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2,6-Dichlorophenyl 4-methylbenzoate

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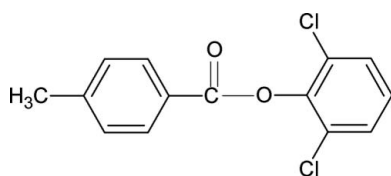
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 Key indicators: single-crystal X-ray study; $T = 299$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.050; wR factor = 0.169; data-to-parameter ratio = 14.3.

The structure of the title compound (26DCP4MeBA), $\text{C}_{14}\text{H}_{10}\text{Cl}_2\text{O}_2$, resembles those of phenyl benzoate (PBA), 2,6-dichlorophenyl benzoate (26DCPBA), 2,4-dichlorophenyl 4-methylbenzoate (24DCP4MeBA) and other aryl benzoates, with similar bond parameters. The dihedral angle between the benzene and benzoyl rings in 26DCP4MeBA is 77.97 (9) $^\circ$, compared with values of 55.7 (PBA), 75.75 (10) (26DCPBA) and 48.13 (5) $^\circ$ (24DCP4MeBA). The molecules in the title compound are packed into zigzag chains in the bc plane.

Related literature

 For related literature, see: Adams & Morsi (1976); Gowda *et al.* (2007a,b); Nayak & Gowda (2008).


Experimental

Crystal data

 $\text{C}_{14}\text{H}_{10}\text{Cl}_2\text{O}_2$
 $M_r = 281.12$
 Monoclinic, $P2_1/n$
 $a = 9.5688$ (8) Å
 $b = 11.1370$ (9) Å
 $c = 13.1947$ (9) Å
 $\beta = 108.898$ (7) $^\circ$
 $V = 1330.33$ (18) Å³
 $Z = 4$
 Cu $K\alpha$ radiation
 $\mu = 4.32$ mm⁻¹
 $T = 299$ (2) K
 $0.60 \times 0.35 \times 0.30$ mm

Data collection

 Enraf–Nonius CAD-4 diffractometer
 Absorption correction: ψ scan (North *et al.*, 1968)
 $T_{\min} = 0.202$, $T_{\max} = 0.273$
 3035 measured reflections

 2366 independent reflections
 2025 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.040$
 3 standard reflections
 frequency: 120 min
 intensity decay: none

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.049$
 $wR(F^2) = 0.168$
 $S = 1.01$
 2366 reflections

 165 parameters
 H-atom parameters constrained
 $\Delta\rho_{\max} = 0.36$ e Å⁻³
 $\Delta\rho_{\min} = -0.43$ e Å⁻³

Data collection: *CAD-4-PC* (Enraf–Nonius, 1996); cell refinement: *CAD-4-PC*; data reduction: *REDU4* (Stoe & Cie, 1987); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); 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: OM2223).

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supplementary materials

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2,6-Dichlorophenyl 4-methylbenzoate

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Comment

In the present work, as part of a study of the substituent effects on the structures of chemically and industrially significant compounds (Gowda *et al.*, 2007*a,b*), the structure of 2,6-dichlorophenyl 4-methylbenzoate (26DCP4MeBA) has been determined. The structure of 26DCP4MeBA (Fig. 1) resembles those of phenyl benzoate (PBA) (Adams & Morsi, 1976), 2,6-dichlorophenyl benzoate (26DCPBA) (Gowda *et al.*, 2007*a*), 2,4-dichlorophenyl 4-methyl benzoate (24DCP4MeBA) (Gowda *et al.*, 2007*b*) and other aryl benzoates. The bond parameters in 26DCP4MeBA are similar to those in PBA, 26DCPBA, 24DCP4MeBA and other benzoates. The dihedral angle between the benzene and benzoyl rings in 26DCP4MeBA is 77.97 (9)°, compared to the values of 55.7° (PBA)(Adams & Morsi, 1976), 75.75 (10)° (26DCPBA)(Gowda *et al.*, 2007*a*) and 48.13 (5)° (24DCP4MeBA)(Gowda *et al.*, 2007*b*). The molecules in 26DCP4MeBA are packed into a zigzag structure with the dichlorophenyl ring being nearly orthogonal to the benzoyl ring (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.

Refinement

The H atoms were positioned with idealized geometry using a riding model (C—H = 0.93–0.96 Å) with $U_{\text{iso}} = 1.2 U_{\text{eq}}$ of the parent atom.

Figures

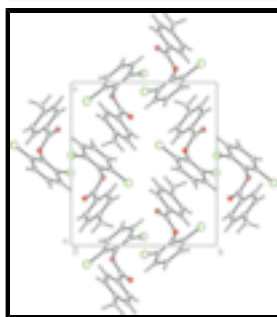
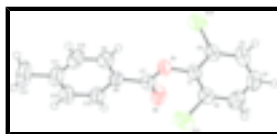
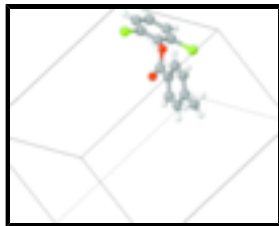


Fig. 1. Molecular structure of the title compound, showing the atom labeling. Displacement ellipsoids are drawn at the 50% probability level.

Fig. 2. Molecular packing of the title compound as viewed down a.



2,6-Dichlorophenyl 4-methylbenzoate

Crystal data

$C_{14}H_{10}Cl_2O_2$

$M_r = 281.12$

Monoclinic, $P2_1/n$

Hall symbol: -P 2yn

$a = 9.5688$ (8) Å

$b = 11.1370$ (9) Å

$c = 13.1947$ (9) Å

$\beta = 108.898$ (7)°

$V = 1330.33$ (18) Å³

$Z = 4$

$F_{000} = 576$

$D_x = 1.404$ Mg m⁻³

Cu $K\alpha$ radiation

$\lambda = 1.54180$ Å

Cell parameters from 25 reflections

$\theta = 5.3$ – 18.7 °

$\mu = 4.32$ mm⁻¹

$T = 299$ (2) K

Rod, colourless

$0.60 \times 0.35 \times 0.30$ mm

Data collection

Enraf–Nonius CAD-4
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 299$ (2) K

$\omega/2\theta$ scans

Absorption correction: ψ scan
(North *et al.*, 1968)

$T_{\min} = 0.202$, $T_{\max} = 0.273$

3035 measured reflections

2366 independent reflections

2025 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.040$

$\theta_{\max} = 67.0$ °

$\theta_{\min} = 5.0$ °

$h = -11 \rightarrow 2$

$k = -13 \rightarrow 0$

$l = -15 \rightarrow 15$

3 standard reflections

every 120 min

intensity decay: none

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.049$

$wR(F^2) = 0.168$

$S = 1.01$

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.1211P)^2 + 0.3061P]$$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.011$

$\Delta\rho_{\max} = 0.36$ e Å⁻³

2366 reflections

$$\Delta\rho_{\min} = -0.43 \text{ e } \text{\AA}^{-3}$$

165 parameters

Extinction correction: SHELXL97 (Sheldrick, 2008),

$$F_c^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$$

Primary atom site location: structure-invariant direct methods

Extinction coefficient: 0.0170 (18)

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 $F^2 > \sigma(F^2)$ 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)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.1987 (2)	0.6943 (2)	0.02446 (17)	0.0490 (5)
C2	0.1627 (3)	0.5987 (2)	-0.0454 (2)	0.0568 (6)
C3	0.0175 (3)	0.5780 (3)	-0.1077 (2)	0.0683 (7)
H3	-0.0065	0.5127	-0.1541	0.082*
C4	-0.0902 (3)	0.6551 (3)	-0.0999 (2)	0.0705 (7)
H4	-0.1879	0.6418	-0.1415	0.085*
C5	-0.0563 (3)	0.7510 (3)	-0.0320 (2)	0.0679 (7)
H5	-0.1304	0.8030	-0.0280	0.082*
C6	0.0887 (3)	0.7707 (2)	0.03086 (19)	0.0547 (6)
C7	0.4023 (2)	0.6546 (2)	0.17553 (18)	0.0499 (5)
C8	0.5626 (2)	0.6726 (2)	0.22269 (17)	0.0484 (5)
C9	0.6386 (3)	0.7563 (2)	0.1830 (2)	0.0636 (7)
H9	0.5881	0.8063	0.1266	0.076*
C10	0.7903 (3)	0.7648 (3)	0.2280 (3)	0.0744 (8)
H10	0.8409	0.8210	0.2009	0.089*
C11	0.8687 (3)	0.6923 (3)	0.3118 (2)	0.0693 (8)
C12	0.7918 (3)	0.6113 (3)	0.3517 (2)	0.0681 (7)
H12	0.8426	0.5620	0.4086	0.082*
C13	0.6393 (3)	0.6016 (2)	0.3082 (2)	0.0574 (6)
H13	0.5887	0.5471	0.3369	0.069*
C14	1.0350 (3)	0.7024 (4)	0.3581 (3)	0.1081 (14)
H14A	1.0606	0.7552	0.4189	0.130*
H14B	1.0733	0.7342	0.3047	0.130*
H14C	1.0766	0.6245	0.3799	0.130*
O1	0.34465 (16)	0.71769 (15)	0.08263 (13)	0.0551 (5)
O2	0.32703 (19)	0.59229 (19)	0.21108 (15)	0.0692 (6)
Cl1	0.30058 (9)	0.50474 (7)	-0.05432 (7)	0.0849 (4)

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C12 0.13347 (8) 0.89253 (7) 0.11604 (6) 0.0796 (3)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0404 (11)	0.0544 (12)	0.0506 (12)	0.0032 (9)	0.0127 (9)	0.0059 (9)
C2	0.0570 (14)	0.0574 (14)	0.0578 (13)	0.0078 (10)	0.0210 (11)	0.0025 (10)
C3	0.0700 (16)	0.0723 (17)	0.0568 (14)	-0.0073 (13)	0.0124 (12)	-0.0048 (12)
C4	0.0492 (13)	0.093 (2)	0.0597 (15)	-0.0064 (13)	0.0040 (11)	0.0035 (14)
C5	0.0443 (12)	0.091 (2)	0.0654 (15)	0.0142 (12)	0.0139 (11)	0.0084 (14)
C6	0.0488 (12)	0.0627 (14)	0.0522 (12)	0.0091 (10)	0.0157 (10)	0.0002 (10)
C7	0.0464 (12)	0.0493 (12)	0.0528 (12)	-0.0002 (9)	0.0143 (9)	0.0007 (9)
C8	0.0424 (11)	0.0485 (12)	0.0538 (12)	-0.0010 (9)	0.0148 (9)	-0.0070 (9)
C9	0.0577 (14)	0.0586 (14)	0.0741 (16)	-0.0067 (11)	0.0206 (12)	0.0040 (12)
C10	0.0577 (15)	0.0775 (19)	0.090 (2)	-0.0224 (13)	0.0267 (14)	-0.0050 (15)
C11	0.0432 (13)	0.091 (2)	0.0695 (16)	-0.0092 (12)	0.0131 (11)	-0.0208 (14)
C12	0.0478 (13)	0.0830 (18)	0.0635 (15)	0.0035 (12)	0.0042 (11)	-0.0020 (13)
C13	0.0479 (13)	0.0621 (14)	0.0597 (14)	-0.0038 (10)	0.0139 (10)	-0.0018 (10)
C14	0.0438 (15)	0.161 (4)	0.110 (3)	-0.0203 (19)	0.0125 (16)	-0.025 (3)
O1	0.0408 (8)	0.0593 (10)	0.0611 (10)	0.0006 (6)	0.0109 (7)	0.0097 (7)
O2	0.0502 (9)	0.0845 (13)	0.0681 (11)	-0.0149 (8)	0.0125 (8)	0.0170 (9)
Cl1	0.0880 (6)	0.0766 (5)	0.0967 (6)	0.0244 (4)	0.0389 (5)	-0.0084 (4)
Cl2	0.0782 (5)	0.0754 (5)	0.0764 (5)	0.0184 (3)	0.0128 (4)	-0.0178 (3)

Geometric parameters (\AA , $^\circ$)

C1—C6	1.377 (3)	C8—C13	1.379 (3)
C1—C2	1.377 (3)	C8—C9	1.385 (3)
C1—O1	1.383 (3)	C9—C10	1.382 (4)
C2—C3	1.386 (4)	C9—H9	0.9300
C2—C11	1.718 (2)	C10—C11	1.379 (4)
C3—C4	1.371 (4)	C10—H10	0.9300
C3—H3	0.9300	C11—C12	1.372 (4)
C4—C5	1.364 (4)	C11—C14	1.513 (4)
C4—H4	0.9300	C12—C13	1.389 (4)
C5—C6	1.384 (4)	C12—H12	0.9300
C5—H5	0.9300	C13—H13	0.9300
C6—Cl2	1.725 (3)	C14—H14A	0.9600
C7—O2	1.199 (3)	C14—H14B	0.9600
C7—O1	1.365 (3)	C14—H14C	0.9600
C7—C8	1.470 (3)		
C6—C1—C2	119.2 (2)	C9—C8—C7	122.4 (2)
C6—C1—O1	120.3 (2)	C10—C9—C8	119.4 (3)
C2—C1—O1	120.4 (2)	C10—C9—H9	120.3
C1—C2—C3	120.8 (2)	C8—C9—H9	120.3
C1—C2—C11	119.07 (19)	C11—C10—C9	121.8 (3)
C3—C2—C11	120.2 (2)	C11—C10—H10	119.1
C4—C3—C2	119.0 (3)	C9—C10—H10	119.1

C4—C3—H3	120.5	C12—C11—C10	118.2 (2)
C2—C3—H3	120.5	C12—C11—C14	121.3 (3)
C5—C4—C3	121.0 (2)	C10—C11—C14	120.5 (3)
C5—C4—H4	119.5	C11—C12—C13	121.0 (3)
C3—C4—H4	119.5	C11—C12—H12	119.5
C4—C5—C6	119.7 (2)	C13—C12—H12	119.5
C4—C5—H5	120.1	C8—C13—C12	120.2 (2)
C6—C5—H5	120.1	C8—C13—H13	119.9
C1—C6—C5	120.2 (2)	C12—C13—H13	119.9
C1—C6—C12	119.48 (19)	C11—C14—H14A	109.5
C5—C6—C12	120.26 (19)	C11—C14—H14B	109.5
O2—C7—O1	122.0 (2)	H14A—C14—H14B	109.5
O2—C7—C8	126.1 (2)	C11—C14—H14C	109.5
O1—C7—C8	111.85 (18)	H14A—C14—H14C	109.5
C13—C8—C9	119.3 (2)	H14B—C14—H14C	109.5
C13—C8—C7	118.3 (2)	C7—O1—C1	116.30 (17)
C6—C1—C2—C3	-0.9 (4)	O2—C7—C8—C9	-172.7 (3)
O1—C1—C2—C3	-177.0 (2)	O1—C7—C8—C9	7.8 (3)
C6—C1—C2—C11	179.23 (18)	C13—C8—C9—C10	1.7 (4)
O1—C1—C2—C11	3.2 (3)	C7—C8—C9—C10	-177.0 (2)
C1—C2—C3—C4	0.8 (4)	C8—C9—C10—C11	-0.2 (5)
C11—C2—C3—C4	-179.3 (2)	C9—C10—C11—C12	-1.0 (5)
C2—C3—C4—C5	-0.1 (4)	C9—C10—C11—C14	179.0 (3)
C3—C4—C5—C6	-0.6 (4)	C10—C11—C12—C13	0.5 (4)
C2—C1—C6—C5	0.2 (4)	C14—C11—C12—C13	-179.4 (3)
O1—C1—C6—C5	176.3 (2)	C9—C8—C13—C12	-2.2 (4)
C2—C1—C6—C12	-178.59 (18)	C7—C8—C13—C12	176.6 (2)
O1—C1—C6—C12	-2.5 (3)	C11—C12—C13—C8	1.0 (4)
C4—C5—C6—C1	0.5 (4)	O2—C7—O1—C1	-8.0 (3)
C4—C5—C6—C12	179.3 (2)	C8—C7—O1—C1	171.58 (18)
O2—C7—C8—C13	8.5 (4)	C6—C1—O1—C7	100.0 (3)
O1—C7—C8—C13	-171.0 (2)	C2—C1—O1—C7	-84.0 (3)

Fig. 1

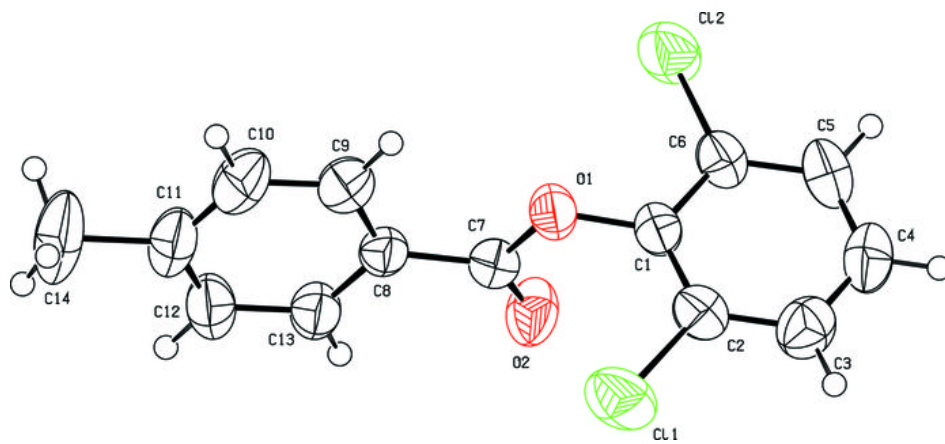


Fig. 2

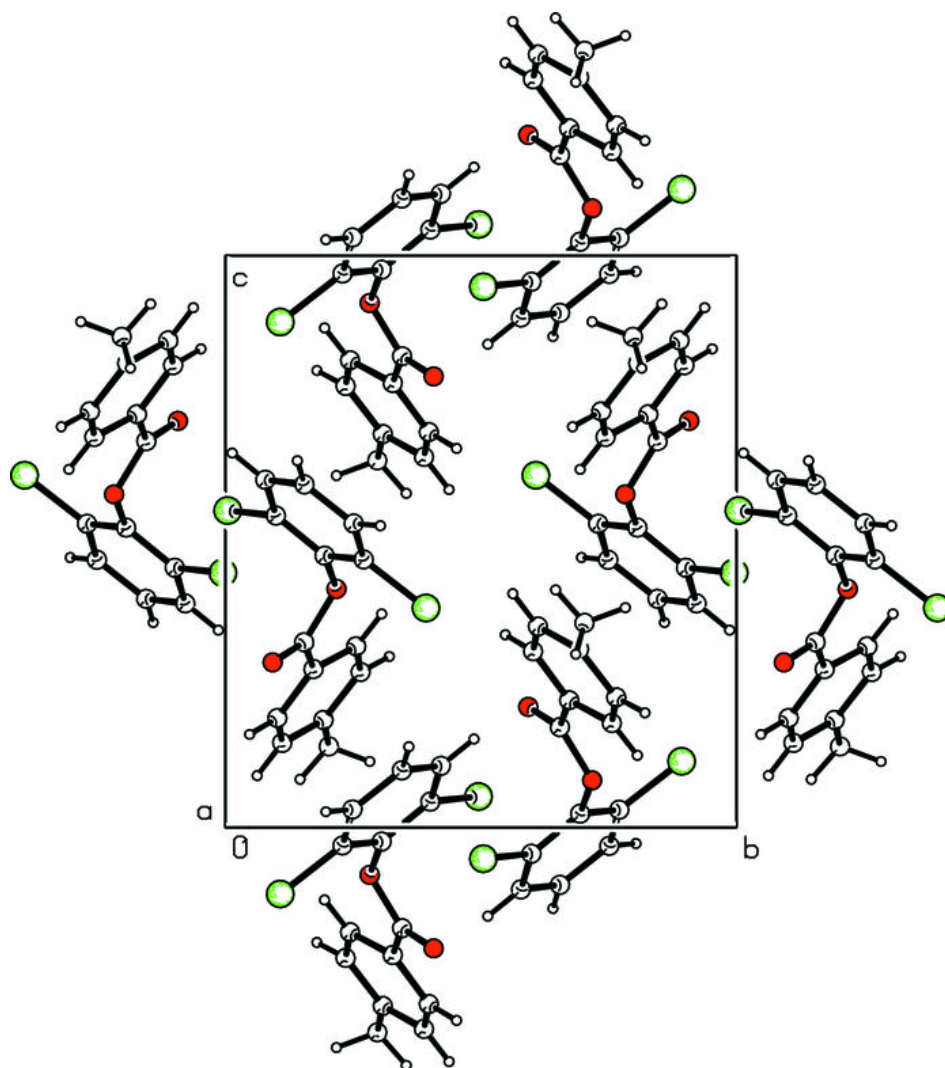


Fig. 3

