Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2,4-Dichloro-5-fluorobenzoic acid

Yun-Feng Zhao

School of Life Sciences, Qufu Normal University, Qufu 273165, People's Republic of China
Correspondence e-mail: zhaoyunfeng69@163.com

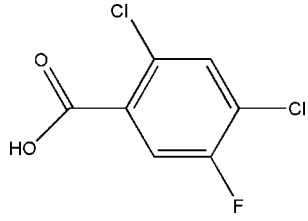
Received 21 October 2007; accepted 21 October 2007

Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.004 Å; R factor = 0.052; wR factor = 0.142; data-to-parameter ratio = 14.0.

In the title compound, $C_7H_3Cl_2FO_2$, the dihedral angle between the carboxyl group and the benzene ring is 49.27 (13)°. In the crystal structure, inversion dimers arise *via* pairs of weak O—H···O hydrogen bonds (H···O = 2.23 Å).

Related literature

For related structures, see: Lalancette *et al.* (1996); Potrzebowski & Chruszcz (2007); Taga *et al.* (1985). For the synthesis, see: Tang *et al.* (1991). For background, see Li & Guo (1992).



Experimental

Crystal data

$C_7H_3Cl_2FO_2$
M_r = 208.99
Monoclinic, $P2_1/n$
a = 5.0438 (19) Å
b = 10.632 (4) Å
c = 15.550 (6) Å
β = 95.515 (5)°
V = 830.0 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.75 mm^{-1}
T = 295 (2) K
0.35 × 0.12 × 0.06 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
T_{min} = 0.779, T_{max} = 0.956
5973 measured reflections
1540 independent reflections
1293 reflections with $I > 2\sigma(I)$
R_{int} = 0.056

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.142
S = 1.06
1540 reflections
110 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.61 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H1···O1^{i}	0.82	2.23	3.034 (3)	167

Symmetry code: (i) $-x+1, -y+2, -z+1$.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

The author thanks the Natural Science Foundation of Shandong Province and Qufu Normal University for supporting this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2604).

References

Bruker (2002). *SADABS*, *SAINT* and *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Lalancette, R. A., Stringer, J. A. & Coté, M. L. (1996). *Acta Cryst.* C**52**, 1801–1804.
Li, M. & Guo, H.-Y. (1992). *Chin. J. Pharm.* **23**, 427–429.
Potrzebowski, W. & Chruszcz, M. (2007). *Acta Cryst.* E**63**, o2754.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Taga, T., Yamamoto, N. & Osaki, K. (1985). *Acta Cryst.* C**41**, 153–154.
Tang, W.-G., Peng, C.-Y. & Huang, Y.-L. (1991). *Chin. J. Pharm.* **22**, 551–552.

 doi:10.1107/S1600536807052130

supplementary materials

Acta Cryst. (2007). E**63**, o4449 [**doi:10.1107/S1600536807052130**]

2,4-Dichloro-5-fluorobenzoic acid

Y.-F. Zhao

Comment

The title compound, (I), is an important intermediate in the syntheis of fluoroquinolone antibiotics (Li & Guo, 1992). We report herein its structure (Fig. 1).

The bond lengths and angles in (I) are within normal ranges (Lalancette *et al.*, 1996; Potrzebowski & Chruszcz, 2007; Taga *et al.*, 1985). The carboxyl group and phenyl ring planes are twisted by 49.27 (13)°, which is caused by steric effects between carboxylic group and *ortho*-chlorine atom. In the crystal, a weak O—H···O hydrogen-bond between inversion related carboxyl groups is formed (Table 1) resulting in an $R^2_2(8)$ ring.

Experimental

The title compound was prepared from 2,4-dichlorofluorobenzene according to the reported method (Tang *et al.*, 1991). Colourless plates of (I) were obtained by slow evaporation of an aqueous solution at room temperature.

Refinement

H atoms were placed at calculated positions and refined in the riding-model approximation, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C), and O—H = 0.82 Å and U_{iso}(H) = 1.5U_{eq}(O).

Figures

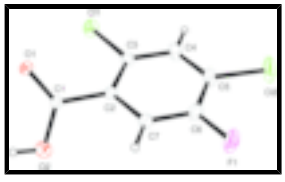


Fig. 1. The structure of (I), with displacement ellipsoids drawn at the 30% probability level for the non-hydrogen atoms.

2,4-Dichloro-5-fluorobenzoic acid

Crystal data

$C_7H_3Cl_2FO_2$	F_{000} = 416
M_r = 208.99	D_x = 1.672 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 1959 reflections
a = 5.0438 (19) Å	θ = 2.3–26.7º
b = 10.632 (4) Å	μ = 0.75 mm^{-1}

c = 15.550 (6) Å	T = 295 (2) K
β = 95.515 (5)º	Plate, colorless
V = 830.0 (5) Å^3	0.35 × 0.12 × 0.06 mm
Z = 4	

Data collection

Bruker SMART APEX CCD diffractometer	1540 independent reflections
Radiation source: fine-focus sealed tube	1293 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.056
T = 295(2) K	θ_{max} = 25.5º
φ and ω scans	θ_{min} = 2.3º
Absorption correction: multi-scan (SADABS; Bruker, 2002)	$h = -6 \rightarrow 6$
T_{min} = 0.779, T_{max} = 0.956	$k = -12 \rightarrow 12$
5973 measured reflections	$l = -18 \rightarrow 18$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.052	$w = 1/[\sigma^2(F_o^2) + (0.0612P)^2 + 0.7105P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.142	$(\Delta/\sigma)_{max} < 0.001$
S = 1.06	$\Delta\rho_{max}$ = 0.61 e Å^{-3}
1540 reflections	$\Delta\rho_{min}$ = −0.37 e Å^{-3}
110 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: 0.151 (12)
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	0.5167 (5)	0.9568 (3)	0.36752 (18)	0.0333 (7)
C2	0.5453 (5)	0.9186 (3)	0.27613 (17)	0.0304 (6)
C3	0.3990 (6)	0.8225 (3)	0.23460 (18)	0.0339 (7)
C4	0.4315 (7)	0.7892 (3)	0.1506 (2)	0.0443 (8)
H9	0.3323	0.7236	0.1242	0.053*
C5	0.6115 (7)	0.8534 (3)	0.1059 (2)	0.0481 (9)
C6	0.7558 (7)	0.9497 (3)	0.1461 (2)	0.0468 (8)
C7	0.7278 (6)	0.9821 (3)	0.2299 (2)	0.0389 (7)
H7	0.8306	1.0466	0.2561	0.047*
O1	0.2963 (4)	0.9777 (2)	0.39280 (13)	0.0423 (6)
O2	0.7417 (5)	0.9684 (3)	0.41719 (17)	0.0760 (10)
H1	0.7099	0.9894	0.4659	0.114*
F1	0.9320 (5)	1.0123 (2)	0.10281 (14)	0.0758 (8)
Cl1	0.17719 (18)	0.73365 (8)	0.28805 (5)	0.0506 (4)
Cl2	0.6602 (3)	0.81275 (13)	0.00154 (6)	0.0861 (5)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0266 (14)	0.0421 (16)	0.0310 (15)	−0.0001 (12)	0.0018 (11)	−0.0062 (12)
C2	0.0286 (14)	0.0331 (15)	0.0294 (14)	0.0048 (11)	0.0024 (11)	−0.0023 (11)
C3	0.0369 (15)	0.0327 (15)	0.0320 (15)	0.0015 (12)	0.0035 (12)	0.0039 (12)
C4	0.058 (2)	0.0380 (17)	0.0367 (17)	−0.0063 (15)	0.0041 (14)	−0.0066 (13)
C5	0.066 (2)	0.0504 (19)	0.0286 (16)	0.0005 (17)	0.0110 (15)	−0.0039 (14)
C6	0.0483 (19)	0.053 (2)	0.0417 (18)	−0.0052 (15)	0.0167 (15)	0.0051 (15)
C7	0.0362 (16)	0.0397 (16)	0.0417 (17)	−0.0039 (13)	0.0085 (13)	−0.0061 (13)
O1	0.0242 (11)	0.0667 (15)	0.0365 (11)	0.0027 (9)	0.0053 (8)	−0.0130 (10)
O2	0.0477 (16)	0.129 (3)	0.0509 (16)	0.0006 (16)	0.0015 (12)	−0.0256 (16)
F1	0.0881 (17)	0.0890 (17)	0.0564 (14)	−0.0316 (14)	0.0390 (12)	−0.0013 (12)
Cl1	0.0604 (6)	0.0461 (5)	0.0470 (5)	−0.0165 (4)	0.0143 (4)	0.0011 (3)
Cl2	0.1285 (11)	0.0979 (9)	0.0369 (6)	−0.0234 (7)	0.0330 (6)	−0.0179 (5)

Geometric parameters (Å, °)

C1—O1	1.234 (3)	C4—H9	0.9300
C1—O2	1.316 (4)	C5—C6	1.371 (5)
C1—C2	1.498 (4)	C5—Cl2	1.720 (3)
C2—C3	1.383 (4)	C6—F1	1.342 (4)
C2—C7	1.395 (4)	C6—C7	1.368 (4)
C3—C4	1.378 (4)	C7—H7	0.9300
C3—Cl1	1.736 (3)	O2—H1	0.8200
C4—C5	1.377 (5)		
O1—C1—O2	123.3 (3)	C3—C4—H9	120.2
O1—C1—C2	121.5 (2)	C6—C5—C4	119.2 (3)

O2—C1—C2	115.2 (2)	C6—C5—Cl2	120.0 (3)
C3—C2—C7	117.8 (3)	C4—C5—Cl2	120.8 (3)
C3—C2—C1	123.2 (3)	F1—C6—C7	119.1 (3)
C7—C2—C1	119.1 (2)	F1—C6—C5	119.3 (3)
C4—C3—C2	121.7 (3)	C7—C6—C5	121.6 (3)
C4—C3—Cl1	117.0 (2)	C6—C7—C2	120.1 (3)
C2—C3—Cl1	121.2 (2)	C6—C7—H7	119.9
C5—C4—C3	119.6 (3)	C2—C7—H7	119.9
C5—C4—H9	120.2	C1—O2—H1	109.5
O1—C1—C2—C3	−49.8 (4)	C3—C4—C5—C6	0.1 (5)
O2—C1—C2—C3	131.5 (3)	C3—C4—C5—Cl2	179.1 (3)
O1—C1—C2—C7	130.3 (3)	C4—C5—C6—F1	179.8 (3)
O2—C1—C2—C7	−48.5 (4)	Cl2—C5—C6—F1	0.8 (5)
C7—C2—C3—C4	0.4 (4)	C4—C5—C6—C7	1.0 (5)
C1—C2—C3—C4	−179.6 (3)	Cl2—C5—C6—C7	−178.0 (3)
C7—C2—C3—Cl1	177.3 (2)	F1—C6—C7—C2	179.8 (3)
C1—C2—C3—Cl1	−2.7 (4)	C5—C6—C7—C2	−1.3 (5)
C2—C3—C4—C5	−0.8 (5)	C3—C2—C7—C6	0.6 (4)
Cl1—C3—C4—C5	−177.8 (3)	C1—C2—C7—C6	−179.4 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H1···O1^{i}	0.82	2.23	3.034 (3)	167

Symmetry codes: (i) −*x*+1, −*y*+2, −*z*+1.

Fig. 1