

## 3-(4-Chlorobenzoyloxy)-4-methoxybenzaldehyde

Chun-Hua Diao\* and Zhi Fan

College of Sciences, Tianjin University of  
Science and Technology, Tianjin 300222,  
People's Republic of ChinaCorrespondence e-mail:  
diao\_chunhua@163.com

## Key indicators

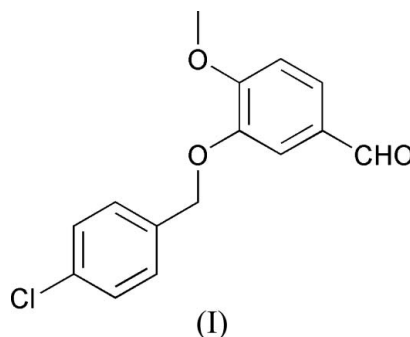
Single-crystal X-ray study  
 $T = 294$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å  
 $R$  factor = 0.047  
 $wR$  factor = 0.111  
Data-to-parameter ratio = 13.5For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.

In the title compound,  $\text{C}_{15}\text{H}_{13}\text{ClO}_3$ , the isovanillin group makes a dihedral angle of  $81.31(8)^\circ$  with the chlorobenzene ring. The crystal structure is stabilized by intermolecular  $\text{C}-\text{H}\cdots\text{O}$  interactions, forming a two-dimensional network.

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## Comment

There has been a steady growth of interest in the structure and reactivity of Schiff bases due to their potential as antibacterial and antitumor agents (Klayman *et al.*, 1979; Santos *et al.*, 2001). As a part of our interest in the coordination properties of Schiff bases functioning as ligands, we have investigated the title compound, (I), which is used as a precursor in the preparation of Schiff bases.



The bond lengths and angles in (I) (Fig. 1) are within their normal ranges (Allen *et al.*, 1987). The isovanillin group (C1–C6/C8/O1/O3) is essentially planar, with an r.m.s. deviation for the fitted atoms of 0.009 Å. This group makes a dihedral angle of  $81.31(8)^\circ$  with the C10–C15 benzene ring.

The crystal packing for (I) is stabilized by weak non-classical intermolecular  $\text{C}-\text{H}\cdots\text{O}=\text{C}$  hydrogen bonds (Table 1), thereby forming a two-dimensional network (Fig. 2).

## Experimental

An anhydrous acetonitrile solution (50 ml) of 3-hydroxy-4-methoxybenzaldehyde (1.52 g, 10 mmol) was added dropwise to a solution (100 ml) of 1-(bromomethyl)-4-chlorobenzene (2.05 g, 10 mmol) and potassium carbonate (1.38 g, 10 mmol) in acetonitrile over a period of 30 min. The mixture was refluxed for 24 h under a nitrogen atmosphere. The solvent was removed and the resultant mixture poured into ice-water (100 ml). The white precipitate was then isolated and recrystallized from acetonitrile, and then dried in a vacuum to give the pure compound in 68% yield. Colorless single crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of an acetonitrile solution.

Crystal data

C<sub>15</sub>H<sub>13</sub>ClO<sub>3</sub>  
*M<sub>r</sub>* = 276.70  
 Monoclinic, *P*2<sub>1</sub>/*c*  
*a* = 10.165 (11) Å  
*b* = 16.752 (18) Å  
*c* = 7.874 (9) Å  
 $\beta$  = 92.54 (2)°  
*V* = 1340 (3) Å<sup>3</sup>

*Z* = 4  
*D<sub>x</sub>* = 1.372 Mg m<sup>-3</sup>  
 Mo *K*α radiation  
 $\mu$  = 0.29 mm<sup>-1</sup>  
*T* = 294 (2) K  
 Block, colorless  
 0.26 × 0.24 × 0.16 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer  
 $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
*T<sub>min</sub>* = 0.912, *T<sub>max</sub>* = 0.955

5172 measured reflections  
 2343 independent reflections  
 1238 reflections with *I* > 2σ(*I*)  
*R<sub>int</sub>* = 0.069  
 $\theta_{max}$  = 25.0°

Refinement

Refinement on *F*<sup>2</sup>  
*R* [*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.047  
*wR* (*F*<sup>2</sup>) = 0.111  
*S* = 1.02  
 2343 reflections  
 173 parameters

H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.04P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{max} = 0.003$   
 $\Delta\rho_{max} = 0.18 \text{ e } \text{Å}^{-3}$   
 $\Delta\rho_{min} = -0.24 \text{ e } \text{Å}^{-3}$

Table 1

Hydrogen-bond geometry (Å, °).

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
C12—H12···O2 <sup>i</sup>	0.93	2.43	3.242 (5)	146
C7—H7B···O2 <sup>ii</sup>	0.96	2.49	3.349 (5)	148

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

The H atoms were included in calculated positions (C—H = 0.93–0.97 Å) and refined as riding, with *U<sub>iso</sub>*(H) = 1.2*U<sub>eq</sub>*(C) or 1.5*U<sub>eq</sub>*(methyl C).

Data collection: SMART (Bruker, 1999); cell refinement: SAINT (Bruker, 1999); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997a); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997a); molecular graphics: SHELXTL (Sheldrick, 1997b); software used to prepare material for publication: SHELXTL.

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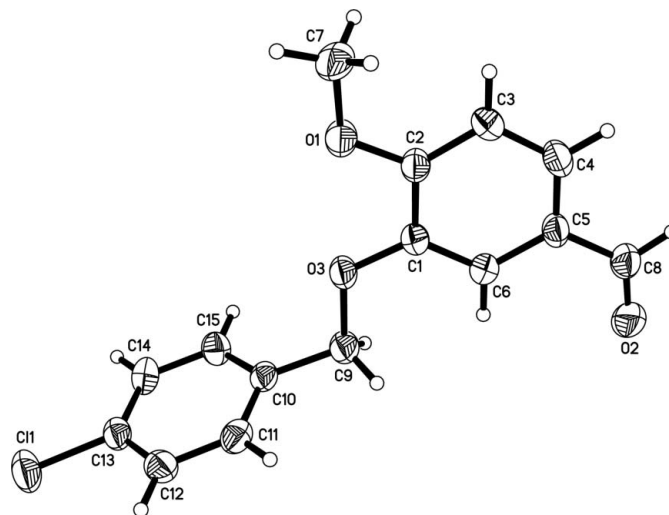


Figure 1 The molecular structure of (I), with displacement ellipsoids for non-H atoms drawn at the 30% probability level.

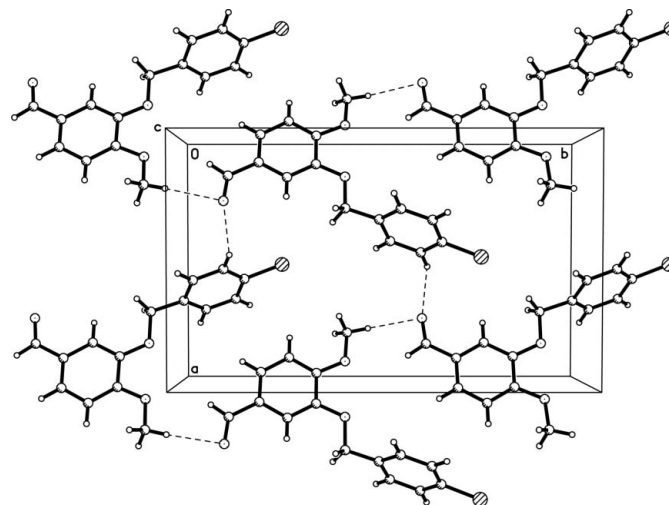


Figure 2 Intermolecular hydrogen-bonding (dashed lines) interactions in (I).

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