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3-Methylphenyl benzoate

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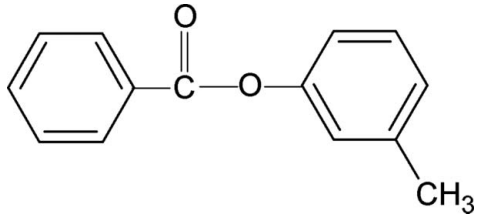
Key indicators: single-crystal X-ray study; T = 299 K; mean σ(C–C) = 0.003 Å; R factor = 0.041; wR factor = 0.131; data-to-parameter ratio = 13.5.

The structure of the title compound, $C_{14}H_{12}O_2$, resembles that of phenyl benzoate and 4-methylphenyl benzoate, with similar geometric parameters. The dihedral angle between the phenyl and benzoyl rings is 79.61 (6)°, compared to values of 55.7° for phenyl benzoate and 60.17 (7)° for 4-methylphenyl benzoate. The molecules in the title compound are packed with the methylphenyl and the benzoyl rings nearly orthogonal to each other.

Related literature

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



Experimental

Crystal data

$C_{14}H_{12}O_2$
M_r = 212.24
Monoclinic, $P2_1/c$
a = 9.530 (1) Å
b = 10.676 (1) Å
c = 11.654 (2) Å
β = 104.04 (1)°
V = 1150.3 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 299 (2) K
0.50 × 0.50 × 0.40 mm

Data collection

Oxford Diffraction Xcalibur single-crystal X-ray diffractometer with a Sapphire CCD detector
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
T_{min} = 0.951, T_{max} = 0.977
8434 measured reflections
2341 independent reflections
1624 reflections with $I > 2\sigma(I)$
R_{int} = 0.013

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.131
S = 1.06
2341 reflections
174 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2003); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2007); data reduction: *CrysAlis RED*; 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: BT2465).

References

Adams, J. M. & Morsi, S. E. (1976). *Acta Cryst.* B**32**, 1345–1347.
Gowda, B. T., Foro, S., Nayak, R. & Fuess, H. (2007*a*). *Acta Cryst.* E**63**, o3507.
Gowda, B. T., Foro, S., Nayak, R. & Fuess, H. (2007*b*). *Acta Cryst.* E**63**, o3563.
Gowda, B. T., Kozisek, J., Svoboda, I. & Fuess, H. (2007). *Z. Naturforsch. Teil A*, **62**, 91–100.
Nayak, R. & Gowda, B. T. (2007). *Z. Naturforsch. Teil A*, **62**. In the press.
Oxford Diffraction (2003). *CrysAlis CCD*. Version 1.170.17. Oxford Diffraction Ltd, Abingdon, Oxfordshire, England.
Oxford Diffraction (2007). *CrysAlis RED*. Version 1.171.32.5. Oxford Diffraction Ltd, Abingdon, Oxfordshire, England.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

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supplementary materials

Acta Cryst. (2007). E**63**, o3756 [**doi:10.1107/S1600536807038585**]

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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*a*, *b*; Gowda, Kozisek *et al.*, 2007), the structure of 3-methylphenyl benzoate (3MePBA) has been determined. The structure of 3MePBA (Fig. 1) is similar to that of phenyl benzoate (PBA) (Adams & Morsi, 1976) and 4-methylphenyl benzoate (4MePBA) (Gowda, Foro *et al.*, 2007*b*). The bond parameters in 3MePBA are similar to those in PBA, 4MePBA and other benzoates. The molecules in the title compound are packed with the methylphenyl and the benzoyl rings nearly orthoganal to each other (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 of the methyl group were positioned with idealized geometry and included in further refinement using a riding model approximation [C—H = 0.96 Å, U_{iso}(H) = 1.2U_{eq}(C)]. In addition, the methyl group was allowed to rotate but not to tip. All other H atoms were located in the difference map, and their positional parameters were refined, whereas their isotropic displacement parameters were set to 1.2 U_{eq} of the parent atom.

Figures

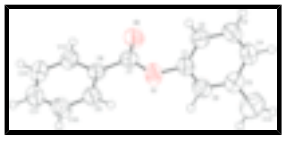

Fig. 1. Molecular structure of the title compound, showing the atom labeling. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented as small spheres of arbitrary radius.

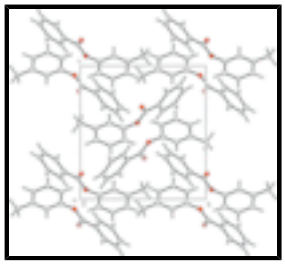

Fig. 2. Molecular packing of the title compound with hydrogen bonding shown as dashed lines.

3-Methylphenyl benzoate

Crystal data

$C_{14}H_{12}O_2$	F_{000} = 448
M_r = 212.24	D_x = 1.226 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 2877 reflections
a = 9.530 (1) Å	θ = 2.1–25.2º
b = 10.676 (1) Å	μ = 0.08 mm^{-1}
c = 11.654 (2) Å	T = 299 (2) K
β = 104.04 (1)º	Prism, colourless
V = 1150.3 (3) Å^3	0.50 × 0.50 × 0.40 mm
Z = 4	

Data collection

Oxford Diffraction Xcalibur single-crystal X-ray diffractometer with a Sapphire CCD detector	2341 independent reflections
Radiation source: fine-focus sealed tube	1624 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.013
T = 299(2) K	θ_{max} = 26.4º
Rotation method data acquisition using ω and φ scans	θ_{min} = 4.1º
Absorption correction: multi-scan (CrysAlis RED; Oxford Diffraction, 2007)	h = −11→11
T_{min} = 0.951, T_{max} = 0.977	k = −13→13
8434 measured reflections	l = −14→14

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
$R[F^2 > 2\sigma(F^2)]$ = 0.041	$w = 1/[\sigma^2(F_o^2) + (0.053P)^2 + 0.3191P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.131	$(\Delta/\sigma)_{max}$ = 0.004
S = 1.06	$\Delta\rho_{max}$ = 0.17 e Å^{-3}
2341 reflections	$\Delta\rho_{min}$ = −0.16 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: 0.039 (4)
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	0.26886 (17)	0.15483 (17)	0.03031 (15)	0.0540 (4)
C2	0.3452 (2)	0.14859 (19)	−0.05466 (17)	0.0602 (5)
H2	0.371 (2)	0.071 (2)	−0.0830 (18)	0.072*
C3	0.3866 (2)	0.2592 (2)	−0.09759 (17)	0.0633 (5)
H3	0.442 (2)	0.2570 (18)	−0.156 (2)	0.076*
C4	0.3513 (2)	0.37200 (19)	−0.05653 (16)	0.0608 (5)
H4	0.382 (2)	0.450 (2)	−0.0862 (18)	0.073*
C5	0.2725 (2)	0.37878 (18)	0.02860 (16)	0.0616 (5)
C6	0.2318 (2)	0.26692 (19)	0.07217 (16)	0.0594 (5)
H6	0.175 (2)	0.2674 (18)	0.1315 (19)	0.071*
C7	0.31272 (17)	−0.01993 (16)	0.15799 (14)	0.0505 (4)
C8	0.24368 (17)	−0.12558 (15)	0.20569 (14)	0.0478 (4)
C9	0.09865 (19)	−0.15503 (18)	0.16453 (16)	0.0578 (5)
H9	0.040 (2)	−0.1072 (18)	0.1003 (18)	0.069*
C10	0.0395 (2)	−0.2517 (2)	0.21564 (19)	0.0673 (5)
H10	−0.062 (3)	−0.268 (2)	0.1874 (19)	0.081*
C11	0.1233 (2)	−0.3176 (2)	0.30867 (18)	0.0674 (5)
H11	0.080 (2)	−0.386 (2)	0.3449 (19)	0.081*
C12	0.2675 (2)	−0.28943 (19)	0.34923 (18)	0.0653 (5)
H12	0.324 (2)	−0.335 (2)	0.4132 (19)	0.078*
C13	0.3281 (2)	−0.19441 (17)	0.29812 (16)	0.0565 (4)
H13	0.429 (2)	−0.1738 (18)	0.3242 (17)	0.068*
C14	0.2329 (3)	0.5024 (2)	0.0733 (3)	0.0986 (8)
H14A	0.1898	0.5551	0.0074	0.118*
H14B	0.3183	0.5420	0.1198	0.118*
H14C	0.1652	0.4891	0.1211	0.118*
O1	0.21733 (13)	0.04446 (13)	0.07312 (12)	0.0681 (4)
O2	0.43703 (13)	0.00903 (13)	0.19029 (12)	0.0684 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}

C1	0.0465 (9)	0.0572 (10)	0.0542 (9)	−0.0076 (8)	0.0044 (7)	0.0100 (8)
C2	0.0587 (11)	0.0589 (11)	0.0636 (11)	0.0005 (9)	0.0162 (8)	−0.0012 (9)
C3	0.0601 (11)	0.0763 (13)	0.0558 (10)	−0.0049 (9)	0.0185 (8)	0.0048 (9)
C4	0.0613 (11)	0.0616 (12)	0.0563 (10)	−0.0106 (9)	0.0078 (8)	0.0091 (9)
C5	0.0611 (11)	0.0608 (11)	0.0579 (10)	−0.0020 (9)	0.0047 (8)	−0.0047 (9)
C6	0.0562 (10)	0.0733 (13)	0.0495 (9)	−0.0033 (9)	0.0142 (8)	0.0013 (9)
C7	0.0463 (9)	0.0546 (10)	0.0500 (8)	0.0002 (7)	0.0105 (7)	−0.0024 (7)
C8	0.0486 (9)	0.0469 (9)	0.0482 (8)	0.0010 (7)	0.0124 (7)	−0.0036 (7)
C9	0.0509 (10)	0.0639 (11)	0.0570 (10)	−0.0022 (8)	0.0100 (8)	0.0073 (9)
C10	0.0558 (11)	0.0741 (13)	0.0720 (12)	−0.0120 (10)	0.0151 (9)	0.0039 (10)
C11	0.0773 (13)	0.0570 (11)	0.0702 (12)	−0.0080 (10)	0.0224 (10)	0.0068 (9)
C12	0.0734 (13)	0.0553 (11)	0.0628 (11)	0.0037 (9)	0.0078 (9)	0.0093 (9)
C13	0.0522 (10)	0.0534 (10)	0.0603 (10)	0.0022 (8)	0.0065 (8)	−0.0003 (8)
C14	0.114 (2)	0.0758 (16)	0.1066 (18)	0.0040 (14)	0.0288 (15)	−0.0192 (14)
O1	0.0533 (7)	0.0690 (8)	0.0754 (8)	−0.0119 (6)	0.0028 (6)	0.0228 (7)
O2	0.0478 (7)	0.0762 (9)	0.0781 (9)	−0.0065 (6)	0.0092 (6)	0.0115 (7)

Geometric parameters (Å, °)

C1—C2	1.365 (3)	C8—C9	1.385 (2)
C1—C6	1.371 (3)	C8—C13	1.388 (2)
C1—O1	1.413 (2)	C9—C10	1.379 (3)
C2—C3	1.377 (3)	C9—H9	0.97 (2)
C2—H2	0.95 (2)	C10—C11	1.374 (3)
C3—C4	1.368 (3)	C10—H10	0.96 (2)
C3—H3	0.96 (2)	C11—C12	1.374 (3)
C4—C5	1.383 (3)	C11—H11	0.98 (2)
C4—H4	0.97 (2)	C12—C13	1.373 (3)
C5—C6	1.389 (3)	C12—H12	0.94 (2)
C5—C14	1.500 (3)	C13—H13	0.96 (2)
C6—H6	0.98 (2)	C14—H14A	0.9600
C7—O2	1.1935 (19)	C14—H14B	0.9600
C7—O1	1.357 (2)	C14—H14C	0.9600
C7—C8	1.480 (2)		
C2—C1—C6	121.98 (17)	C13—C8—C7	117.90 (15)
C2—C1—O1	120.48 (17)	C10—C9—C8	119.92 (17)
C6—C1—O1	117.43 (16)	C10—C9—H9	120.6 (11)
C1—C2—C3	118.14 (18)	C8—C9—H9	119.5 (11)
C1—C2—H2	121.4 (12)	C11—C10—C9	120.23 (19)
C3—C2—H2	120.5 (12)	C11—C10—H10	121.3 (13)
C4—C3—C2	120.76 (18)	C9—C10—H10	118.4 (13)
C4—C3—H3	119.7 (12)	C12—C11—C10	120.09 (19)
C2—C3—H3	119.5 (12)	C12—C11—H11	120.2 (12)
C3—C4—C5	121.29 (18)	C10—C11—H11	119.7 (12)
C3—C4—H4	120.4 (12)	C13—C12—C11	120.23 (18)
C5—C4—H4	118.3 (12)	C13—C12—H12	120.3 (13)
C4—C5—C6	117.74 (18)	C11—C12—H12	119.5 (13)
C4—C5—C14	121.39 (19)	C12—C13—C8	120.13 (17)
C6—C5—C14	120.87 (19)	C12—C13—H13	121.7 (12)

C1—C6—C5	120.09 (17)	C8—C13—H13	118.1 (12)
C1—C6—H6	119.5 (12)	C5—C14—H14A	109.5
C5—C6—H6	120.4 (12)	C5—C14—H14B	109.5
O2—C7—O1	122.47 (16)	H14A—C14—H14B	109.5
O2—C7—C8	125.20 (15)	C5—C14—H14C	109.5
O1—C7—C8	112.31 (13)	H14A—C14—H14C	109.5
C9—C8—C13	119.38 (16)	H14B—C14—H14C	109.5
C9—C8—C7	122.69 (15)	C7—O1—C1	116.81 (13)
C6—C1—C2—C3	0.7 (3)	O1—C7—C8—C13	−176.29 (15)
O1—C1—C2—C3	176.76 (15)	C13—C8—C9—C10	0.2 (3)
C1—C2—C3—C4	−0.4 (3)	C7—C8—C9—C10	−177.56 (17)
C2—C3—C4—C5	−0.3 (3)	C8—C9—C10—C11	1.1 (3)
C3—C4—C5—C6	0.7 (3)	C9—C10—C11—C12	−1.7 (3)
C3—C4—C5—C14	−179.64 (19)	C10—C11—C12—C13	0.8 (3)
C2—C1—C6—C5	−0.3 (3)	C11—C12—C13—C8	0.5 (3)
O1—C1—C6—C5	−176.50 (15)	C9—C8—C13—C12	−1.0 (3)
C4—C5—C6—C1	−0.4 (3)	C7—C8—C13—C12	176.86 (16)
C14—C5—C6—C1	179.97 (18)	O2—C7—O1—C1	−5.0 (3)
O2—C7—C8—C9	−179.88 (17)	C8—C7—O1—C1	173.70 (14)
O1—C7—C8—C9	1.5 (2)	C2—C1—O1—C7	82.1 (2)
O2—C7—C8—C13	2.3 (3)	C6—C1—O1—C7	−101.67 (18)

Fig. 1

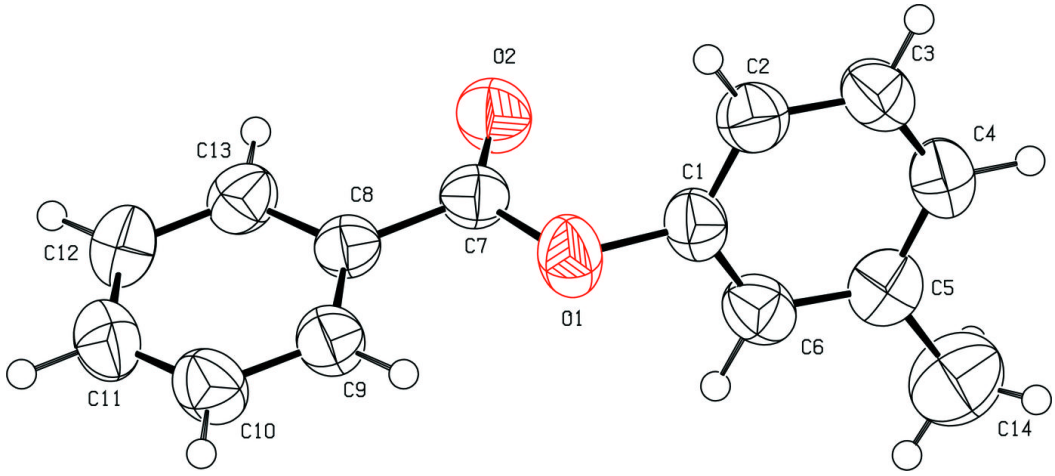

Fig. 2