (4)
C9	0.26051 (7)	0.0089 (2)	0.45387 (14)	0.0529 (4)
H9	0.2236	−0.0433	0.4668	0.063*
C10	0.32965 (7)	−0.02856 (18)	0.53609 (13)	0.0474 (3)
H10	0.3387	−0.1072	0.6027	0.057*
C11	0.17032 (9)	0.1623 (3)	0.26113 (19)	0.0739 (5)
H11A	0.1696	0.2622	0.2109	0.111*
H11B	0.1425	0.1841	0.3093	0.111*
H11C	0.1509	0.0656	0.2050	0.111*
O1	0.50637 (5)	0.12345 (12)	0.62240 (9)	0.0503 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0579 (8)	0.0333 (6)	0.0742 (10)	−0.0053 (6)	0.0195 (7)	−0.0101 (6)
C2	0.0496 (7)	0.0405 (7)	0.0470 (7)	−0.0063 (5)	0.0091 (6)	−0.0084 (5)
C3	0.0360 (5)	0.0337 (6)	0.0368 (6)	−0.0015 (4)	0.0088 (5)	−0.0008 (4)
C4	0.0414 (6)	0.0359 (6)	0.0318 (6)	−0.0023 (4)	0.0100 (5)	−0.0016 (4)

C5	0.0405 (6)	0.0371 (6)	0.0324 (6)	0.0011 (4)	0.0097 (5)	−0.0003 (4)
C6	0.0487 (7)	0.0482 (7)	0.0442 (7)	0.0033 (5)	0.0167 (6)	0.0096 (5)
C7	0.0557 (8)	0.0531 (8)	0.0437 (7)	0.0116 (6)	0.0125 (6)	0.0121 (6)
C8	0.0450 (7)	0.0493 (7)	0.0471 (7)	0.0084 (6)	0.0079 (6)	−0.0061 (5)
C9	0.0418 (7)	0.0575 (8)	0.0566 (8)	−0.0040 (6)	0.0176 (6)	−0.0025 (6)
C10	0.0484 (7)	0.0482 (7)	0.0416 (7)	−0.0025 (5)	0.0143 (5)	0.0049 (5)
C11	0.0483 (8)	0.0751 (11)	0.0757 (11)	0.0150 (7)	0.0028 (8)	−0.0027 (9)
O1	0.0479 (5)	0.0442 (5)	0.0487 (5)	−0.0100 (4)	0.0098 (4)	0.0032 (4)

Geometric parameters (Å, °)

C1—C1^{i}	1.374 (3)	C6—H6	0.9300
C1—C2	1.379 (2)	C7—C8	1.383 (2)
C1—H1	0.9300	C7—H7	0.9300
C2—C3	1.3890 (16)	C8—C9	1.384 (2)
C2—H2	0.9300	C8—C11	1.507 (2)
C3—C3^{i}	1.396 (2)	C9—C10	1.383 (2)
C3—C4	1.4975 (16)	C9—H9	0.9300
C4—O1	1.2128 (15)	C10—H10	0.9300
C4—C5	1.4832 (16)	C11—H11A	0.9600
C5—C10	1.3872 (18)	C11—H11B	0.9600
C5—C6	1.3887 (17)	C11—H11C	0.9600
C6—C7	1.3778 (19)		
C1^{i}—C1—C2	120.07 (8)	C6—C7—C8	121.50 (13)
C1^{i}—C1—H1	120.0	C6—C7—H7	119.2
C2—C1—H1	120.0	C8—C7—H7	119.2
C1—C2—C3	120.60 (12)	C7—C8—C9	118.11 (12)
C1—C2—H2	119.7	C7—C8—C11	120.53 (14)
C3—C2—H2	119.7	C9—C8—C11	121.36 (15)
C2—C3—C3^{i}	119.31 (7)	C10—C9—C8	120.95 (13)
C2—C3—C4	119.89 (10)	C10—C9—H9	119.5
C3^{i}—C3—C4	120.54 (6)	C8—C9—H9	119.5
O1—C4—C5	121.61 (11)	C9—C10—C5	120.58 (12)
O1—C4—C3	119.89 (10)	C9—C10—H10	119.7
C5—C4—C3	118.48 (10)	C5—C10—H10	119.7
C10—C5—C6	118.59 (11)	C8—C11—H11A	109.5
C10—C5—C4	122.14 (11)	C8—C11—H11B	109.5
C6—C5—C4	119.21 (11)	H11A—C11—H11B	109.5
C7—C6—C5	120.25 (13)	C8—C11—H11C	109.5
C7—C6—H6	119.9	H11A—C11—H11C	109.5
C5—C6—H6	119.9	H11B—C11—H11C	109.5
C1^{i}—C1—C2—C3	1.0 (3)	C10—C5—C6—C7	−1.1 (2)
C1—C2—C3—C3^{i}	1.0 (2)	C4—C5—C6—C7	−178.36 (12)
C1—C2—C3—C4	175.06 (13)	C5—C6—C7—C8	1.4 (2)
C2—C3—C4—O1	−125.83 (13)	C6—C7—C8—C9	−0.5 (2)
C3^{i}—C3—C4—O1	48.2 (2)	C6—C7—C8—C11	179.79 (14)
C2—C3—C4—C5	52.62 (16)	C7—C8—C9—C10	−0.8 (2)

C3^{i}—C3—C4—C5	−133.37 (15)	C11—C8—C9—C10	178.91 (14)
O1—C4—C5—C10	−156.10 (13)	C8—C9—C10—C5	1.2 (2)
C3—C4—C5—C10	25.47 (17)	C6—C5—C10—C9	−0.2 (2)
O1—C4—C5—C6	21.08 (18)	C4—C5—C10—C9	177.00 (12)
C3—C4—C5—C6	−157.35 (12)		

Symmetry codes: (i) −*x*+1, *y*, −*z*+3/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1···O1^{ii}	0.93	2.62	3.4305 (17)	145.

Symmetry codes: (ii) *x*, *y*−1, *z*.

Fig. 1

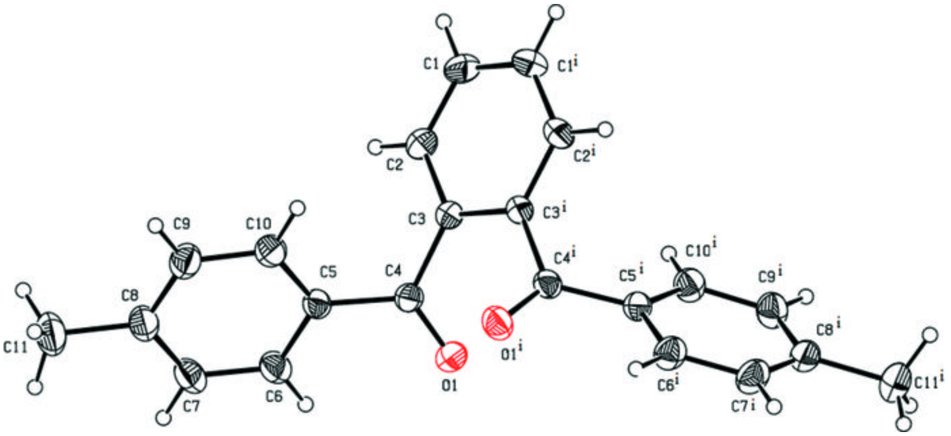
C1
C1i
C2
C2i
C3
C3i
C4
C4i
C5
C5i
C6
C6i
C7
C7i
C8
C8i
C9
C9i
C10
C10i
C11
C11i
O1
O1i

Fig. 2