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

# 2,4-Dimethylphenyl benzoate

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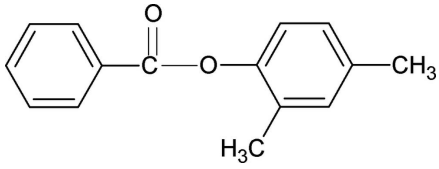
Received 5 June 2008; accepted 10 June 2008

Key indicators: single-crystal X-ray study; $T$ = 295 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.054; $wR$ factor = 0.135; data-to-parameter ratio = 15.8.

The crystal structure of the title compound (24DMPBA), $C_{15}H_{14}O_2$, resembles those of 4-methylphenyl benzoate, 2,3-dimethylphenyl benzoate and other aryl benzoates, with similar bond parameters. The central –O—C—O– group in 24DMPBA makes dihedral angles of 85.81 (5) and 5.71 (13)°, respectively, with the benzoyl and phenyl rings, while the two aromatic rings form a dihedral angle of 80.25 (5)°. The molecules are packed with their axes parallel to the $a$-axis direction.

## Related literature

For related literature, see: Gowda *et al.* (2007, 2008); Nayak & Gowda (2008).




## Experimental

### Crystal data

$C_{15}H_{14}O_2$
$M_r$ = 226.26
Monoclinic, $P2_1/c$
$a$ = 7.9813 (2) Å
$b$ = 14.3260 (3) Å
$c$ = 11.0932 (2) Å
$\beta$ = 94.028 (2)°
$V$ = 1265.26 (5) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.08 mm$^{-1}$
$T$ = 295 (2) K
0.48 × 0.38 × 0.21 mm

### Data collection

Oxford Diffraction Xcalibur diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
$T_{min}$ = 0.965, $T_{max}$ = 0.987
28657 measured reflections
2471 independent reflections
2056 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.031

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.134
$S$ = 1.08
2471 reflections
156 parameters
4 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.16 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.14 e Å$^{-3}$

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2007); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2007); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 2002); software used to prepare material for publication: *SHELXL97*, *PLATON* (Spek, 2003) and *WinGX* (Farrugia, 1999).

BTG thanks the Alexander von Humboldt Foundation, Bonn, Germany, for extensions of his research fellowship. MT and JK thank the Grant Agency of the Slovak Republic (grant No. VEGA 1/0817/08) and the Structural Funds, Interreg IIIA, for financial support in the purchase of the diffractometer.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2614).

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# supplementary materials

*Acta Cryst.* (2008). E**64**, o1280 [ **doi:10.1107/S1600536808017480** ]

## 2,4-Dimethylphenyl benzoate

**B. T. Gowda, M. Tokarcík, J. Kozísek, K. S. Babitha and H. Fuess**

### Comment

In the present work, as part of a study of the substituent effects on the solid state geometries of aryl benzoates (Gowda *et al.*, 2007, 2008), the structure of 2,4-dimethylphenyl benzoate (24DMPBA) has been determined. The structure of 24DMPBA (Fig. 1) is similar to those of 4-methylphenyl benzoate (4MePBA)(Gowda *et al.*, 2007), 2,3-dimethylphenyl benzoate (23DMPBA) (Gowda *et al.*, 2008) and other aryl benzoates. The central –O—C—O– group in 24DMPBA makes a dihedral angle of 85.81 (5)° with the benzoyl phenyl ring and 5.71 (13)° with the phenyl ring. The two aromatic rings in 24DMPBA form a dihedral angle of 80.25 (5)°. The bond parameters in 24DMPBA are similar to those in 4MePBA, 23DMPBA and other aryl benzoates. Part of the crystal structure of the title compound as viewed along the *a* axis is shown in Fig.2.

### Experimental

The title compound was prepared according to a literature method (Nayak & Gowda, 2008). The purity of the compound was checked by determining its melting point. It was characterized by recording its infrared and NMR spectra (Nayak & Gowda, 2008). Single crystals of the title compound were obtained by slow evaporation of an ethanolic solution and used for X-ray diffraction studies at room temperature.

### Refinement

H atoms were placed in calculated positions and treated as riding with C-H = 0.93Å (aromatic) or 0.96Å (methyl), and $U_{iso}$(H) = 1.2 $U_{eq}$(CH) and 1.5$U_{eq}$($CH_3$). The methyl groups (C14,C15) are disordered over two different orientations. The occupancy factor for the major orientation refined to 0.56 (3) for the C14-methyl group and 0.67 (3) for the C15-methyl group.

### Figures

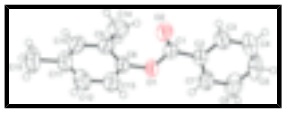

Fig. 1. Molecular structure of the title compound, showing the atom labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented as small spheres of arbitrary radii.

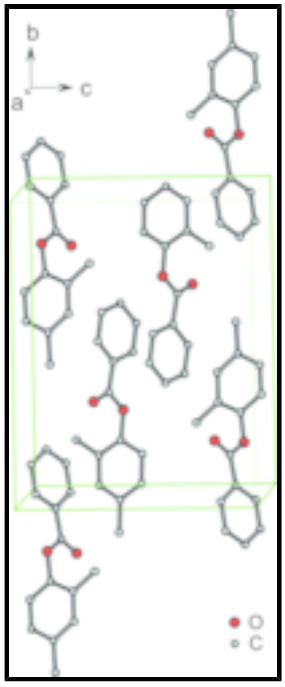


Fig. 2. Part of the crystal structure of the title compound as viewed along the *a* axis. H atoms have been omitted for the sake of clarity.

**2,4-Dimethylphenyl benzoate**

*Crystal data*

| | |
|---|---|
| $C_{15}H_{14}O_2$ | $F_{000}$ = 480 |
| $M_r$ = 226.26 | $D_x$ = 1.188 Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation<br>λ = 0.71073 Å |
| Hall symbol: -P 2ybc | Cell parameters from 12993 reflections |
| $a$ = 7.9813 (2) Å | θ = 3.2–29.3º |
| $b$ = 14.3260 (3) Å | μ = 0.08 mm$^{-1}$ |
| $c$ = 11.0932 (2) Å | $T$ = 295 (2) K |
| β = 94.028 (2)º | Block, colourless |
| $V$ = 1265.26 (5) Å$^3$ | 0.48 × 0.38 × 0.21 mm |
| $Z$ = 4 | |

*Data collection*

| | |
|---|---|
| Oxford Diffraction Xcalibur diffractometer | 2471 independent reflections |
| Monochromator: graphite | 2056 reflections with $I > 2\sigma(I)$ |
| Detector resolution: 10.434 pixels mm$^{-1}$ | $R_{int}$ = 0.031 |
| $T$ = 295(2) K | $\theta_{max}$ = 26.0º |
| ω scans with κ offsets | $\theta_{min}$ = 5.9º |
| Absorption correction: multi-scan (CrysAlis RED; Oxford Diffraction, 2007) | $h$ = −9→9 |
| $T_{min}$ = 0.965, $T_{max}$ = 0.987 | $k$ = −17→17 |

28657 measured reflections

$l = -13 \rightarrow 13$

*Refinement*

Refinement on $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.053$

$wR(F^2) = 0.134$

$S = 1.08$

2471 reflections

156 parameters

4 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

$w = 1/[\sigma^2(F_o^2) + (0.0541P)^2 + 0.2483P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 0.16$ e Å$^{-3}$

$\Delta\rho_{min} = -0.14$ e Å$^{-3}$

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 $F^2 > \sigma(F^2)$ 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* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| O1 | 0.77410 (13) | 0.30501 (7) | 0.43628 (10) | 0.0642 (3) | |
| O2 | 0.56045 (16) | 0.31504 (8) | 0.29564 (11) | 0.0795 (4) | |
| C1 | 0.65706 (18) | 0.35245 (10) | 0.36678 (13) | 0.0540 (4) | |
| C2 | 0.66645 (18) | 0.45392 (10) | 0.38934 (13) | 0.0529 (4) | |
| C3 | 0.5646 (2) | 0.51221 (12) | 0.31812 (17) | 0.0750 (5) | |
| H3 | 0.4919 | 0.4871 | 0.2574 | 0.09* | |
| C4 | 0.5690 (3) | 0.60709 (14) | 0.3358 (2) | 0.0901 (6) | |
| H4 | 0.5004 | 0.6458 | 0.2865 | 0.108* | |
| C5 | 0.6720 (3) | 0.64395 (12) | 0.4237 (3) | 0.0912 (7) | |
| H5 | 0.6748 | 0.7082 | 0.4353 | 0.109* | |
| C6 | 0.7731 (3) | 0.58741 (14) | 0.4966 (2) | 0.0971 (7) | |
| H6 | 0.8437 | 0.6134 | 0.5579 | 0.116* | |
| C7 | 0.7711 (2) | 0.49201 (12) | 0.47963 (18) | 0.0738 (5) | |
| H7 | 0.8402 | 0.4537 | 0.5292 | 0.089* | |
| C8 | 0.77716 (18) | 0.20698 (10) | 0.42443 (13) | 0.0552 (4) | |
| C9 | 0.8731 (2) | 0.16674 (11) | 0.34018 (14) | 0.0623 (4) | |

| | | | | | |
|---|---|---|---|---|---|
| C10 | 0.8778 (2) | 0.06901 (12) | 0.33938 (17) | 0.0732 (5) | |
| H10 | 0.9403 | 0.0392 | 0.2831 | 0.088* | |
| C11 | 0.7940 (2) | 0.01520 (12) | 0.41818 (18) | 0.0759 (5) | |
| C12 | 0.7035 (2) | 0.05916 (12) | 0.50064 (19) | 0.0786 (5) | |
| H12 | 0.6473 | 0.0239 | 0.5555 | 0.094* | |
| C13 | 0.6936 (2) | 0.15527 (12) | 0.50441 (16) | 0.0682 (4) | |
| H13 | 0.6306 | 0.1845 | 0.5609 | 0.082* | |
| C14 | 0.9689 (3) | 0.22412 (17) | 0.2560 (2) | 0.0964 (6) | |
| H14A | 0.9884 | 0.1881 | 0.1854 | 0.145* | 0.56 (3) |
| H14B | 1.0745 | 0.2423 | 0.2958 | 0.145* | 0.56 (3) |
| H14C | 0.9052 | 0.2789 | 0.2328 | 0.145* | 0.56 (3) |
| H14D | 0.9904 | 0.2847 | 0.2906 | 0.145* | 0.44 (3) |
| H14E | 0.9042 | 0.2305 | 0.1802 | 0.145* | 0.44 (3) |
| H14F | 1.0735 | 0.1939 | 0.2432 | 0.145* | 0.44 (3) |
| C15 | 0.8030 (3) | −0.09032 (13) | 0.4133 (3) | 0.1179 (10) | |
| H15A | 0.771 | −0.1159 | 0.4884 | 0.177* | 0.67 (3) |
| H15B | 0.9157 | −0.1092 | 0.4002 | 0.177* | 0.67 (3) |
| H15C | 0.7279 | −0.1128 | 0.3484 | 0.177* | 0.67 (3) |
| H15D | 0.8387 | −0.1094 | 0.3362 | 0.177* | 0.33 (3) |
| H15E | 0.6941 | −0.1161 | 0.4244 | 0.177* | 0.33 (3) |
| H15F | 0.8818 | −0.1124 | 0.4762 | 0.177* | 0.33 (3) |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0729 (7) | 0.0412 (5) | 0.0751 (7) | 0.0067 (5) | −0.0183 (5) | −0.0071 (5) |
| O2 | 0.0873 (8) | 0.0582 (7) | 0.0878 (8) | 0.0055 (6) | −0.0314 (7) | −0.0134 (6) |
| C1 | 0.0571 (8) | 0.0488 (8) | 0.0553 (8) | 0.0039 (6) | −0.0018 (7) | −0.0026 (6) |
| C2 | 0.0542 (8) | 0.0450 (7) | 0.0601 (8) | 0.0017 (6) | 0.0072 (6) | 0.0017 (6) |
| C3 | 0.0791 (11) | 0.0585 (10) | 0.0857 (12) | 0.0119 (8) | −0.0066 (9) | 0.0087 (8) |
| C4 | 0.0900 (14) | 0.0574 (11) | 0.1237 (17) | 0.0170 (10) | 0.0124 (13) | 0.0235 (11) |
| C5 | 0.0875 (13) | 0.0391 (9) | 0.151 (2) | −0.0004 (9) | 0.0357 (14) | 0.0035 (11) |
| C6 | 0.1008 (15) | 0.0578 (11) | 0.1305 (18) | −0.0126 (10) | −0.0065 (13) | −0.0219 (11) |
| C7 | 0.0802 (11) | 0.0480 (9) | 0.0906 (12) | −0.0014 (8) | −0.0120 (9) | −0.0058 (8) |
| C8 | 0.0599 (9) | 0.0420 (7) | 0.0614 (9) | 0.0049 (6) | −0.0113 (7) | −0.0057 (6) |
| C9 | 0.0636 (9) | 0.0620 (9) | 0.0598 (9) | 0.0067 (7) | −0.0077 (7) | −0.0058 (7) |
| C10 | 0.0728 (11) | 0.0665 (10) | 0.0775 (11) | 0.0210 (8) | −0.0152 (8) | −0.0246 (8) |
| C11 | 0.0760 (11) | 0.0466 (9) | 0.0998 (13) | 0.0052 (7) | −0.0321 (9) | −0.0061 (8) |
| C12 | 0.0782 (12) | 0.0592 (10) | 0.0962 (13) | −0.0084 (8) | −0.0077 (9) | 0.0118 (9) |
| C13 | 0.0691 (10) | 0.0601 (10) | 0.0752 (11) | 0.0040 (8) | 0.0039 (8) | −0.0023 (8) |
| C14 | 0.1010 (15) | 0.1049 (16) | 0.0852 (13) | 0.0047 (12) | 0.0189 (11) | 0.0038 (12) |
| C15 | 0.1271 (19) | 0.0463 (10) | 0.170 (2) | 0.0118 (10) | −0.0637 (18) | −0.0131 (12) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| O1—C1 | 1.3519 (17) | C10—C11 | 1.374 (3) |
| O1—C8 | 1.4108 (17) | C10—H10 | 0.93 |
| O2—C1 | 1.1913 (17) | C11—C12 | 1.359 (3) |
| C1—C2 | 1.476 (2) | C11—C15 | 1.514 (2) |

| | | | |
|---|---|---|---|
| C2—C7 | 1.371 (2) | C12—C13 | 1.380 (2) |
| C2—C3 | 1.376 (2) | C12—H12 | 0.93 |
| C3—C4 | 1.373 (3) | C13—H13 | 0.93 |
| C3—H3 | 0.93 | C14—H14A | 0.96 |
| C4—C5 | 1.339 (3) | C14—H14B | 0.96 |
| C4—H4 | 0.93 | C14—H14C | 0.96 |
| C5—C6 | 1.367 (3) | C14—H14D | 0.96 |
| C5—H5 | 0.93 | C14—H14E | 0.96 |
| C6—C7 | 1.379 (3) | C14—H14F | 0.96 |
| C6—H6 | 0.93 | C15—H15A | 0.96 |
| C7—H7 | 0.93 | C15—H15B | 0.96 |
| C8—C13 | 1.365 (2) | C15—H15C | 0.96 |
| C8—C9 | 1.376 (2) | C15—H15D | 0.96 |
| C9—C10 | 1.401 (2) | C15—H15E | 0.96 |
| C9—C14 | 1.494 (3) | C15—H15F | 0.96 |
| C1—O1—C8 | 117.59 (11) | C9—C14—H14B | 109.5 |
| O2—C1—O1 | 122.74 (14) | H14A—C14—H14B | 109.5 |
| O2—C1—C2 | 125.32 (14) | C9—C14—H14C | 109.5 |
| O1—C1—C2 | 111.93 (12) | H14A—C14—H14C | 109.5 |
| C7—C2—C3 | 118.87 (15) | H14B—C14—H14C | 109.5 |
| C7—C2—C1 | 122.47 (14) | C9—C14—H14D | 109.5 |
| C3—C2—C1 | 118.65 (14) | H14A—C14—H14D | 141.1 |
| C4—C3—C2 | 120.70 (19) | H14B—C14—H14D | 56.3 |
| C4—C3—H3 | 119.7 | H14C—C14—H14D | 56.3 |
| C2—C3—H3 | 119.7 | C9—C14—H14E | 109.5 |
| C5—C4—C3 | 120.17 (19) | H14A—C14—H14E | 56.3 |
| C5—C4—H4 | 119.9 | H14B—C14—H14E | 141.1 |
| C3—C4—H4 | 119.9 | H14C—C14—H14E | 56.3 |
| C4—C5—C6 | 120.23 (17) | H14D—C14—H14E | 109.5 |
| C4—C5—H5 | 119.9 | C9—C14—H14F | 109.5 |
| C6—C5—H5 | 119.9 | H14A—C14—H14F | 56.3 |
| C5—C6—C7 | 120.4 (2) | H14B—C14—H14F | 56.3 |
| C5—C6—H6 | 119.8 | H14C—C14—H14F | 141.1 |
| C7—C6—H6 | 119.8 | H14D—C14—H14F | 109.5 |
| C2—C7—C6 | 119.64 (18) | H14E—C14—H14F | 109.5 |
| C2—C7—H7 | 120.2 | C11—C15—H15A | 109.5 |
| C6—C7—H7 | 120.2 | C11—C15—H15B | 109.5 |
| C13—C8—C9 | 122.33 (15) | H15A—C15—H15B | 109.5 |
| C13—C8—O1 | 117.84 (14) | C11—C15—H15C | 109.5 |
| C9—C8—O1 | 119.64 (14) | H15A—C15—H15C | 109.5 |
| C8—C9—C10 | 116.07 (16) | H15B—C15—H15C | 109.5 |
| C8—C9—C14 | 121.84 (16) | C11—C15—H15D | 109.5 |
| C10—C9—C14 | 122.09 (17) | H15A—C15—H15D | 141.1 |
| C11—C10—C9 | 122.86 (16) | H15B—C15—H15D | 56.3 |
| C11—C10—H10 | 118.6 | H15C—C15—H15D | 56.3 |
| C9—C10—H10 | 118.6 | C11—C15—H15E | 109.5 |
| C12—C11—C10 | 118.26 (16) | H15A—C15—H15E | 56.3 |
| C12—C11—C15 | 121.0 (2) | H15B—C15—H15E | 141.1 |
| C10—C11—C15 | 120.7 (2) | H15C—C15—H15E | 56.3 |

| | | | |
|---|---|---|---|
| C11—C12—C13 | 121.14 (18) | H15D—C15—H15E | 109.5 |
| C11—C12—H12 | 119.4 | C11—C15—H15F | 109.5 |
| C13—C12—H12 | 119.4 | H15A—C15—H15F | 56.3 |
| C8—C13—C12 | 119.34 (17) | H15B—C15—H15F | 56.3 |
| C8—C13—H13 | 120.3 | H15C—C15—H15F | 141.1 |
| C12—C13—H13 | 120.3 | H15D—C15—H15F | 109.5 |
| C9—C14—H14A | 109.5 | H15E—C15—H15F | 109.5 |
| C8—O1—C1—O2 | −1.4 (2) | C1—O1—C8—C9 | 89.23 (17) |
| C8—O1—C1—C2 | 179.25 (12) | C13—C8—C9—C10 | 1.2 (2) |
| O2—C1—C2—C7 | 174.36 (17) | O1—C8—C9—C10 | 176.08 (13) |
| O1—C1—C2—C7 | −6.4 (2) | C13—C8—C9—C14 | −177.81 (16) |
| O2—C1—C2—C3 | −4.7 (2) | O1—C8—C9—C14 | −2.9 (2) |
| O1—C1—C2—C3 | 174.61 (14) | C8—C9—C10—C11 | −0.7 (2) |
| C7—C2—C3—C4 | 0.9 (3) | C14—C9—C10—C11 | 178.30 (17) |
| C1—C2—C3—C4 | −179.98 (17) | C9—C10—C11—C12 | −0.3 (3) |
| C2—C3—C4—C5 | −0.6 (3) | C9—C10—C11—C15 | 179.91 (16) |
| C3—C4—C5—C6 | −0.1 (3) | C10—C11—C12—C13 | 0.9 (3) |
| C4—C5—C6—C7 | 0.5 (3) | C15—C11—C12—C13 | −179.29 (17) |
| C3—C2—C7—C6 | −0.5 (3) | C9—C8—C13—C12 | −0.7 (2) |
| C1—C2—C7—C6 | −179.57 (18) | O1—C8—C13—C12 | −175.61 (14) |
| C5—C6—C7—C2 | −0.2 (3) | C11—C12—C13—C8 | −0.5 (3) |
| C1—O1—C8—C13 | −95.67 (17) | | |

**Fig. 1**

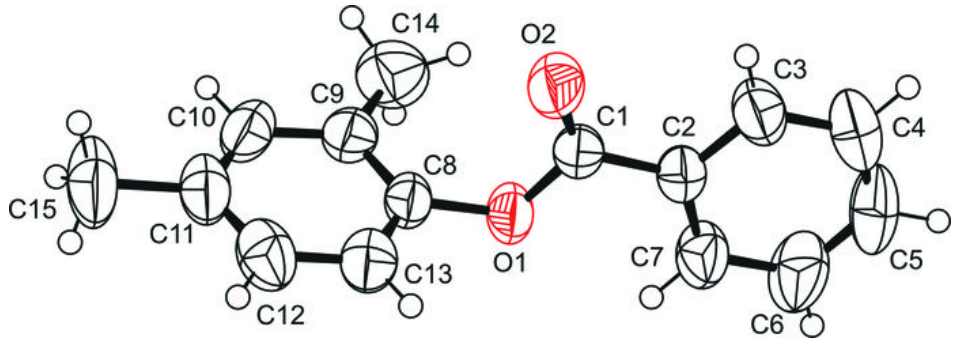

**Fig. 2**