

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

Phenyl 4-methylbenzoate

B. Thimme Gowda,^{a*} Miroslav Tokarčík,^b Jozef Kožíšek,^b
P. A. Suchetan^a and Hartmut Fuess^c^aDepartment of Chemistry, Mangalore University, Mangalagangotri 574 199, Mangalore, India, ^bFaculty of Chemical and Food Technology, Slovak Technical University, Radlinského 9, SK-812 37 Bratislava, Slovak Republic, and ^cInstitute of Materials Science, Darmstadt University of Technology, Petersenstrasse 23, D-64287 Darmstadt, Germany

Correspondence e-mail: gowdabt@yahoo.com

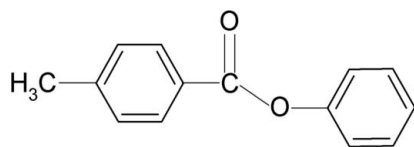
Received 15 September 2009; accepted 28 September 2009

Key indicators: single-crystal X-ray study; $T = 295$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.046; wR factor = 0.145; data-to-parameter ratio = 14.6.

The structure of the title compound, $\text{C}_{14}\text{H}_{12}\text{O}_2$, resembles those of phenyl benzoate and 4-methylphenyl benzoate, with similar bond parameters. The two aromatic rings make a dihedral angle of $76.0(1)^\circ$. The plane of the central $-\text{C}(=\text{O})-\text{O}-$ group is twisted by $9.4(2)^\circ$ out of the plane of the benzoyl ring, and by $83.3(1)^\circ$ out of the plane of the phenyl ring. The crystal structure exhibits weak parallel stacking of the benzoyl rings, with an interplanar distance of 3.65 Å and an offset of 1.84 Å. The methyl group shows orientational disorder.

Related literature

For preparation of the compound, see: Nayak & Gowda (2009). For background to our study of the effects of substituents on the crystal structures of aryl benzoates and for related structures, see: Gowda *et al.* (2007*a,b*, 2008). For phenyl benzoate, see: Adams & Morsi (1976);



Experimental

Crystal data

$\text{C}_{14}\text{H}_{12}\text{O}_2$
 $M_r = 212.24$
 Monoclinic, $P2_1/c$
 $a = 12.3440(4)$ Å
 $b = 8.1332(2)$ Å
 $c = 12.1545(4)$ Å
 $\beta = 110.911(4)^\circ$

$V = 1139.89(6)$ Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.08$ mm⁻¹
 $T = 295$ K
 $0.52 \times 0.46 \times 0.32$ mm

Data collection

Oxford Diffraction Xcalibur diffractometer with a Ruby (Gemini Mo) detector
 Absorption correction: multi-scan (*CrysAlis RED*; Oxford)

Diffraction, 2009
 $T_{\min} = 0.96$, $T_{\max} = 0.98$
 20946 measured reflections
 2138 independent reflections
 1468 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.027$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.046$
 $wR(F^2) = 0.145$
 $S = 1.03$
 2138 reflections

146 parameters
 H-atom parameters constrained
 $\Delta\rho_{\max} = 0.23$ e Å⁻³
 $\Delta\rho_{\min} = -0.16$ e Å⁻³

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2009); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2009); 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, 2009) and *WinGX* (Farrugia, 1999).

MT and JK thank the Grant Agency of the Slovak Republic (VEGA 1/0817/08) and 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: OM2279).

References

- Adams, J. M. & Morsi, S. E. (1976). *Acta Cryst.* **B32**, 1345–1347.
 Brandenburg, K. (2002). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
 Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
 Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
 Gowda, B. T., Foro, S., Babitha, K. S. & Fuess, H. (2007*a*). *Acta Cryst.* **E63**, o3867.
 Gowda, B. T., Foro, S., Babitha, K. S. & Fuess, H. (2008). *Acta Cryst.* **E64**, o1581.
 Gowda, B. T., Foro, S., Nayak, R. & Fuess, H. (2007*b*). *Acta Cryst.* **E63**, o3563.
 Nayak, R. & Gowda, B. T. (2009). *Z. Naturforsch. Teil A*, **63**. In preparation.
 Oxford Diffraction (2009). *CrysAlis CCD* and *CrysAlis RED*. Oxford Diffraction Ltd, Yarnton, England.
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
 Spek, A. L. (2009). *Acta Cryst.* **D65**, 148–155.

supporting information

Acta Cryst. (2009). E65, o2620 [https://doi.org/10.1107/S1600536809039361]

Phenyl 4-methylbenzoate

B. Thimme Gowda, Miroslav Tokarčík, Jozef Kožíšek, P. A. Suchetan and Hartmut Fues

S1. Comment

In the present work, as a part of the study of the substituent effects on the crystal structures of aryl benzoates (Gowda *et al.*, 2007*a, b*; 2008), the structure of phenyl-4-methylbenzoate (I) has been determined. The structure of (I) (Fig. 1) is similar to those of phenyl benzoate (II) (Adams & Morsi, 1976), 4-methylphenyl benzoate (III) (Gowda *et al.*, 2007*b*), 4-methylphenyl 2-methylbenzoate (IV) (Gowda *et al.*, 2008), 4-methylphenyl 4-methylbenzoate (V) (Gowda *et al.*, 2007*a*) and other aryl benzoates. The two benzene rings make a dihedral angle of 76.0 (1)°, compared to the values of 55.7° for (II), 60.17 (7)° (III), 73.04 (8)° (IV) and 63.57 (5)° (V). The plane of the central –C(=O)–O– group in (I) is twisted 9.4 (2)° out of the plane of the benzoyl ring, and 83.3 (1)° out of the plane of the phenyl ring. The crystal structure exhibits weak parallel stacking of benzoyl rings, with interplanar distance of 3.65 Å and offset 1.84 Å. In the crystal structure, there are no classical hydrogen bonds. The molecules in the structure are packed into chains as viewed in the *ac* plane (Fig. 2).

S2. Experimental

The title compound was prepared according to a literature method (Nayak & Gowda, 2009). The purity of the compound was checked by determination of its melting point. It was characterized by infrared and NMR spectra (Nayak & Gowda, 2009). Colorless single crystals of the title compound were obtained by slow evaporation of its ethanol solution.

S3. Refinement

All hydrogen atoms were placed in calculated positions with C–H distances 0.93 or 0.96 Å. The C14 methyl group shows orientational disorder in the hydrogen atom positions. The two sets of methyl hydrogen atoms were refined with equal occupancy. The $U_{\text{iso}}(\text{H})$ values were set at 1.2 $U_{\text{eq}}(\text{C-aromatic})$ or 1.5 $U_{\text{eq}}(\text{C-methyl})$.

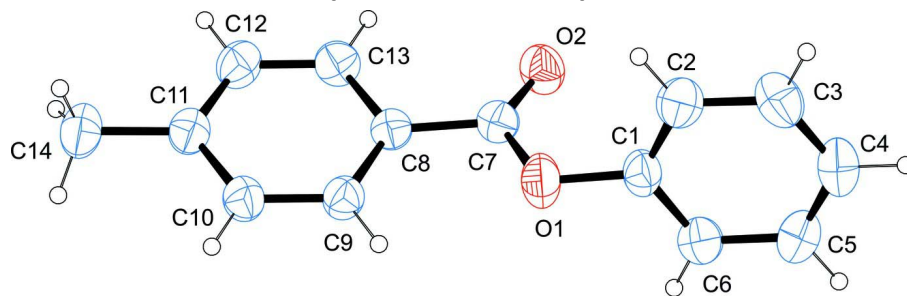


Figure 1

Molecular structure of the title compound showing the atom labelling scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are represented as small spheres of arbitrary radii.

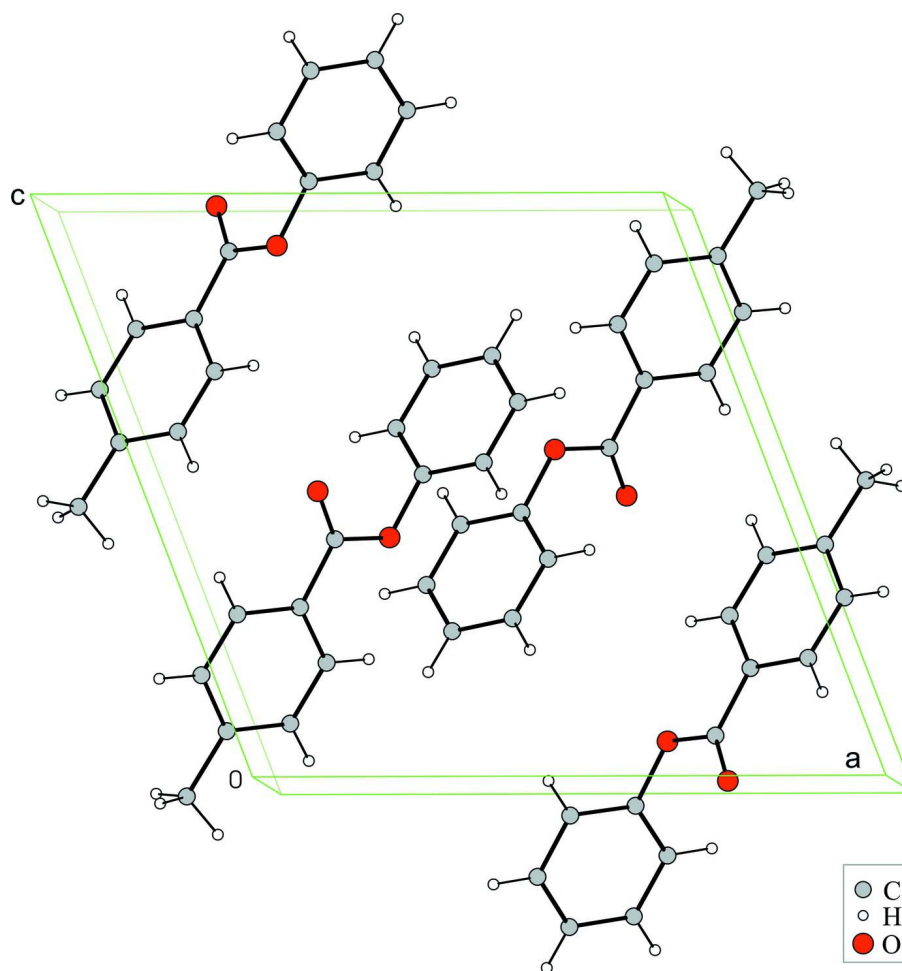


Figure 2
Molecular packing of the title compound.

Phenyl 4-methylbenzoate

Crystal data

$C_{14}H_{12}O_2$

$M_r = 212.24$

Monoclinic, $P2_1/c$

Hall symbol: $-P\ 2_1/c$

$a = 12.3440\ (4)\ \text{\AA}$

$b = 8.1332\ (2)\ \text{\AA}$

$c = 12.1545\ (4)\ \text{\AA}$

$\beta = 110.911\ (4)^\circ$

$V = 1139.89\ (6)\ \text{\AA}^3$

$Z = 4$

$F(000) = 448$

$D_x = 1.237\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 9248 reflections

$\theta = 3.1\text{--}29.3^\circ$

$\mu = 0.08\ \text{mm}^{-1}$

$T = 295\ \text{K}$

Block, colourless

$0.52 \times 0.46 \times 0.32\ \text{mm}$

Data collection

Oxford Diffraction Xcalibur
diffractometer with a Ruby (Gemini Mo)
detector

Graphite monochromator

Detector resolution: $10.434\ \text{pixels mm}^{-1}$

ω scans

Absorption correction: multi-scan

(*CrysAlis RED*; Oxford Diffraction, 2009)

$T_{\min} = 0.96$, $T_{\max} = 0.98$

20946 measured reflections

2138 independent reflections
 1468 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.027$
 $\theta_{\text{max}} = 25.6^\circ$, $\theta_{\text{min}} = 3.1^\circ$

$h = -15 \rightarrow 15$
 $k = -9 \rightarrow 9$
 $l = -14 \rightarrow 14$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.046$
 $wR(F^2) = 0.145$
 $S = 1.03$
 2138 reflections
 146 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
 $w = 1/[\sigma^2(F_o^2) + (0.0889P)^2 + 0.0575P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.23 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.16 \text{ e } \text{\AA}^{-3}$

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
C1	0.44050 (14)	0.7055 (2)	0.52718 (13)	0.0649 (4)	
C2	0.42337 (16)	0.6054 (2)	0.60914 (16)	0.0826 (5)	
H2	0.3509	0.559	0.5955	0.099*	
C3	0.51407 (17)	0.5731 (2)	0.71233 (15)	0.0847 (6)	
H3	0.503	0.5045	0.7686	0.102*	
C4	0.61978 (16)	0.6415 (2)	0.73202 (15)	0.0809 (5)	
H4	0.681	0.6201	0.8019	0.097*	
C5	0.63602 (14)	0.7415 (2)	0.64933 (16)	0.0792 (5)	
H5	0.7085	0.7882	0.6634	0.095*	
C6	0.54637 (15)	0.7745 (2)	0.54505 (15)	0.0737 (5)	
H6	0.5577	0.8419	0.4883	0.088*	
C7	0.26747 (13)	0.84141 (18)	0.41132 (13)	0.0602 (4)	
C8	0.17152 (12)	0.83643 (17)	0.29559 (12)	0.0558 (4)	
C9	0.17601 (13)	0.74161 (18)	0.20301 (13)	0.0629 (4)	
H9	0.2427	0.6822	0.2108	0.075*	
C10	0.08196 (13)	0.73479 (19)	0.09922 (14)	0.0660 (4)	
H10	0.0868	0.6716	0.0374	0.079*	
C11	-0.01947 (13)	0.81929 (18)	0.08448 (13)	0.0633 (4)	
C12	-0.02227 (14)	0.9156 (2)	0.17716 (15)	0.0718 (5)	
H12	-0.0889	0.9754	0.1691	0.086*	
C13	0.07132 (14)	0.92496 (18)	0.28101 (14)	0.0679 (4)	

H13	0.0674	0.9911	0.3419	0.082*	
C14	-0.12267 (15)	0.8048 (2)	-0.02748 (15)	0.0835 (5)	
H14A	-0.1656	0.906	-0.042	0.125*	0.5
H14B	-0.1715	0.7167	-0.0203	0.125*	0.5
H14C	-0.097	0.7825	-0.0918	0.125*	0.5
H14D	-0.1924	0.8088	-0.0098	0.125*	0.5
H14E	-0.1192	0.7023	-0.0652	0.125*	0.5
H14F	-0.1224	0.8941	-0.0791	0.125*	0.5
O1	0.35063 (10)	0.72961 (15)	0.41782 (10)	0.0865 (4)	
O2	0.27223 (9)	0.92969 (13)	0.49154 (9)	0.0758 (4)	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0612 (9)	0.0712 (10)	0.0534 (8)	0.0089 (8)	0.0095 (7)	-0.0108 (7)
C2	0.0734 (11)	0.0913 (12)	0.0790 (11)	-0.0181 (9)	0.0221 (9)	-0.0136 (10)
C3	0.1043 (15)	0.0767 (11)	0.0670 (11)	-0.0104 (10)	0.0230 (10)	0.0040 (8)
C4	0.0817 (12)	0.0714 (10)	0.0689 (11)	0.0066 (9)	0.0016 (9)	-0.0025 (8)
C5	0.0599 (10)	0.0815 (12)	0.0842 (12)	-0.0029 (8)	0.0110 (9)	-0.0022 (9)
C6	0.0729 (11)	0.0763 (11)	0.0705 (10)	0.0036 (9)	0.0238 (9)	0.0047 (8)
C7	0.0624 (9)	0.0576 (8)	0.0608 (9)	-0.0016 (7)	0.0222 (7)	-0.0014 (7)
C8	0.0562 (8)	0.0526 (8)	0.0581 (8)	-0.0029 (6)	0.0198 (7)	0.0001 (6)
C9	0.0572 (9)	0.0656 (9)	0.0629 (9)	0.0044 (7)	0.0178 (7)	-0.0038 (7)
C10	0.0642 (10)	0.0704 (10)	0.0597 (9)	-0.0018 (8)	0.0176 (8)	-0.0059 (7)
C11	0.0589 (9)	0.0602 (9)	0.0651 (9)	-0.0043 (7)	0.0153 (7)	0.0109 (7)
C12	0.0622 (10)	0.0683 (10)	0.0806 (11)	0.0143 (8)	0.0204 (8)	0.0094 (8)
C13	0.0733 (10)	0.0615 (9)	0.0697 (10)	0.0077 (8)	0.0264 (8)	-0.0012 (7)
C14	0.0669 (10)	0.0899 (12)	0.0778 (11)	-0.0072 (9)	0.0063 (9)	0.0131 (9)
O1	0.0739 (8)	0.1056 (9)	0.0623 (7)	0.0271 (7)	0.0024 (6)	-0.0195 (6)
O2	0.0821 (8)	0.0734 (7)	0.0660 (7)	0.0022 (6)	0.0193 (6)	-0.0148 (5)

Geometric parameters (Å, °)

C1—C2	1.361 (2)	C8—C13	1.387 (2)
C1—C6	1.366 (2)	C9—C10	1.377 (2)
C1—O1	1.4082 (18)	C9—H9	0.93
C2—C3	1.376 (2)	C10—C11	1.383 (2)
C2—H2	0.93	C10—H10	0.93
C3—C4	1.359 (2)	C11—C12	1.383 (2)
C3—H3	0.93	C11—C14	1.500 (2)
C4—C5	1.362 (2)	C12—C13	1.376 (2)
C4—H4	0.93	C12—H12	0.93
C5—C6	1.379 (2)	C13—H13	0.93
C5—H5	0.93	C14—H14A	0.96
C6—H6	0.93	C14—H14B	0.96
C7—O2	1.1954 (16)	C14—H14C	0.96
C7—O1	1.3524 (18)	C14—H14D	0.96
C7—C8	1.481 (2)	C14—H14E	0.96

C8—C9	1.381 (2)	C14—H14F	0.96
C2—C1—C6	121.27 (15)	C8—C9—H9	119.9
C2—C1—O1	119.90 (15)	C9—C10—C11	121.80 (14)
C6—C1—O1	118.65 (15)	C9—C10—H10	119.1
C1—C2—C3	119.54 (17)	C11—C10—H10	119.1
C1—C2—H2	120.2	C12—C11—C10	117.44 (14)
C3—C2—H2	120.2	C12—C11—C14	121.56 (15)
C4—C3—C2	120.02 (17)	C10—C11—C14	121.00 (15)
C4—C3—H3	120	C13—C12—C11	121.45 (15)
C2—C3—H3	120	C13—C12—H12	119.3
C3—C4—C5	119.96 (16)	C11—C12—H12	119.3
C3—C4—H4	120	C12—C13—C8	120.48 (15)
C5—C4—H4	120	C12—C13—H13	119.8
C4—C5—C6	120.86 (17)	C8—C13—H13	119.8
C4—C5—H5	119.6	C11—C14—H14A	109.5
C6—C5—H5	119.6	C11—C14—H14B	109.5
C1—C6—C5	118.34 (16)	H14A—C14—H14B	109.5
C1—C6—H6	120.8	C11—C14—H14C	109.5
C5—C6—H6	120.8	H14A—C14—H14C	109.5
O2—C7—O1	122.75 (13)	H14B—C14—H14C	109.5
O2—C7—C8	125.51 (14)	C11—C14—H14D	109.5
O1—C7—C8	111.72 (12)	C11—C14—H14E	109.5
C9—C8—C13	118.62 (14)	H14D—C14—H14E	109.5
C9—C8—C7	122.54 (13)	C11—C14—H14F	109.5
C13—C8—C7	118.79 (13)	H14D—C14—H14F	109.5
C10—C9—C8	120.18 (14)	H14E—C14—H14F	109.5
C10—C9—H9	119.9	C7—O1—C1	118.32 (11)
C6—C1—C2—C3	0.3 (3)	C7—C8—C9—C10	176.63 (14)
O1—C1—C2—C3	175.36 (15)	C8—C9—C10—C11	-0.9 (2)
C1—C2—C3—C4	0.2 (3)	C9—C10—C11—C12	1.8 (2)
C2—C3—C4—C5	-0.3 (3)	C9—C10—C11—C14	-177.47 (14)
C3—C4—C5—C6	-0.1 (3)	C10—C11—C12—C13	-1.2 (2)
C2—C1—C6—C5	-0.7 (3)	C14—C11—C12—C13	178.09 (15)
O1—C1—C6—C5	-175.82 (14)	C11—C12—C13—C8	-0.3 (2)
C4—C5—C6—C1	0.6 (3)	C9—C8—C13—C12	1.3 (2)
O2—C7—C8—C9	174.22 (14)	C7—C8—C13—C12	-176.12 (14)
O1—C7—C8—C9	-7.1 (2)	O2—C7—O1—C1	6.3 (2)
O2—C7—C8—C13	-8.5 (2)	C8—C7—O1—C1	-172.34 (13)
O1—C7—C8—C13	170.12 (13)	C2—C1—O1—C7	82.15 (19)
C13—C8—C9—C10	-0.6 (2)	C6—C1—O1—C7	-102.63 (18)