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# 2-Chloro-3-hydroxy-4-methoxybenzaldehyde

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**Key indicators**

Single-crystal X-ray study
*T* = 293 K
Mean σ(C–C) = 0.003 Å
*R* factor = 0.036
*wR* factor = 0.098
Data-to-parameter ratio = 12.7

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.



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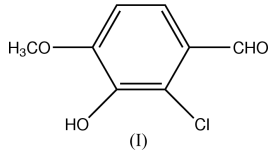
The molecule of the title compound, $C_8H_7ClO_3$, is almost planar, and there are intramolecular O—H···O, C—H···O and C—H···Cl interactions. The molecules are connected by O—H···O and C—H···O interactions, forming two-dimensional networks.

## Comment

The title compound, (I), is an important intermediate in the syntheses of antihypertensives (Lebow & Tremper, 1986) and herbicides (Michelotti *et al.*, 1999). It can be prepared as the main product from 3-hydroxy-4-methoxybenzaldehyde by chlorination (Joseph, 1983). This paper reports the structure analysis of (I).




(I)

The molecular structure of (I) is shown in Fig. 1. The C—C bond lengths in the benzene ring are 1.373 (2)–1.407 (2) Å, and the bond angles 117.61 (15)–122.01 (16)° (Table 1); these are not distorted as seriously as in other similar compounds (Ferreira *et al.*, 2001; Boudjada *et al.*, 2001). The aromatic ring is essentially planar, and other substituent groups lie almost in the same plane, as can be seen from the torsion angles listed in Table 1.

There are intramolecular O2—H2···O1 hydrogen bonds, and C6—H6···O3 and C7—H7···Cl short contacts (Table 2). The intermolecular interactions of O2—H2···O3$^{i}$, C7—

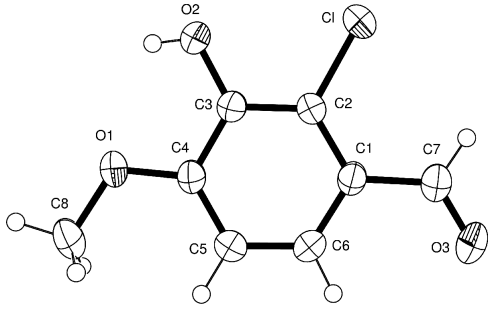



**Figure 1**
The molecular structure of (I), showing the atomic numbering. Displacement ellipsoids are drawn at the 50% probability level for non-H atoms.

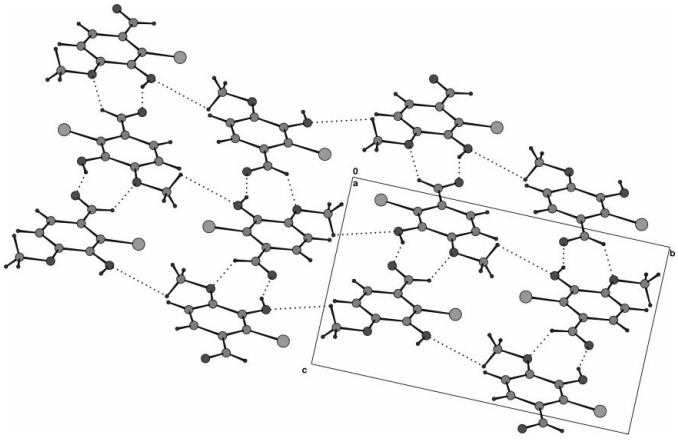


**Figure 2**
Packing diagram of (I), viewed along the *a* axis, showing the hydrogen bonds and short contacts as dashed lines.

H7···O1$^{ii}$ and C8—H8*A*···O2$^{iii}$ (symmetry codes in Table 2) generate two-dimensional networks (Fig. 2).

## Experimental

The title compound was synthesized in our laboratory (Michelotti *et al.*, 1999). Crystals suitable for X-ray analysis were obtained by slow evaporation of a saturated aqueous solution at room temperature.

*Crystal data*

$C_8H_7ClO_3$
$M_r$ = 186.59
Monoclinic, $P2_1/c$
$a$ = 6.4910 (5) Å
$b$ = 14.2605 (13) Å
$c$ = 8.5148 (9) Å
$\beta$ = 98.457 (3)°
$V$ = 779.60 (12) Å$^3$
$Z$ = 4
$D_x$ = 1.590 Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 7841 reflections
$\theta$ = 3.5–27.3°
$\mu$ = 0.45 mm$^{-1}$
$T$ = 293 (2) K
Prism, colorless
0.26 × 0.22 × 0.18 mm

*Data collection*

Rigaku R-AXIS RAPID diffractometer
$\omega$ scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min}$ = 0.888, $T_{max}$ = 0.923
3309 measured reflections
1755 independent reflections
1391 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.026
$\theta_{max}$ = 27.3°
$h = -8 \rightarrow 8$
$k = -18 \rightarrow 18$
$l = -10 \rightarrow 10$

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.098
$S$ = 1.01
1755 reflections
138 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0509P)^2 + 0.1956P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.28 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.23 e Å$^{-3}$
Extinction correction: *SHELXL*97
Extinction coefficient: 0.0081 (19)

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| Cl—C2 | 1.7322 (16) | C6—C5 | 1.373 (2) |
| C1—C7 | 1.464 (2) | C6—C1 | 1.385 (2) |
| C2—C3 | 1.383 (2) | C8—O1 | 1.433 (2) |
| C2—C1 | 1.402 (2) | O1—C4 | 1.357 (2) |
| C3—C4 | 1.407 (2) | O2—C3 | 1.344 (2) |
| C4—C5 | 1.381 (2) | O3—C7 | 1.208 (2) |
| | | | |
| C2—C3—C4 | 118.27 (15) | C5—C6—C1 | 122.01 (16) |
| C3—C2—C1 | 121.90 (15) | C6—C1—C2 | 117.61 (15) |
| C5—C4—C3 | 120.55 (15) | C6—C5—C4 | 119.64 (16) |
| | | | |
| C6—C1—C7—O3 | −0.4 (3) | C8—O1—C4—C5 | 3.5 (3) |

**Table 2**
Hydrogen-bonding geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O2—H2···O1 | 0.77 (3) | 2.29 (3) | 2.6802 (18) | 113 (2) |
| O2—H2···O3$^{i}$ | 0.77 (3) | 2.00 (3) | 2.7044 (18) | 152 (3) |
| C6—H6···O3 | 0.92 (2) | 2.56 (2) | 2.814 (2) | 96.4 (14) |
| C7—H7···Cl | 0.94 (2) | 2.74 (2) | 3.101 (2) | 103.3 (17) |
| C7—H7···O1$^{ii}$ | 0.94 (2) | 2.64 (2) | 3.280 (2) | 125.6 (18) |
| C8—H8*A*···O2$^{iii}$ | 0.98 (3) | 2.90 (3) | 3.229 (3) | 101.0 (17) |

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

All H atoms were located in difference Fourier maps and refined isotropically. Refined distances were C—H = 0.92 (2)–0.98 (2) Å and O—H = 0.77 (3) Å.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC & Rigaku, 2002); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 *for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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