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4-Methylphenyl 4-chlorobenzoate

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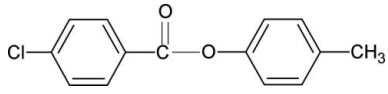
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.034; wR factor = 0.096; data-to-parameter ratio = 15.5.

The crystal structure of the title compound, $C_{14}H_{11}ClO_2$, is similar to those of phenyl benzoate, 4-methylphenyl benzoate and 4-methylphenyl 4-methylbenzoate. The dihedral angle between the phenyl and benzene rings is 51.86 (4)°. The molecules crystallize in planes parallel to ($\bar{1}$02).

Related literature

For related literature, see: Adams & Morsi (1976); Gowda, Foro, Babitha & Fuess (2007*a*,*b*,*c*,*d*,*e*); Gowda, Foro, Nayak & Fuess (2007*a*,*b*); Nayak & Gowda (2007).



Experimental

Crystal data

$C_{14}H_{11}ClO_2$
M_r = 246.68
Monoclinic, $P2_1/c$
a = 14.6932 (4) Å
b = 11.3269 (3) Å
c = 7.2386 (2) Å
β = 101.050 (3)°
V = 1182.37 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.31 mm^{-1}
T = 100 (2) K
0.40 × 0.28 × 0.08 mm

Data collection

Oxford Diffraction Xcalibur diffractometer with Sapphire CCD detector
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2006)
T_{min} = 0.887, T_{max} = 0.976
17127 measured reflections
2407 independent reflections
1889 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.096
S = 1.04
2407 reflections
155 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.04 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis RED*; 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) and *ORTEP-3* (Farrugia, 1997); 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: BT2647).

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supporting information

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4-Methylphenyl 4-chlorobenzoate

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S1. Comment

In the present work, the structure of 4-methylphenyl 4-chlorobenzoate (4MP4CBA) has been determined, as part of a study of substituent effects on the structures of industrially significant compounds (Gowda, Foro, Babitha & Fuess, 2007*a*, 2007*b*; Gowda, Foro, Nayak & Fuess, 2007*a*, 2007*b*). The structure of 4MP4CBA (Fig. 1) resembles those of phenyl benzoate (PBA)(Adams & Morsi, 1976), 4-methylphenyl benzoate (4MPBA) (Gowda, Foro, Nayak & Fuess, 2007*b*), 4-methylphenyl 4-methylbenzoate (4MP4MBA)(Gowda, Foro, Babitha & Fuess, 2007*b*) and other aryl benzoates (Gowda, Foro, Babitha & Fuess, 2007*a*; Gowda, Foro, Nayak & Fuess, 2007*a*). The bond parameters in 4MP4CBA are similar to those in PBA, 4MPBA, 4MP4MBA and other benzoates (Gowda, Foro, Babitha & Fuess, 2007*a*, 2007*b*; Gowda, Foro, Nayak & Fuess, 2007*a*, 2007*b*). The molecules in the title compound are packed into plane parallel to (-1 0 2) (Fig. 2).

S2. 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.

S3. Refinement

The H atoms of the methyl groups were positioned with idealized geometry using a riding model with C—H = 0.98 Å. The other H atoms were located in difference map and their positions refined.

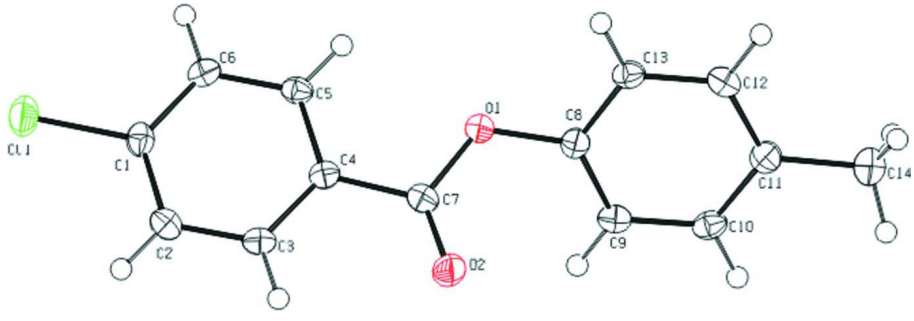

Figure 1

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.

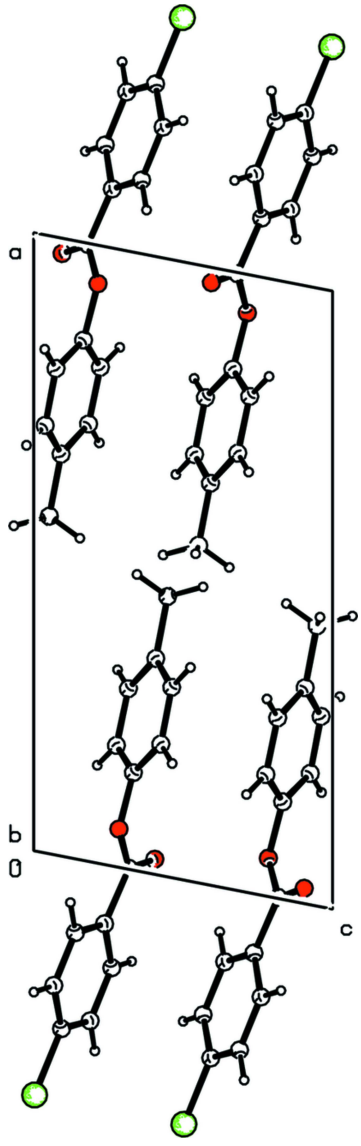

Figure 2

Molecular packing of the title compound.

4-Methylphenyl 4-chlorobenzoate

Crystal data

$C_{14}H_{11}ClO_2$
$M_r = 246.68$
Monoclinic, $P2_1/c$
Hall symbol: -P2ybc
$a = 14.6932\ (4)$ Å
$b = 11.3269\ (3)$ Å
$c = 7.2386\ (2)$ Å
$\beta = 101.050\ (3)°$
$V = 1182.37\ (6)$ Å^3
$Z = 4$

$F(000) = 512$
$D_x = 1.386$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5716 reflections
$\theta = 2.2–26.9°$
$\mu = 0.31$ mm^{-1}
$T = 100$ K
Prism, colourless
0.40 × 0.28 × 0.08 mm

Data collection

Oxford Diffraction Xcalibur diffractometer with Sapphire CCD detector
Radiation source: Enhance (Mo) X-ray Source
Graphite monochromator
Detector resolution: 8.4012 pixels mm^{-1}
Rotation method data acquisition using ω scans.
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2006)
T_{min} = 0.887, T_{max} = 0.976

17127 measured reflections
2407 independent reflections
1889 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 26.4°, θ_{min} = 2.3°
h = −18→18
k = −13→14
l = −9→9

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.096
S = 1.04
2407 reflections
155 parameters
0 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0437P)^2 + 0.873P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.04 e $Å^{-3}$
$\Delta\rho_{min}$ = −0.29 e $Å^{-3}$

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 ($Å^2$)

	x	y	z	U_{iso}*/U_{eq}
Cl1	−0.39495 (3)	0.43951 (5)	0.00266 (7)	0.03131 (16)
O1	0.06211 (8)	0.40950 (10)	0.28512 (17)	0.0203 (3)
O2	0.02463 (9)	0.23571 (11)	0.40524 (18)	0.0264 (3)
C1	−0.27915 (12)	0.40681 (16)	0.0929 (2)	0.0204 (4)
C2	−0.25731 (12)	0.30158 (16)	0.1886 (2)	0.0214 (4)
H2	−0.3045	0.2473	0.2043	0.026*
C3	−0.16463 (12)	0.27738 (15)	0.2611 (2)	0.0193 (4)
H3	−0.1481	0.2058	0.3275	0.023*
C4	−0.09585 (11)	0.35718 (15)	0.2371 (2)	0.0172 (3)
C5	−0.11937 (12)	0.46239 (15)	0.1393 (2)	0.0184 (4)
H5	−0.0723	0.5167	0.1224	0.022*
C6	−0.21182 (12)	0.48738 (15)	0.0668 (2)	0.0196 (4)
H6	−0.2287	0.5588	0.0002	0.024*
C7	0.00171 (12)	0.32497 (15)	0.3186 (2)	0.0188 (4)
C8	0.15790 (11)	0.38716 (16)	0.3334 (2)	0.0185 (4)
C9	0.19650 (12)	0.28504 (15)	0.2769 (2)	0.0197 (4)

H9	0.1583	0.2245	0.2123	0.024*
C10	0.29215 (12)	0.27312 (15)	0.3169 (2)	0.0208 (4)
H10	0.3193	0.2028	0.2806	0.025*
C11	0.34947 (12)	0.36115 (16)	0.4084 (2)	0.0222 (4)
C12	0.30820 (12)	0.46299 (16)	0.4619 (2)	0.0224 (4)
H12	0.3462	0.5244	0.5243	0.027*
C13	0.21257 (12)	0.47634 (15)	0.4254 (2)	0.0199 (4)
H13	0.1851	0.5460	0.4633	0.024*
C14	0.45367 (13)	0.34475 (18)	0.4483 (3)	0.0327 (5)
H14A	0.4683	0.2603	0.4581	0.049*
H14B	0.4805	0.3840	0.5669	0.049*
H14C	0.4797	0.3794	0.3457	0.049*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0190 (2)	0.0368 (3)	0.0365 (3)	0.00206 (19)	0.00115 (18)	0.0060 (2)
O1	0.0181 (6)	0.0181 (6)	0.0245 (6)	−0.0002 (5)	0.0033 (5)	0.0019 (5)
O2	0.0240 (7)	0.0247 (7)	0.0303 (7)	0.0022 (5)	0.0044 (5)	0.0110 (6)
C1	0.0170 (8)	0.0249 (9)	0.0192 (9)	0.0012 (7)	0.0032 (7)	−0.0033 (7)
C2	0.0224 (9)	0.0220 (9)	0.0200 (9)	−0.0038 (7)	0.0049 (7)	−0.0003 (7)
C3	0.0254 (9)	0.0158 (8)	0.0168 (8)	−0.0002 (7)	0.0043 (7)	0.0003 (7)
C4	0.0206 (8)	0.0167 (8)	0.0149 (8)	0.0011 (7)	0.0052 (6)	−0.0018 (7)
C5	0.0221 (8)	0.0160 (8)	0.0184 (8)	−0.0012 (7)	0.0070 (7)	−0.0010 (7)
C6	0.0239 (9)	0.0168 (8)	0.0190 (8)	0.0033 (7)	0.0062 (7)	0.0012 (7)
C7	0.0215 (8)	0.0184 (9)	0.0171 (8)	−0.0022 (7)	0.0051 (7)	−0.0016 (7)
C8	0.0183 (8)	0.0209 (9)	0.0167 (8)	0.0008 (7)	0.0047 (7)	0.0041 (7)
C9	0.0252 (9)	0.0173 (9)	0.0166 (8)	−0.0010 (7)	0.0043 (7)	0.0000 (7)
C10	0.0265 (9)	0.0178 (9)	0.0200 (8)	0.0031 (7)	0.0087 (7)	0.0009 (7)
C11	0.0221 (9)	0.0234 (9)	0.0226 (9)	0.0010 (7)	0.0080 (7)	0.0037 (7)
C12	0.0241 (9)	0.0200 (9)	0.0231 (9)	−0.0041 (7)	0.0045 (7)	−0.0005 (7)
C13	0.0239 (9)	0.0166 (8)	0.0205 (9)	0.0013 (7)	0.0074 (7)	−0.0002 (7)
C14	0.0221 (9)	0.0310 (11)	0.0448 (12)	0.0012 (8)	0.0061 (8)	0.0015 (9)

Geometric parameters (Å, º)

Cl1—C1	1.7414 (17)	C8—C13	1.380 (2)
O1—C7	1.359 (2)	C8—C9	1.384 (2)
O1—C8	1.407 (2)	C9—C10	1.386 (2)
O2—C7	1.203 (2)	C9—H9	0.9500
C1—C2	1.385 (3)	C10—C11	1.389 (3)
C1—C6	1.385 (3)	C10—H10	0.9500
C2—C3	1.390 (2)	C11—C12	1.392 (3)
C2—H2	0.9500	C11—C14	1.514 (2)
C3—C4	1.391 (2)	C12—C13	1.387 (2)
C3—H3	0.9500	C12—H12	0.9500
C4—C5	1.395 (2)	C13—H13	0.9500
C4—C7	1.487 (2)	C14—H14A	0.9800

C5—C6	1.388 (2)	C14—H14B	0.9800
C5—H5	0.9500	C14—H14C	0.9800
C6—H6	0.9500		

C7—O1—C8	119.05 (13)	C13—C8—O1	116.77 (15)
C2—C1—C6	122.14 (16)	C9—C8—O1	121.61 (15)
C2—C1—Cl1	119.12 (14)	C8—C9—C10	118.44 (16)
C6—C1—Cl1	118.74 (14)	C8—C9—H9	120.8
C1—C2—C3	118.36 (16)	C10—C9—H9	120.8
C1—C2—H2	120.8	C9—C10—C11	121.84 (16)
C3—C2—H2	120.8	C9—C10—H10	119.1
C2—C3—C4	120.50 (16)	C11—C10—H10	119.1
C2—C3—H3	119.8	C10—C11—C12	118.09 (16)
C4—C3—H3	119.8	C10—C11—C14	120.10 (16)
C3—C4—C5	120.19 (16)	C12—C11—C14	121.81 (17)
C3—C4—C7	117.33 (15)	C13—C12—C11	121.12 (17)
C5—C4—C7	122.48 (15)	C13—C12—H12	119.4
C6—C5—C4	119.67 (16)	C11—C12—H12	119.4
C6—C5—H5	120.2	C8—C13—C12	119.11 (16)
C4—C5—H5	120.2	C8—C13—H13	120.4
C1—C6—C5	119.14 (16)	C12—C13—H13	120.4
C1—C6—H6	120.4	C11—C14—H14A	109.5
C5—C6—H6	120.4	C11—C14—H14B	109.5
O2—C7—O1	123.92 (15)	H14A—C14—H14B	109.5
O2—C7—C4	124.41 (15)	C11—C14—H14C	109.5
O1—C7—C4	111.66 (14)	H14A—C14—H14C	109.5
C13—C8—C9	121.39 (16)	H14B—C14—H14C	109.5

C6—C1—C2—C3	0.4 (3)	C3—C4—C7—O1	179.72 (14)
Cl1—C1—C2—C3	−179.45 (13)	C5—C4—C7—O1	−0.1 (2)
C1—C2—C3—C4	−0.2 (3)	C7—O1—C8—C13	−134.88 (16)
C2—C3—C4—C5	−0.2 (3)	C7—O1—C8—C9	50.6 (2)
C2—C3—C4—C7	−179.97 (15)	C13—C8—C9—C10	0.8 (3)
C3—C4—C5—C6	0.3 (2)	O1—C8—C9—C10	174.97 (14)
C7—C4—C5—C6	−179.89 (15)	C8—C9—C10—C11	−1.1 (3)
C2—C1—C6—C5	−0.2 (3)	C9—C10—C11—C12	0.6 (3)
Cl1—C1—C6—C5	179.59 (13)	C9—C10—C11—C14	−179.67 (17)
C4—C5—C6—C1	−0.1 (3)	C10—C11—C12—C13	0.2 (3)
C8—O1—C7—O2	7.9 (2)	C14—C11—C12—C13	−179.55 (17)
C8—O1—C7—C4	−172.71 (14)	C9—C8—C13—C12	0.0 (3)
C3—C4—C7—O2	−0.9 (3)	O1—C8—C13—C12	−174.50 (15)
C5—C4—C7—O2	179.27 (17)	C11—C12—C13—C8	−0.5 (3)