Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# Benzoylmethyl 4-methoxybenzoate

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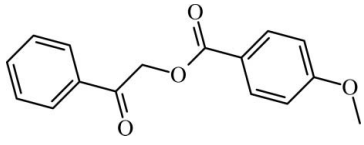
Received 17 October 2007; accepted 1 November 2007

Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.035; $wR$ factor = 0.092; data-to-parameter ratio = 14.4.

The title compound, $C_{16}H_{14}O_4$, was obtained by the reaction of 4-methoxybenzoic acid and phenacyl bromide. The dihedral angle between the two aromatic rings is 71.21 (6)°. The molecules are linked into a two-dimensional network parallel to the *ab* plane by C—H···O and C—H···$\pi$ interactions.

## Related literature

For related literature, see: Hendrickson & Kandall (1970).



## Experimental

### Crystal data

$C_{16}H_{14}O_4$
$M_r$ = 270.27
Monoclinic, $P2_1/n$
$a$ = 8.0618 (2) Å
$b$ = 9.6671 (3) Å
$c$ = 17.1819 (5) Å
$\beta$ = 91.535 (3)°
$V$ = 1338.58 (7) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.10 mm$^{-1}$
$T$ = 298 (2) K
0.40 × 0.27 × 0.17 mm

### Data collection

Bruker APEX area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min}$ = 0.962, $T_{max}$ = 0.984
9851 measured reflections
2615 independent reflections
1873 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.023

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.092
$S$ = 1.02
2615 reflections
181 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.11 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.17 e Å$^{-3}$

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

*Cg*1 is the centroid of the C2–C7 ring.

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C8—H8$B$···O1$^{i}$ | 0.97 | 2.28 | 3.2447 (17) | 172 |
| C12—H12···O3$^{ii}$ | 0.93 | 2.55 | 3.2973 (16) | 137 |
| C11—H11···*Cg*1$^{ii}$ | 0.93 | 2.86 | 3.6552 (15) | 144 |

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

The authors thank the Key Foundation of Science and Technology Project of Fujian Province, China (key grant No. 2002H011), for supporting this work. We also thank Mr R.-B. Huang for technical assistance.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2491).

## References

Bruker (2001). *SAINT* (Version 6.22), *SMART* (Version 5.625) and *SADABS* (Version 2.03). Bruker AXS Inc., Madison, Wisconsin, USA.
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  doi:10.1107/S1600536807055250 

# supplementary materials

*Acta Cryst.* (2007). E**63**, o4766 [ **doi:10.1107/S1600536807055250** ]

# Benzoylmethyl 4-methoxybenzoate

**T. Ji, X.-L. Wang, Y.-X. Gao, G. Tang and Y.-F. Zhao**

## Comment

The title compound was synthesized for a study of protection of carboxyl group. The phenacyl group has proved to be an important reagent for protecting carboxyl functions during organic synthesis in presence of other esters (Hendrickson & Kandall, 1970).

The molecular structure of the title compound is shown in Fig. 1. The dihedral angle between the two aromatic rings is 71.21 (6)°. Weak C—H···O hydrogen bonds and C—H···π interactions help to stabilize the crystal structure (Table 1). The molecules are linked into a two-dimensional network parallel to the *ab* plane by the above interactions.

## Experimental

4-Methoxybenzoic acid (0.76 g, 5 mmol) was dissolved in tetrahydrofuran (20 ml). Triethylamine (0.7 ml) and phenacyl bromide (0.989 g, 5 mmol) were added to the solution with stirring. The stirring was continued for overnight at room temperature. The tetrahydrofuran was removed *in vacuo* and the residue was recrystallized from ethyl acetate to give the title compound in 88% yield.

## Refinement

H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H = 0.93 Å (aromatic), 0.97 Å (methylene), 0.96 Å (methyl), and with $U_{iso}$(H) = 1.2$U_{eq}$($c$) for aromatic and methylene H atoms or 1.5$U_{eq}$($c$) for methyl H atoms.

## Figures

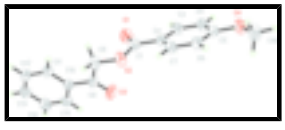

Fig. 1. The molecular structure of the title compound, showing 50% probability displacement ellipsoids.

## Benzoylmethyl 4-methoxybenzoate

*Crystal data*

| | |
|---|---|
| $C_{16}H_{14}O_4$ | $F_{000}$ = 568 |
| $M_r$ = 270.27 | $D_x$ = 1.341 Mg m$^{-3}$ |
| Monoclinic, $P2_1/n$ | Mo $K\alpha$ radiation<br>λ = 0.71073 Å |
| Hall symbol: -P 2yn | Cell parameters from 3973 reflections |

| | |
|---|---|
| $a$ = 8.0618 (2) Å | θ = 2.4–32.5º |
| $b$ = 9.6671 (3) Å | μ = 0.10 mm$^{-1}$ |
| $c$ = 17.1819 (5) Å | $T$ = 298 (2) K |
| β = 91.535 (3)º | Plate, colourless |
| $V$ = 1338.58 (7) Å$^3$ | 0.40 × 0.27 × 0.17 mm |
| $Z$ = 4 | |

*Data collection*

| | |
|---|---|
| Bruker APEX area-detector diffractometer | 2615 independent reflections |
| Radiation source: fine-focus sealed tube | 1873 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int}$ = 0.023 |
| $T$ = 298(2) K | $\theta_{max}$ = 26.0º |
| φ and ω scans | $\theta_{min}$ = 2.4º |
| Absorption correction: multi-scan (SADABS; Bruker, 2001) | $h = -9 \rightarrow 9$ |
| $T_{min}$ = 0.962, $T_{max}$ = 0.984 | $k = -11 \rightarrow 11$ |
| 9851 measured reflections | $l = -20 \rightarrow 21$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)]$ = 0.035 | H-atom parameters constrained |
| $wR(F^2)$ = 0.092 | $w = 1/[\sigma^2(F_o^2) + (0.0534P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S$ = 1.02 | $(\Delta/\sigma)_{max}$ = 0.001 |
| 2615 reflections | $\Delta\rho_{max}$ = 0.11 e Å$^{-3}$ |
| 181 parameters | $\Delta\rho_{min}$ = −0.17 e Å$^{-3}$ |
| Primary atom site location: structure-invariant direct methods | 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 $F^2 > 2$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 | 0.06068 (12) | 0.25236 (10) | 0.22525 (6) | 0.0523 (3) |
| O2 | 0.06074 (10) | 0.02414 (9) | 0.24485 (6) | 0.0428 (3) |
| O3 | 0.10480 (11) | 0.11666 (13) | 0.39171 (6) | 0.0625 (3) |
| O4 | −0.64971 (11) | 0.09532 (10) | 0.08808 (6) | 0.0478 (3) |
| C1 | −0.00852 (15) | 0.14235 (13) | 0.21933 (7) | 0.0350 (3) |
| C2 | −0.17527 (15) | 0.12207 (12) | 0.18382 (7) | 0.0318 (3) |
| C3 | −0.26981 (16) | 0.23871 (13) | 0.16601 (8) | 0.0366 (3) |
| H3 | −0.2260 | 0.3262 | 0.1758 | 0.044* |
| C4 | −0.42681 (16) | 0.22643 (14) | 0.13417 (8) | 0.0389 (3) |
| H4 | −0.4891 | 0.3051 | 0.1227 | 0.047* |
| C5 | −0.49259 (15) | 0.09587 (13) | 0.11908 (7) | 0.0343 (3) |
| C6 | −0.39972 (16) | −0.02145 (13) | 0.13555 (8) | 0.0368 (3) |
| H6 | −0.4431 | −0.1088 | 0.1250 | 0.044* |
| C7 | −0.24165 (15) | −0.00732 (13) | 0.16797 (7) | 0.0352 (3) |
| H7 | −0.1790 | −0.0859 | 0.1793 | 0.042* |
| C8 | 0.22653 (15) | 0.03720 (15) | 0.27621 (8) | 0.0434 (4) |
| H8A | 0.2892 | 0.0978 | 0.2429 | 0.052* |
| H8B | 0.2795 | −0.0529 | 0.2762 | 0.052* |
| C9 | 0.23180 (15) | 0.09397 (14) | 0.35776 (8) | 0.0376 (3) |
| C10 | 0.39810 (15) | 0.11977 (12) | 0.39404 (7) | 0.0324 (3) |
| C11 | 0.54325 (15) | 0.09679 (13) | 0.35428 (8) | 0.0359 (3) |
| H11 | 0.5378 | 0.0654 | 0.3031 | 0.043* |
| C12 | 0.69576 (16) | 0.12042 (14) | 0.39048 (8) | 0.0399 (3) |
| H12 | 0.7926 | 0.1042 | 0.3637 | 0.048* |
| C13 | 0.70499 (17) | 0.16773 (14) | 0.46575 (8) | 0.0438 (4) |
| H13 | 0.8079 | 0.1839 | 0.4898 | 0.053* |
| C14 | 0.56132 (17) | 0.19132 (15) | 0.50589 (8) | 0.0438 (3) |
| H14 | 0.5676 | 0.2239 | 0.5568 | 0.053* |
| C15 | 0.40934 (16) | 0.16673 (13) | 0.47056 (8) | 0.0391 (3) |
| H15 | 0.3131 | 0.1816 | 0.4980 | 0.047* |
| C16 | −0.72513 (18) | −0.03507 (16) | 0.07032 (9) | 0.0534 (4) |
| H16A | −0.8352 | −0.0203 | 0.0492 | 0.080* |
| H16B | −0.7306 | −0.0894 | 0.1169 | 0.080* |
| H16C | −0.6602 | −0.0831 | 0.0328 | 0.080* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0448 (6) | 0.0426 (6) | 0.0688 (7) | −0.0108 (4) | −0.0098 (5) | 0.0053 (5) |
| O2 | 0.0345 (5) | 0.0390 (5) | 0.0544 (6) | 0.0035 (4) | −0.0112 (4) | −0.0043 (5) |
| O3 | 0.0300 (6) | 0.1046 (9) | 0.0532 (7) | 0.0026 (5) | 0.0080 (5) | −0.0067 (6) |
| O4 | 0.0396 (5) | 0.0473 (6) | 0.0557 (6) | −0.0031 (4) | −0.0139 (5) | 0.0018 (5) |
| C1 | 0.0340 (7) | 0.0357 (7) | 0.0353 (7) | −0.0011 (6) | 0.0030 (6) | −0.0010 (6) |
| C2 | 0.0323 (7) | 0.0335 (7) | 0.0296 (6) | −0.0013 (5) | 0.0029 (5) | 0.0011 (6) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C3 | 0.0410 (7) | 0.0294 (7) | 0.0394 (8) | −0.0027 (5) | −0.0012 (6) | 0.0010 (6) |
| C4 | 0.0406 (7) | 0.0335 (7) | 0.0425 (8) | 0.0045 (6) | −0.0026 (6) | 0.0038 (6) |
| C5 | 0.0332 (7) | 0.0403 (7) | 0.0294 (6) | −0.0012 (5) | −0.0015 (5) | 0.0018 (6) |
| C6 | 0.0414 (7) | 0.0310 (7) | 0.0379 (7) | −0.0040 (5) | −0.0012 (6) | −0.0020 (6) |
| C7 | 0.0382 (7) | 0.0305 (7) | 0.0368 (7) | 0.0029 (5) | 0.0002 (6) | 0.0012 (6) |
| C8 | 0.0292 (7) | 0.0498 (9) | 0.0509 (9) | 0.0062 (6) | −0.0061 (6) | −0.0086 (7) |
| C9 | 0.0311 (7) | 0.0400 (8) | 0.0418 (8) | 0.0028 (5) | 0.0025 (6) | 0.0039 (6) |
| C10 | 0.0307 (6) | 0.0311 (7) | 0.0354 (7) | 0.0021 (5) | 0.0020 (5) | 0.0031 (6) |
| C11 | 0.0326 (7) | 0.0420 (8) | 0.0330 (7) | 0.0010 (5) | 0.0016 (5) | −0.0005 (6) |
| C12 | 0.0305 (7) | 0.0458 (8) | 0.0435 (8) | −0.0031 (6) | 0.0027 (6) | 0.0015 (7) |
| C13 | 0.0375 (8) | 0.0451 (8) | 0.0483 (9) | −0.0053 (6) | −0.0100 (6) | 0.0011 (7) |
| C14 | 0.0532 (9) | 0.0424 (8) | 0.0356 (8) | 0.0020 (6) | −0.0044 (6) | −0.0046 (6) |
| C15 | 0.0405 (8) | 0.0403 (8) | 0.0366 (7) | 0.0070 (6) | 0.0061 (6) | 0.0006 (6) |
| C16 | 0.0457 (8) | 0.0581 (10) | 0.0557 (9) | −0.0105 (7) | −0.0099 (7) | −0.0085 (8) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| O1—C1 | 1.2040 (15) | C8—H8A | 0.97 |
| O2—C1 | 1.3406 (15) | C8—H8B | 0.97 |
| O2—C8 | 1.4331 (15) | C9—C10 | 1.4844 (18) |
| O3—C9 | 1.2119 (15) | C10—C11 | 1.3886 (16) |
| O4—C5 | 1.3609 (15) | C10—C15 | 1.3916 (18) |
| O4—C16 | 1.4289 (17) | C11—C12 | 1.3820 (18) |
| C1—C2 | 1.4743 (18) | C11—H11 | 0.93 |
| C2—C7 | 1.3847 (17) | C12—C13 | 1.3719 (19) |
| C2—C3 | 1.3906 (17) | C12—H12 | 0.93 |
| C3—C4 | 1.3705 (18) | C13—C14 | 1.3828 (19) |
| C3—H3 | 0.93 | C13—H13 | 0.93 |
| C4—C5 | 1.3907 (18) | C14—C15 | 1.3735 (19) |
| C4—H4 | 0.93 | C14—H14 | 0.93 |
| C5—C6 | 1.3840 (18) | C15—H15 | 0.93 |
| C6—C7 | 1.3838 (18) | C16—H16A | 0.96 |
| C6—H6 | 0.93 | C16—H16B | 0.96 |
| C7—H7 | 0.93 | C16—H16C | 0.96 |
| C8—C9 | 1.504 (2) | | |
| C1—O2—C8 | 115.09 (10) | H8A—C8—H8B | 107.8 |
| C5—O4—C16 | 118.25 (11) | O3—C9—C10 | 122.19 (13) |
| O1—C1—O2 | 122.50 (12) | O3—C9—C8 | 120.75 (12) |
| O1—C1—C2 | 124.59 (12) | C10—C9—C8 | 117.07 (10) |
| O2—C1—C2 | 112.90 (11) | C11—C10—C15 | 118.86 (12) |
| C7—C2—C3 | 118.85 (12) | C11—C10—C9 | 122.01 (12) |
| C7—C2—C1 | 123.02 (12) | C15—C10—C9 | 119.13 (11) |
| C3—C2—C1 | 118.13 (11) | C12—C11—C10 | 120.23 (12) |
| C4—C3—C2 | 120.83 (12) | C12—C11—H11 | 119.9 |
| C4—C3—H3 | 119.6 | C10—C11—H11 | 119.9 |
| C2—C3—H3 | 119.6 | C13—C12—C11 | 120.30 (12) |
| C3—C4—C5 | 119.77 (12) | C13—C12—H12 | 119.8 |
| C3—C4—H4 | 120.1 | C11—C12—H12 | 119.8 |
| C5—C4—H4 | 120.1 | C12—C13—C14 | 120.01 (13) |

| | | | |
|---|---|---|---|
| O4—C5—C6 | 124.72 (12) | C12—C13—H13 | 120.0 |
| O4—C5—C4 | 115.01 (11) | C14—C13—H13 | 120.0 |
| C6—C5—C4 | 120.27 (12) | C15—C14—C13 | 120.01 (13) |
| C7—C6—C5 | 119.26 (12) | C15—C14—H14 | 120.0 |
| C7—C6—H6 | 120.4 | C13—C14—H14 | 120.0 |
| C5—C6—H6 | 120.4 | C14—C15—C10 | 120.58 (12) |
| C6—C7—C2 | 121.02 (12) | C14—C15—H15 | 119.7 |
| C6—C7—H7 | 119.5 | C10—C15—H15 | 119.7 |
| C2—C7—H7 | 119.5 | O4—C16—H16A | 109.5 |
| O2—C8—C9 | 112.64 (10) | O4—C16—H16B | 109.5 |
| O2—C8—H8A | 109.1 | H16A—C16—H16B | 109.5 |
| C9—C8—H8A | 109.1 | O4—C16—H16C | 109.5 |
| O2—C8—H8B | 109.1 | H16A—C16—H16C | 109.5 |
| C9—C8—H8B | 109.1 | H16B—C16—H16C | 109.5 |
| C8—O2—C1—O1 | −2.97 (18) | C1—C2—C7—C6 | 179.11 (11) |
| C8—O2—C1—C2 | 176.88 (10) | C1—O2—C8—C9 | 78.38 (14) |
| O1—C1—C2—C7 | 170.58 (12) | O2—C8—C9—O3 | 3.89 (19) |
| O2—C1—C2—C7 | −9.26 (17) | O2—C8—C9—C10 | −176.36 (11) |
| O1—C1—C2—C3 | −9.79 (19) | O3—C9—C10—C11 | −178.42 (13) |
| O2—C1—C2—C3 | 170.36 (10) | C8—C9—C10—C11 | 1.84 (18) |
| C7—C2—C3—C4 | 0.77 (19) | O3—C9—C10—C15 | 2.43 (19) |
| C1—C2—C3—C4 | −178.87 (11) | C8—C9—C10—C15 | −177.31 (12) |
| C2—C3—C4—C5 | −0.3 (2) | C15—C10—C11—C12 | −0.02 (19) |
| C16—O4—C5—C6 | −0.60 (18) | C9—C10—C11—C12 | −179.17 (12) |
| C16—O4—C5—C4 | 179.44 (11) | C10—C11—C12—C13 | −0.5 (2) |
| C3—C4—C5—O4 | 179.48 (11) | C11—C12—C13—C14 | 0.3 (2) |
| C3—C4—C5—C6 | −0.47 (19) | C12—C13—C14—C15 | 0.3 (2) |
| O4—C5—C6—C7 | −179.23 (11) | C13—C14—C15—C10 | −0.8 (2) |
| C4—C5—C6—C7 | 0.72 (18) | C11—C10—C15—C14 | 0.68 (19) |
| C5—C6—C7—C2 | −0.22 (19) | C9—C10—C15—C14 | 179.86 (12) |
| C3—C2—C7—C6 | −0.52 (18) | | |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C8—H8B···O1$^{i}$ | 0.97 | 2.28 | 3.2447 (17) | 172 |
| C12—H12···O3$^{ii}$ | 0.93 | 2.55 | 3.2973 (16) | 137 |
| C11—H11···Cg1$^{ii}$ | 0.93 | 2.86 | 3.6552 (15) | 144 |

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

**Fig. 1**