Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# 4-Chlorophenyl 4-chlorobenzoate

**B. Thimme Gowda,[a]* Sabine Foro,[b] K. S. Babitha[a] and Hartmut Fuess[b]**

[a]Department of Chemistry, Mangalore University, Mangalagangotri 574 199, Mangalore, India, and [b]Institute of Materials Science, Darmstadt University of Technology, Petersenstrasse 23, D-64287 Darmstadt, Germany
Correspondence e-mail: gowdabt@yahoo.com

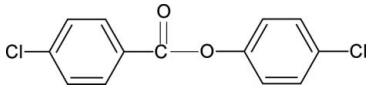
Received 18 July 2008; accepted 20 July 2008

Key indicators: single-crystal X-ray study; $T$ = 299 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.048; $wR$ factor = 0.139; data-to-parameter ratio = 11.8.

The structure of the title compound (4CP4CBA), $C_{13}H_8Cl_2O_2$, resembles those of 4-methylphenyl 4-chlorobenzoate (4MP4CBA), 4-chlorophenyl 4-methylbenzoate (4CP4MBA) and 4-methylphenyl 4-methylbenzoate (4MP4MBA), with similar bond parameters. The dihedral angle between the two benzene rings in 4CP4CBA is 47.98 (7)°, compared with 51.86 (4)° in 4MP4CBA, 63.89 (8)° in 4CP4MBA and 63.57 (5)° in 4MP4MBA. In the crystal structure, molecules are linked into helical chains running along the $b$ axis by C—H—O hydrogen bonds.

## Related literature

For related literature, see: Gowda *et al.* (2007); Gowda, Foro *et al.* (2008); Gowda, Svoboda *et al.* (2008); Nayak & Gowda (2008).



## Experimental

### *Crystal data*

$C_{13}H_8Cl_2O_2$
$M_r$ = 267.09
Monoclinic, $P2_1/n$
$a$ = 15.370 (2) Å
$b$ = 3.9528 (4) Å
$c$ = 19.465 (2) Å
$\beta$ = 91.804 (9)°
$V$ = 1182.0 (2) Å$^3$
$Z$ = 4
Cu $K\alpha$ radiation
$\mu$ = 4.83 mm$^{-1}$
$T$ = 299 (2) K
0.45 × 0.23 × 0.18 mm

### *Data collection*

Enraf–Nonius CAD-4 diffractometer
Absorption correction: $\psi$ scan (North *et al.*, 1968)
$T_{min}$ = 0.194, $T_{max}$ = 0.420
4211 measured reflections
2109 independent reflections
1724 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.080
3 standard reflections
frequency: 120 min
intensity decay: 1.0%

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.139
$S$ = 1.05
2109 reflections
178 parameters
Only H-atom coordinates refined
$\Delta\rho_{max}$ = 0.39 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.33 e Å$^{-3}$

**Table 1**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C5—H5···O2$^{i}$ | 0.92 (3) | 2.58 (3) | 3.168 (3) | 123 (2) |

Symmetry code: (i) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$.

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*.

BTG thanks the Alexander von Humboldt Foundation, Bonn, Germany, for extensions of his research fellowship.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2640).

## References

Enraf–Nonius (1996). *CAD-4-PC*. Enraf–Nonius, Delft, The Netherlands.
Gowda, B. T., Foro, S., Babitha, K. S. & Fuess, H. (2007). *Acta Cryst.* E**63**, o3867.
Gowda, B. T., Foro, S., Babitha, K. S. & Fuess, H. (2008). *Acta Cryst.* E**64**, o1518.
Gowda, B. T., Svoboda, I., Babitha, K. S. & Fuess, H. (2008). *Acta Cryst.* E**64**, o88.
Nayak, R. & Gowda, B. T. (2008). *Z. Naturforsch. Teil A*, **63**. In the press.
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Stoe & Cie (1987). *REDU4*. Stoe & Cie GmbH, Darmstadt, Germany.

# supporting information

*Acta Cryst.* (2008). E**64**, o1582 [doi:10.1107/S1600536808022800]

## 4-Chlorophenyl 4-chlorobenzoate

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

### S1. Comment

As part of a study of the substituent effects on the solid state structures of aryl benzoates (Gowda *et al.*, 2007; Gowda, Foro *et al.*, 2008; Gowda, Svoboda *et al.*, 2008), the crystal structure of 4-chlorophenyl 4-chlorobenzoate (4CP4CBA) has been determined. The structure (Fig. 1) is similar to those of 4-methylphenyl 4-chlorobenzoate (4MP4CBA) (Gowda, Svoboda *et al.*, 2008), 4-chlorophenyl 4-methylbenzoate (4CP4MBA) (Gowda, Foro *et al.*, 2008) and 4-methylphenyl 4-methylbenzoate (4MP4MBA) (Gowda *et al.*, 2007). The bond parameters in 4CP4CBA are similar to those in afore mentioned 4MP4CBA, 4CP4MBA, 4MP4MBA and other aryl benzoates (Gowda *et al.*, 2007; Gowda, Foro *et al.*, 2008; Gowda, Svoboda *et al.*, 2008). The dihedral angle between the benzene and benzoyl rings in 4CP4CBA is 47.98 (7)°, compared to the values of 51.86 (4)° in 4MP4CBA, 63.89 (8)° in 4CP4MBA and 63.57 (5)° in 4MP4MBA.

In the crystal structure, the molecules are linked into helical chains (Fig. 2) running along the *b* axis by C—H—O hydrogen bonds (Table 1).

### S2. 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 used in X-ray diffraction studies were obtained by slow evaporation of its ethanol solution.

### S3. Refinement

H atoms were located in a difference map and their positional parameters were refined [C-H = 0.90 (3)–0.97 (3) Å] with $U_{iso}$(H) = 1.2$U_{eq}$(C).

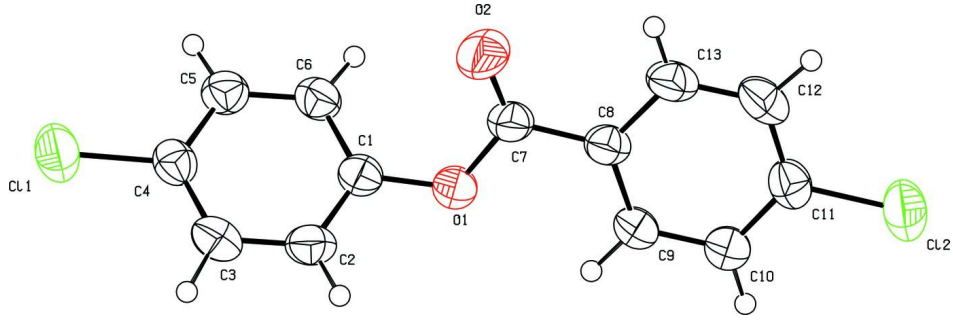



**Figure 1**

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.

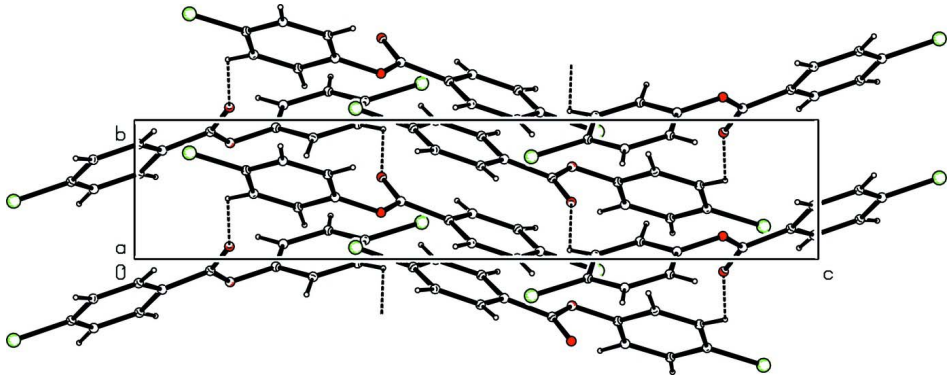



**Figure 2**

Molecular packing of the title compound.

### 4-Chlorophenyl 4-chlorobenzoate

*Crystal data*

$C_{13}H_8Cl_2O_2$
$M_r = 267.09$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 15.370$ (2) Å
$b = 3.9528$ (4) Å
$c = 19.465$ (2) Å
$\beta = 91.804$ (9)°
$V = 1182.0$ (2) Å$^3$
$Z = 4$
$F(000) = 544$
$D_x = 1.501$ Mg m$^{-3}$
Cu $K\alpha$ radiation, $\lambda = 1.54180$ Å
Cell parameters from 25 reflections
$\theta = 11.5$–$24.3°$
$\mu = 4.83$ mm$^{-1}$
$T = 299$ K
Rod, colourless
0.45 × 0.23 × 0.18 mm

*Data collection*

Enraf–Nonius CAD-4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega/2\theta$ scans
Absorption correction: $\psi$ scan (North *et al.*, 1968)
$T_{min} = 0.194$, $T_{max} = 0.420$
4211 measured reflections
2109 independent reflections
1724 reflections with $I > 2\sigma(I)$
$R_{int} = 0.080$
$\theta_{max} = 67.0°$, $\theta_{min} = 3.6°$
$h = -18 \rightarrow 18$
$k = -4 \rightarrow 0$
$l = -23 \rightarrow 23$
3 standard reflections every 120 min
intensity decay: 1.0%

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.139$
$S = 1.05$
2109 reflections
178 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
Only H-atom coordinates refined
$w = 1/[\sigma^2(F_o^2) + (0.0736P)^2 + 0.2805P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.021$
$\Delta\rho_{max} = 0.39$ e Å$^{-3}$
$\Delta\rho_{min} = -0.33$ 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 (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cl1 | 0.49228 (5) | 0.7640 (2) | 0.08027 (4) | 0.0690 (3) |
| Cl2 | 0.72347 (5) | −0.0839 (2) | 0.67678 (3) | 0.0704 (3) |
| O1 | 0.59363 (10) | 0.3353 (5) | 0.36024 (9) | 0.0529 (5) |
| O2 | 0.72448 (12) | 0.5904 (7) | 0.36130 (10) | 0.0737 (7) |
| C1 | 0.57335 (13) | 0.4453 (6) | 0.29332 (12) | 0.0444 (5) |
| C2 | 0.49523 (15) | 0.6088 (7) | 0.28247 (14) | 0.0518 (6) |
| H2 | 0.4603 (19) | 0.657 (8) | 0.3193 (16) | 0.062* |
| C3 | 0.46945 (15) | 0.7062 (7) | 0.21667 (15) | 0.0546 (6) |
| H3 | 0.4132 (19) | 0.820 (9) | 0.2133 (15) | 0.066* |
| C4 | 0.52292 (14) | 0.6377 (6) | 0.16294 (13) | 0.0469 (5) |
| C5 | 0.60108 (15) | 0.4709 (7) | 0.17399 (13) | 0.0492 (6) |
| H5 | 0.6337 (18) | 0.438 (8) | 0.1358 (16) | 0.059* |
| C6 | 0.62658 (14) | 0.3724 (7) | 0.23892 (13) | 0.0488 (6) |
| H6 | 0.6762 (19) | 0.246 (8) | 0.2482 (15) | 0.059* |
| C7 | 0.67225 (14) | 0.4158 (7) | 0.38938 (12) | 0.0482 (6) |
| C8 | 0.68345 (13) | 0.2812 (6) | 0.45961 (12) | 0.0452 (5) |
| C9 | 0.61746 (15) | 0.1152 (8) | 0.49299 (14) | 0.0530 (6) |
| H9 | 0.5619 (19) | 0.089 (8) | 0.4691 (16) | 0.064* |
| C10 | 0.62957 (16) | 0.0048 (8) | 0.55961 (13) | 0.0538 (6) |
| H10 | 0.584 (2) | −0.108 (8) | 0.5807 (16) | 0.065* |
| C11 | 0.70901 (15) | 0.0570 (7) | 0.59276 (13) | 0.0494 (6) |
| C12 | 0.77573 (16) | 0.2151 (8) | 0.56050 (15) | 0.0579 (7) |
| H12 | 0.826 (2) | 0.225 (9) | 0.5856 (17) | 0.069* |
| C13 | 0.76306 (14) | 0.3276 (8) | 0.49402 (14) | 0.0534 (6) |
| H13 | 0.8067 (19) | 0.428 (9) | 0.4718 (16) | 0.064* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cl1 | 0.0694 (4) | 0.0793 (5) | 0.0574 (4) | 0.0037 (3) | −0.0138 (3) | 0.0097 (4) |
| Cl2 | 0.0777 (5) | 0.0819 (6) | 0.0507 (4) | 0.0114 (4) | −0.0142 (3) | 0.0012 (3) |
| O1 | 0.0419 (8) | 0.0685 (12) | 0.0480 (9) | −0.0142 (8) | −0.0015 (6) | 0.0071 (9) |
| O2 | 0.0623 (11) | 0.0998 (18) | 0.0589 (11) | −0.0387 (11) | 0.0032 (9) | 0.0064 (11) |
| C1 | 0.0394 (10) | 0.0469 (13) | 0.0469 (12) | −0.0087 (9) | 0.0002 (9) | −0.0007 (11) |
| C2 | 0.0404 (11) | 0.0604 (16) | 0.0553 (14) | −0.0009 (10) | 0.0094 (10) | −0.0063 (12) |
| C3 | 0.0395 (11) | 0.0581 (15) | 0.0659 (16) | 0.0061 (11) | −0.0023 (10) | −0.0024 (13) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C4 | 0.0447 (11) | 0.0462 (13) | 0.0492 (12) | −0.0044 (10) | −0.0046 (9) | 0.0006 (11) |
| C5 | 0.0451 (11) | 0.0537 (14) | 0.0491 (13) | 0.0034 (10) | 0.0054 (10) | −0.0044 (12) |
| C6 | 0.0393 (11) | 0.0553 (14) | 0.0518 (13) | 0.0056 (10) | 0.0007 (9) | −0.0009 (12) |
| C7 | 0.0378 (10) | 0.0605 (15) | 0.0463 (12) | −0.0070 (10) | 0.0038 (9) | −0.0042 (11) |
| C8 | 0.0367 (10) | 0.0513 (13) | 0.0477 (13) | −0.0032 (9) | 0.0027 (9) | −0.0065 (11) |
| C9 | 0.0368 (10) | 0.0715 (17) | 0.0504 (13) | −0.0101 (11) | −0.0043 (9) | 0.0033 (12) |
| C10 | 0.0428 (11) | 0.0678 (16) | 0.0507 (13) | −0.0070 (12) | 0.0003 (10) | 0.0049 (13) |
| C11 | 0.0514 (12) | 0.0502 (14) | 0.0460 (12) | 0.0065 (10) | −0.0064 (10) | −0.0059 (11) |
| C12 | 0.0413 (11) | 0.0657 (17) | 0.0659 (16) | 0.0002 (11) | −0.0123 (11) | −0.0106 (14) |
| C13 | 0.0356 (10) | 0.0625 (16) | 0.0622 (15) | −0.0079 (11) | 0.0026 (10) | −0.0057 (13) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cl1—C4 | 1.736 (3) | C5—H5 | 0.92 (3) |
| Cl2—C11 | 1.735 (3) | C6—H6 | 0.93 (3) |
| O1—C7 | 1.356 (3) | C7—C8 | 1.472 (3) |
| O1—C1 | 1.399 (3) | C8—C9 | 1.387 (3) |
| O2—C7 | 1.203 (3) | C8—C13 | 1.389 (3) |
| C1—C2 | 1.374 (3) | C9—C10 | 1.375 (4) |
| C1—C6 | 1.389 (3) | C9—H9 | 0.96 (3) |
| C2—C3 | 1.383 (4) | C10—C11 | 1.379 (3) |
| C2—H2 | 0.93 (3) | C10—H10 | 0.93 (3) |
| C3—C4 | 1.377 (4) | C11—C12 | 1.370 (4) |
| C3—H3 | 0.97 (3) | C12—C13 | 1.376 (4) |
| C4—C5 | 1.381 (3) | C12—H12 | 0.90 (3) |
| C5—C6 | 1.368 (4) | C13—H13 | 0.90 (3) |
| | | | |
| C7—O1—C1 | 119.07 (17) | O2—C7—C8 | 124.7 (2) |
| C2—C1—C6 | 120.9 (2) | O1—C7—C8 | 112.34 (19) |
| C2—C1—O1 | 117.2 (2) | C9—C8—C13 | 118.9 (2) |
| C6—C1—O1 | 121.7 (2) | C9—C8—C7 | 122.7 (2) |
| C1—C2—C3 | 119.8 (2) | C13—C8—C7 | 118.4 (2) |
| C1—C2—H2 | 120.1 (19) | C10—C9—C8 | 120.8 (2) |
| C3—C2—H2 | 120.1 (19) | C10—C9—H9 | 120.8 (18) |
| C4—C3—C2 | 119.2 (2) | C8—C9—H9 | 118.3 (18) |
| C4—C3—H3 | 126.1 (17) | C11—C10—C9 | 119.0 (2) |
| C2—C3—H3 | 114.7 (17) | C11—C10—H10 | 122 (2) |
| C3—C4—C5 | 120.8 (2) | C9—C10—H10 | 119 (2) |
| C3—C4—Cl1 | 119.77 (19) | C12—C11—C10 | 121.2 (2) |
| C5—C4—Cl1 | 119.41 (19) | C12—C11—Cl2 | 120.19 (19) |
| C6—C5—C4 | 120.1 (2) | C10—C11—Cl2 | 118.6 (2) |
| C6—C5—H5 | 124.0 (19) | C11—C12—C13 | 119.5 (2) |
| C4—C5—H5 | 115.8 (19) | C11—C12—H12 | 114 (2) |
| C5—C6—C1 | 119.1 (2) | C13—C12—H12 | 126 (2) |
| C5—C6—H6 | 123.0 (18) | C12—C13—C8 | 120.5 (2) |
| C1—C6—H6 | 117.8 (18) | C12—C13—H13 | 121 (2) |
| O2—C7—O1 | 122.9 (2) | C8—C13—H13 | 119 (2) |

| | | | |
|---|---|---|---|
| C7—O1—C1—C2 | −129.5 (3) | O2—C7—C8—C9 | 172.1 (3) |
| C7—O1—C1—C6 | 55.0 (3) | O1—C7—C8—C9 | −4.8 (4) |
| C6—C1—C2—C3 | −0.8 (4) | O2—C7—C8—C13 | −6.9 (4) |
| O1—C1—C2—C3 | −176.3 (2) | O1—C7—C8—C13 | 176.2 (2) |
| C1—C2—C3—C4 | −0.1 (4) | C13—C8—C9—C10 | 1.5 (4) |
| C2—C3—C4—C5 | 0.7 (4) | C7—C8—C9—C10 | −177.5 (3) |
| C2—C3—C4—Cl1 | −179.0 (2) | C8—C9—C10—C11 | −0.9 (4) |
| C3—C4—C5—C6 | −0.3 (4) | C9—C10—C11—C12 | −0.2 (4) |
| Cl1—C4—C5—C6 | 179.4 (2) | C9—C10—C11—Cl2 | −179.9 (2) |
| C4—C5—C6—C1 | −0.6 (4) | C10—C11—C12—C13 | 0.7 (4) |
| C2—C1—C6—C5 | 1.1 (4) | Cl2—C11—C12—C13 | −179.5 (2) |
| O1—C1—C6—C5 | 176.5 (2) | C11—C12—C13—C8 | −0.1 (4) |
| C1—O1—C7—O2 | 3.2 (4) | C9—C8—C13—C12 | −1.0 (4) |
| C1—O1—C7—C8 | −179.9 (2) | C7—C8—C13—C12 | 178.0 (3) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C5—H5···O2$^{i}$ | 0.92 (3) | 2.58 (3) | 3.168 (3) | 123 (2) |

Symmetry code: (i) −*x*+3/2, *y*−1/2, −*z*+1/2.