Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

4-(4-Chlorobenzyloxy)-3-methoxybenzaldehyde

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

[a]College of Chemical and Pharmaceutical Engineering, Hebei University of Science and Technology, Shijiazhuang 050018, People's Republic of China, and [b]College of Sciences, Hebei University of Science and Technology, Shijiazhuang 050018, People's Republic of China
Correspondence e-mail: liu_shouxin@163.com

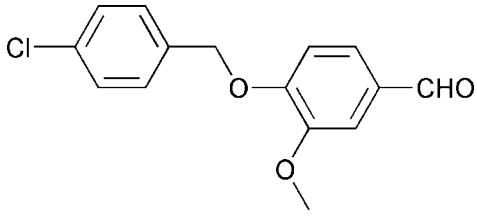
Received 15 October 2007; accepted 24 October 2007

Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.005 Å; R factor = 0.054; wR factor = 0.157; data-to-parameter ratio = 13.8.

In the title compound, $C_{15}H_{13}ClO_3$, the vanillin group makes a dihedral angle of 72.79 (9)° with the chlorobenzene ring. The crystal structure is stabilized by weak non-classical intermolecular C—H···O hydrogen bonds that form centrosymmetric dimers.

Related literature

For general background, see: Allen *et al.* (1987); Jones *et al.* (1979); Larson & Pecoraro (1991); Santos *et al.* (2001).



Experimental

Crystal data

$C_{15}H_{13}ClO_3$
M_r = 276.70
Monoclinic, $P2_1/c$
a = 9.054 (3) Å
b = 8.535 (2) Å
c = 17.828 (5) Å
β = 90.10 (2)°
V = 1377.7 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.28 mm^{-1}
T = 294 (2) K
0.28 × 0.22 × 0.20 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.912, T_{max} = 0.946
6675 measured reflections
2383 independent reflections
1124 reflections with $I > 2\sigma(I)$
R_{int} = 0.048

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.157
S = 1.08
2383 reflections
173 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C14—H14···O2^{i}	0.93	2.56	3.423 (5)	154

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

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*.

This project was supported by the Foundation of the Education Department of Hebei Province (grant No. 606022).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BQ2040).

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.
Jones, R. D., Summerville, D. A. & Basolo, F. (1979). *Chem. Rev.* **17**, 139–179.
Larson, E. J. & Pecoraro, V. L. (1991). *J. Am. Chem. Soc.* **113**, 3810–3818.
Santos, M. L. P., Bagatin, I. A., Pereira, E. M. & Ferreira, A. M. D. C. (2001). *J. Chem. Soc. Dalton Trans.* pp. 838–844.
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.

‡ Additional contact author: email: han_jianrong@163.com.

 doi:10.1107/S1600536807052853

supplementary materials

Acta Cryst. (2007). E**63**, o4481 [**doi:10.1107/S1600536807052853**]

4-(4-Chlorobenzyloxy)-3-methoxybenzaldehyde

S.-X. Liu, X. Tian, X.-L. Zhen, Z.-C. Li and J.-R. Han

Comment

There has been a steady growth of interest in the synthesis, structure, and reactivity of Schiff bases due to their potential applications in areas such as biological modelling, catalysis, and molecular magnets (Jones *et al.*, 1979; Larson & Pecoraro, 1991). Consequently, a significant effort has been devoted to the synthesis of new Schiff base derivatives (Santos *et al.*, 2001).

As a part of our interest in the coordination properties of Schiff bases functioning as ligands, we investigated the title compound, (I), used as a precursor in the preparation of Schiff bases.

In the title molecule (Fig. 1), bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The vanillin group (C1—C6/C8/O1/O2) is essentially planar, with an r.m.s. deviation for fitted atoms of 0.0090 Å. This group makes a dihedral angle of 72.79 (9)° with the benzene ring (C10—C15).

The crystal structure is stabilized by weak non-classical intermolecular C14—H14···O2 hydrogen bonds that forms centrosymmetric dimers (Table 1, Fig. 2).

Experimental

An anhydrous acetonitrile solution (50 ml) of 4-hydroxy-3-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, in 30 min., and the mixture refluxed for 48 h under 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 65% yield. Colorless single crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of an acetonitrile solution.

Refinement

The H atoms were included in calculated positions and refined using a riding model approximation. Constrained C—H and N—H bond lengths and isotropic U parameters: 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C) for Csp^2—H; 0.97 Å and U_{iso}(H) = 1.2U_{eq}(C) for methylene C—H; 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C) for methyl C—H.

Figures

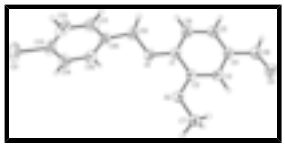


Fig. 1. The structure of (I) with displacement ellipsoids for non-H atoms drawn at the 30% probability level.

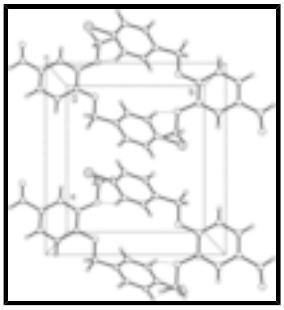


Fig. 2. Intermolecular hydrogen bonding interactions (dashed lines).

4-(4-Chlorobenzyloxy)-3-methoxybenzaldehyde

Crystal data

$C_{15}H_{13}ClO_3$	F_{000} = 576
M_r = 276.70	D_x = 1.334 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 1181 reflections
a = 9.054 (3) Å	θ = 2.3–21.1º
b = 8.535 (2) Å	μ = 0.28 mm^{-1}
c = 17.828 (5) Å	T = 294 (2) K
β = 90.10 (2)º	Block, colorless
V = 1377.7 (7) Å^3	0.28 × 0.22 × 0.20 mm
Z = 4	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	2383 independent reflections
Radiation source: fine-focus sealed tube	1124 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.048
T = 294(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 2.3º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −5→10
T_{min} = 0.912, T_{max} = 0.946	k = −10→10
6675 measured reflections	l = −20→21

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.054	H-atom parameters constrained
$wR(F^2)$ = 0.157	$w = 1/[\sigma^2(F_o^2) + (0.064P)^2 + 0.0805P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.08	$(\Delta/\sigma)_{max}$ = 0.001

2383 reflections	$\Delta\rho_{max} = 0.38$ e Å^{-3}
173 parameters	$\Delta\rho_{min} = -0.39$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2\sigma(F^2)$ 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}
Cl1	0.59471 (15)	−0.34118 (12)	0.00262 (10)	0.1423 (8)
O1	0.9350 (2)	0.3047 (2)	0.11555 (14)	0.0664 (8)
O2	1.1901 (2)	0.2923 (2)	0.17769 (15)	0.0688 (8)
O3	1.3242 (3)	0.8721 (3)	0.23371 (18)	0.0879 (10)
C1	0.9921 (3)	0.4453 (4)	0.13587 (19)	0.0542 (9)
C2	1.1324 (4)	0.4386 (4)	0.17014 (19)	0.0539 (9)
C3	1.1999 (4)	0.5747 (4)	0.1921 (2)	0.0593 (10)
H3	1.2936	0.5707	0.2135	0.071*
C4	1.1305 (4)	0.7187 (4)	0.1830 (2)	0.0560 (10)
C5	0.9929 (4)	0.7241 (4)	0.1508 (2)	0.0648 (11)
H5	0.9454	0.8200	0.1454	0.078*
C6	0.9239 (4)	0.5888 (4)	0.1265 (2)	0.0672 (11)
H6	0.8315	0.5943	0.1038	0.081*
C7	1.3303 (4)	0.2813 (4)	0.2140 (3)	0.0829 (13)
H7A	1.4013	0.3429	0.1870	0.124*
H7B	1.3616	0.1739	0.2149	0.124*
H7C	1.3223	0.3198	0.2644	0.124*
C8	1.2026 (5)	0.8637 (4)	0.2065 (2)	0.0670 (11)
H8	1.1506	0.9567	0.2001	0.080*
C9	0.7940 (4)	0.3070 (4)	0.0790 (2)	0.0767 (12)
H9A	0.8002	0.3664	0.0328	0.092*
H9B	0.7215	0.3566	0.1112	0.092*
C10	0.7489 (4)	0.1425 (4)	0.0626 (2)	0.0554 (10)
C11	0.6410 (4)	0.0703 (5)	0.1033 (2)	0.0744 (11)
H11	0.5989	0.1227	0.1437	0.089*
C12	0.5926 (4)	−0.0802 (6)	0.0857 (3)	0.0843 (14)
H12	0.5184	−0.1286	0.1133	0.101*
C13	0.6582 (6)	−0.1550 (4)	0.0260 (3)	0.0778 (14)

C14	0.7666 (5)	−0.0873 (5)	−0.0142 (3)	0.0786 (12)
H14	0.8106	−0.1407	−0.0537	0.094*
C15	0.8108 (4)	0.0606 (4)	0.0039 (2)	0.0665 (10)
H15	0.8850	0.1077	−0.0242	0.080*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.1369 (12)	0.0565 (7)	0.2331 (18)	−0.0265 (6)	−0.1169 (11)	0.0205 (8)
O1	0.0558 (15)	0.0491 (13)	0.094 (2)	−0.0021 (11)	−0.0285 (13)	−0.0118 (13)
O2	0.0572 (16)	0.0501 (13)	0.099 (2)	0.0064 (11)	−0.0255 (14)	−0.0154 (13)
O3	0.0724 (19)	0.0621 (17)	0.129 (3)	−0.0115 (13)	−0.0257 (18)	−0.0126 (15)
C1	0.050 (2)	0.054 (2)	0.059 (3)	−0.0026 (16)	−0.0079 (17)	−0.0058 (18)
C2	0.051 (2)	0.049 (2)	0.062 (3)	−0.0003 (16)	−0.0071 (17)	−0.0057 (18)
C3	0.044 (2)	0.056 (2)	0.077 (3)	−0.0016 (17)	−0.0096 (17)	−0.008 (2)
C4	0.054 (2)	0.050 (2)	0.064 (3)	−0.0048 (17)	−0.0062 (19)	−0.0051 (18)
C5	0.070 (3)	0.045 (2)	0.080 (3)	0.0047 (18)	−0.012 (2)	−0.0033 (19)
C6	0.063 (2)	0.055 (2)	0.083 (3)	0.0038 (18)	−0.025 (2)	−0.003 (2)
C7	0.064 (3)	0.061 (2)	0.123 (4)	0.0113 (19)	−0.036 (2)	−0.013 (2)
C8	0.073 (3)	0.050 (2)	0.078 (3)	−0.0015 (19)	−0.002 (2)	−0.0049 (18)
C9	0.070 (3)	0.062 (2)	0.097 (3)	−0.0031 (18)	−0.038 (2)	−0.002 (2)
C10	0.050 (2)	0.055 (2)	0.061 (3)	−0.0015 (17)	−0.0189 (19)	−0.0009 (19)
C11	0.064 (3)	0.093 (3)	0.066 (3)	0.009 (2)	−0.009 (2)	0.001 (2)
C12	0.057 (3)	0.096 (4)	0.100 (4)	−0.024 (2)	−0.021 (2)	0.046 (3)
C13	0.076 (3)	0.050 (2)	0.107 (4)	−0.010 (2)	−0.052 (3)	0.011 (2)
C14	0.083 (3)	0.068 (3)	0.085 (3)	−0.004 (2)	−0.023 (2)	−0.017 (2)
C15	0.061 (2)	0.074 (3)	0.064 (3)	−0.017 (2)	−0.0031 (19)	0.000 (2)

Geometric parameters (Å, °)

Cl1—C13	1.741 (4)	C7—H7B	0.9600
O1—C1	1.355 (4)	C7—H7C	0.9600
O1—C9	1.432 (4)	C8—H8	0.9300
O2—C2	1.360 (4)	C9—C10	1.491 (4)
O2—C7	1.427 (4)	C9—H9A	0.9700
O3—C8	1.204 (4)	C9—H9B	0.9700
C1—C6	1.381 (4)	C10—C11	1.365 (5)
C1—C2	1.410 (4)	C10—C15	1.378 (5)
C2—C3	1.369 (4)	C11—C12	1.393 (5)
C3—C4	1.390 (4)	C11—H11	0.9300
C3—H3	0.9300	C12—C13	1.376 (6)
C4—C5	1.371 (5)	C12—H12	0.9300
C4—C8	1.461 (4)	C13—C14	1.347 (6)
C5—C6	1.383 (4)	C14—C15	1.363 (5)
C5—H5	0.9300	C14—H14	0.9300
C6—H6	0.9300	C15—H15	0.9300
C7—H7A	0.9600		
C1—O1—C9	116.7 (2)	O3—C8—H8	117.5

C2—O2—C7	116.5 (2)	C4—C8—H8	117.5
O1—C1—C6	125.6 (3)	O1—C9—C10	108.7 (3)
O1—C1—C2	115.0 (3)	O1—C9—H9A	110.0
C6—C1—C2	119.4 (3)	C10—C9—H9A	110.0
O2—C2—C3	125.4 (3)	O1—C9—H9B	110.0
O2—C2—C1	115.2 (3)	C10—C9—H9B	110.0
C3—C2—C1	119.4 (3)	H9A—C9—H9B	108.3
C2—C3—C4	121.0 (3)	C11—C10—C15	117.9 (3)
C2—C3—H3	119.5	C11—C10—C9	121.1 (4)
C4—C3—H3	119.5	C15—C10—C9	121.0 (4)
C5—C4—C3	119.3 (3)	C10—C11—C12	121.4 (4)
C5—C4—C8	119.8 (3)	C10—C11—H11	119.3
C3—C4—C8	120.9 (3)	C12—C11—H11	119.3
C4—C5—C6	120.8 (3)	C13—C12—C11	117.8 (4)
C4—C5—H5	119.6	C13—C12—H12	121.1
C6—C5—H5	119.6	C11—C12—H12	121.1
C1—C6—C5	120.1 (3)	C14—C13—C12	121.9 (4)
C1—C6—H6	120.0	C14—C13—Cl1	120.3 (4)
C5—C6—H6	120.0	C12—C13—Cl1	117.8 (4)
O2—C7—H7A	109.5	C13—C14—C15	119.0 (4)
O2—C7—H7B	109.5	C13—C14—H14	120.5
H7A—C7—H7B	109.5	C15—C14—H14	120.5
O2—C7—H7C	109.5	C14—C15—C10	122.0 (4)
H7A—C7—H7C	109.5	C14—C15—H15	119.0
H7B—C7—H7C	109.5	C10—C15—H15	119.0
O3—C8—C4	125.0 (3)		
C9—O1—C1—C6	2.2 (5)	C4—C5—C6—C1	1.4 (6)
C9—O1—C1—C2	−178.7 (3)	C5—C4—C8—O3	−178.3 (4)
C7—O2—C2—C3	2.3 (5)	C3—C4—C8—O3	1.2 (6)
C7—O2—C2—C1	−178.4 (3)	C1—O1—C9—C10	−178.9 (3)
O1—C1—C2—O2	0.1 (5)	O1—C9—C10—C11	106.1 (4)
C6—C1—C2—O2	179.3 (3)	O1—C9—C10—C15	−76.4 (4)
O1—C1—C2—C3	179.5 (3)	C15—C10—C11—C12	−1.1 (5)
C6—C1—C2—C3	−1.3 (5)	C9—C10—C11—C12	176.4 (3)
O2—C2—C3—C4	−179.0 (3)	C10—C11—C12—C13	0.6 (6)
C1—C2—C3—C4	1.7 (5)	C11—C12—C13—C14	0.6 (6)
C2—C3—C4—C5	−0.6 (5)	C11—C12—C13—Cl1	−178.5 (3)
C2—C3—C4—C8	179.9 (4)	C12—C13—C14—C15	−1.2 (6)
C3—C4—C5—C6	−1.0 (6)	Cl1—C13—C14—C15	177.9 (3)
C8—C4—C5—C6	178.5 (3)	C13—C14—C15—C10	0.6 (6)
O1—C1—C6—C5	178.9 (3)	C11—C10—C15—C14	0.5 (5)
C2—C1—C6—C5	−0.3 (6)	C9—C10—C15—C14	−177.0 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C14—H14···O2^{i}	0.93	2.56	3.423 (5)	154

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

Fig. 1

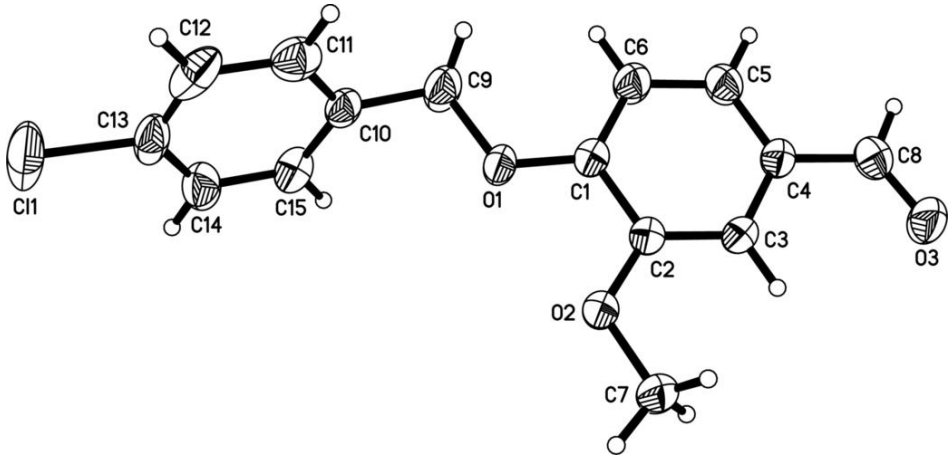


Fig. 2