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## Structure Reports

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## 2,4-Dichlorophenyl benzoate

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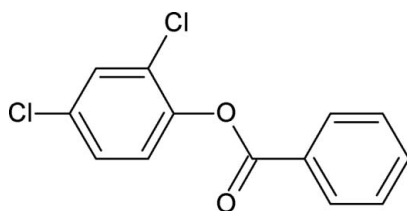
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 Key indicators: single-crystal X-ray study;  $T = 295$  K; mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å;  $R$  factor = 0.023;  $wR$  factor = 0.059; data-to-parameter ratio = 13.8.

The crystal structure of the title compound,  $\text{C}_{13}\text{H}_8\text{Cl}_2\text{O}_2$ , resembles those of 2,3-dichlorophenyl benzoate, 2,4-dimethylphenyl benzoate and other aryl benzoates, with similar bond parameters. The plane of central  $-\text{C}(=\text{O})-\text{O}-$  group is inclined at the angle of  $9.1(2)^\circ$  with respect to the benzoate ring. The two aromatic rings make a dihedral angle of  $47.8(1)^\circ$ . In the crystal structure there are no classical hydrogen bonds. The molecules in the structure are packed into chains diagonally in the  $bc$  plane.

## Related literature

For the preparation of the compound, see: Nayak & Gowda (2009); For related structures, see: Gowda *et al.* (2007, 2008, 2009).



## Experimental

## Crystal data

 $\text{C}_{13}\text{H}_8\text{Cl}_2\text{O}_2$   
 $M_r = 267.09$ 

 Orthorhombic,  $P2_12_12_1$   
 $a = 3.9722(1)$  Å

 $b = 11.9458(3)$  Å  
 $c = 24.9407(5)$  Å  
 $V = 1183.46(5)$  Å<sup>3</sup>  
 $Z = 4$ 

 Mo  $K\alpha$  radiation  
 $\mu = 0.53$  mm<sup>-1</sup>  
 $T = 295$  K  
 $0.47 \times 0.11 \times 0.10$  mm

## Data collection

 Oxford Diffraction Xcalibur diffractometer with a Ruby (Gemini Mo) detector  
 Absorption correction: multi-scan (*CrysAlis RED*; Oxford)

 Diffraction, 2009)  
 $T_{\min} = 0.751$ ,  $T_{\max} = 0.943$   
 20045 measured reflections  
 2202 independent reflections  
 1961 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.027$ 

## Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.023$   
 $wR(F^2) = 0.059$   
 $S = 1.03$   
 2202 reflections  
 160 parameters  
 2 restraints

 H atoms treated by a mixture of independent and constrained refinement  
 $\Delta\rho_{\max} = 0.13$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.15$  e Å<sup>-3</sup>  
 Absolute structure: Flack (1983), 861 Friedel pairs  
 Flack parameter: 0.02 (5)

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2009); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2009); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 2002); software used to prepare material for publication: *SHELXL97*, *PLATON* (Spek, 2009) and *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2919).

## References

- Brandenburg, K. (2002). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.  
 Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.  
 Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.  
 Flack, H. D. (1983). *Acta Cryst.* **A39**, 876–881.  
 Gowda, B. T., Foro, S., Babitha, K. S. & Fuess, H. (2007). *Acta Cryst.* **E63**, o4286.  
 Gowda, B. T., Tokarčík, M., Kožíšek, J., Babitha, K. S. & Fuess, H. (2008). *Acta Cryst.* **E64**, o1280.  
 Gowda, B. T., Tokarčík, M., Kožíšek, J., Suchetan, P. A. & Fuess, H. (2009). *Acta Cryst.* **E65**, o915.  
 Nayak, R. & Gowda, B. T. (2009). *Z. Naturforsch. Teil A*, **63**. In preparation.  
 Oxford Diffraction (2009). *CrysAlis CCD* and *CrysAlis RED*. Oxford Diffraction Ltd, Abingdon, England.  
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.  
 Spek, A. L. (2009). *Acta Cryst.* **D65**, 148–155.

**supplementary materials**

*Acta Cryst.* (2009). E65, o947 [ doi:10.1107/S1600536809011763 ]

## 2,4-Dichlorophenyl benzoate

**B. T. Gowda, M. Tokarcík, J. Kozísek, P. A. Suchetan and H. Fues**

### Comment

In the present work, as a part of studying the substituent effects on the crystal structures of aryl benzoates (Gowda *et al.*, 2007, 2008, 2009), the structure of 2,4-dichlorophenyl benzoate has been determined. The structure (Fig. 1) is similar to those of 2,3-dichlorophenylbenzoate (Gowda *et al.*, 2007), 2,4-dimethylphenyl benzoate (Gowda *et al.*, 2008) and other aryl benzoates (Gowda *et al.*, 2009). The two aromatic rings make a dihedral angle of 47.8 (1)°. The plane of the –C(=O)–O– group is inclined at an angle of 9.1 (2)° to the benzoate ring. In the crystal structure, there are no classical hydrogen bonds. The molecules in the structure are packed into chains as viewed down the *bc* plane (Fig. 2).

### Experimental

The title compound was prepared according to a literature method (Nayak & Gowda, 2009). The purity of the compound was checked by determining its melting point. It was characterized by recording its infrared and NMR spectra (Nayak & Gowda, 2009). Single crystals of the title compound were obtained by slow evaporation of its ethanol solution. The X-ray diffraction studies were made at room temperature.

### Refinement

H atoms were positioned geometrically and refined using a riding model with C—H distances of 0.93 Å, except for H atoms bound to C4 and C5, which were subject to the restraint on the C—H distance (set to 0.95 (4) Å). This measure improved the anisotropic displacement parameters of the atoms C4, C5 and enabled to remove the alert\_C regarding the Hirshfeld-test. All H atoms were refined with  $U_{\text{iso}}(\text{H}) = 1.2$  times  $U_{\text{eq}}(\text{C})$ .

### Figures

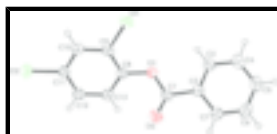


Fig. 1. Molecular structure of the title compound showing the atom labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are represented as small spheres of arbitrary radii.

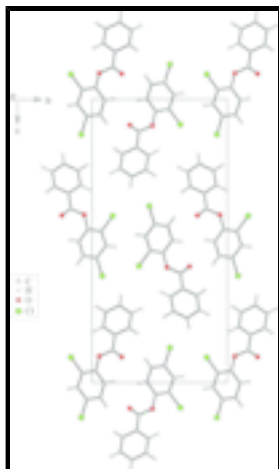


Fig. 2. The packing of the title compound viewed down the *a* axis.

## 2,4-Dichlorophenyl benzoate

### Crystal data

$C_{13}H_8Cl_2O_2$

$M_r = 267.09$

Orthorhombic,  $P2_12_12_1$

Hall symbol: P 2ac 2ab

$a = 3.97220 (10) \text{ \AA}$

$b = 11.9458 (3) \text{ \AA}$

$c = 24.9407 (5) \text{ \AA}$

$V = 1183.46 (5) \text{ \AA}^3$

$Z = 4$

$F_{000} = 544$

$D_x = 1.499 \text{ Mg m}^{-3}$

Mo  $K\alpha$  radiation

$\lambda = 0.71073 \text{ \AA}$

Cell parameters from 10923 reflections

$\theta = 3.3\text{--}29.5^\circ$

$\mu = 0.53 \text{ mm}^{-1}$

$T = 295 \text{ K}$

Needle, colourless

$0.47 \times 0.11 \times 0.10 \text{ mm}$

### Data collection

Oxford Diffraction Xcalibur diffractometer with a Ruby (Gemini Mo) detector

Monochromator: graphite

Detector resolution:  $10.434 \text{ pixels mm}^{-1}$

$T = 295 \text{ K}$

$\omega$  scans

Absorption correction: multi-scan (CrysAlis RED; Oxford Diffraction, 2009)

$T_{\min} = 0.751$ ,  $T_{\max} = 0.943$

20045 measured reflections

2202 independent reflections

1961 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.027$

$\theta_{\max} = 25.5^\circ$

$\theta_{\min} = 3.3^\circ$

$h = -4 \rightarrow 4$

$k = -14 \rightarrow 14$

$l = -30 \rightarrow 30$

### Refinement

Refinement on  $F^2$

Least-squares matrix: full

Hydrogen site location: inferred from neighbouring sites

H atoms treated by a mixture of independent and constrained refinement

$R[F^2 > 2\sigma(F^2)] = 0.023$	$w = 1/[\sigma^2(F_o^2) + (0.0343P)^2 + 0.0694P]$
$wR(F^2) = 0.059$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{\max} < 0.001$
2202 reflections	$\Delta\rho_{\max} = 0.13 \text{ e } \text{\AA}^{-3}$
160 parameters	$\Delta\rho_{\min} = -0.15 \text{ e } \text{\AA}^{-3}$
2 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983), 861 Friedel pairs
Secondary atom site location: difference Fourier map	Flack parameter: 0.02 (5)

### 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 ( $\text{\AA}^2$ )

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.4499 (4)	0.34482 (14)	0.11405 (6)	0.0475 (4)
C2	0.5855 (4)	0.32994 (13)	0.16904 (6)	0.0454 (4)
C3	0.7373 (5)	0.41579 (15)	0.19708 (7)	0.0532 (4)
H3	0.7648	0.4856	0.1811	0.064*
C4	0.8484 (6)	0.39790 (19)	0.24887 (7)	0.0649 (5)
H4	0.947 (5)	0.4659 (16)	0.2689 (8)	0.078*
C5	0.8127 (6)	0.29517 (19)	0.27219 (8)	0.0671 (5)
H5	0.884 (6)	0.2847 (17)	0.3063 (8)	0.081*
C6	0.6657 (6)	0.20918 (18)	0.24438 (8)	0.0709 (6)
H6	0.6437	0.1393	0.2604	0.085*
C7	0.5496 (5)	0.22556 (15)	0.19272 (7)	0.0603 (5)
H7	0.4485	0.1672	0.174	0.072*
C8	0.4313 (4)	0.47198 (13)	0.04142 (6)	0.0439 (4)
C9	0.2560 (4)	0.56988 (13)	0.03415 (6)	0.0436 (4)
C10	0.1619 (4)	0.60433 (13)	-0.01650 (6)	0.0466 (4)
H10	0.0463	0.6712	-0.0215	0.056*
C11	0.2437 (4)	0.53692 (13)	-0.05937 (6)	0.0457 (4)
C12	0.4179 (4)	0.43887 (13)	-0.05300 (6)	0.0489 (4)
H12	0.4704	0.3947	-0.0825	0.059*
C13	0.5148 (4)	0.40651 (14)	-0.00208 (7)	0.0489 (4)
H13	0.636	0.3407	0.0028	0.059*
O1	0.5392 (3)	0.44515 (9)	0.09308 (4)	0.0522 (3)

## supplementary materials

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O2	0.2813 (4)	0.27886 (11)	0.09054 (5)	0.0749 (4)
C11	0.14820 (14)	0.65271 (4)	0.088572 (17)	0.06409 (15)
C12	0.11922 (13)	0.57737 (4)	-0.123305 (17)	0.06442 (15)

### Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1	0.0547 (10)	0.0419 (8)	0.0460 (8)	-0.0075 (9)	0.0057 (8)	-0.0025 (7)
C2	0.0474 (9)	0.0440 (9)	0.0450 (8)	-0.0005 (8)	0.0081 (7)	-0.0007 (7)
C3	0.0588 (10)	0.0515 (10)	0.0493 (9)	-0.0038 (9)	0.0020 (8)	0.0003 (8)
C4	0.0657 (12)	0.0814 (14)	0.0477 (10)	-0.0034 (12)	-0.0026 (9)	-0.0054 (9)
C5	0.0699 (13)	0.0840 (14)	0.0474 (10)	0.0095 (12)	0.0021 (10)	0.0095 (11)
C6	0.0816 (14)	0.0657 (12)	0.0654 (12)	0.0070 (13)	0.0145 (11)	0.0207 (10)
C7	0.0742 (13)	0.0497 (10)	0.0571 (11)	-0.0025 (10)	0.0093 (10)	0.0030 (8)
C8	0.0467 (9)	0.0394 (8)	0.0455 (8)	-0.0080 (8)	-0.0019 (7)	0.0002 (6)
C9	0.0466 (9)	0.0371 (8)	0.0470 (9)	-0.0076 (7)	0.0047 (7)	-0.0072 (7)
C10	0.0479 (9)	0.0401 (8)	0.0517 (9)	0.0020 (8)	0.0019 (8)	-0.0005 (7)
C11	0.0460 (9)	0.0485 (9)	0.0425 (8)	-0.0045 (8)	0.0005 (7)	0.0036 (7)
C12	0.0518 (10)	0.0482 (9)	0.0468 (9)	0.0031 (9)	0.0063 (8)	-0.0060 (7)
C13	0.0516 (9)	0.0411 (9)	0.0541 (9)	0.0043 (8)	0.0012 (8)	0.0009 (7)
O1	0.0667 (8)	0.0424 (6)	0.0475 (6)	-0.0113 (6)	-0.0117 (6)	0.0031 (5)
O2	0.1069 (11)	0.0634 (8)	0.0546 (7)	-0.0411 (8)	-0.0074 (8)	-0.0019 (6)
Cl1	0.0868 (3)	0.0509 (2)	0.0545 (2)	-0.0017 (2)	0.0102 (2)	-0.0149 (2)
Cl2	0.0754 (3)	0.0715 (3)	0.0464 (2)	0.0074 (3)	-0.0040 (2)	0.0055 (2)

### Geometric parameters ( $\text{\AA}$ , $^\circ$ )

C1—O2	1.189 (2)	C7—H7	0.93
C1—O1	1.355 (2)	C8—C9	1.373 (2)
C1—C2	1.484 (2)	C8—C13	1.378 (2)
C2—C3	1.380 (2)	C8—O1	1.3951 (19)
C2—C7	1.387 (2)	C9—C10	1.380 (2)
C3—C4	1.382 (3)	C9—Cl1	1.7334 (15)
C3—H3	0.93	C10—C11	1.378 (2)
C4—C5	1.365 (3)	C10—H10	0.93
C4—H4	1.031 (19)	C11—C12	1.370 (2)
C5—C6	1.370 (3)	C11—Cl2	1.7380 (16)
C5—H5	0.905 (19)	C12—C13	1.382 (2)
C6—C7	1.382 (3)	C12—H12	0.93
C6—H6	0.93	C13—H13	0.93
O2—C1—O1	122.91 (15)	C2—C7—H7	120.3
O2—C1—C2	125.52 (15)	C9—C8—C13	120.10 (14)
O1—C1—C2	111.57 (13)	C9—C8—O1	118.25 (13)
C3—C2—C7	119.82 (16)	C13—C8—O1	121.53 (14)
C3—C2—C1	122.54 (14)	C8—C9—C10	120.81 (14)
C7—C2—C1	117.63 (15)	C8—C9—Cl1	120.54 (12)
C2—C3—C4	119.89 (17)	C10—C9—Cl1	118.65 (13)
C2—C3—H3	120.1	C11—C10—C9	118.18 (15)

C4—C3—H3	120.1	C11—C10—H10	120.9
C5—C4—C3	120.3 (2)	C9—C10—H10	120.9
C5—C4—H4	122.8 (11)	C12—C11—C10	121.94 (15)
C3—C4—H4	116.8 (11)	C12—C11—C12	119.22 (13)
C4—C5—C6	120.16 (19)	C10—C11—C12	118.85 (12)
C4—C5—H5	119.4 (14)	C11—C12—C13	119.11 (15)
C6—C5—H5	120.4 (14)	C11—C12—H12	120.4
C5—C6—C7	120.52 (18)	C13—C12—H12	120.4
C5—C6—H6	119.7	C8—C13—C12	119.85 (16)
C7—C6—H6	119.7	C8—C13—H13	120.1
C6—C7—C2	119.33 (19)	C12—C13—H13	120.1
C6—C7—H7	120.3	C1—O1—C8	118.64 (12)
O2—C1—C2—C3	-170.23 (18)	O1—C8—C9—C11	-4.3 (2)
O1—C1—C2—C3	9.2 (2)	C8—C9—C10—C11	1.0 (2)
O2—C1—C2—C7	8.5 (3)	C11—C9—C10—C11	-178.90 (13)
O1—C1—C2—C7	-172.04 (15)	C9—C10—C11—C12	-0.9 (2)
C7—C2—C3—C4	-1.0 (3)	C9—C10—C11—C12	178.61 (13)
C1—C2—C3—C4	177.77 (17)	C10—C11—C12—C13	0.0 (2)
C2—C3—C4—C5	0.9 (3)	C12—C11—C12—C13	-179.58 (13)
C3—C4—C5—C6	-0.2 (3)	C9—C8—C13—C12	-0.8 (3)
C4—C5—C6—C7	-0.5 (3)	O1—C8—C13—C12	-176.67 (15)
C5—C6—C7—C2	0.4 (3)	C11—C12—C13—C8	0.9 (3)
C3—C2—C7—C6	0.3 (3)	O2—C1—O1—C8	-0.6 (3)
C1—C2—C7—C6	-178.49 (18)	C2—C1—O1—C8	179.94 (14)
C13—C8—C9—C10	-0.2 (2)	C9—C8—O1—C1	125.12 (16)
O1—C8—C9—C10	175.80 (14)	C13—C8—O1—C1	-59.0 (2)
C13—C8—C9—C11	179.76 (13)		

Fig. 1

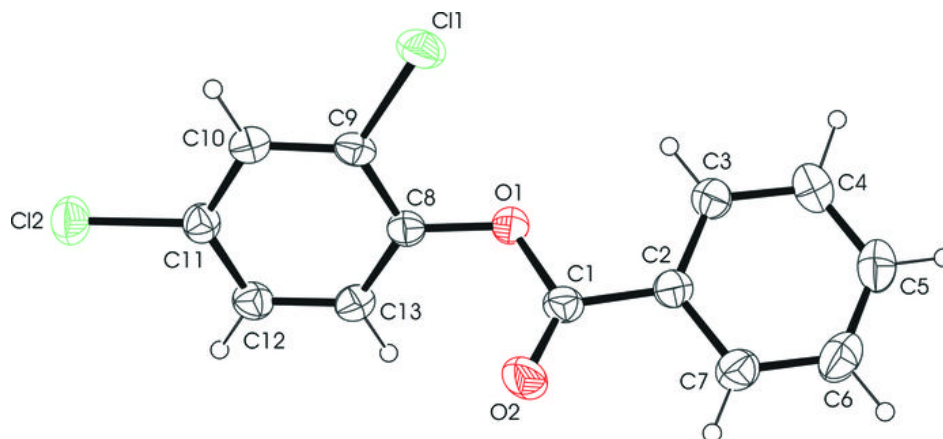


Fig. 2

