Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-[2-(Cyclohexylcarbonyl)phenyl]-1-phenylethanone

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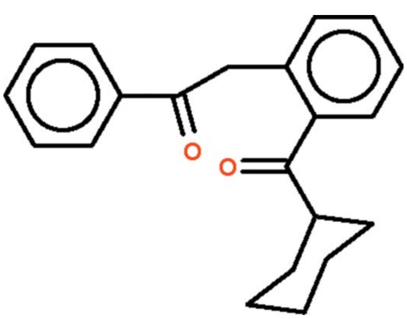
Received 8 October 2009; accepted 9 October 2009

Key indicators: single-crystal X-ray study; T = 290 K; mean σ(C–C) = 0.004 Å; R factor = 0.074; wR factor = 0.183; data-to-parameter ratio = 14.3.

The title diketone, $C_{21}H_{22}O_2$, features a phenylene ring having benzoylmethyl and cyclohexanoyl substituents *ortho* to each other. The cyclohexyl ring adopts a chair conformation with the ketonic group occupying an equatorial position; the four-atom –C(O)–C ketonic unit is twisted out of the plane of the phenylene ring by 34.9 (1)°.

Related literature

For the synthesis of this and other 1,2-phenylethanones from isocoumarins, see: Manivel *et al.* (2008).



Experimental

Crystal data

$C_{21}H_{22}O_2$	V = 1693.35 (17) Å^3
M_r = 306.39	Z = 4
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
a = 10.4012 (6) Å	μ = 0.08 mm^{-1}
b = 10.1132 (6) Å	T = 290 K
c = 16.0981 (9) Å	0.25 × 0.22 × 0.18 mm
β = 90.038 (1)°	

Data collection

Bruker SMART area-detector diffractometer	2984 independent reflections
Absorption correction: none	2797 reflections with $I > 2\sigma(I)$
11930 measured reflections	R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.074	208 parameters
$wR(F^2)$ = 0.183	H-atom parameters constrained
S = 1.32	$\Delta\rho_{max}$ = 0.18 e Å^{-3}
2984 reflections	$\Delta\rho_{min}$ = −0.18 e Å^{-3}

Data collection: *SMART* (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: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2009).

We thank the Department of Science and Technology, India, for use of the diffraction facility at IISc under the IRHPA-DST program. FNK thanks the DST for Fast Track Proposal funding. We thank VIT University and the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2553).

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supplementary materials

Acta Cryst. (2009). E**65**, o2745 [**doi:10.1107/S1600536809041270**]

2-[2-(Cyclohexylcarbonyl)phenyl]-1-phenylethanone

F. N. Khan, P. Manivel, K. Prabakaran, V. R. Hathwar and S. W. Ng

Experimental

The compound was synthesized as described by Manivel *et al.* (2008). Single crystals were grown from its solution in ether.

Refinement

Carbon-bound H-atoms were placed in calculated positions (C–H 0.93–0.98 Å) and were included in the refinement in the riding model approximation with U_{iso}(H) set to 1.2U_{eq}(C).

Figures

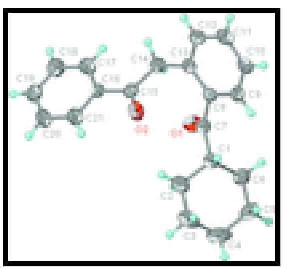


Fig. 1. Thermal ellipsoid plot (Barbour, 2001) of $C_{21}H_{22}O_2$ at the 50% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

2-[2-(Cyclohexylcarbonyl)phenyl]-1-phenylethanone

Crystal data

$C_{21}H_{22}O_2$	F_{000} = 656
M_r = 306.39	D_x = 1.202 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo *K*α radiation, λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 878 reflections
a = 10.4012 (6) Å	θ = 2.4–25.3°
b = 10.1132 (6) Å	μ = 0.08 mm^{-1}
c = 16.0981 (9) Å	*T* = 290 K
β = 90.038 (1)°	Block, colorless
V = 1693.35 (17) Å^3	0.25 × 0.22 × 0.18 mm
Z = 4	

Data collection

Bruker SMART area-detector diffractometer	2797 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.025

Monochromator: graphite	θ_{max} = 25.0°
T = 290 K	θ_{min} = 2.0°
φ and ω scans	$h = -12 \rightarrow 12$
Absorption correction: None	$k = -12 \rightarrow 12$
11930 measured reflections	$l = -18 \rightarrow 19$
2984 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.074$	H-atom parameters constrained
$wR(F^2) = 0.183$	$w = 1/[\sigma^2(F_o^2) + (0.068P)^2 + 0.5871P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.32	$(\Delta/\sigma)_{max}$ = 0.001
2984 reflections	$\Delta\rho_{max}$ = 0.18 e Å^{-3}
208 parameters	$\Delta\rho_{min}$ = −0.18 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
O1	0.63291 (18)	0.81169 (19)	0.64919 (12)	0.0603 (6)
O2	0.83697 (18)	0.5709 (2)	0.67129 (13)	0.0649 (6)
C1	0.8136 (2)	0.9209 (2)	0.70629 (15)	0.0444 (6)
H1	0.8661	0.9089	0.7563	0.053*
C2	0.8988 (3)	0.8982 (3)	0.63032 (19)	0.0617 (8)
H2A	0.9350	0.8099	0.6326	0.074*
H2B	0.8472	0.9047	0.5803	0.074*
C3	1.0069 (3)	0.9992 (4)	0.6269 (2)	0.0772 (10)
H3A	1.0633	0.9868	0.6743	0.093*
H3B	1.0570	0.9855	0.5769	0.093*
C4	0.9553 (4)	1.1381 (4)	0.6276 (2)	0.0855 (11)
H4A	0.9063	1.1536	0.5772	0.103*
H4B	1.0264	1.2001	0.6285	0.103*
C5	0.8704 (3)	1.1617 (3)	0.7022 (2)	0.0737 (9)
H5A	0.8346	1.2501	0.6993	0.088*
H5B	0.9216	1.1555	0.7524	0.088*
C6	0.7621 (3)	1.0616 (3)	0.7059 (2)	0.0593 (7)
H6A	0.7062	1.0736	0.6582	0.071*
H6B	0.7116	1.0764	0.7556	0.071*
C7	0.7044 (2)	0.8228 (2)	0.70871 (15)	0.0426 (6)
C8	0.6826 (2)	0.7417 (2)	0.78542 (14)	0.0405 (6)
C9	0.7074 (2)	0.7974 (3)	0.86283 (15)	0.0468 (6)
H9	0.7392	0.8832	0.8655	0.056*
C10	0.6862 (3)	0.7290 (3)	0.93556 (16)	0.0543 (7)

H10	0.7033	0.7683	0.9866	0.065*
C11	0.6397 (3)	0.6023 (3)	0.93171 (17)	0.0574 (7)
H11	0.6245	0.5551	0.9803	0.069*
C12	0.6154 (2)	0.5451 (3)	0.85552 (18)	0.0520 (7)
H12	0.5841	0.4590	0.8538	0.062*
C13	0.6361 (2)	0.6117 (2)	0.78134 (15)	0.0432 (6)
C14	0.6148 (2)	0.5387 (3)	0.70076 (17)	0.0499 (7)
H14A	0.5514	0.5862	0.6681	0.060*
H14B	0.5800	0.4519	0.7130	0.060*
C15	0.7363 (2)	0.5223 (2)	0.64918 (16)	0.0440 (6)
C16	0.7295 (2)	0.4449 (2)	0.57069 (15)	0.0421 (6)
C17	0.6237 (3)	0.3730 (3)	0.54615 (18)	0.0631 (8)
H17	0.5501	0.3733	0.5788	0.076*
C18	0.6259 (3)	0.3006 (3)	0.4736 (2)	0.0720 (9)
H18	0.5537	0.2525	0.4578	0.086*
C19	0.7325 (3)	0.2990 (3)	0.42538 (18)	0.0636 (8)
H19	0.7339	0.2490	0.3769	0.076*
C20	0.8376 (3)	0.3707 (3)	0.4480 (2)	0.0706 (9)
H20	0.9102	0.3711	0.4144	0.085*
C21	0.8365 (3)	0.4425 (3)	0.52045 (19)	0.0633 (8)
H21	0.9091	0.4903	0.5358	0.076*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0612 (12)	0.0688 (13)	0.0509 (11)	−0.0129 (10)	−0.0135 (10)	0.0076 (9)
O2	0.0428 (10)	0.0826 (15)	0.0694 (13)	−0.0102 (10)	0.0025 (9)	−0.0298 (11)
C1	0.0458 (14)	0.0501 (15)	0.0374 (13)	−0.0036 (11)	−0.0054 (10)	0.0045 (11)
C2	0.0532 (16)	0.072 (2)	0.0597 (18)	−0.0021 (14)	0.0077 (13)	−0.0045 (15)
C3	0.0565 (18)	0.108 (3)	0.067 (2)	−0.0182 (19)	0.0109 (15)	0.0035 (19)
C4	0.087 (2)	0.095 (3)	0.075 (2)	−0.043 (2)	−0.0039 (19)	0.022 (2)
C5	0.087 (2)	0.0552 (18)	0.079 (2)	−0.0176 (16)	−0.0054 (18)	0.0040 (16)
C6	0.0614 (17)	0.0513 (17)	0.0653 (18)	−0.0026 (13)	0.0027 (14)	0.0011 (14)
C7	0.0435 (13)	0.0449 (14)	0.0394 (13)	0.0032 (11)	−0.0036 (11)	−0.0012 (11)
C8	0.0337 (12)	0.0465 (14)	0.0412 (13)	0.0018 (10)	0.0023 (10)	−0.0029 (11)
C9	0.0506 (14)	0.0468 (14)	0.0431 (14)	0.0009 (11)	0.0014 (11)	−0.0050 (11)
C10	0.0537 (16)	0.0687 (19)	0.0407 (14)	0.0036 (14)	0.0055 (12)	−0.0033 (13)
C11	0.0555 (16)	0.0702 (19)	0.0466 (16)	0.0046 (14)	0.0087 (13)	0.0116 (14)
C12	0.0455 (15)	0.0500 (15)	0.0606 (17)	−0.0017 (12)	0.0069 (12)	0.0055 (13)
C13	0.0342 (12)	0.0483 (14)	0.0472 (14)	0.0014 (10)	0.0060 (10)	−0.0024 (11)
C14	0.0442 (14)	0.0488 (15)	0.0567 (16)	−0.0082 (11)	0.0024 (12)	−0.0057 (12)
C15	0.0400 (13)	0.0416 (13)	0.0503 (15)	−0.0039 (11)	−0.0025 (11)	−0.0032 (11)
C16	0.0452 (13)	0.0355 (13)	0.0457 (14)	−0.0013 (10)	−0.0016 (11)	−0.0003 (10)
C17	0.0546 (17)	0.076 (2)	0.0592 (18)	−0.0195 (15)	0.0067 (13)	−0.0189 (15)
C18	0.070 (2)	0.080 (2)	0.065 (2)	−0.0255 (17)	−0.0016 (16)	−0.0239 (17)
C19	0.087 (2)	0.0557 (17)	0.0480 (16)	−0.0083 (16)	0.0014 (15)	−0.0103 (13)
C20	0.070 (2)	0.079 (2)	0.0626 (19)	−0.0104 (17)	0.0167 (16)	−0.0213 (17)
C21	0.0504 (16)	0.0703 (19)	0.0693 (19)	−0.0135 (14)	0.0090 (14)	−0.0198 (16)

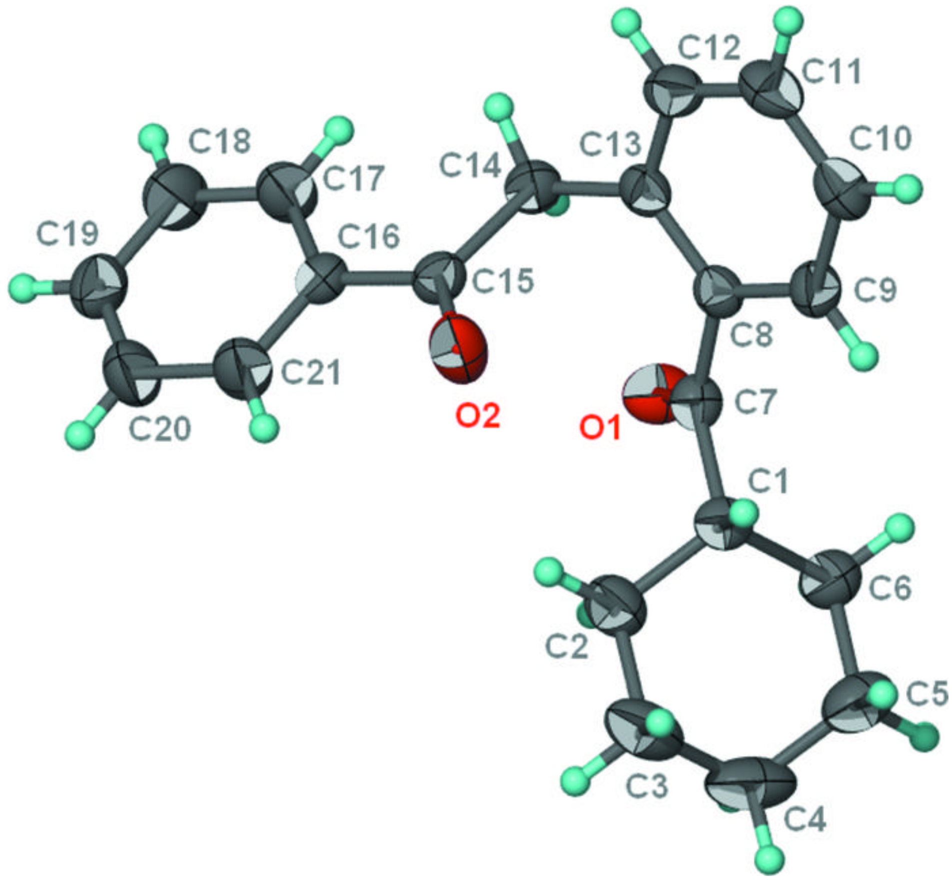
Geometric parameters (Å, °)

O1—C7	1.218 (3)	C9—H9	0.9300
O2—C15	1.210 (3)	C10—C11	1.371 (4)
C1—C7	1.509 (3)	C10—H10	0.9300
C1—C6	1.520 (4)	C11—C12	1.380 (4)
C1—C2	1.528 (4)	C11—H11	0.9300
C1—H1	0.9800	C12—C13	1.388 (4)
C2—C3	1.520 (4)	C12—H12	0.9300
C2—H2A	0.9700	C13—C14	1.509 (4)
C2—H2B	0.9700	C14—C15	1.521 (4)
C3—C4	1.504 (5)	C14—H14A	0.9700
C3—H3A	0.9700	C14—H14B	0.9700
C3—H3B	0.9700	C15—C16	1.488 (3)
C4—C5	1.510 (5)	C16—C21	1.376 (4)
C4—H4A	0.9700	C16—C17	1.376 (4)
C4—H4B	0.9700	C17—C18	1.378 (4)
C5—C6	1.515 (4)	C17—H17	0.9300
C5—H5A	0.9700	C18—C19	1.355 (4)
C5—H5B	0.9700	C18—H18	0.9300
C6—H6A	0.9700	C19—C20	1.361 (4)
C6—H6B	0.9700	C19—H19	0.9300
C7—C8	1.500 (3)	C20—C21	1.374 (4)
C8—C9	1.392 (3)	C20—H20	0.9300
C8—C13	1.402 (4)	C21—H21	0.9300
C9—C10	1.378 (4)		
C7—C1—C6	110.5 (2)	C10—C9—C8	121.9 (2)
C7—C1—C2	111.0 (2)	C10—C9—H9	119.1
C6—C1—C2	110.0 (2)	C8—C9—H9	119.1
C7—C1—H1	108.4	C11—C10—C9	119.2 (3)
C6—C1—H1	108.4	C11—C10—H10	120.4
C2—C1—H1	108.4	C9—C10—H10	120.4
C3—C2—C1	110.9 (2)	C10—C11—C12	119.8 (3)
C3—C2—H2A	109.5	C10—C11—H11	120.1
C1—C2—H2A	109.5	C12—C11—H11	120.1
C3—C2—H2B	109.5	C11—C12—C13	122.2 (3)
C1—C2—H2B	109.5	C11—C12—H12	118.9
H2A—C2—H2B	108.1	C13—C12—H12	118.9
C4—C3—C2	111.4 (3)	C12—C13—C8	118.0 (2)
C4—C3—H3A	109.4	C12—C13—C14	118.6 (2)
C2—C3—H3A	109.4	C8—C13—C14	123.3 (2)
C4—C3—H3B	109.4	C13—C14—C15	113.7 (2)
C2—C3—H3B	109.4	C13—C14—H14A	108.8
H3A—C3—H3B	108.0	C15—C14—H14A	108.8
C3—C4—C5	111.2 (3)	C13—C14—H14B	108.8
C3—C4—H4A	109.4	C15—C14—H14B	108.8
C5—C4—H4A	109.4	H14A—C14—H14B	107.7
C3—C4—H4B	109.4	O2—C15—C16	120.3 (2)

C5—C4—H4B	109.4	O2—C15—C14	120.9 (2)
H4A—C4—H4B	108.0	C16—C15—C14	118.8 (2)
C4—C5—C6	111.1 (3)	C21—C16—C17	117.9 (2)
C4—C5—H5A	109.4	C21—C16—C15	118.0 (2)
C6—C5—H5A	109.4	C17—C16—C15	124.0 (2)
C4—C5—H5B	109.4	C18—C17—C16	120.7 (3)
C6—C5—H5B	109.4	C18—C17—H17	119.6
H5A—C5—H5B	108.0	C16—C17—H17	119.6
C5—C6—C1	111.3 (2)	C19—C18—C17	120.4 (3)
C5—C6—H6A	109.4	C19—C18—H18	119.8
C1—C6—H6A	109.4	C17—C18—H18	119.8
C5—C6—H6B	109.4	C18—C19—C20	119.8 (3)
C1—C6—H6B	109.4	C18—C19—H19	120.1
H6A—C6—H6B	108.0	C20—C19—H19	120.1
O1—C7—C8	120.3 (2)	C19—C20—C21	120.1 (3)
O1—C7—C1	120.0 (2)	C19—C20—H20	119.9
C8—C7—C1	119.7 (2)	C21—C20—H20	119.9
C9—C8—C13	119.0 (2)	C20—C21—C16	121.0 (3)
C9—C8—C7	119.2 (2)	C20—C21—H21	119.5
C13—C8—C7	121.8 (2)	C16—C21—H21	119.5

C7—C1—C2—C3	178.6 (2)	C11—C12—C13—C14	176.2 (2)
C6—C1—C2—C3	56.0 (3)	C9—C8—C13—C12	0.9 (3)
C1—C2—C3—C4	−56.3 (4)	C7—C8—C13—C12	−178.3 (2)
C2—C3—C4—C5	55.9 (4)	C9—C8—C13—C14	−175.6 (2)
C3—C4—C5—C6	−55.8 (4)	C7—C8—C13—C14	5.3 (3)
C4—C5—C6—C1	56.4 (4)	C12—C13—C14—C15	−116.1 (3)
C7—C1—C6—C5	−179.2 (2)	C8—C13—C14—C15	60.3 (3)
C2—C1—C6—C5	−56.3 (3)	C13—C14—C15—O2	−3.5 (4)
C6—C1—C7—O1	67.7 (3)	C13—C14—C15—C16	176.3 (2)
C2—C1—C7—O1	−54.6 (3)	O2—C15—C16—C21	−6.8 (4)
C6—C1—C7—C8	−110.8 (3)	C14—C15—C16—C21	173.3 (3)
C2—C1—C7—C8	126.9 (2)	O2—C15—C16—C17	171.7 (3)
O1—C7—C8—C9	−143.9 (2)	C14—C15—C16—C17	−8.2 (4)
C1—C7—C8—C9	34.6 (3)	C21—C16—C17—C18	0.3 (5)
O1—C7—C8—C13	35.2 (3)	C15—C16—C17—C18	−178.2 (3)
C1—C7—C8—C13	−146.2 (2)	C16—C17—C18—C19	0.1 (5)
C13—C8—C9—C10	−0.8 (4)	C17—C18—C19—C20	−0.9 (5)
C7—C8—C9—C10	178.4 (2)	C18—C19—C20—C21	1.3 (5)
C8—C9—C10—C11	0.2 (4)	C19—C20—C21—C16	−0.9 (5)
C9—C10—C11—C12	0.3 (4)	C17—C16—C21—C20	0.1 (5)
C10—C11—C12—C13	−0.2 (4)	C15—C16—C21—C20	178.6 (3)
C11—C12—C13—C8	−0.4 (4)		

Fig. 1


C12
C11
C18
C17
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C13
C10
C19
C16
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C9
C8
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O2
O1
C7
C20
C1
C6
C2
C5
C3
C4