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2-Chlorophenyl 4-methylbenzoate

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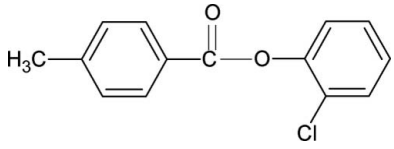
Key indicators: single-crystal X-ray study; T = 299 K; mean σ(C–C) = 0.005 Å; R factor = 0.035; wR factor = 0.116; data-to-parameter ratio = 14.4.

The conformation of the C=O bond in the title compound, $C_{14}H_{11}ClO_2$, is *anti* to the Cl atom, similar to what was observed in 2-methylphenyl 4-methylbenzoate. The dihedral angle between the two aromatic rings is 59.36 (7)°.

Related literature

For related literature, see: Gowda *et al.* (2008*a*,*b*,*c*); Nayak & Gowda (2008).



Experimental

Crystal data

$C_{14}H_{11}ClO_2$
M_r = 246.68
Monoclinic, $P2_1$
a = 4.0538 (8) Å
b = 13.661 (3) Å
c = 10.975 (2) Å
β = 91.70 (2)°
V = 607.5 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.30 mm^{-1}
T = 299 (2) K
0.48 × 0.24 × 0.16 mm

Data collection

Oxford Diffraction Xcalibur diffractometer with a Sapphire CCD detector
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
T_{min} = 0.869, T_{max} = 0.954
4160 measured reflections
2238 independent reflections
1632 reflections with $I > 2\sigma(I)$
R_{int} = 0.012

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.116
S = 1.15
2238 reflections
155 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}
Absolute structure: Flack (1983), 957 Friedel pairs
Flack parameter: −0.09 (9)

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2004); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2007); data reduction: *CrysAlis RED*; 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: BT2750).

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supporting information

Acta Cryst. (2008). E**64**, o1546 [doi:10.1107/S1600536808022290]

2-Chlorophenyl 4-methylbenzoate

B. Thimme Gowda, Sabine Foro, K. S. Babitha and Hartmut Fuess

S1. Comment

As part of a study of the substituent effects on the crystal structures of aryl benzoates (Gowda *et al.*, 2008*a*, 2008*b*, 2008*c*), in the present work, the structure of 2-chlorophenyl 4-methylbenzoate (2CP4MBA) has been determined. The conformation of the C=O bond in 2CP4MBA is *anti* to the *ortho*-chloro group in the phenolic benzene ring (Fig. 1), similar to what is observed in 2-methylphenyl 4-methylbenzoate (2MP4MBA) (Gowda *et al.*, 2008*c*). The dihedral angle between the benzene and benzoyl rings in 2CP4MBA is 59.36 (7)°, compared with the values of 71.75 (7)° in 3CP4MBA (Gowda *et al.*, 2008*a*), 63.89 (8)° in 4CP4MBA (Gowda *et al.*, 2008*b*) and 73.04 (8)° in 2MP4MBA (Gowda *et al.*, 2008*c*). Further, the bond parameters in 2CP4MBA are similar to those in 2MP4MBA and other aryl benzoates (Gowda *et al.*, 2008*a, b, c*). The packing diagram is shown in Fig. 2.

S2. Experimental

The title compound was prepared according to a method of 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 used in X-ray diffraction studies were obtained by slow evaporation of ethanolic solution of the title compound.

S3. Refinement

The H atoms were positioned with idealized geometry and refined using a riding model with $C_{aromatic}$—H = 0.93Å or C_{methyl}—H = 0.96 Å and with isotropic displacement parameters set to 1.2 U_{eq}(C) or 1.5U_{eq}(C_{methyl}). The methyl group was allowed to rotate but not to tip.

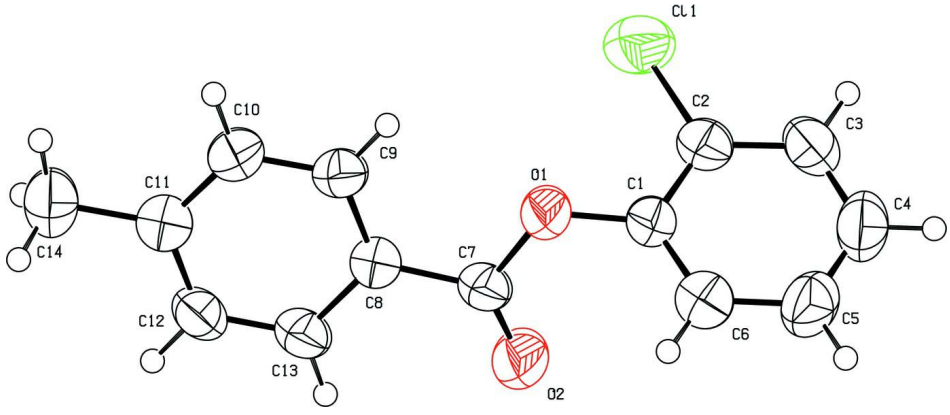

Figure 1

Molecular structure of the title compound, showing the atom labeling scheme. The displacement ellipsoids are drawn at the 50% probability level. The H atoms are represented as small spheres of arbitrary radii.

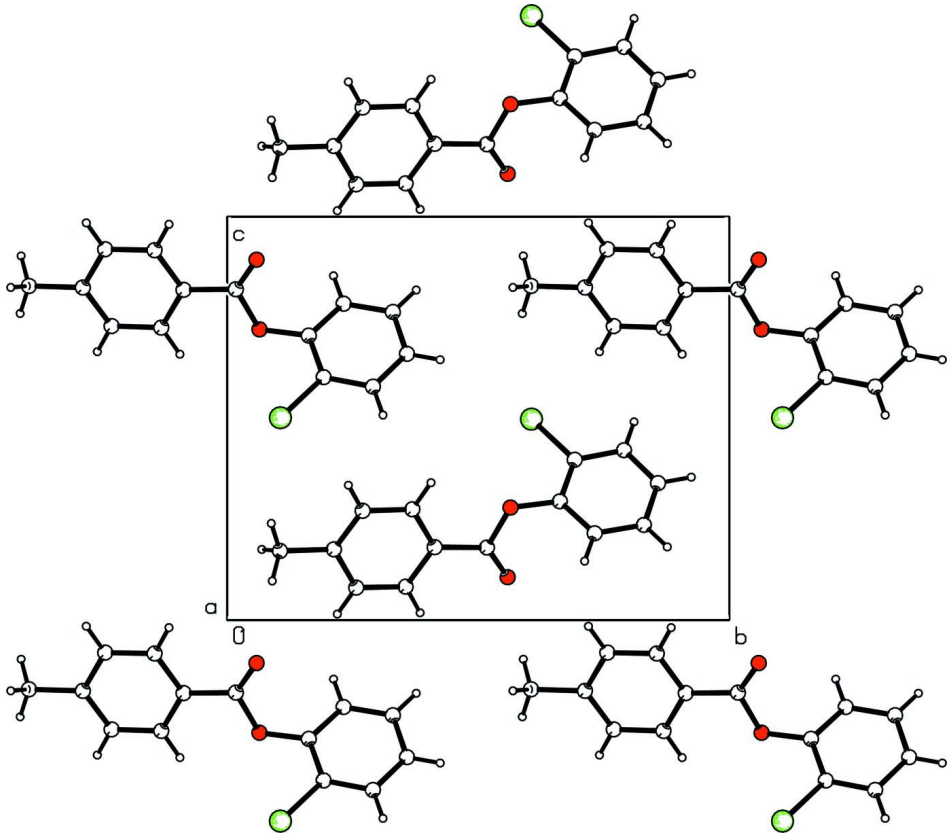

Figure 2

Packing diagram of the title compound.

2-Chlorophenyl 4-methylbenzoate

Crystal data

$C_{14}H_{11}ClO_2$
$M_r = 246.68$
Monoclinic, $P2_1$
Hall symbol: P 2yb
$a = 4.0538\ (8)$ Å
$b = 13.661\ (3)$ Å
$c = 10.975\ (2)$ Å
$\beta = 91.70\ (2)°$
$V = 607.5\ (2)$ Å^3
$Z = 2$
$F(000) = 256$
$D_x = 1.349$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1136 reflections
$\theta = 2.4–27.8°$
$\mu = 0.30$ mm^{-1}
$T = 299$ K
Long needle, colourless
0.48 × 0.24 × 0.16 mm

Data collection

Oxford Diffraction Xcalibur diffractometer with a Sapphire CCD detector
Radiation source: fine-focus sealed tube
Graphite monochromator
Rotation method data acquisition using ω and φ scans
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
$T_{min} = 0.869$, $T_{max} = 0.954$
4160 measured reflections
2238 independent reflections
1632 reflections with $I > 2\sigma(I)$
$R_{int} = 0.012$
$\theta_{max} = 26.4°$, $\theta_{min} = 2.4°$
$h = -5\rightarrow5$
$k = -17\rightarrow15$
$l = -13\rightarrow7$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.116$
$S = 1.15$
2238 reflections
155 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.0644P)^2 + 0.0085P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.018$
$\Delta\rho_{max} = 0.36$ e Å^{-3}
$\Delta\rho_{min} = -0.34$ e Å^{-3}
Absolute structure: Flack (1983), 957 Friedel pairs
Absolute structure parameter: −0.09 (9)

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.7402 (8)	0.6625 (2)	0.2945 (2)	0.0525 (7)
C2	0.5813 (7)	0.6919 (2)	0.3974 (2)	0.0570 (8)
C3	0.5373 (9)	0.7904 (3)	0.4209 (3)	0.0699 (10)
H3	0.4350	0.8104	0.4914	0.084*
C4	0.6454 (10)	0.8581 (3)	0.3396 (3)	0.0801 (11)
H4	0.6107	0.9243	0.3544	0.096*
C5	0.8047 (9)	0.8300 (3)	0.2364 (4)	0.0751 (10)
H5	0.8796	0.8765	0.1819	0.090*
C6	0.8512 (9)	0.7319 (3)	0.2154 (3)	0.0677 (8)
H6	0.9600	0.7122	0.1461	0.081*
C7	0.6657 (7)	0.5173 (2)	0.1796 (2)	0.0513 (7)
C8	0.7526 (7)	0.4132 (2)	0.1815 (2)	0.0460 (6)
C9	0.9317 (7)	0.3687 (2)	0.2745 (2)	0.0527 (7)
H9	1.0084	0.4057	0.3406	0.063*
C10	0.9986 (7)	0.2701 (2)	0.2709 (3)	0.0579 (7)
H10	1.1216	0.2417	0.3345	0.069*
C11	0.8878 (7)	0.2126 (2)	0.1756 (3)	0.0548 (7)
C12	0.7055 (7)	0.2569 (2)	0.0806 (2)	0.0562 (8)
H12	0.6276	0.2192	0.0153	0.067*
C13	0.6405 (7)	0.3554 (2)	0.0827 (2)	0.0552 (7)
H13	0.5216	0.3841	0.0184	0.066*
C14	0.9603 (8)	0.1054 (3)	0.1717 (3)	0.0726 (8)
H14A	1.1020	0.0880	0.2399	0.087*

H14B	1.0677	0.0900	0.0973	0.087*
H14C	0.7577	0.0693	0.1754	0.087*
O1	0.7986 (5)	0.56428 (14)	0.27927 (18)	0.0615 (6)
O2	0.4938 (7)	0.55841 (16)	0.1064 (2)	0.0776 (7)
Cl1	0.4406 (2)	0.60598 (9)	0.49831 (7)	0.0834 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0659 (17)	0.0460 (19)	0.0452 (14)	0.0061 (14)	−0.0050 (12)	−0.0011 (12)
C2	0.0682 (19)	0.055 (2)	0.0468 (15)	−0.0031 (15)	−0.0084 (13)	−0.0042 (13)
C3	0.088 (2)	0.067 (3)	0.0541 (17)	0.0134 (19)	−0.0046 (16)	−0.0151 (16)
C4	0.103 (3)	0.047 (2)	0.089 (2)	0.008 (2)	−0.022 (2)	−0.008 (2)
C5	0.092 (3)	0.050 (2)	0.082 (2)	−0.0120 (19)	−0.0133 (19)	0.0066 (17)
C6	0.083 (2)	0.061 (2)	0.0597 (16)	−0.0017 (17)	−0.0004 (15)	−0.0015 (15)
C7	0.0616 (17)	0.0522 (19)	0.0397 (12)	−0.0047 (14)	−0.0037 (12)	−0.0034 (13)
C8	0.0517 (15)	0.0460 (18)	0.0405 (12)	−0.0052 (12)	0.0039 (11)	−0.0023 (11)
C9	0.0592 (18)	0.054 (2)	0.0442 (12)	−0.0002 (14)	−0.0031 (12)	0.0047 (12)
C10	0.0649 (18)	0.055 (2)	0.0529 (15)	0.0061 (15)	−0.0060 (13)	0.0039 (13)
C11	0.0583 (15)	0.046 (2)	0.0602 (16)	−0.0030 (14)	0.0119 (13)	−0.0024 (12)
C12	0.0686 (18)	0.057 (2)	0.0431 (14)	−0.0091 (15)	0.0048 (13)	−0.0107 (13)
C13	0.0638 (18)	0.0587 (19)	0.0427 (12)	−0.0029 (16)	−0.0052 (12)	−0.0060 (14)
C14	0.080 (2)	0.054 (2)	0.084 (2)	0.000 (2)	0.0041 (16)	−0.0060 (19)
O1	0.0858 (15)	0.0461 (12)	0.0514 (11)	0.0094 (10)	−0.0167 (10)	−0.0022 (8)
O2	0.1052 (17)	0.0570 (14)	0.0686 (13)	0.0119 (13)	−0.0286 (13)	−0.0011 (11)
Cl1	0.1042 (7)	0.0856 (6)	0.0608 (4)	−0.0113 (6)	0.0082 (4)	0.0093 (4)

Geometric parameters (Å, º)

C1—C6	1.370 (5)	C8—C9	1.376 (4)
C1—O1	1.374 (3)	C8—C13	1.406 (4)
C1—C2	1.376 (4)	C9—C10	1.375 (4)
C2—C3	1.382 (4)	C9—H9	0.9300
C2—Cl1	1.723 (3)	C10—C11	1.373 (4)
C3—C4	1.366 (5)	C10—H10	0.9300
C3—H3	0.9300	C11—C12	1.398 (4)
C4—C5	1.375 (6)	C11—C14	1.495 (5)
C4—H4	0.9300	C12—C13	1.372 (4)
C5—C6	1.373 (5)	C12—H12	0.9300
C5—H5	0.9300	C13—H13	0.9300
C6—H6	0.9300	C14—H14A	0.9600
C7—O2	1.188 (3)	C14—H14B	0.9600
C7—O1	1.365 (3)	C14—H14C	0.9600
C7—C8	1.465 (4)		
C6—C1—O1	122.5 (3)	C13—C8—C7	117.5 (2)
C6—C1—C2	119.3 (3)	C10—C9—C8	120.8 (3)
O1—C1—C2	118.1 (3)	C10—C9—H9	119.6

C1—C2—C3	120.2 (3)	C8—C9—H9	119.6
C1—C2—Cl1	120.1 (2)	C11—C10—C9	121.5 (3)
C3—C2—Cl1	119.7 (2)	C11—C10—H10	119.3
C4—C3—C2	119.4 (3)	C9—C10—H10	119.3
C4—C3—H3	120.3	C10—C11—C12	118.3 (3)
C2—C3—H3	120.3	C10—C11—C14	121.5 (3)
C3—C4—C5	121.1 (4)	C12—C11—C14	120.2 (3)
C3—C4—H4	119.5	C13—C12—C11	120.6 (2)
C5—C4—H4	119.5	C13—C12—H12	119.7
C6—C5—C4	118.8 (4)	C11—C12—H12	119.7
C6—C5—H5	120.6	C12—C13—C8	120.4 (2)
C4—C5—H5	120.6	C12—C13—H13	119.8
C1—C6—C5	121.3 (3)	C8—C13—H13	119.8
C1—C6—H6	119.4	C11—C14—H14A	109.5
C5—C6—H6	119.4	C11—C14—H14B	109.5
O2—C7—O1	121.9 (3)	H14A—C14—H14B	109.5
O2—C7—C8	127.2 (2)	C11—C14—H14C	109.5
O1—C7—C8	110.8 (2)	H14A—C14—H14C	109.5
C9—C8—C13	118.3 (3)	H14B—C14—H14C	109.5
C9—C8—C7	124.1 (2)	C7—O1—C1	119.4 (2)

C6—C1—C2—C3	−0.6 (4)	C13—C8—C9—C10	−0.2 (4)
O1—C1—C2—C3	175.5 (3)	C7—C8—C9—C10	178.8 (3)
C6—C1—C2—Cl1	−179.8 (2)	C8—C9—C10—C11	−0.5 (4)
O1—C1—C2—Cl1	−3.7 (4)	C9—C10—C11—C12	0.5 (4)
C1—C2—C3—C4	1.7 (5)	C9—C10—C11—C14	−180.0 (3)
Cl1—C2—C3—C4	−179.1 (3)	C10—C11—C12—C13	0.2 (4)
C2—C3—C4—C5	−1.7 (5)	C14—C11—C12—C13	−179.3 (3)
C3—C4—C5—C6	0.6 (5)	C11—C12—C13—C8	−0.9 (4)
O1—C1—C6—C5	−176.4 (3)	C9—C8—C13—C12	0.9 (4)
C2—C1—C6—C5	−0.4 (5)	C7—C8—C13—C12	−178.2 (3)
C4—C5—C6—C1	0.4 (5)	O2—C7—O1—C1	−1.7 (4)
O2—C7—C8—C9	−174.5 (3)	C8—C7—O1—C1	−179.1 (3)
O1—C7—C8—C9	2.7 (4)	C6—C1—O1—C7	−64.4 (4)
O2—C7—C8—C13	4.5 (5)	C2—C1—O1—C7	119.6 (3)
O1—C7—C8—C13	−178.3 (2)		