Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

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

F. Nawaz Khan,[a] P. Manivel,[a] K. Prabakaran,[a] Venkatesha R. Hathwar[b] and Seik Weng Ng[c]*

[a]Chemistry Division, School of Science and Humanities, VIT University, Vellore 632 014, Tamil Nadu, India, [b]Solid State and Structural Chemistry Unit, Indian Institute of Science, Bangalore 560 012, Karnataka, India, and [c]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia
Correspondence e-mail: seikweng@um.edu.my

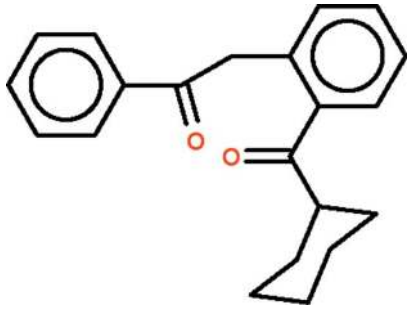
Received 8 October 2009; accepted 9 October 2009

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

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

Data collection

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

Refinement

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

References

Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Bruker (2004). *SAINT* and *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.
Manivel, P., Roopan, S. M. & Khan, F. N. (2008). *Indian J. Heterocycl. Chem.* **18**, 21–24.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Westrip, S. P. (2009). *publCIF*. In preparation.

supporting information

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

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

F. Nawaz Khan, P. Manivel, K. Prabakaran, Venkatesha R. Hathwar and Seik Weng Ng

S1. Experimental

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

S2. 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).

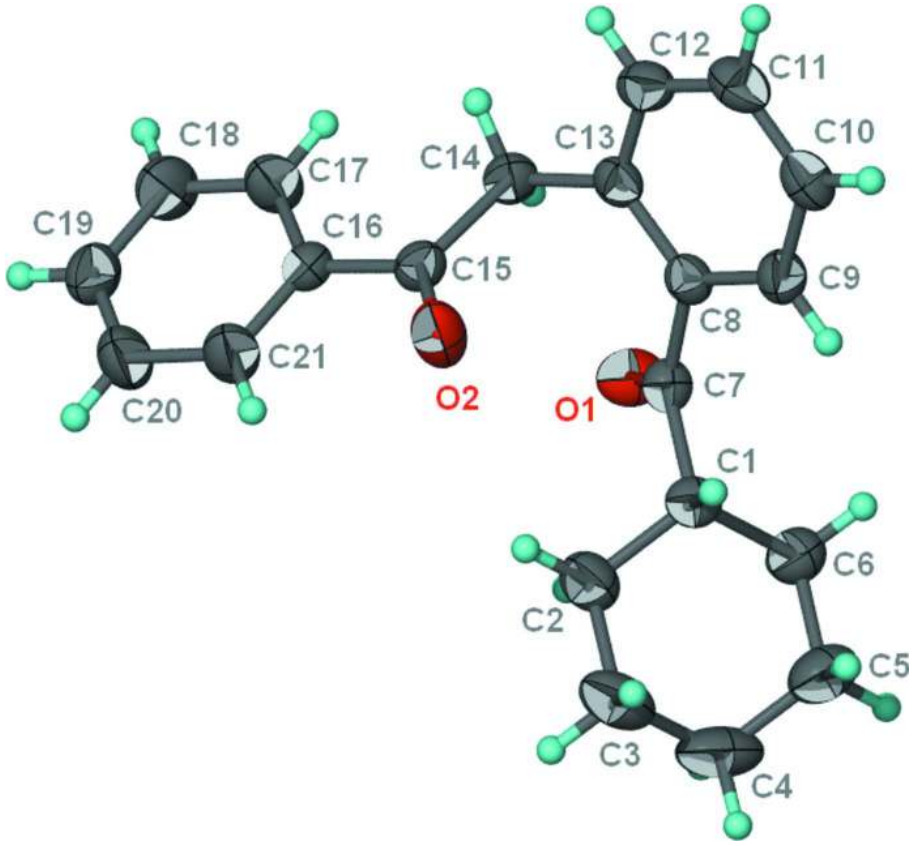


Figure 1

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

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

Data collection

Bruker SMART area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
11930 measured reflections
2984 independent reflections
2797 reflections with $I > 2\sigma(I)$
$R_{int} = 0.025$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.0°$
$h = -12 \rightarrow 12$
$k = -12 \rightarrow 12$
$l = -18 \rightarrow 19$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.074$
$wR(F^2) = 0.183$
$S = 1.32$
2984 reflections
208 parameters
0 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
$w = 1/[\sigma^2(F_o^2) + (0.068P)^2 + 0.5871P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.18$ e Å^{-3}
$\Delta\rho_{min} = -0.18$ e Å^{-3}

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 (Å²)

	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, º)

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)		