# 4-Methoxy-3-methylbenzophenone

R. S. Rathore,[a]*
T. Narasimhamurthy,[b] T. Vijay,[c]
H. S. Yathirajan,[d]
H. G. Anilkumar[d] and
Y. B. Basavaraju[d]

[a]Oriental Organization of Molecular & Structural Biology, 203, Agarwal Bhavan, Malleshwaram, Bangalore 560 055, India, [b]D210, Indian Institute of Science, Bangalore 560 012, India, [c]Solid State and Structural Chemistry Unit, Indian Institute of Science, Bangalore 560 012, India, and [d]Department of Studies in Chemistry, University of Mysore, Manasagangotri, Mysore 570 006, India

Correspondence e-mail:
ravindranath_rathore@yahoo.com

The molecule of the title compound, $C_{15}H_{14}O_2$, is non-planar and the planes of the benzene rings intersect at an angle of 59.8 (1)°. The crystal structure exhibits a significant short intermolecular $\pi$–$\pi$ contact.

## Comment

The title compound, (I), a benzophenone derivative, is an intermediate for the preparation of antimitiotic $\beta$-apopicropodophyllin (Basavaraju & Anjanamurthy, 2003). Over 300 crystal structures of benzophenone derivatives in the Cambridge Structural Database (CSD, Version 5.26; Allen, 2002) highlight the importance of structural studies on such pharmaceutically useful compounds. The synthesis and structure of (I) are reported here.



(I)
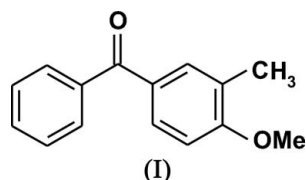
A projection of (I) with the numbering scheme is shown in Fig. 1. Relevant geometric details are given in Table 1. The structure of (I), similar to other benzophenone analogues (Malathy Sony et al., 2005; Mahendra et al., 2005; Khanum et al., 2005), is non-planar due to the strains associated with the overlapping of adjacent H atoms of aromatic rings. The planes through C7–C13 and O2/C1–C7/C14/C15 intersect at an angle of 59.1 (1)°, whereas the planes of benzene rings (C1–C6 and C8–C13) intersect at 59.8 (1)°. Atom O1 is displaced by −0.226 (2) and 0.960 (2)Å with respect to aromatic rings C1–C6 and C8–C13. The dihedral angles between the planes associated with the carbonyl group O1/C1/C7/C8 and adjacent benzene rings C1–C6 and C8–C13 are 8.9 (1) and 53.0 (1)°, respectively. The conformation of the
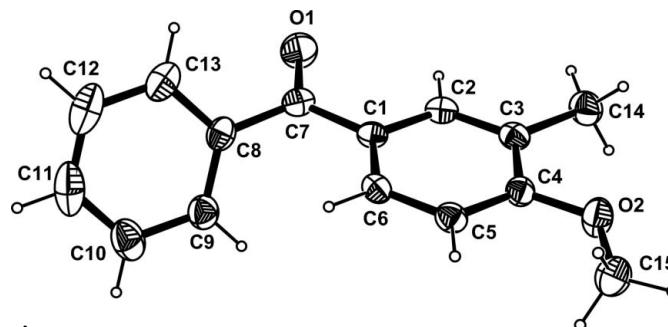


**Figure 1**
The molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level.
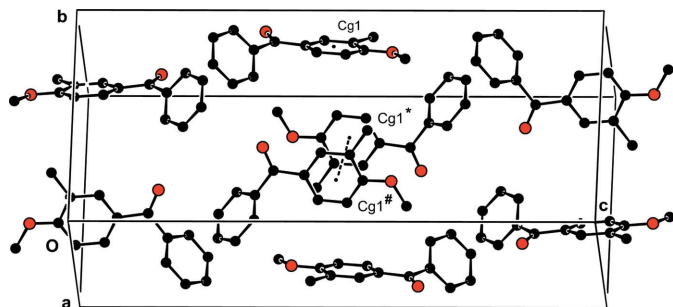
**Figure 2**
The crystal packing of (I). The short $\pi$–$\pi$ contact is shown as a dashed line. *Cg*1 is the centroid of aromatic ring C1–C6. The asterisk (*) and hash (#) symbols indicate that the molecules are located at the symmetry positions ($\frac{1}{2} + x, \frac{3}{2} - y, 1 - z$) and ($\frac{1}{2} - x, -\frac{1}{2} + y, z$), respectively.

molecule as a whole is essentially described by the torsion angles about the C1—C7 and C7—C8 bonds: C2—C1—C7—O1 = $-7.0$ (3)°, O1—C7—C8—C13 = $-50.7$ (3)°, C2—C1—C7—C8 = 173.61 (16)° and C1—C7—C8—C13 = 128.68 (19)°. In contrast, the values of the corresponding torsion angles in an isomeric compound crystallizing in $P2_1/c$ (2-methoxy-5-methylphenyl phenyl ketone; Malathy Sony *et al.*, 2005) are: C6—C1—C7—O8 = 51.7 (3)°, O8—C7—C9—C10 = 17.5 (4)°, C6—C1—C7—C9 = $-124.9$ (3)° and C1—C7—C9—C10 = $-166.0$ (2)°.

A view of the crystal packing is shown in Fig. 2. The crystal structure displays a significant short intermolecular $\pi$–$\pi$ contact of face-to-face type, where the $Cg1\cdots Cg1^i$ [symmetry code: (i) $-x, 2 - y, 1 - z$; *Cg*1 is the centroid of the ring C1–C6] separation and perpendicular distances are 3.55 and 3.48Å, respectively. The rest of the short intermolecular contacts are in the range of van der Waals interactions.

## Experimental

A solution of *o*-methylanisole (2 g, 0.0163 mol) in dry dichloromethane (15 ml) was treated with anhydrous aluminium chloride (2.183 g, 0.0163 mol). The reaction mixture was stirred continuously for 30 min. A solution of benzoyl chloride (2.3 g, 0.01637 mol) in dichloromethane (15 ml) was added dropwise over a period of 1 h to the reaction mixture at 298 K. After 24 h, 6 ml of concentrated HCl was added over 30 min. The reaction mixture was stirred for 24 h. Aqueous NaCl solution (10%) was added to break up the emulsion and the lower organic layer was separated and washed twice with 50 ml of 10% NaOH. The excess of dichloromethane was distilled off and the concentrated solution was left to stand overnight. Pale-yellow crystalline solids were separated and recrystallized from methanol (yield, 90%; m.p. 343 K).

### Crystal data

| | |
|---|---|
| $C_{15}H_{14}O_2$ | $Z = 8$ |
| $M_r = 226.26$ | $D_x = 1.241$ Mg m$^{-3}$ |
| Orthorhombic, $Pbca$ | Mo $K\alpha$ radiation |
| $a = 8.582$ (2) Å | $\mu = 0.08$ mm$^{-1}$ |
| $b = 11.314$ (3) Å | $T = 295$ (2) K |
| $c = 24.941$ (7) Å | Block, colourless |
| $V = 2421.5$ (12) Å$^3$ | $0.34 \times 0.31 \times 0.25$ mm |

### Data collection

| | |
|---|---|
| Bruker SMART CCD area-detector diffractometer | 17509 measured reflections |
| $\varphi$ and $\omega$ scans | 2380 independent reflections |
| Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996) | 1630 reflections with $I > 2\sigma(I)$ |
| $T_{min} = 0.960$, $T_{max} = 0.988$ | $R_{int} = 0.048$ |
| | $\theta_{max} = 26.0°$ |

### Refinement

| | |
|---|---|
| Refinement on $F^2$ | $w = 1/[\sigma^2(F_o^2) + (0.0423P)^2 + 0.4398P]$ |
| $R[F^2 > 2\sigma(F^2)] = 0.053$ | where $P = (F_o^2 + 2F_c^2)/3$ |
| $wR(F^2) = 0.119$ | $(\Delta/\sigma)_{max} < 0.001$ |
| $S = 1.10$ | $\Delta\rho_{max} = 0.14$ e Å$^{-3}$ |
| 2380 reflections | $\Delta\rho_{min} = -0.14$ e Å$^{-3}$ |
| 156 parameters | |
| H-atom parameters constrained | |

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| O1—C7 | 1.222 (2) | C1—C7 | 1.480 (3) |
| O2—C4 | 1.361 (2) | C3—C14 | 1.503 (3) |
| O2—C15 | 1.425 (2) | C7—C8 | 1.499 (3) |
| | | | |
| C4—O2—C15 | 119.04 (16) | O2—C4—C3 | 114.75 (16) |
| C6—C1—C7 | 122.92 (17) | O1—C7—C1 | 121.16 (18) |
| C2—C1—C7 | 119.31 (16) | C1—C7—C8 | 119.93 (16) |
| C2—C3—C14 | 121.87 (17) | C9—C8—C7 | 122.07 (17) |
| C4—C3—C14 | 120.42 (17) | C13—C8—C7 | 118.60 (19) |
| O2—C4—C5 | 124.29 (17) | | |

All H atoms were positioned geometrically and were refined as riding on their carrier atoms, with $C_{ar}$—H = 0.93Å with $U_{iso}(H) = 1.2U_{eq}(C_{ar})$, and $C_{methyl}$—H = 0.96Å with $U_{iso}(H) = 1.5U_{eq}(C_{methyl})$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997) ans *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *PLATON*.

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