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4-(2,4-Dichlorobenzyloxy)-3-methoxybenzaldehyde

Shou-Xin Liu,[a]* Jian-Rong Han,[b]‡ Xiao-Li Zhen[b] and Xia Tian[b]

[a]College of Chemical & Pharmaceutical Engineering, Hebei University of Science & Technology, Shijiazhuang 050018, People's Republic of China, and [b]College of Sciences, Hebei University of Science & Technology, Shijiazhuang 050018, People's Republic of China

‡ Second contact author, email: han_jianrong@163.com

Correspondence e-mail: liu_shouxin@163.com

Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.003 Å
R factor = 0.044
wR factor = 0.104
Data-to-parameter ratio = 16.2

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

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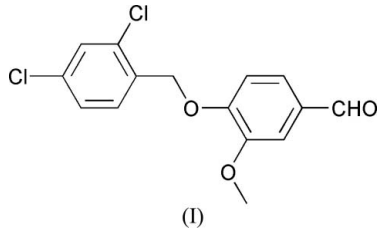
In the title compound, $C_{15}H_{12}Cl_2O_3$, the vanillin group makes a dihedral angle of 4.47 (8)° with the dichlorobenzene ring. Intermolecular C—H···O hydrogen bonds help to consolidate the crystal structure.

Comment

As 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.



(I)

In (I) (Fig. 1), the bond lengths and angles are within their normal ranges (Allen *et al.*, 1987). The vanillin group (atoms C1–C6/C8/O1/O2) is almost planar, with an r.m.s. deviation for the fitted atoms of 0.016 Å. This plane makes a dihedral angle of 4.47 (8)° with the mean plane of the C10–C15 benzene ring.

The crystal structure is stabilized by weak C—H···O interactions that link adjacent molecules into one-dimensional chains running along the *b* axis (Table 1 and Fig. 2).

Experimental

An anhydrous acetonitrile solution (50 ml) of 4-hydroxy-3-methoxybenzaldehyde (1.52 g, 10 mmol) was added dropwise to a

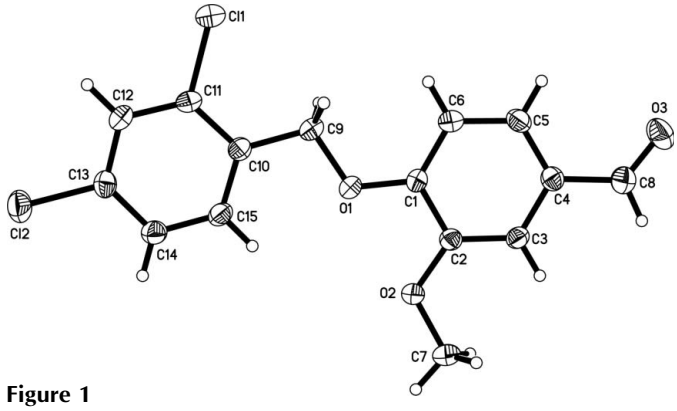


Figure 1
The molecular structure of (I), with displacement ellipsoids for the non-H atoms drawn at the 30% probability level.

solution (100 ml) of 1-(bromomethyl)-2,4-dichlorobenzene (2.40 g, 10 mmol) and potassium carbonate (1.38 g, 10 mmol) in acetonitrile, over a period of 30 min, and 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 resulting white precipitate was isolated and recrystallized from acetonitrile, and then dried in a vacuum to give the pure compound in 52% yield. Colorless single crystals of (I) suitable for X-ray crystallographic analysis were obtained by slow evaporation of an acetonitrile solution.

Crystal data

$C_{15}H_{12}Cl_2O_3$
M_r = 311.15
Monoclinic, $P2_1/c$
a = 7.507 (4) Å
b = 24.436 (15) Å
c = 8.386 (5) Å
β = 109.945 (9)°
V = 1446.1 (15) Å^3
Z = 4
D_x = 1.429 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.45 mm^{-1}
T = 294 (2) K
Block, colorless
0.20 × 0.16 × 0.10 mm

Data collection

Bruker SMART APEX CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.903, T_{max} = 0.956
8038 measured reflections
2952 independent reflections
1663 reflections with $I > 2\sigma(I)$
R_{int} = 0.045
θ_{max} = 26.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.104
S = 1.03
2952 reflections
182 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0423P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.003
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C12—H12···O3^{i}	0.93	2.62	3.512 (3)	161

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

The H atoms were included in calculated positions (C—H = 0.93–0.97 Å) and refined as riding, with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

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

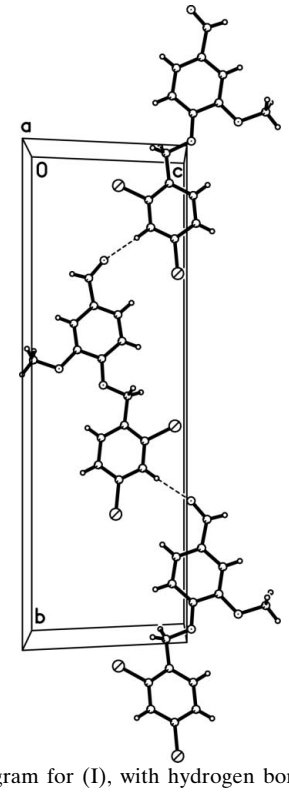


Figure 2
Partial packing diagram for (I), with hydrogen bonds shown as dashed lines.

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References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Bruker (1999). *SMART* (Version 5.0) and *SAINT* (Version 4.0) for Windows NT. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*a*). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*b*). *SHELXTL*. Version 5.10 for Windows NT. Bruker AXS Inc., Madison, Wisconsin, USA.