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4-Methoxyphenyl benzoate

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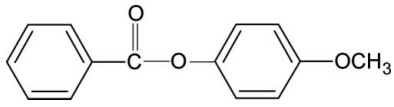
Key indicators: single-crystal X-ray study; T = 299 K; mean σ(C–C) = 0.002 Å; R factor = 0.033; wR factor = 0.095; data-to-parameter ratio = 10.8.

The structure of the title compound (4MPBA), $C_{14}H_{12}O_3$, resembles that of phenyl benzoate (PBA), with similar geometric parameters. The dihedral angle between the phenyl and benzene rings in 4MPBA is 56.42 (3)°, compared with 55.7° observed for PBA. The molecules in the title compound pack in layers parallel to the *ac* plane and in columns parallel to the *c* axis.

Related literature

For related literature, see: Adams & Morsi (1976); Gowda, Kozisek, Tokarcik *et al.* (2007*a*, 2007*b*); Gowda, Foro & Fuess (2007); Gowda, Kozisek, Svoboda *et al.* (2007); Gowda, Nayak *et al.* (2007); Gowda, Svoboda *et al.* (2007); Nayak & Gowda (2007).



Experimental

Crystal data

$C_{14}H_{12}O_3$
M_r = 228.24
Orthorhombic, *Pbca*
a = 14.303 (1) Å
b = 6.4799 (7) Å
c = 25.113 (2) Å
V = 2327.5 (4) Å^3
Z = 8
Cu $K\alpha$ radiation
μ = 0.75 mm^{-1}
T = 299 (2) K
0.60 × 0.50 × 0.43 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.648, T_{max} = 0.727
3699 measured reflections
2067 independent reflections
1876 reflections with $I > 2\sigma(I)$
R_{int} = 0.017
3 standard reflections
frequency: 120 min
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.095
S = 1.06
2067 reflections
191 parameters
Only H-atom coordinates refined
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.11 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: WN2169).

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supplementary materials

Acta Cryst. (2007). E**63**, o3507 [**doi:10.1107/S160053680703406X**]

4-Methoxyphenyl benzoate

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Comment

As part of a study of substituent effects on the solid state structures of chemically and biologically significant compounds (Gowda, Foro & Fuess, 2007; Gowda, Kozisek, Svoboda & Fuess, 2007; Gowda, Kozisek *et al.*, 2007*a*, *b*; Gowda, Nayak *et al.*, 2007; Gowda, Svoboda & Fuess, 2007) the structure of 4-methoxyphenyl benzoate (4MPBA) has been determined. The structure of 4MPBA (Fig. 1) resembles that of phenyl benzoate (PBA) (Adams & Morsi, 1976). The bond parameters in 4MPBA are similar to those in PBA and other benzoates. The molecules in the title compound pack in layers parallel to the *ac* plane and columns parallel to the *c* axis (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 H atoms were located in difference map and their positions refined, with U_{iso}(H) = 1.2U_{eq}(parent atom). The range of refined C—H distances was 0.94 (1) − 1.01 (2) Å.

Figures

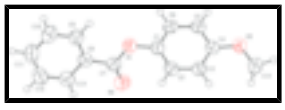

Fig. 1. Molecular structure of the title compound, showing the atom labeling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented as small spheres of arbitrary radius.

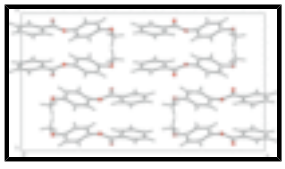

Fig. 2. Packing diagram of the title compound, as viewed perpendicular to the *ac* plane.

4-Methoxyphenyl benzoate

Crystal data

$C_{14}H_{12}O_3$	F_{000} = 960
M_r = 228.24	D_x = 1.303 Mg m^{-3}
Orthorhombic, *Pbca*	Cu *K*α radiation

	λ = 1.54180 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 25 reflections
a = 14.303 (1) Å	θ = 4.7–21.7º
b = 6.4799 (7) Å	μ = 0.75 mm^{-1}
c = 25.113 (2) Å	T = 299 (2) K
V = 2327.5 (4) Å^3	Prism, colourless
Z = 8	0.60 × 0.50 × 0.43 mm

Data collection

Enraf–Nonius CAD-4 diffractometer	R_{int} = 0.017
Radiation source: fine-focus sealed tube	θ_{max} = 66.9º
Monochromator: graphite	θ_{min} = 3.5º
T = 299(2) K	h = −17→0
ω/2θ scans	k = −7→0
Absorption correction: ψ scan (North *et al.*, 1968)	l = −19→29
T_{min} = 0.648, T_{max} = 0.727	3 standard reflections
3699 measured reflections	every 120 min
2067 independent reflections	intensity decay: none
1876 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	Only H-atom coordinates refined
$R[F^2 > 2\sigma(F^2)]$ = 0.033	$w = 1/[\sigma^2(F_o^2) + (0.0479P)^2 + 0.3393P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.095	$(\Delta/\sigma)_{max}$ = 0.005
S = 1.06	$\Delta\rho_{max}$ = 0.14 e Å^{-3}
2067 reflections	$\Delta\rho_{min}$ = −0.11 e Å^{-3}
191 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: 0.0102 (5)
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 calculat-

ing *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	0.12046 (8)	−0.07468 (18)	0.77616 (5)	0.0468 (3)
C2	0.16769 (8)	0.10896 (19)	0.77077 (5)	0.0514 (3)
H2	0.1991 (10)	0.164 (2)	0.8005 (6)	0.062*
C3	0.16764 (8)	0.21005 (19)	0.72225 (5)	0.0503 (3)
H3	0.2002 (10)	0.342 (2)	0.7183 (5)	0.060*
C4	0.12047 (8)	0.12494 (18)	0.67947 (4)	0.0455 (3)
C5	0.07270 (8)	−0.06046 (18)	0.68560 (5)	0.0493 (3)
H5	0.0400 (10)	−0.118 (2)	0.6556 (5)	0.059*
C6	0.07288 (8)	−0.16024 (19)	0.73398 (5)	0.0494 (3)
H6	0.0408 (10)	−0.290 (2)	0.7388 (5)	0.059*
C7	0.09183 (8)	−0.11004 (19)	0.86903 (5)	0.0501 (3)
C8	0.10711 (8)	−0.24883 (19)	0.91488 (5)	0.0492 (3)
C9	0.14336 (10)	−0.4464 (2)	0.90924 (6)	0.0584 (3)
H9	0.1586 (11)	−0.496 (2)	0.8733 (6)	0.070*
C10	0.15736 (11)	−0.5668 (3)	0.95396 (7)	0.0716 (4)
H10	0.1801 (12)	−0.702 (3)	0.9493 (7)	0.086*
C11	0.13484 (12)	−0.4930 (3)	1.00365 (7)	0.0790 (5)
H11	0.1452 (12)	−0.582 (3)	1.0353 (8)	0.095*
C12	0.09794 (14)	−0.2973 (3)	1.00923 (6)	0.0800 (5)
H12	0.0753 (12)	−0.247 (3)	1.0449 (7)	0.096*
C13	0.08494 (11)	−0.1753 (2)	0.96511 (5)	0.0649 (4)
H13	0.0600 (11)	−0.038 (3)	0.9686 (6)	0.078*
C14	0.16889 (14)	0.3934 (3)	0.62070 (7)	0.0706 (4)
H14A	0.2357 (14)	0.377 (3)	0.6281 (6)	0.085*
H14B	0.1605 (12)	0.420 (3)	0.5825 (7)	0.085*
H14C	0.1478 (12)	0.500 (3)	0.6441 (7)	0.085*
O1	0.12642 (6)	−0.19084 (13)	0.82345 (3)	0.0558 (3)
O2	0.05426 (8)	0.05500 (15)	0.87100 (4)	0.0733 (3)
O3	0.11796 (7)	0.20889 (14)	0.62955 (3)	0.0607 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0468 (6)	0.0470 (6)	0.0467 (6)	0.0065 (5)	0.0050 (5)	0.0006 (5)
C2	0.0504 (6)	0.0552 (7)	0.0485 (6)	−0.0045 (5)	−0.0054 (5)	−0.0059 (5)
C3	0.0504 (6)	0.0470 (6)	0.0536 (7)	−0.0091 (5)	−0.0024 (5)	−0.0029 (5)
C4	0.0450 (6)	0.0466 (6)	0.0450 (6)	0.0004 (5)	0.0003 (4)	−0.0030 (5)
C5	0.0485 (6)	0.0491 (6)	0.0502 (6)	−0.0050 (5)	−0.0025 (5)	−0.0084 (5)
C6	0.0475 (6)	0.0432 (6)	0.0574 (7)	−0.0041 (5)	0.0058 (5)	−0.0040 (5)
C7	0.0483 (6)	0.0499 (7)	0.0521 (7)	0.0042 (5)	0.0041 (5)	−0.0026 (5)
C8	0.0464 (6)	0.0516 (6)	0.0496 (6)	−0.0012 (5)	0.0013 (5)	−0.0001 (5)
C9	0.0626 (8)	0.0550 (7)	0.0577 (7)	0.0047 (6)	0.0021 (6)	0.0028 (6)

C10	0.0758 (9)	0.0622 (9)	0.0769 (10)	0.0045 (7)	−0.0038 (8)	0.0158 (7)
C11	0.0899 (11)	0.0854 (11)	0.0616 (9)	−0.0134 (9)	−0.0111 (8)	0.0216 (8)
C12	0.1012 (12)	0.0885 (12)	0.0504 (8)	−0.0148 (10)	0.0035 (8)	0.0003 (8)
C13	0.0774 (9)	0.0632 (8)	0.0542 (7)	−0.0018 (7)	0.0088 (6)	−0.0033 (6)
C14	0.0887 (11)	0.0603 (8)	0.0629 (9)	−0.0134 (8)	−0.0013 (8)	0.0120 (7)
O1	0.0679 (5)	0.0518 (5)	0.0477 (5)	0.0130 (4)	0.0081 (4)	0.0031 (4)
O2	0.0954 (8)	0.0579 (6)	0.0666 (6)	0.0280 (5)	0.0150 (5)	0.0029 (4)
O3	0.0765 (6)	0.0567 (5)	0.0489 (5)	−0.0113 (4)	−0.0083 (4)	0.0042 (4)

Geometric parameters (Å, °)

C1—C2	1.3751 (17)	C8—C13	1.3852 (18)
C1—C6	1.3756 (17)	C8—C9	1.3886 (18)
C1—O1	1.4086 (14)	C9—C10	1.382 (2)
C2—C3	1.3832 (17)	C9—H9	0.983 (15)
C2—H2	0.943 (14)	C10—C11	1.375 (2)
C3—C4	1.3833 (16)	C10—H10	0.942 (18)
C3—H3	0.979 (14)	C11—C12	1.381 (3)
C4—O3	1.3671 (14)	C11—H11	0.992 (19)
C4—C5	1.3906 (16)	C12—C13	1.374 (2)
C5—C6	1.3764 (17)	C12—H12	1.007 (18)
C5—H5	0.963 (14)	C13—H13	0.961 (17)
C6—H6	0.964 (15)	C14—O3	1.4176 (17)
C7—O2	1.1978 (15)	C14—H14A	0.98 (2)
C7—O1	1.3524 (14)	C14—H14B	0.982 (18)
C7—C8	1.4774 (17)	C14—H14C	0.956 (19)
C2—C1—C6	121.06 (11)	C10—C9—C8	119.45 (14)
C2—C1—O1	121.05 (11)	C10—C9—H9	122.0 (9)
C6—C1—O1	117.63 (11)	C8—C9—H9	118.5 (9)
C1—C2—C3	119.76 (11)	C11—C10—C9	120.48 (15)
C1—C2—H2	118.9 (8)	C11—C10—H10	121.1 (11)
C3—C2—H2	121.3 (8)	C9—C10—H10	118.4 (11)
C4—C3—C2	119.70 (11)	C10—C11—C12	120.08 (15)
C4—C3—H3	120.2 (8)	C10—C11—H11	119.3 (11)
C2—C3—H3	120.1 (8)	C12—C11—H11	120.7 (11)
O3—C4—C3	124.50 (11)	C13—C12—C11	119.90 (15)
O3—C4—C5	115.61 (10)	C13—C12—H12	119.2 (11)
C3—C4—C5	119.87 (11)	C11—C12—H12	120.7 (11)
C6—C5—C4	120.17 (11)	C12—C13—C8	120.36 (15)
C6—C5—H5	120.6 (8)	C12—C13—H13	120.5 (10)
C4—C5—H5	119.2 (8)	C8—C13—H13	119.1 (10)
C1—C6—C5	119.43 (11)	O3—C14—H14A	112.3 (11)
C1—C6—H6	119.3 (8)	O3—C14—H14B	103.8 (10)
C5—C6—H6	121.3 (8)	H14A—C14—H14B	108.9 (14)
O2—C7—O1	123.00 (11)	O3—C14—H14C	110.6 (11)
O2—C7—C8	125.29 (11)	H14A—C14—H14C	105.6 (14)
O1—C7—C8	111.71 (10)	H14B—C14—H14C	115.8 (15)
C13—C8—C9	119.71 (12)	C7—O1—C1	118.98 (9)
C13—C8—C7	117.80 (12)	C4—O3—C14	117.76 (10)

C9—C8—C7	122.48 (11)		
C6—C1—C2—C3	0.00 (18)	C13—C8—C9—C10	−0.4 (2)
O1—C1—C2—C3	173.98 (10)	C7—C8—C9—C10	178.90 (13)
C1—C2—C3—C4	−0.36 (18)	C8—C9—C10—C11	0.6 (2)
C2—C3—C4—O3	−178.21 (11)	C9—C10—C11—C12	0.0 (3)
C2—C3—C4—C5	0.62 (18)	C10—C11—C12—C13	−0.9 (3)
O3—C4—C5—C6	178.39 (11)	C11—C12—C13—C8	1.1 (3)
C3—C4—C5—C6	−0.54 (17)	C9—C8—C13—C12	−0.5 (2)
C2—C1—C6—C5	0.08 (17)	C7—C8—C13—C12	−179.82 (14)
O1—C1—C6—C5	−174.10 (10)	O2—C7—O1—C1	1.65 (19)
C4—C5—C6—C1	0.18 (17)	C8—C7—O1—C1	−177.86 (10)
O2—C7—C8—C13	−6.8 (2)	C2—C1—O1—C7	64.57 (15)
O1—C7—C8—C13	172.67 (12)	C6—C1—O1—C7	−121.25 (12)
O2—C7—C8—C9	173.90 (14)	C3—C4—O3—C14	1.48 (19)
O1—C7—C8—C9	−6.61 (17)	C5—C4—O3—C14	−177.40 (12)

Fig. 1

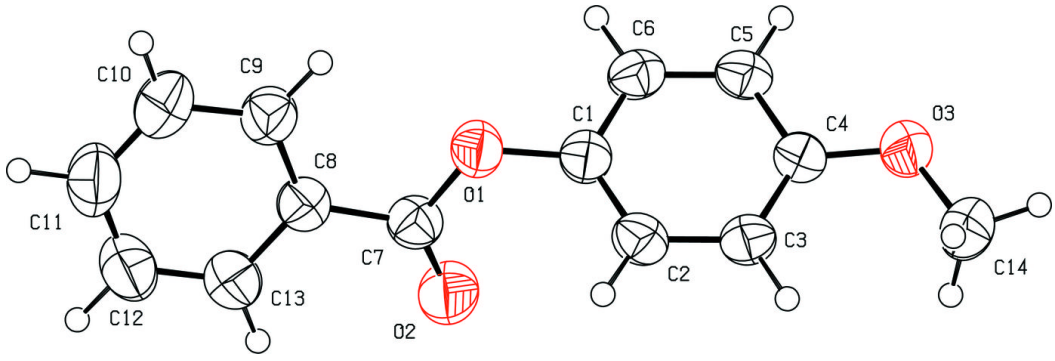

Fig. 2