# 2-(4-Bromo-phen-yl)-2-oxoethyl 2-meth-oxy-benzoate

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# 2-(4-Bromophenyl)-2-oxoethyl 2-methoxybenzoate

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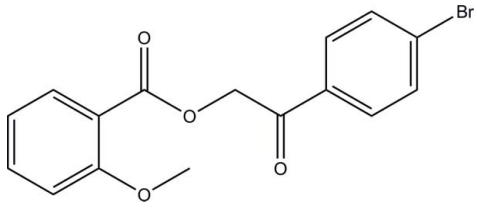
Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.037; $wR$ factor = 0.095; data-to-parameter ratio = 24.9.

In the title molecule, $C_{16}H_{13}BrO_4$, the dihedral angle between the benzene rings is 85.92 (10)°. In the crystal, molecules are linked into chains along [100] *via* weak intermolecular C—H···O hydrogen bonds.

## Related literature

For general background to and applications of phenacyl benzoate derivatives, see: Rather & Reid (1919); Sheehan & Umezaw (1973); Ruzicka *et al.* (2002); Litera *et al.* (2006); Huang *et al.* (1996); Gandhi *et al.* (1995). For standard bond-length data, see: Allen *et al.* (1987).




## Experimental

### Crystal data

$C_{16}H_{13}BrO_4$
$M_r$ = 349.17
Orthorhombic, *Pbca*
$a$ = 7.8424 (5) Å
$b$ = 14.6799 (9) Å
$c$ = 25.7677 (14) Å
$V$ = 2966.5 (3) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 2.78 mm$^{-1}$
$T$ = 296 K
0.56 × 0.25 × 0.12 mm

### Data collection

Bruker SMART APEXII DUO CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min}$ = 0.306, $T_{max}$ = 0.733
19358 measured reflections
4731 independent reflections
2916 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.035

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.095
$S$ = 1.00
4731 reflections
190 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.51 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.54 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C2—H2$A$···O1$^{i}$ | 0.93 | 2.45 | 3.360 (3) | 165 |

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5263).

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§ Thomson Reuters ResearcherID: A-5525-2009.

# supplementary materials

*Acta Cryst.* (2011). E**67**, o1724 [ **doi:10.1107/S1600536811023002** ]

# 2-(4-Bromophenyl)-2-oxoethyl 2-methoxybenzoate

**H.-K. Fun, C. K. Quah, B. Garudachari, A. M. Isloor and M. N. Satyanarayan**

## Comment

Phenacyl benzoates derivatives are very important in the identification of organic acids (Rather & Reid, 1919). They undergo photolysis in neutral and mild conditions (Sheehan & Umezaw, 1973; Ruzicka *et al.*, 2002; Litera *et al.*, 2006). They find applications in the field of synthetic chemistry for the synthesis of oxazoles, imidazoles (Huang *et al.*, 1996), benzoxazepine (Gandhi *et al.*, 1995). We report herein the crystal structure of 2-(4-bromophenyl)-2-oxoethyl 2-methoxybenzoate which is potentially of commercial importance.

The molecular structure of the title compound is shown in Fig. 1. The benzene rings (C1-C6 and C10-C15) form a dihedral angle of 85.92 (10) ° . Bond lengths (Allen *et al.*, 1987) and angles are within normal ranges. In the crystal (Fig. 2), the molecules are linked into one-dimensional chains along [100] *via* weak intermolecular C2–H2A···O1$^{i}$ hydrogen bonds (Table 1).

## Experimental

A mixture of 2-methoxybenzoic acid (1.00 g, 0.0065 mol) potassium carbonate (0.98 g, 0.0071 mol) and 2-bromo-1-(4-bromophenyl)ethanone (1.80 g, 0.0065 mol) in dimethylformamide (10 ml) was stirred at room temperature for 2 h. On cooling, colorless needle shaped crystals of 2-(4-bromophenyl)-2-oxoethyl 2-methoxybenzoate began to separate. These were collected by filtration and recrystallized from ethanol. Yield: 2.15 g, 93.8 %, *m.p.* : 388-389 K.

## Refinement

All H atoms were positioned geometrically and refined using a riding model with C—H = 0.93 – 0.96 Å and $U_{iso}$(H) = 1.2 or 1.5 $U_{eq}$(C). The highest residual electron density peak is located at 0.79 Å and the deepest hole is located at 0.78 Å from Br1, respectively.

## Figures

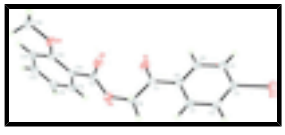

Fig. 1. The molecular structure of the title compound showing 20% probability displacement ellipsoids for non-H atoms.

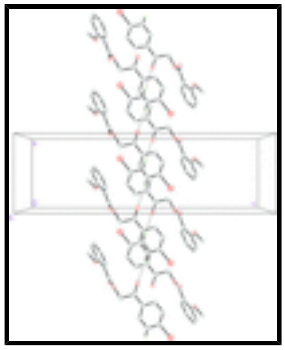

Fig. 2. Part of the crystal structure of the title compound, viewed along the *b* axis. H atoms not involved in hydrogen bonds (dashed lines) have been omitted for clarity.

**2-(4-Bromophenyl)-2-oxoethyl 2-methoxybenzoate**

*Crystal data*

| | |
|---|---|
| $C_{16}H_{13}BrO_4$ | $F(000) = 1408$ |
| $M_r = 349.17$ | $D_x = 1.564$ Mg m$^{-3}$ |
| Orthorhombic, *Pbca* | Mo *K*α radiation, λ = 0.71073 Å |
| Hall symbol: -P 2ac 2ab | Cell parameters from 3938 reflections |
| $a = 7.8424$ (5) Å | θ = 2.8–26.5° |
| $b = 14.6799$ (9) Å | μ = 2.78 mm$^{-1}$ |
| $c = 25.7677$ (14) Å | $T = 296$ K |
| $V = 2966.5$ (3) Å$^3$ | Needle, colourless |
| $Z = 8$ | 0.56 × 0.25 × 0.12 mm |

*Data collection*

| | |
|---|---|
| Bruker SMART APEXII DUO CCD area-detector diffractometer | 4731 independent reflections |
| Radiation source: fine-focus sealed tube | 2916 reflections with $I > 2\sigma(I)$ |
| graphite | $R_{int} = 0.035$ |
| φ and ω scans | $\theta_{max} = 31.0°$, $\theta_{min} = 2.8°$ |
| Absorption correction: multi-scan (*SADABS*; Bruker, 2009) | $h = -11 \rightarrow 11$ |
| $T_{min} = 0.306$, $T_{max} = 0.733$ | $k = -21 \rightarrow 14$ |
| 19358 measured reflections | $l = -37 \rightarrow 37$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Primary atom site location: structure-invariant direct methods |
| Least-squares matrix: full | Secondary atom site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)] = 0.037$ | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.095$ | H-atom parameters constrained |
| $S = 1.00$ | $w = 1/[\sigma^2(F_o^2) + (0.0329P)^2 + 1.2401P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| 4731 reflections | $(\Delta/\sigma)_{max} = 0.001$ |

| | |
|---|---|
| 190 parameters | $\Delta\rho_{max} = 0.51$ e Å$^{-3}$ |
| 0 restraints | $\Delta\rho_{min} = -0.54$ e Å$^{-3}$ |

*Special details*

**Geometry**. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2\text{sigma}(F^2)$ 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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Br1 | 1.19995 (4) | 0.063553 (17) | 0.603716 (11) | 0.07024 (11) |
| O1 | 0.4583 (2) | 0.13020 (14) | 0.46925 (7) | 0.0717 (5) |
| O2 | 0.4899 (2) | 0.19606 (9) | 0.37415 (6) | 0.0579 (4) |
| O3 | 0.4628 (2) | 0.04790 (10) | 0.35626 (6) | 0.0604 (4) |
| O4 | 0.19571 (19) | 0.00663 (10) | 0.29651 (6) | 0.0544 (4) |
| C1 | 0.9183 (3) | 0.14467 (14) | 0.47702 (8) | 0.0488 (5) |
| H1A | 0.9406 | 0.1695 | 0.4445 | 0.059* |
| C2 | 1.0517 (3) | 0.12695 (15) | 0.51036 (8) | 0.0517 (5) |
| H2A | 1.1635 | 0.1396 | 0.5007 | 0.062* |
| C3 | 1.0158 (3) | 0.09006 (13) | 0.55825 (8) | 0.0487 (5) |
| C4 | 0.8516 (3) | 0.07055 (14) | 0.57344 (8) | 0.0538 (5) |
| H4A | 0.8302 | 0.0457 | 0.6060 | 0.065* |
| C5 | 0.7199 (3) | 0.08825 (15) | 0.53991 (8) | 0.0504 (5) |
| H5A | 0.6087 | 0.0749 | 0.5498 | 0.060* |
| C6 | 0.7504 (3) | 0.12584 (13) | 0.49133 (7) | 0.0428 (4) |
| C7 | 0.6034 (3) | 0.14284 (14) | 0.45588 (8) | 0.0470 (4) |
| C8 | 0.6423 (3) | 0.17663 (14) | 0.40202 (8) | 0.0496 (5) |
| H8A | 0.7113 | 0.2313 | 0.4042 | 0.059* |
| H8B | 0.7073 | 0.1308 | 0.3835 | 0.059* |
| C9 | 0.4043 (3) | 0.12319 (13) | 0.35557 (7) | 0.0444 (4) |
| C10 | 0.2356 (3) | 0.15108 (13) | 0.33476 (7) | 0.0420 (4) |
| C11 | 0.1753 (3) | 0.23898 (15) | 0.34381 (8) | 0.0540 (5) |
| H11A | 0.2411 | 0.2790 | 0.3633 | 0.065* |
| C12 | 0.0207 (3) | 0.26793 (17) | 0.32457 (9) | 0.0654 (6) |
| H12A | −0.0176 | 0.3268 | 0.3311 | 0.078* |
| C13 | −0.0762 (3) | 0.20873 (18) | 0.29561 (9) | 0.0643 (6) |
| H13A | −0.1803 | 0.2280 | 0.2823 | 0.077* |
| C14 | −0.0216 (3) | 0.12187 (16) | 0.28619 (8) | 0.0551 (5) |
| H14A | −0.0894 | 0.0827 | 0.2668 | 0.066* |
| C15 | 0.1337 (3) | 0.09149 (13) | 0.30522 (7) | 0.0442 (4) |

| | | | | |
|---|---|---|---|---|
| C16 | 0.0967 (4) | −0.05475 (17) | 0.26574 (11) | 0.0735 (7) |
| H16A | 0.1556 | −0.1118 | 0.2627 | 0.110* |
| H16B | 0.0799 | −0.0292 | 0.2318 | 0.110* |
| H16C | −0.0120 | −0.0644 | 0.2820 | 0.110* |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Br1 | 0.07526 (19) | 0.05554 (15) | 0.07991 (18) | 0.00639 (12) | −0.03345 (13) | −0.00558 (11) |
| O1 | 0.0385 (8) | 0.1055 (14) | 0.0713 (10) | −0.0059 (9) | 0.0015 (8) | −0.0039 (10) |
| O2 | 0.0574 (9) | 0.0434 (8) | 0.0729 (9) | −0.0015 (7) | −0.0214 (8) | 0.0012 (7) |
| O3 | 0.0584 (9) | 0.0481 (8) | 0.0746 (10) | 0.0109 (7) | −0.0218 (8) | −0.0110 (7) |
| O4 | 0.0577 (9) | 0.0459 (7) | 0.0595 (8) | −0.0012 (7) | −0.0141 (7) | −0.0071 (6) |
| C1 | 0.0433 (11) | 0.0560 (11) | 0.0472 (10) | −0.0059 (10) | 0.0009 (9) | −0.0014 (9) |
| C2 | 0.0372 (10) | 0.0562 (12) | 0.0617 (12) | −0.0049 (9) | −0.0018 (9) | −0.0084 (10) |
| C3 | 0.0535 (12) | 0.0381 (9) | 0.0544 (11) | 0.0025 (9) | −0.0136 (10) | −0.0098 (8) |
| C4 | 0.0634 (14) | 0.0506 (11) | 0.0474 (10) | −0.0032 (11) | −0.0006 (10) | −0.0014 (9) |
| C5 | 0.0430 (11) | 0.0542 (11) | 0.0540 (11) | −0.0053 (10) | 0.0062 (9) | −0.0046 (9) |
| C6 | 0.0381 (9) | 0.0421 (10) | 0.0481 (10) | −0.0023 (8) | 0.0013 (8) | −0.0093 (8) |
| C7 | 0.0398 (11) | 0.0466 (10) | 0.0547 (11) | −0.0035 (9) | −0.0017 (9) | −0.0102 (8) |
| C8 | 0.0444 (11) | 0.0434 (10) | 0.0608 (12) | −0.0064 (9) | −0.0111 (9) | 0.0010 (9) |
| C9 | 0.0505 (12) | 0.0430 (10) | 0.0398 (9) | 0.0012 (9) | −0.0048 (8) | −0.0011 (8) |
| C10 | 0.0453 (10) | 0.0437 (9) | 0.0371 (8) | 0.0042 (8) | −0.0024 (8) | 0.0010 (7) |
| C11 | 0.0603 (14) | 0.0510 (11) | 0.0508 (11) | 0.0078 (10) | −0.0030 (10) | −0.0057 (9) |
| C12 | 0.0679 (15) | 0.0613 (14) | 0.0671 (14) | 0.0228 (13) | −0.0041 (12) | −0.0009 (11) |
| C13 | 0.0505 (13) | 0.0780 (16) | 0.0646 (13) | 0.0163 (12) | −0.0071 (11) | 0.0099 (12) |
| C14 | 0.0486 (12) | 0.0654 (14) | 0.0513 (11) | −0.0005 (11) | −0.0093 (10) | 0.0052 (10) |
| C15 | 0.0475 (11) | 0.0490 (10) | 0.0362 (8) | 0.0017 (9) | 0.0003 (8) | 0.0040 (7) |
| C16 | 0.0819 (18) | 0.0597 (14) | 0.0788 (16) | −0.0071 (13) | −0.0264 (15) | −0.0160 (11) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Br1—C3 | 1.900 (2) | C7—C8 | 1.505 (3) |
| O1—C7 | 1.203 (3) | C8—H8A | 0.9700 |
| O2—C9 | 1.351 (2) | C8—H8B | 0.9700 |
| O2—C8 | 1.423 (2) | C9—C10 | 1.485 (3) |
| O3—C9 | 1.197 (2) | C10—C11 | 1.394 (3) |
| O4—C15 | 1.356 (2) | C10—C15 | 1.408 (3) |
| O4—C16 | 1.430 (3) | C11—C12 | 1.377 (3) |
| C1—C2 | 1.378 (3) | C11—H11A | 0.9300 |
| C1—C6 | 1.395 (3) | C12—C13 | 1.375 (3) |
| C1—H1A | 0.9300 | C12—H12A | 0.9300 |
| C2—C3 | 1.377 (3) | C13—C14 | 1.367 (3) |
| C2—H2A | 0.9300 | C13—H13A | 0.9300 |
| C3—C4 | 1.376 (3) | C14—C15 | 1.386 (3) |
| C4—C5 | 1.371 (3) | C14—H14A | 0.9300 |
| C4—H4A | 0.9300 | C16—H16A | 0.9600 |
| C5—C6 | 1.389 (3) | C16—H16B | 0.9600 |
| C5—H5A | 0.9300 | C16—H16C | 0.9600 |

| | | | |
|---|---|---|---|
| C6—C7 | 1.492 (3) | | |
| C9—O2—C8 | 115.94 (15) | H8A—C8—H8B | 108.0 |
| C15—O4—C16 | 118.42 (17) | O3—C9—O2 | 122.39 (19) |
| C2—C1—C6 | 120.95 (19) | O3—C9—C10 | 126.97 (18) |
| C2—C1—H1A | 119.5 | O2—C9—C10 | 110.63 (16) |
| C6—C1—H1A | 119.5 | C11—C10—C15 | 118.24 (19) |
| C3—C2—C1 | 118.55 (19) | C11—C10—C9 | 119.80 (18) |
| C3—C2—H2A | 120.7 | C15—C10—C9 | 121.96 (17) |
| C1—C2—H2A | 120.7 | C12—C11—C10 | 121.6 (2) |
| C4—C3—C2 | 121.9 (2) | C12—C11—H11A | 119.2 |
| C4—C3—Br1 | 119.56 (16) | C10—C11—H11A | 119.2 |
| C2—C3—Br1 | 118.56 (17) | C13—C12—C11 | 119.2 (2) |
| C5—C4—C3 | 119.1 (2) | C13—C12—H12A | 120.4 |
| C5—C4—H4A | 120.5 | C11—C12—H12A | 120.4 |
| C3—C4—H4A | 120.5 | C14—C13—C12 | 120.8 (2) |
| C4—C5—C6 | 120.9 (2) | C14—C13—H13A | 119.6 |
| C4—C5—H5A | 119.5 | C12—C13—H13A | 119.6 |
| C6—C5—H5A | 119.5 | C13—C14—C15 | 120.8 (2) |
| C5—C6—C1 | 118.64 (19) | C13—C14—H14A | 119.6 |
| C5—C6—C7 | 119.04 (18) | C15—C14—H14A | 119.6 |
| C1—C6—C7 | 122.30 (18) | O4—C15—C14 | 123.50 (19) |
| O1—C7—C6 | 121.99 (19) | O4—C15—C10 | 117.17 (17) |
| O1—C7—C8 | 120.4 (2) | C14—C15—C10 | 119.32 (19) |
| C6—C7—C8 | 117.61 (18) | O4—C16—H16A | 109.5 |
| O2—C8—C7 | 111.19 (18) | O4—C16—H16B | 109.5 |
| O2—C8—H8A | 109.4 | H16A—C16—H16B | 109.5 |
| C7—C8—H8A | 109.4 | O4—C16—H16C | 109.5 |
| O2—C8—H8B | 109.4 | H16A—C16—H16C | 109.5 |
| C7—C8—H8B | 109.4 | H16B—C16—H16C | 109.5 |
| C6—C1—C2—C3 | 0.1 (3) | C8—O2—C9—C10 | 171.08 (17) |
| C1—C2—C3—C4 | 0.1 (3) | O3—C9—C10—C11 | 170.4 (2) |
| C1—C2—C3—Br1 | 178.86 (15) | O2—C9—C10—C11 | −10.3 (3) |
| C2—C3—C4—C5 | 0.1 (3) | O3—C9—C10—C15 | −10.5 (3) |
| Br1—C3—C4—C5 | −178.69 (15) | O2—C9—C10—C15 | 168.90 (17) |
| C3—C4—C5—C6 | −0.4 (3) | C15—C10—C11—C12 | −0.2 (3) |
| C4—C5—C6—C1 | 0.5 (3) | C9—C10—C11—C12 | 179.0 (2) |
| C4—C5—C6—C7 | 179.23 (18) | C10—C11—C12—C13 | −0.2 (3) |
| C2—C1—C6—C5 | −0.4 (3) | C11—C12—C13—C14 | 0.5 (4) |
| C2—C1—C6—C7 | −179.03 (19) | C12—C13—C14—C15 | −0.6 (4) |
| C5—C6—C7—O1 | 4.6 (3) | C16—O4—C15—C14 | 0.5 (3) |
| C1—C6—C7—O1 | −176.7 (2) | C16—O4—C15—C10 | −178.7 (2) |
| C5—C6—C7—C8 | −175.25 (18) | C13—C14—C15—O4 | −179.0 (2) |
| C1—C6—C7—C8 | 3.4 (3) | C13—C14—C15—C10 | 0.2 (3) |
| C9—O2—C8—C7 | −76.7 (2) | C11—C10—C15—O4 | 179.39 (17) |
| O1—C7—C8—O2 | 4.4 (3) | C9—C10—C15—O4 | 0.2 (3) |
| C6—C7—C8—O2 | −175.70 (16) | C11—C10—C15—C14 | 0.1 (3) |
| C8—O2—C9—O3 | −9.5 (3) | C9—C10—C15—C14 | −179.03 (18) |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C2—H2A···O1$^{i}$ | 0.93 | 2.45 | 3.360 (3) | 165 |

Symmetry codes: (i) *x*+1, *y*, *z*.

**Fig. 1**

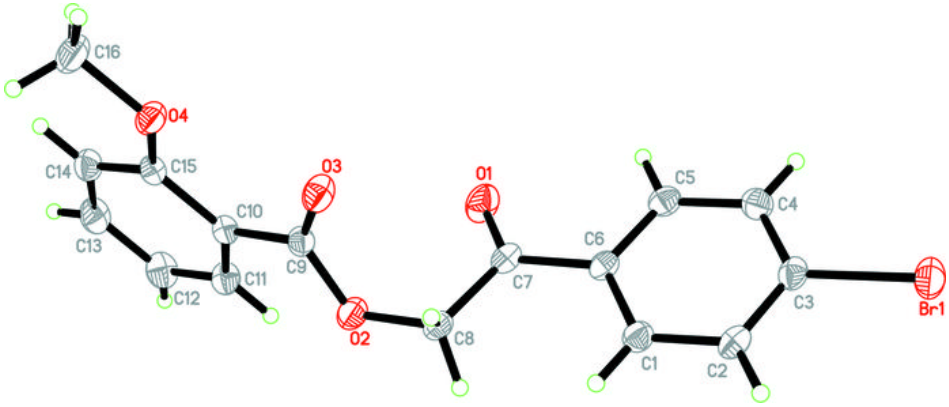
C16
O4
C14
C15
O3
C10
C13
C11
C9
C12
O2
C8
O1
C7
C6
C5
C4
C3
Br1
C1
C2

**Fig. 2**