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2,4-Dichlorobenzaldehyde

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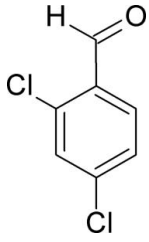
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.001 Å; R factor = 0.036; wR factor = 0.114; data-to-parameter ratio = 34.9.

In the crystal structure of the title compound, $C_7H_4Cl_2O$, the molecules form a network of weak C—H···O interactions involving the aldehyde O atom and the *ortho*-H atom on the benzene ring together with C—H···O interactions between the formyl groups. Together, these connect the molecules into $(10\bar{1})$ layers, which are stabilized additionally by π–π stacking interactions of the benzene rings [centroid–centroid distance = 3.772 (1) Å]. The aldehyde group is twisted relative to the benzene ring by 7.94 (13)°.

Related literature

For applications of the title compound, see: Katagi (1988); Wang *et al.* (2004). For a related structure, see: Gawlicka-Chruszcz *et al.* (2006).



Experimental

Crystal data

$C_7H_4Cl_2O$
M_r = 175.01
Monoclinic, $P2_1/n$
a = 13.100 (1) Å
b = 3.772 (1) Å
c = 15.332 (1) Å
β = 113.797 (2)°
V = 693.2 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.85 mm^{-1}
T = 100 K
0.40 × 0.10 × 0.10 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (Otwinowski *et al.*, 2003)
T_{min} = 0.90, T_{max} = 0.92
6924 measured reflections
3737 independent reflections
3221 reflections with $I > 2\sigma(I)$
R_{int} = 0.063

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.114
S = 1.10
3737 reflections
107 parameters
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.67 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C7—H7···O1^{i}	0.946 (17)	2.533 (17)	3.4289 (11)	158.0 (14)
C6—H6···O1^{ii}	0.950 (19)	2.512 (17)	3.2774 (11)	137.8 (12)

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

Data collection: *HKL-2000* (Otwinowski & Minor, 1997); cell refinement: *HKL-2000*; data reduction: *HKL-2000*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008) and *HKL-3000SM* (Minor *et al.*, 2006); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008) and *HKL-3000SM*; molecular graphics: *HKL-3000SM*, *ORTEPIII* (Burnett & Johnson, 1996), *ORTEP-3* (Farrugia, 1997), *Mercury* (Macrae *et al.*, 2006) and *POV-RAY* (The *POV-RAY* Team, 2004); software used to prepare material for publication: *HKL-3000SM*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GK2246).

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2,4-Dichlorobenzaldehyde

Ricardo Cabello, Maksymilian Chruszcz and Wladek Minor

S1. Comment

2,4-Dichlorobenzaldehyde is primarily used in the preparation of dyes, insecticides, herbicides, antiseptics and disinfectants (Wang *et al.*, 2004). It is also used as an intermediate of organic synthesis of fungicide diniconazole (Katagi, 1988).

In the crystal structure of 2,4-dichlorobenzaldehyde (Fig. 1), the aldehyde group is twisted relative to the benzene ring with torsion angles C6—C1—C7—O1 and C2—C1—C7—O1 being -7.94 (13)° and 170.86 (9)°. These torsion angles are significantly smaller in comparison to the corresponding angles in 2,6-dichlorobenzaldehyde (Gawlicka-Chruszcz *et al.*, 2006) which are -27.3° and 152.6° respectively. Significantly bigger twist of the aldehyde group in the case of 2,6-dichlorobenzaldehyde is caused by presence of the chlorine atoms in ortho positions.

The change of the position of chlorine atom causes that interactions in which chlorine atoms are involved in 2,4-dichlorobenzaldehyde and 2,6-dichlorobenzaldehyde differ significantly. In the case of 2,6-dichlorobenzaldehyde Cl2 was involved in weak interaction with hydrogen atom from neighboring benzene ring, while in 2,4-dichlorobenzaldehyde structure such interactions are not observed for any of the chlorine atoms. However, in the case of 2,4-dichlorobenzaldehyde, the chlorine atoms from neighboring molecules form short contacts with Cl1···Cl2 (1/2 + *x*,1/2 - *y*,1/2 + *z*) distance being 3.442Å (Fig. 2).

The weak O···H—C interactions (Table 1) between the aldehyde oxygen and the benzene hydrogen atoms connect molecules to form layers, which are additionally stabilized by stacking of benzene rings (Fig. 2). The oxygen atom from the aldehyde group plays a central role in the formation of weak interactions, and O1···H6—C6 (1 - *x*,-1 - *y*,1 - *z*) and O1···H7—C7 (1,5 - *x*,-1/2 + *y*,1.5 - *z*) distances are 2.51Å and 2.53Å respectively.

S2. Experimental

2,4-dichlorobenzaldehyde was purchased from ALDRICH (99% purity, lot 08722CD). The compound was provided in crystalline form.

S3. Refinement

All hydrogen atoms were localized using the difference density Fourier map. Their positions and isotropic displacement parameters were refined.

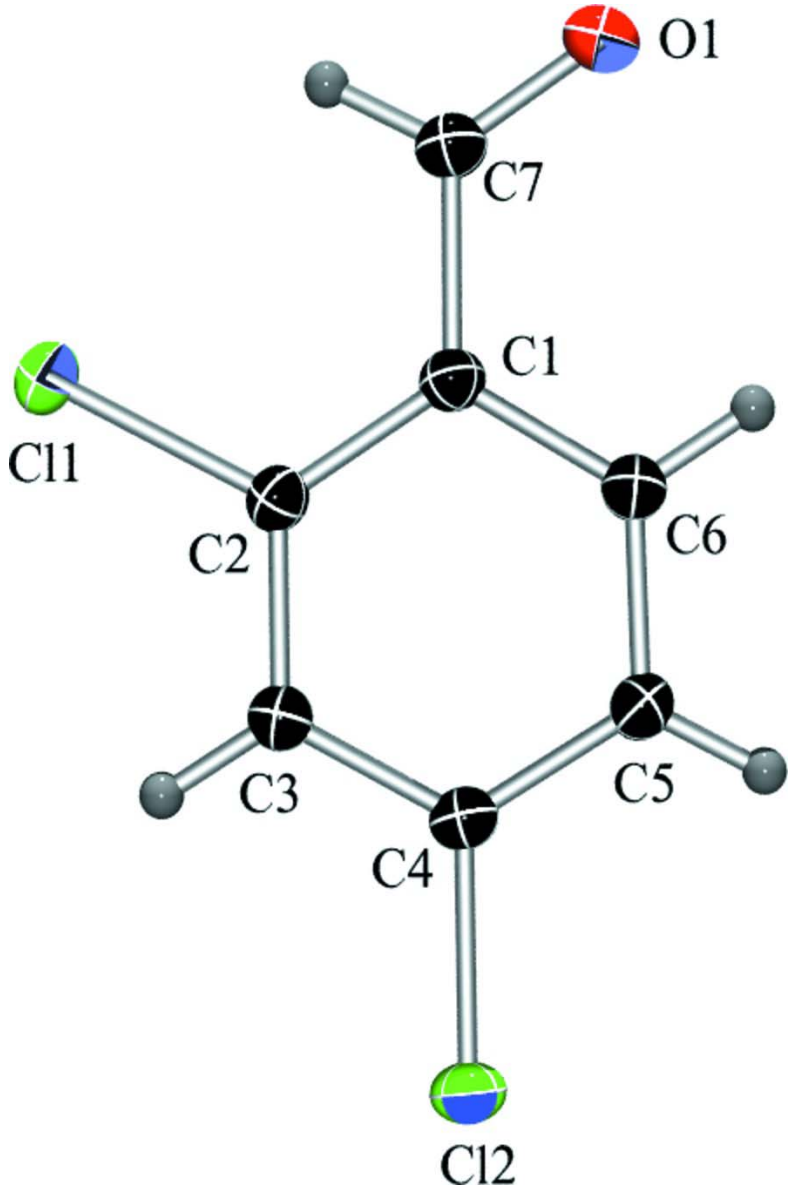

Figure 1

The asymmetric unit of the reported structure. Displacement ellipsoids are drawn at the 50% probability level and hydrogen atoms are drawn as grey spheres of an arbitrary radius.

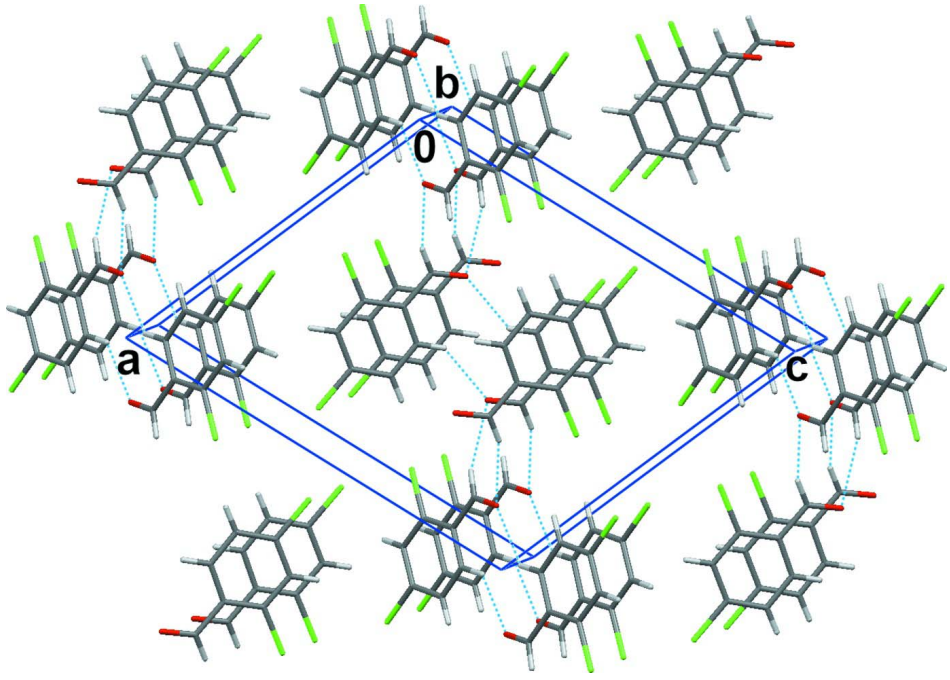

Figure 2

The molecular packing of 2,4-dichlorobenzaldehyde. Weak interactions, in which the oxygen atom participates, are shown as blue, dashed lines.

2,4-Dichlorobenzaldehyde

Crystal data

$C_7H_4Cl_2O$
$M_r = 175.01$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 13.100$ (1) Å
$b = 3.772$ (1) Å
$c = 15.332$ (1) Å
$\beta = 113.797$ (2)°
$V = 693.2$ (3) Å^3
$Z = 4$

$F(000) = 352$
$D_x = 1.677$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71074$ Å
Cell parameters from 31891 reflections
$\theta = 1.0$–$37.8°$
$\mu = 0.85$ mm^{-1}
$T = 100$ K
Block, colorless
0.40 × 0.10 × 0.10 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 10 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (Otwinowski *et al.*, 2003)
$T_{min} = 0.90$, $T_{max} = 0.92$

6924 measured reflections
3737 independent reflections
3221 reflections with $I > 2\sigma(I)$
$R_{int} = 0.063$
$\theta_{max} = 37.8°$, $\theta_{min} = 1.0°$
$h = -22 \rightarrow 22$
$k = -6 \rightarrow 6$
$l = -26 \rightarrow 24$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.114$
$S = 1.10$
3737 reflections
107 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0708P)^2 + 0.0197P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.67$ e Å^{-3}
$\Delta\rho_{min} = -0.41$ 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}
Cl2	0.138241 (15)	0.17792 (6)	0.579292 (15)	0.02422 (7)
Cl1	0.558151 (16)	0.15135 (6)	0.840216 (14)	0.02526 (7)
C1	0.49878 (6)	−0.1166 (2)	0.66074 (6)	0.01968 (13)
C3	0.35318 (6)	0.1385 (2)	0.70157 (6)	0.02006 (14)
C2	0.46410 (6)	0.0484 (2)	0.72565 (5)	0.01980 (13)
C6	0.41880 (6)	−0.1866 (2)	0.56890 (6)	0.02060 (14)
C5	0.30765 (6)	−0.0964 (2)	0.54240 (6)	0.02080 (13)
C4	0.27652 (6)	0.0634 (2)	0.60987 (5)	0.01992 (13)
O1	0.64561 (5)	−0.4059 (2)	0.63526 (5)	0.02975 (14)
C7	0.61622 (6)	−0.2245 (2)	0.68671 (6)	0.02340 (14)
H3	0.3319 (13)	0.260 (4)	0.7450 (12)	0.038 (3)*
H5	0.2576 (13)	−0.150 (4)	0.4813 (13)	0.042 (4)*
H6	0.4423 (13)	−0.293 (5)	0.5239 (12)	0.046 (4)*
H7	0.6686 (14)	−0.131 (4)	0.7449 (13)	0.041 (4)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl2	0.01697 (10)	0.02944 (12)	0.02558 (11)	0.00285 (6)	0.00789 (8)	0.00236 (6)
Cl1	0.02130 (11)	0.02926 (12)	0.02104 (11)	−0.00059 (6)	0.00422 (8)	−0.00518 (6)
C1	0.0165 (3)	0.0207 (3)	0.0213 (3)	−0.0005 (2)	0.0071 (2)	−0.0007 (2)
C3	0.0190 (3)	0.0209 (3)	0.0206 (3)	0.0003 (2)	0.0083 (3)	−0.0003 (2)
C2	0.0182 (3)	0.0203 (3)	0.0195 (3)	−0.0014 (2)	0.0062 (2)	−0.0017 (2)
C6	0.0189 (3)	0.0226 (3)	0.0206 (3)	−0.0002 (2)	0.0082 (2)	−0.0008 (2)
C5	0.0185 (3)	0.0229 (3)	0.0195 (3)	−0.0007 (2)	0.0061 (2)	−0.0008 (2)

C4	0.0168 (3)	0.0209 (3)	0.0215 (3)	0.0001 (2)	0.0071 (2)	0.0016 (2)
O1	0.0214 (3)	0.0378 (3)	0.0304 (3)	0.0045 (2)	0.0108 (2)	−0.0046 (3)
C7	0.0178 (3)	0.0266 (3)	0.0251 (3)	−0.0001 (3)	0.0080 (3)	−0.0013 (3)

Geometric parameters (Å, º)

Cl2—C4	1.7327 (7)	C3—H3	0.939 (17)
Cl1—C2	1.7343 (8)	C6—C5	1.3869 (11)
C1—C2	1.3961 (11)	C6—H6	0.950 (19)
C1—C6	1.3999 (11)	C5—C4	1.3930 (11)
C1—C7	1.4820 (11)	C5—H5	0.923 (18)
C3—C4	1.3877 (11)	O1—C7	1.2180 (11)
C3—C2	1.3893 (11)	C7—H7	0.946 (17)
C2—C1—C6	118.32 (7)	C1—C6—H6	118.6 (9)
C2—C1—C7	122.14 (7)	C6—C5—C4	118.43 (7)
C6—C1—C7	119.53 (7)	C6—C5—H5	118.4 (10)
C4—C3—C2	118.11 (7)	C4—C5—H5	123.2 (10)
C4—C3—H3	121.2 (10)	C3—C4—C5	122.11 (7)
C2—C3—H3	120.6 (10)	C3—C4—Cl2	118.26 (6)
C3—C2—C1	121.73 (7)	C5—C4—Cl2	119.62 (6)
C3—C2—Cl1	116.99 (6)	O1—C7—C1	123.05 (8)
C1—C2—Cl1	121.28 (6)	O1—C7—H7	121.4 (10)
C5—C6—C1	121.30 (7)	C1—C7—H7	115.5 (10)
C5—C6—H6	120.0 (9)		
C4—C3—C2—C1	−0.72 (12)	C1—C6—C5—C4	−0.68 (12)
C4—C3—C2—Cl1	179.11 (6)	C2—C3—C4—C5	−0.19 (12)
C6—C1—C2—C3	0.90 (12)	C2—C3—C4—Cl2	−179.59 (6)
C7—C1—C2—C3	−177.92 (8)	C6—C5—C4—C3	0.88 (12)
C6—C1—C2—Cl1	−178.92 (6)	C6—C5—C4—Cl2	−179.73 (6)
C7—C1—C2—Cl1	2.26 (11)	C2—C1—C7—O1	170.86 (9)
C2—C1—C6—C5	−0.18 (12)	C6—C1—C7—O1	−7.94 (13)
C7—C1—C6—C5	178.67 (7)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7···O1^{i}	0.946 (17)	2.533 (17)	3.4289 (11)	158.0 (14)
C6—H6···O1^{ii}	0.950 (19)	2.512 (17)	3.2774 (11)	137.8 (12)

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