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4-Methylphenyl benzoate

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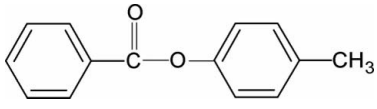
Key indicators: single-crystal X-ray study; T = 299 K; mean σ(C–C) = 0.002 Å; R factor = 0.049; wR factor = 0.142; data-to-parameter ratio = 12.0.

The structure of the title compound (4MePBA), $C_{14}H_{12}O_2$, resembles those of phenyl benzoate (PBA) and 4-methoxyphenyl benzoate (4MeOPBA), with similar geometric parameters. The dihedral angle between the phenyl and benzene rings in 4MePBA is 60.17 (7)°, compared with the values of 55.7° for PBA and 56.42 (3)° for 4MeOPBA. The molecules in the title compound are packed with the methylphenyl rings parallel to the *bc* plane and the benzoyl rings perpendicular to this plane.

Related literature

For related literature, see: Adams & Morsi (1976); Gowda, Foro *et al.* (2007); Gowda, Kožíšek, Svoboda & Fuess (2007); Gowda, Kožíšek, Tokarčík & Fuess (2007); Gowda, Nayak *et al.* (2007); Gowda, Svoboda & Fuess (2007); Gowda, Tokarčík *et al.* (2007); Nayak & Gowda (2007).



Experimental

Crystal data

$C_{14}H_{12}O_2$
M_r = 212.24
Triclinic, $P\overline{1}$
a = 8.1488 (9) Å
b = 9.052 (1) Å
c = 9.299 (1) Å
α = 76.99 (2)°
β = 68.73 (1)°
γ = 66.87 (1)°
V = 585.08 (11) Å^3
Z = 2
Cu $K\alpha$ radiation
μ = 0.64 mm^{-1}
T = 299 (2) K
0.60 × 0.48 × 0.40 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.671, T_{max} = 0.773
3995 measured reflections
2082 independent reflections
1903 reflections with $I > 2\sigma(I)$
R_{int} = 0.049
3 standard reflections
frequency: 120 min
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.142
S = 1.06
2082 reflections
174 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

Data collection: *CAD-4-PC Software* (Enraf–Nonius, 1996); cell refinement: *CAD-4-PC Software*; data reduction: *REDU4* (Stoe & Cie, 1987); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WN2173).

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supplementary materials

Acta Cryst. (2007). E**63**, o3563 [**doi:10.1107/S1600536807034848**]

4-Methylphenyl benzoate

B. T. Gowda, S. Foro, R. Nayak and H. Fuess

Comment

In the present work, as part of a study of substituent effects on the solid state structures of chemically and industrially significant compounds (Gowda, Foro *et al.*, 2007; Gowda, Kožíšek, Svoboda & Fuess, 2007; Gowda, Kožíšek, Tokarčík & Fuess, 2007; Gowda, Nayak *et al.*, 2007; Gowda, Svoboda & Fuess, 2007; Gowda, Tokarčík *et al.*, 2007) the structure of 4-methylphenyl benzoate (4MePBA) has been determined. The structure of 4MePBA (Fig. 1) is similar to that of phenyl benzoate (PBA) (Adams & Morsi, 1976) and 4-methoxylphenyl benzoate (4MeOPBA) (Gowda, Foro *et al.*, 2007). The bond parameters in 4MePBA are similar to those in PBA and other benzoates. The molecules in the title compound are packed with the methylphenyl rings parallel to the *bc* plane and the benzoyl rings perpendicular to this plane (Fig. 2).

Experimental

The title compound was prepared according to a literature method (Nayak & Gowda, 2007). The purity of the compound was checked by determining its melting point. It was characterized by recording its infrared and NMR spectra (Nayak & Gowda, 2007). 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

The methyl H atoms were positioned with idealized geometry and refined using a riding model, with C—H = 0.96 Å. All other H atoms were located in a difference map and their positions refined freely [C—H = 0.93 (2)–1.01 (2) Å]. U_{iso}(H) values were set equal to 1.2U_{eq} of the parent atom.

Figures

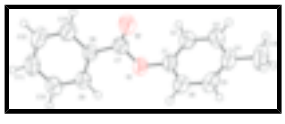

Fig. 1. Molecular structure of the title compound, showing the atom labeling. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented as small spheres of arbitrary radius.

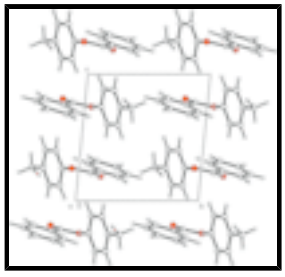

Fig. 2. Molecular packing of the title compound.

4-Methylphenyl benzoate

Crystal data

$C_{14}H_{12}O_2$	$Z = 2$
$M_r = 212.24$	$F_{000} = 224$
Triclinic, $P\overline{1}$	$D_x = 1.205$ Mg m^{-3}
Hall symbol: -P 1	Cu $K\alpha$ radiation $\lambda = 1.54180$ Å
$a = 8.1488$ (9) Å	Cell parameters from 25 reflections
$b = 9.052$ (1) Å	$\theta = 6.2$–25.2º
$c = 9.299$ (1) Å	$\mu = 0.64$ mm^{-1}
$\alpha = 76.99$ (2)º	$T = 299$ (2) K
$\beta = 68.73$ (1)º	Prism, colourless
$\gamma = 66.87$ (1)º	0.60 × 0.48 × 0.40 mm
$V = 585.08$ (11) Å^3	

Data collection

Enraf–Nonius CAD-4 diffractometer	$R_{int} = 0.049$
Radiation source: fine-focus sealed tube	$\theta_{max} = 66.9$º
Monochromator: graphite	$\theta_{min} = 5.1$º
$T = 299(2)$ K	$h = -9 \rightarrow 8$
$\omega/2\theta$ scans	$k = -10 \rightarrow 10$
Absorption correction: ψ scan (North *et al.*, 1968)	$l = -11 \rightarrow 11$
$T_{min} = 0.671$, $T_{max} = 0.773$	3 standard reflections
3995 measured reflections	every 120 min
2082 independent reflections	intensity decay: none
1903 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.049$	$w = 1/[\sigma^2(F_o^2) + (0.0629P)^2 + 0.0783P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.142$	$(\Delta/\sigma)_{max} = 0.003$
$S = 1.06$	$\Delta\rho_{max} = 0.15$ e Å^{-3}
2082 reflections	$\Delta\rho_{min} = -0.24$ e Å^{-3}
174 parameters	Extinction correction: SHELXL97, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.173 (9)

Secondary atom site location: difference Fourier map

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 $F^2 > 2\text{sigma}(F^2)$ 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}
C1	0.31783 (19)	0.13239 (16)	0.74315 (17)	0.0559 (4)
C2	0.3400 (2)	0.14401 (19)	0.87892 (18)	0.0641 (4)
H2	0.275 (2)	0.092 (2)	0.978 (2)	0.077*
C3	0.4548 (2)	0.2249 (2)	0.8743 (2)	0.0678 (5)
H3	0.476 (3)	0.230 (2)	0.965 (2)	0.081*
C4	0.5471 (2)	0.29397 (17)	0.7360 (2)	0.0664 (5)
C5	0.5191 (2)	0.28167 (19)	0.6023 (2)	0.0714 (5)
H5	0.591 (3)	0.328 (2)	0.501 (2)	0.086*
C6	0.4059 (2)	0.20075 (19)	0.60421 (19)	0.0657 (4)
H6	0.385 (2)	0.197 (2)	0.512 (2)	0.079*
C7	0.24839 (19)	−0.10521 (17)	0.77574 (17)	0.0554 (4)
C8	0.11334 (17)	−0.16976 (16)	0.76323 (15)	0.0513 (4)
C9	−0.0320 (2)	−0.07552 (19)	0.70380 (18)	0.0586 (4)
H9	−0.051 (2)	0.035 (2)	0.6694 (19)	0.070*
C10	−0.1494 (2)	−0.1426 (2)	0.6884 (2)	0.0717 (5)
H10	−0.259 (3)	−0.071 (2)	0.651 (2)	0.086*
C11	−0.1205 (3)	−0.3043 (2)	0.7315 (2)	0.0759 (5)
H11	−0.202 (3)	−0.347 (2)	0.718 (2)	0.091*
C12	0.0232 (3)	−0.3988 (2)	0.7912 (2)	0.0769 (5)
H12	0.049 (3)	−0.513 (3)	0.821 (2)	0.092*
C13	0.1401 (2)	−0.33226 (19)	0.8085 (2)	0.0665 (4)
H13	0.241 (3)	−0.397 (2)	0.852 (2)	0.080*
C14	0.6715 (3)	0.3822 (2)	0.7336 (3)	0.0987 (7)
H14A	0.7406	0.3255	0.8056	0.118*
H14B	0.5957	0.4894	0.7624	0.118*
H14C	0.7573	0.3878	0.6311	0.118*
O1	0.19668 (14)	0.05681 (12)	0.74249 (14)	0.0658 (4)
O2	0.39043 (16)	−0.18510 (13)	0.80612 (16)	0.0797 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0542 (8)	0.0488 (8)	0.0726 (9)	−0.0214 (6)	−0.0256 (6)	−0.0032 (6)
C2	0.0688 (9)	0.0665 (10)	0.0645 (9)	−0.0329 (8)	−0.0210 (7)	−0.0014 (7)
C3	0.0751 (10)	0.0653 (10)	0.0781 (10)	−0.0277 (8)	−0.0346 (8)	−0.0101 (8)
C4	0.0583 (8)	0.0481 (8)	0.0975 (12)	−0.0215 (7)	−0.0233 (8)	−0.0108 (7)
C5	0.0809 (11)	0.0580 (9)	0.0749 (10)	−0.0359 (8)	−0.0124 (8)	−0.0026 (7)
C6	0.0837 (11)	0.0579 (9)	0.0645 (9)	−0.0316 (8)	−0.0279 (8)	−0.0004 (7)
C7	0.0514 (7)	0.0518 (8)	0.0671 (9)	−0.0184 (6)	−0.0232 (6)	−0.0034 (6)
C8	0.0475 (7)	0.0504 (8)	0.0579 (8)	−0.0201 (6)	−0.0150 (6)	−0.0042 (6)
C9	0.0587 (8)	0.0540 (8)	0.0702 (9)	−0.0243 (7)	−0.0262 (7)	0.0008 (6)
C10	0.0687 (10)	0.0750 (11)	0.0891 (11)	−0.0327 (8)	−0.0387 (8)	−0.0016 (8)
C11	0.0757 (11)	0.0762 (11)	0.0965 (13)	−0.0438 (9)	−0.0292 (9)	−0.0095 (9)
C12	0.0784 (11)	0.0546 (9)	0.1036 (13)	−0.0337 (8)	−0.0254 (9)	−0.0026 (8)
C13	0.0612 (9)	0.0531 (9)	0.0868 (11)	−0.0214 (7)	−0.0269 (8)	0.0009 (7)
C14	0.0816 (12)	0.0713 (12)	0.161 (2)	−0.0391 (10)	−0.0371 (12)	−0.0209 (12)
O1	0.0635 (6)	0.0525 (6)	0.0964 (8)	−0.0260 (5)	−0.0406 (6)	0.0030 (5)
O2	0.0681 (7)	0.0609 (7)	0.1268 (11)	−0.0191 (5)	−0.0553 (7)	−0.0029 (6)

Geometric parameters (Å, °)

C1—C2	1.370 (2)	C8—C9	1.380 (2)
C1—C6	1.372 (2)	C8—C13	1.387 (2)
C1—O1	1.4070 (16)	C9—C10	1.378 (2)
C2—C3	1.382 (2)	C9—H9	0.947 (18)
C2—H2	0.996 (18)	C10—C11	1.375 (3)
C3—C4	1.384 (2)	C10—H10	1.01 (2)
C3—H3	0.93 (2)	C11—C12	1.372 (3)
C4—C5	1.378 (2)	C11—H11	0.94 (2)
C4—C14	1.509 (2)	C12—C13	1.380 (2)
C5—C6	1.379 (2)	C12—H12	0.97 (2)
C5—H5	1.011 (19)	C13—H13	0.97 (2)
C6—H6	0.940 (19)	C14—H14A	0.9600
C7—O2	1.1958 (17)	C14—H14B	0.9600
C7—O1	1.3524 (17)	C14—H14C	0.9600
C7—C8	1.4814 (18)		
C2—C1—C6	121.18 (14)	C13—C8—C7	117.90 (13)
C2—C1—O1	121.05 (13)	C10—C9—C8	120.23 (15)
C6—C1—O1	117.70 (13)	C10—C9—H9	118.6 (10)
C1—C2—C3	118.91 (15)	C8—C9—H9	121.1 (10)
C1—C2—H2	119.4 (10)	C11—C10—C9	119.77 (16)
C3—C2—H2	121.7 (10)	C11—C10—H10	120.9 (11)
C2—C3—C4	121.39 (15)	C9—C10—H10	119.3 (11)
C2—C3—H3	120.3 (12)	C12—C11—C10	120.43 (15)
C4—C3—H3	118.3 (12)	C12—C11—H11	121.9 (12)
C5—C4—C3	117.96 (14)	C10—C11—H11	117.7 (12)

C5—C4—C14	121.49 (17)	C11—C12—C13	120.19 (16)
C3—C4—C14	120.54 (18)	C11—C12—H12	122.5 (12)
C4—C5—C6	121.57 (15)	C13—C12—H12	117.3 (12)
C4—C5—H5	117.8 (11)	C12—C13—C8	119.63 (16)
C6—C5—H5	120.6 (11)	C12—C13—H13	121.6 (11)
C1—C6—C5	118.99 (15)	C8—C13—H13	118.8 (11)
C1—C6—H6	121.0 (11)	C4—C14—H14A	109.5
C5—C6—H6	120.0 (11)	C4—C14—H14B	109.5
O2—C7—O1	122.91 (13)	H14A—C14—H14B	109.5
O2—C7—C8	125.03 (13)	C4—C14—H14C	109.5
O1—C7—C8	112.01 (11)	H14A—C14—H14C	109.5
C9—C8—C13	119.73 (13)	H14B—C14—H14C	109.5
C9—C8—C7	122.33 (13)	C7—O1—C1	117.67 (10)
C6—C1—C2—C3	−0.6 (2)	O1—C7—C8—C13	−174.01 (13)
O1—C1—C2—C3	−177.45 (13)	C13—C8—C9—C10	−0.5 (2)
C1—C2—C3—C4	0.0 (3)	C7—C8—C9—C10	177.25 (14)
C2—C3—C4—C5	0.9 (2)	C8—C9—C10—C11	−0.4 (3)
C2—C3—C4—C14	179.86 (15)	C9—C10—C11—C12	0.7 (3)
C3—C4—C5—C6	−1.2 (2)	C10—C11—C12—C13	0.0 (3)
C14—C4—C5—C6	179.82 (16)	C11—C12—C13—C8	−0.9 (3)
C2—C1—C6—C5	0.3 (2)	C9—C8—C13—C12	1.2 (3)
O1—C1—C6—C5	177.24 (13)	C7—C8—C13—C12	−176.67 (14)
C4—C5—C6—C1	0.6 (3)	O2—C7—O1—C1	0.5 (2)
O2—C7—C8—C9	−169.30 (15)	C8—C7—O1—C1	−177.13 (11)
O1—C7—C8—C9	8.2 (2)	C2—C1—O1—C7	−70.34 (18)
O2—C7—C8—C13	8.5 (2)	C6—C1—O1—C7	112.73 (16)

Fig. 1

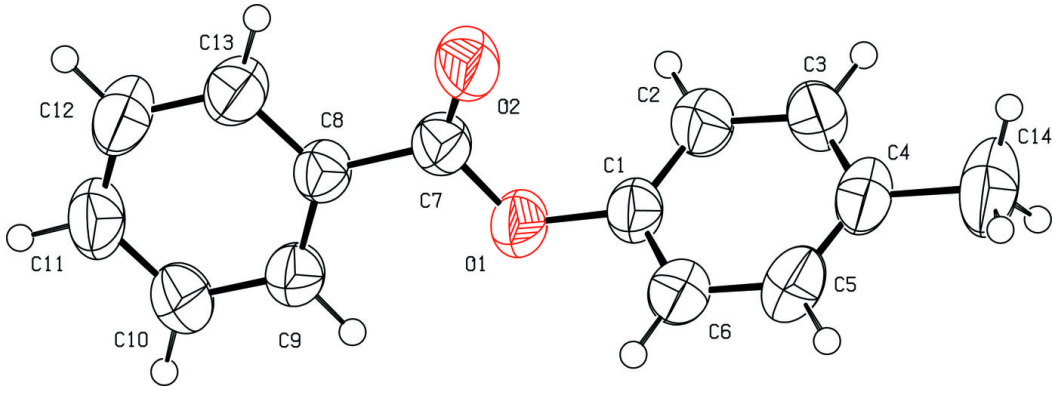

Fig. 2