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2,4-Dichlorophenyl 4-methylbenzoate

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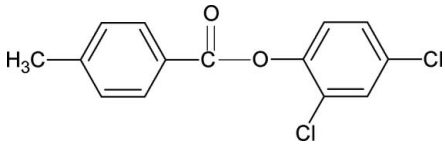
Key indicators: single-crystal X-ray study; T = 299 K; mean σ(C–C) = 0.003 Å; R factor = 0.044; wR factor = 0.130; data-to-parameter ratio = 13.7.

The structure of the title compound (24DCP4MeBA), $C_{14}H_{10}Cl_2O_2$, resembles that of phenyl benzoate (PBA), 4-methylphenyl benzoate (4MePBA) and 4-methylphenyl 4-methylbenzoate (4MeP4MeBA), with similar bond parameters. The dihedral angle between the benzene and benzoyl rings in 24DCP4MeBA is 48.13 (5)°, compared with values in the other compounds of 55.7 (PBA), 60.17 (7) (4MePBA) and 63.57 (5)° (4MeP4MeBA). The molecules of 24DCP4MeBA are packed into column-like infinite chains in the direction of the a axis.

Related literature

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



Experimental

Crystal data

$C_{14}H_{10}Cl_2O_2$
M_r = 281.12
Monoclinic, $P2_1/n$
a = 11.854 (1) Å
b = 7.2039 (9) Å
c = 15.653 (2) Å
β = 108.670 (9)°
V = 1266.3 (3) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 4.53 mm^{-1}
T = 299 (2) K
0.55 × 0.53 × 0.18 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.159, T_{max} = 0.443
4377 measured reflections
2265 independent reflections
2027 reflections with $I > 2\sigma(I)$
R_{int} = 0.034
3 standard reflections
frequency: 120 min
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.130
S = 1.05
2265 reflections
165 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.40 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 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: WN2195).

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supplementary materials

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2,4-Dichlorophenyl 4-methylbenzoate

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Comment

In the present work, as part of a study of substituent effects on the crystal structures of aromatic esters (Gowda *et al.*, 2007*a*,*b*,*c*; Gowda *et al.*, 2007), the structure of 2,4-dichlorophenyl 4-methyl benzoate (24DCP4MeBA) has been determined. The structure of 24DCP4MeBA (Fig. 1) is similar to those of phenyl benzoate (PBA) (Adams & Morsi, 1976), 4-methylphenyl benzoate (4MePBA) (Gowda *et al.*, 2007) and 4-methylphenyl 4-methylbenzoate (4MeP4MeBA) (Gowda *et al.*, 2007*c*). The bond parameters in 24DCP4MeBA are similar to those in PBA, 4MePBA, 4MeP4MeBA and other aryl benzoates (Adams & Morsi, 1976; Gowda *et al.*, 2007*a*,*b*,*c*; Gowda *et al.*, 2007). The dihedral angle between the benzene and benzoyl rings in 24DCP4MeBA is 48.13 (5)°, compared to the values of 55.7° (PBA), 60.17 (7)° (4MePBA) and 63.57 (5)° (4MeP4MeBA). The molecules in 24DCP4MeBA are packed into column-like infinite chains in the direction of the *a* 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 positioned with idealized geometry and refined using a riding model (C—H = 0.93–0.96 Å), with U_{iso}(H) = 1.2U_{eq}(parent atom).

Figures

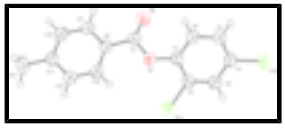

Fig. 1. Molecular structure of the title compound, showing the atom labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented as small spheres of arbitrary radius.

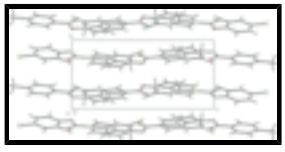

Fig. 2. Molecular packing in the title compound.

2,4-Dichlorophenyl 4-methylbenzoate

Crystal data

$C_{14}H_{10}Cl_2O_2$	F_{000} = 576
M_r = 281.12	D_x = 1.475 Mg m^{-3}
Monoclinic, $P2_1/n$	Cu $K\alpha$ radiation λ = 1.54180 Å
Hall symbol: -P 2yn	Cell parameters from 25 reflections
a = 11.854 (1) Å	θ = 5.7–23.9º
b = 7.2039 (9) Å	μ = 4.53 mm^{-1}
c = 15.653 (2) Å	T = 299 (2) K
β = 108.670 (9)º	Plate, colourless
V = 1266.3 (3) Å^3	0.55 × 0.53 × 0.18 mm
Z = 4	

Data collection

Enraf–Nonius CAD-4 diffractometer	R_{int} = 0.034
Radiation source: fine-focus sealed tube	θ_{max} = 66.9º
Monochromator: graphite	θ_{min} = 4.1º
T = 299(2) K	h = −14→11
ω/2θ scans	k = −8→0
Absorption correction: ψ scan (North *et al.*, 1968)	l = −18→18
T_{min} = 0.159, T_{max} = 0.443	3 standard reflections
4377 measured reflections	every 120 min
2265 independent reflections	intensity decay: none
2027 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.044	$w = 1/[\sigma^2(F_o^2) + (0.0785P)^2 + 0.3594P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.130	$(\Delta/\sigma)_{max}$ = 0.044
S = 1.05	$\Delta\rho_{max}$ = 0.40 e Å^{-3}
2265 reflections	$\Delta\rho_{min}$ = −0.41 e Å^{-3}
165 parameters	Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0072 (8)
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	1.10692 (18)	0.3187 (3)	0.58894 (13)	0.0423 (5)
C2	1.00700 (19)	0.2403 (3)	0.60261 (14)	0.0430 (5)
C3	1.00055 (19)	0.2195 (3)	0.68847 (14)	0.0468 (5)
H3	0.9346	0.1640	0.6977	0.056*
C4	1.0936 (2)	0.2824 (3)	0.76021 (14)	0.0467 (5)
C5	1.1917 (2)	0.3657 (4)	0.74797 (15)	0.0518 (5)
H5	1.2532	0.4095	0.7972	0.062*
C6	1.19799 (19)	0.3834 (3)	0.66157 (14)	0.0494 (5)
H6	1.2640	0.4393	0.6526	0.059*
C7	1.19791 (18)	0.2587 (3)	0.47727 (14)	0.0435 (5)
C8	1.16867 (18)	0.2425 (3)	0.37893 (13)	0.0414 (5)
C9	1.25501 (19)	0.1698 (3)	0.34566 (15)	0.0477 (5)
H9	1.3292	0.1373	0.3853	0.057*
C10	1.2311 (2)	0.1459 (3)	0.25453 (15)	0.0516 (5)
H10	1.2895	0.0959	0.2333	0.062*
C11	1.1218 (2)	0.1949 (3)	0.19339 (15)	0.0476 (5)
C12	1.0350 (2)	0.2662 (3)	0.22694 (15)	0.0488 (5)
H12	0.9607	0.2982	0.1872	0.059*
C13	1.05811 (19)	0.2900 (3)	0.31857 (14)	0.0453 (5)
H13	0.9994	0.3381	0.3400	0.054*
C14	1.0983 (3)	0.1717 (4)	0.09364 (16)	0.0683 (7)
H14A	1.1379	0.0622	0.0830	0.082*
H14B	1.1278	0.2782	0.0706	0.082*
H14C	1.0141	0.1601	0.0638	0.082*
O1	1.10552 (13)	0.3344 (2)	0.50051 (9)	0.0475 (4)
O2	1.28845 (15)	0.2095 (3)	0.53218 (11)	0.0657 (5)
Cl1	0.88757 (5)	0.17361 (9)	0.51123 (4)	0.0578 (2)
Cl2	1.08550 (6)	0.25810 (11)	0.86852 (4)	0.0663 (3)

Atomic displacement parameters (Å^2)

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

C1	0.0423 (11)	0.0501 (11)	0.0367 (10)	0.0031 (9)	0.0156 (9)	0.0014 (8)
C2	0.0395 (11)	0.0474 (11)	0.0395 (11)	0.0011 (8)	0.0092 (9)	−0.0015 (8)
C3	0.0432 (11)	0.0534 (12)	0.0472 (12)	0.0009 (9)	0.0191 (10)	0.0026 (9)
C4	0.0473 (12)	0.0579 (12)	0.0374 (11)	0.0079 (10)	0.0173 (9)	0.0031 (9)
C5	0.0461 (12)	0.0662 (14)	0.0395 (11)	−0.0022 (11)	0.0087 (9)	−0.0052 (10)
C6	0.0427 (11)	0.0618 (13)	0.0448 (11)	−0.0077 (10)	0.0153 (9)	−0.0017 (10)
C7	0.0361 (10)	0.0530 (12)	0.0422 (11)	−0.0051 (8)	0.0134 (9)	−0.0009 (8)
C8	0.0389 (11)	0.0463 (11)	0.0401 (11)	−0.0034 (8)	0.0144 (9)	0.0006 (8)
C9	0.0373 (10)	0.0585 (13)	0.0485 (12)	0.0010 (9)	0.0156 (9)	0.0021 (9)
C10	0.0479 (12)	0.0603 (13)	0.0545 (13)	0.0012 (10)	0.0273 (10)	−0.0027 (10)
C11	0.0526 (12)	0.0521 (12)	0.0421 (11)	−0.0049 (10)	0.0210 (10)	−0.0032 (9)
C12	0.0428 (11)	0.0593 (13)	0.0424 (11)	0.0017 (10)	0.0108 (9)	−0.0001 (9)
C13	0.0410 (11)	0.0544 (12)	0.0440 (11)	0.0037 (9)	0.0185 (9)	0.0006 (9)
C14	0.0794 (18)	0.0868 (19)	0.0411 (13)	−0.0041 (15)	0.0227 (12)	−0.0068 (12)
O1	0.0447 (8)	0.0631 (10)	0.0360 (7)	0.0046 (7)	0.0150 (6)	0.0030 (6)
O2	0.0422 (9)	0.1043 (14)	0.0445 (9)	0.0114 (9)	0.0054 (7)	−0.0046 (9)
Cl1	0.0448 (3)	0.0756 (5)	0.0471 (3)	−0.0110 (3)	0.0066 (2)	−0.0050 (2)
Cl2	0.0661 (4)	0.0979 (6)	0.0391 (3)	0.0083 (3)	0.0225 (3)	0.0052 (3)

Geometric parameters (Å, °)

C1—C6	1.375 (3)	C8—C9	1.391 (3)
C1—O1	1.384 (2)	C8—C13	1.391 (3)
C1—C2	1.389 (3)	C9—C10	1.373 (3)
C2—C3	1.379 (3)	C9—H9	0.9300
C2—Cl1	1.728 (2)	C10—C11	1.388 (3)
C3—C4	1.375 (3)	C10—H10	0.9300
C3—H3	0.9300	C11—C12	1.394 (3)
C4—C5	1.375 (3)	C11—C14	1.505 (3)
C4—Cl2	1.738 (2)	C12—C13	1.382 (3)
C5—C6	1.384 (3)	C12—H12	0.9300
C5—H5	0.9300	C13—H13	0.9300
C6—H6	0.9300	C14—H14A	0.9600
C7—O2	1.194 (3)	C14—H14B	0.9600
C7—O1	1.373 (3)	C14—H14C	0.9600
C7—C8	1.470 (3)		
C6—C1—O1	123.66 (19)	C13—C8—C7	123.14 (19)
C6—C1—C2	119.54 (19)	C10—C9—C8	120.3 (2)
O1—C1—C2	116.72 (18)	C10—C9—H9	119.9
C3—C2—C1	120.70 (19)	C8—C9—H9	119.9
C3—C2—Cl1	119.37 (17)	C9—C10—C11	121.4 (2)
C1—C2—Cl1	119.91 (16)	C9—C10—H10	119.3
C4—C3—C2	118.7 (2)	C11—C10—H10	119.3
C4—C3—H3	120.7	C10—C11—C12	118.22 (19)
C2—C3—H3	120.7	C10—C11—C14	120.6 (2)
C3—C4—C5	121.55 (19)	C12—C11—C14	121.2 (2)
C3—C4—Cl2	118.88 (17)	C13—C12—C11	120.8 (2)
C5—C4—Cl2	119.56 (17)	C13—C12—H12	119.6
C4—C5—C6	119.3 (2)	C11—C12—H12	119.6

C4—C5—H5	120.4	C12—C13—C8	120.3 (2)
C6—C5—H5	120.4	C12—C13—H13	119.8
C1—C6—C5	120.2 (2)	C8—C13—H13	119.8
C1—C6—H6	119.9	C11—C14—H14A	109.5
C5—C6—H6	119.9	C11—C14—H14B	109.5
O2—C7—O1	122.5 (2)	H14A—C14—H14B	109.5
O2—C7—C8	125.9 (2)	C11—C14—H14C	109.5
O1—C7—C8	111.61 (17)	H14A—C14—H14C	109.5
C9—C8—C13	118.99 (19)	H14B—C14—H14C	109.5
C9—C8—C7	117.83 (18)	C7—O1—C1	118.52 (16)
C6—C1—C2—C3	−2.9 (3)	O1—C7—C8—C13	−3.1 (3)
O1—C1—C2—C3	−179.89 (19)	C13—C8—C9—C10	0.1 (3)
C6—C1—C2—Cl1	175.41 (18)	C7—C8—C9—C10	177.9 (2)
O1—C1—C2—Cl1	−1.6 (3)	C8—C9—C10—C11	0.7 (4)
C1—C2—C3—C4	1.8 (3)	C9—C10—C11—C12	−1.2 (4)
Cl1—C2—C3—C4	−176.53 (17)	C9—C10—C11—C14	178.6 (2)
C2—C3—C4—C5	0.3 (3)	C10—C11—C12—C13	0.9 (3)
C2—C3—C4—Cl2	179.53 (17)	C14—C11—C12—C13	−178.9 (2)
C3—C4—C5—C6	−1.2 (4)	C11—C12—C13—C8	−0.2 (3)
Cl2—C4—C5—C6	179.54 (18)	C9—C8—C13—C12	−0.4 (3)
O1—C1—C6—C5	178.7 (2)	C7—C8—C13—C12	−178.0 (2)
C2—C1—C6—C5	1.9 (3)	O2—C7—O1—C1	−13.5 (3)
C4—C5—C6—C1	0.1 (4)	C8—C7—O1—C1	164.82 (18)
O2—C7—C8—C9	−2.5 (3)	C6—C1—O1—C7	57.5 (3)
O1—C7—C8—C9	179.25 (18)	C2—C1—O1—C7	−125.6 (2)
O2—C7—C8—C13	175.1 (2)		

Fig. 1

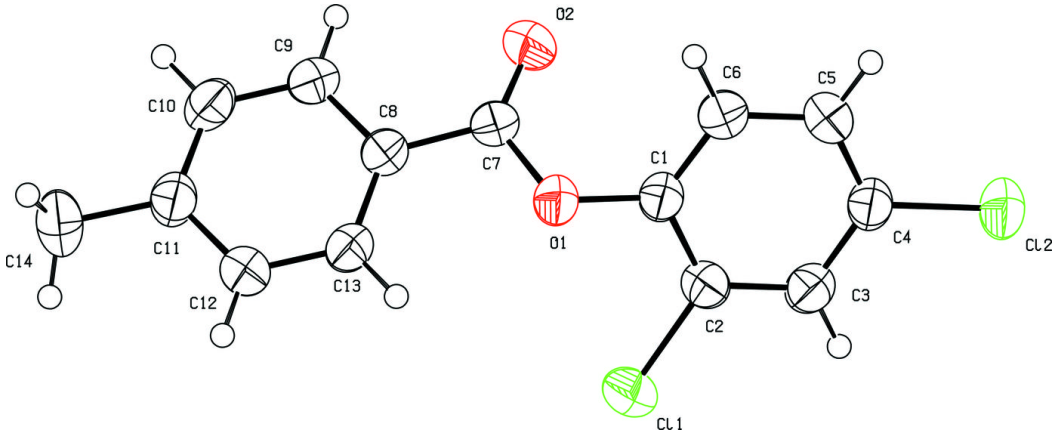

Fig. 2