Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

4-Methoxy-3-(methoxymethyl)benzaldehyde

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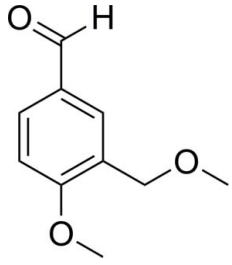
Received 7 December 2012; accepted 11 December 2012

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.063; wR factor = 0.165; data-to-parameter ratio = 14.7.

In the title compound, $C_{10}H_{12}O_3$, the dihedral angle between the benzene ring and the methoxymethyl side chain is 9.7 (2)°. The O atom of the aldehyde group and the C atom of the methoxy group deviate from the plane of the ring by 0.039 (3) and 0.338 (4) Å, respectively. The only intermolecular interactions are very weak C—H$\cdots\pi$ interactions.

Related literature

For the synthesis and applications of the title compound see: Jonali *et al.* (2003).



Experimental

Crystal data

$C_{10}H_{12}O_3$
M_r = 180.20
Monoclinic, $P2_1/c$
a = 7.8100 (16) Å
b = 8.3970 (17) Å
c = 14.510 (3) Å
β = 98.01 (3)°
V = 942.3 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 293 K
0.30 × 0.20 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.973, T_{max} = 0.991
1860 measured reflections
1729 independent reflections
860 reflections with $I > 2\sigma(I)$
R_{int} = 0.099
3 standard reflections every 200 reflections
intensity decay: 1%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.063
$wR(F^2)$ = 0.165
S = 1.01
1729 reflections
118 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

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

*Cg*1 is the centroid of the C1–C6 ring.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C7—H7*B*$\cdots$*Cg*1^{i}	0.96	2.84	3.650 (5)	143
C8—H8*A*$\cdots$*Cg*1^{ii}	0.97	2.97	3.731 (3)	136

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

Data collection: *CAD-4 Software* (Enraf–Nonius, 1985); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

The authors thank the Center of Testing and Analysis, Nanjing University, for the data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB7010).

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Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

Acta Cryst. (2013). E**69**, o112 [https://doi.org/10.1107/S1600536812050350]

4-Methoxy-3-(methoxymethyl)benzaldehyde

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S1. Experimental

The title compound, (I) was prepared by the literature method (Jonali *et al.* 2003). Colourless blocks were obtained by dissolving (I) (0.18 g, 1.0 mmol) in acetone (25 ml) and evaporating the solvent slowly at room temperature for about 7 d.

S2. Refinement

H atoms were positioned geometrically and refined as riding groups with U_{iso}(H) = xU_{eq}(C), where x = 1.2 for aromatic H, and x = 1.5 for other H.

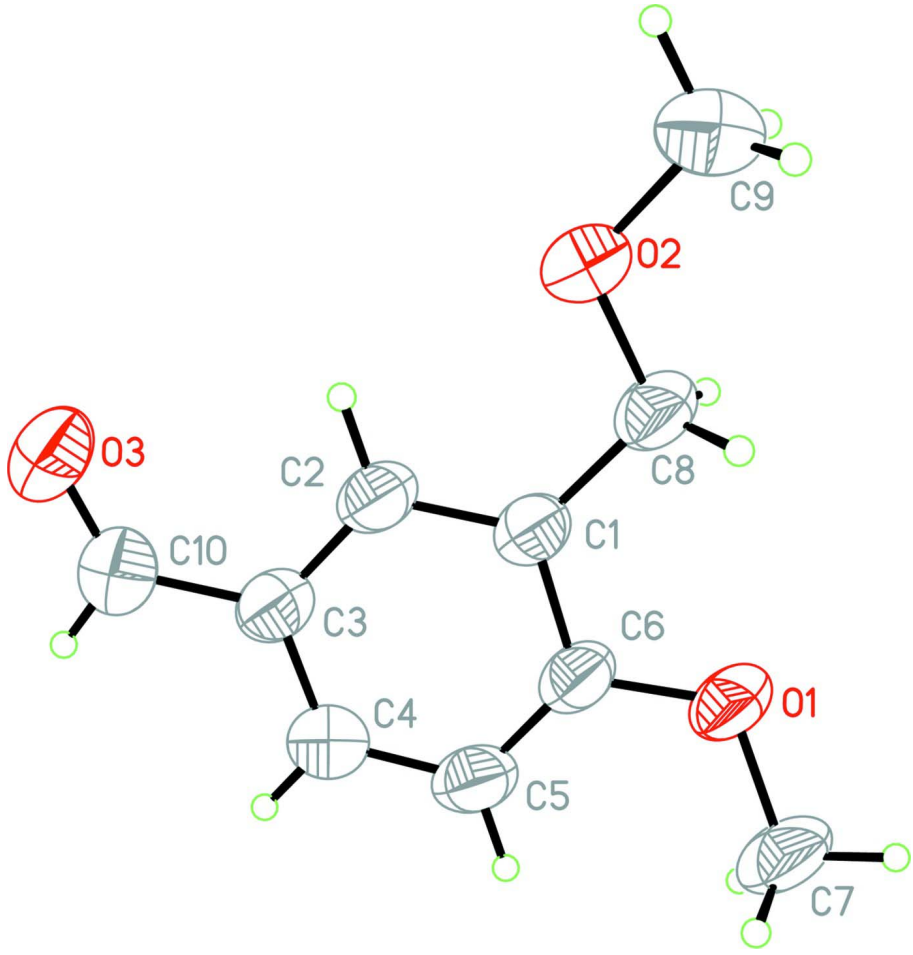

Figure 1

The molecular structure of (I), with displacement ellipsoids drawn at the 50% probability level.

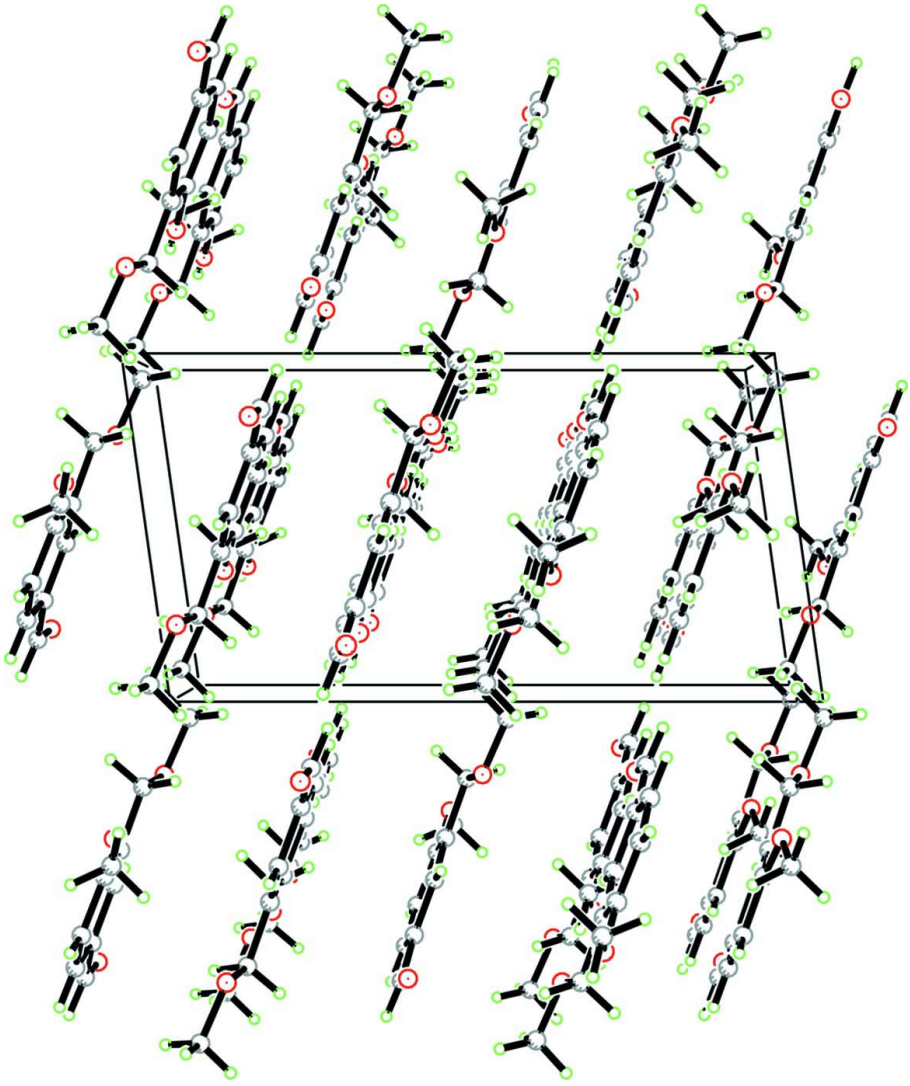

Figure 2

A packing diagram of (I).

4-Methoxy-3-(methoxymethyl)benzaldehyde

Crystal data

$C_{10}H_{12}O_3$
$M_r = 180.20$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 7.8100$ (16) Å
$b = 8.3970$ (17) Å
$c = 14.510$ (3) Å
$\beta = 98.01$ (3)°
$V = 942.3$ (3) Å^3
$Z = 4$
$F(000) = 384$
$D_x = 1.270$ Mg m^{-3}
Melting point: 341 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 9$–13°
$\mu = 0.09$ mm^{-1}
$T = 293$ K
Block, colourless
0.30 × 0.20 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.973, T_{max} = 0.991
1860 measured reflections
1729 independent reflections
860 reflections with $I > 2\sigma(I)$
R_{int} = 0.099
θ_{max} = 25.4°, θ_{min} = 2.6°
h = 0→9
k = 0→10
l = −17→17
3 standard reflections every 200 reflections
intensity decay: 1%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.063
$wR(F^2)$ = 0.165
S = 1.01
1729 reflections
118 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.070P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 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}
O1	0.3742 (3)	−0.2060 (2)	0.10208 (17)	0.0606 (7)
C1	0.4323 (4)	0.0653 (3)	0.1125 (2)	0.0449 (8)
O2	0.2282 (3)	0.2507 (3)	0.03860 (18)	0.0736 (8)
C2	0.5453 (4)	0.1885 (4)	0.1380 (2)	0.0512 (9)
H2A	0.5092	0.2927	0.1250	0.061*
O3	0.8048 (3)	0.4313 (3)	0.1968 (2)	0.0838 (10)
C3	0.7125 (5)	0.1612 (4)	0.1829 (2)	0.0531 (9)
C4	0.7648 (4)	0.0059 (4)	0.2027 (3)	0.0608 (10)
H4A	0.8752	−0.0133	0.2339	0.073*
C5	0.6561 (5)	−0.1209 (4)	0.1772 (3)	0.0579 (10)
H5A	0.6928	−0.2248	0.1904	0.070*
C6	0.4919 (4)	−0.0912 (3)	0.1318 (2)	0.0494 (9)
C7	0.4335 (5)	−0.3667 (4)	0.1007 (3)	0.0688 (12)
H7A	0.3380	−0.4353	0.0791	0.103*
H7B	0.4826	−0.3978	0.1624	0.103*

H7C	0.5196	−0.3749	0.0598	0.103*
C8	0.2523 (4)	0.0900 (3)	0.0654 (2)	0.0547 (9)
H8A	0.2307	0.0221	0.0110	0.066*
H8B	0.1709	0.0614	0.1075	0.066*
C9	0.0623 (5)	0.2781 (4)	−0.0121 (3)	0.0835 (13)
H9A	0.0509	0.3887	−0.0286	0.125*
H9B	−0.0248	0.2497	0.0256	0.125*
H9C	0.0485	0.2145	−0.0676	0.125*
C10	0.8314 (5)	0.2919 (5)	0.2107 (3)	0.0680 (11)
H10A	0.9390	0.2644	0.2425	0.082*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0666 (16)	0.0309 (13)	0.0856 (18)	−0.0025 (11)	0.0151 (13)	−0.0033 (11)
C1	0.050 (2)	0.0358 (18)	0.052 (2)	−0.0002 (16)	0.0158 (16)	−0.0018 (14)
O2	0.0662 (17)	0.0371 (14)	0.112 (2)	0.0032 (13)	−0.0070 (15)	0.0046 (13)
C2	0.058 (2)	0.0342 (17)	0.063 (2)	0.0024 (16)	0.0133 (18)	0.0005 (15)
O3	0.082 (2)	0.0481 (16)	0.118 (3)	−0.0127 (14)	0.0024 (17)	−0.0007 (16)
C3	0.058 (2)	0.0404 (19)	0.062 (2)	0.0006 (18)	0.0120 (18)	−0.0036 (17)
C4	0.055 (2)	0.053 (2)	0.075 (3)	0.0049 (19)	0.0107 (19)	−0.0041 (19)
C5	0.064 (2)	0.040 (2)	0.073 (3)	0.0082 (18)	0.019 (2)	0.0009 (18)
C6	0.057 (2)	0.0321 (18)	0.061 (2)	−0.0024 (16)	0.0157 (19)	−0.0034 (15)
C7	0.084 (3)	0.0297 (18)	0.097 (3)	0.0005 (18)	0.029 (2)	−0.0046 (18)
C8	0.060 (2)	0.0332 (18)	0.072 (3)	−0.0042 (16)	0.0143 (19)	0.0049 (16)
C9	0.066 (3)	0.062 (3)	0.119 (4)	0.016 (2)	0.000 (3)	0.004 (2)
C10	0.060 (2)	0.058 (2)	0.084 (3)	−0.007 (2)	0.006 (2)	−0.003 (2)

Geometric parameters (Å, º)

O1—C6	1.360 (4)	C4—H4A	0.9300
O1—C7	1.427 (3)	C5—C6	1.380 (4)
C1—C2	1.376 (4)	C5—H5A	0.9300
C1—C6	1.409 (4)	C7—H7A	0.9600
C1—C8	1.490 (4)	C7—H7B	0.9600
O2—C8	1.410 (3)	C7—H7C	0.9600
O2—C9	1.416 (4)	C8—H8A	0.9700
C2—C3	1.395 (5)	C8—H8B	0.9700
C2—H2A	0.9300	C9—H9A	0.9600
O3—C10	1.201 (4)	C9—H9B	0.9600
C3—C4	1.385 (4)	C9—H9C	0.9600
C3—C10	1.457 (5)	C10—H10A	0.9300
C4—C5	1.380 (4)		
C6—O1—C7	118.0 (3)	O1—C7—H7B	109.5
C2—C1—C6	117.8 (3)	H7A—C7—H7B	109.5
C2—C1—C8	123.2 (3)	O1—C7—H7C	109.5
C6—C1—C8	119.0 (3)	H7A—C7—H7C	109.5

C8—O2—C9	112.1 (3)	H7B—C7—H7C	109.5
C1—C2—C3	121.7 (3)	O2—C8—C1	109.9 (3)
C1—C2—H2A	119.2	O2—C8—H8A	109.7
C3—C2—H2A	119.2	C1—C8—H8A	109.7
C4—C3—C2	118.8 (3)	O2—C8—H8B	109.7
C4—C3—C10	119.6 (3)	C1—C8—H8B	109.7
C2—C3—C10	121.6 (3)	H8A—C8—H8B	108.2
C5—C4—C3	121.2 (3)	O2—C9—H9A	109.5
C5—C4—H4A	119.4	O2—C9—H9B	109.5
C3—C4—H4A	119.4	H9A—C9—H9B	109.5
C4—C5—C6	119.0 (3)	O2—C9—H9C	109.5
C4—C5—H5A	120.5	H9A—C9—H9C	109.5
C6—C5—H5A	120.5	H9B—C9—H9C	109.5
O1—C6—C5	124.4 (3)	O3—C10—C3	126.8 (4)
O1—C6—C1	114.1 (3)	O3—C10—H10A	116.6
C5—C6—C1	121.5 (3)	C3—C10—H10A	116.6
O1—C7—H7A	109.5		

C6—C1—C2—C3	−1.0 (5)	C4—C5—C6—C1	−1.0 (5)
C8—C1—C2—C3	179.3 (3)	C2—C1—C6—O1	−178.2 (3)
C1—C2—C3—C4	−0.6 (5)	C8—C1—C6—O1	1.5 (4)
C1—C2—C3—C10	−179.4 (3)	C2—C1—C6—C5	1.8 (5)
C2—C3—C4—C5	1.4 (5)	C8—C1—C6—C5	−178.4 (3)
C10—C3—C4—C5	−179.8 (3)	C9—O2—C8—C1	176.0 (3)
C3—C4—C5—C6	−0.6 (5)	C2—C1—C8—O2	9.5 (4)
C7—O1—C6—C5	−13.0 (5)	C6—C1—C8—O2	−170.2 (3)
C7—O1—C6—C1	167.1 (3)	C4—C3—C10—O3	178.7 (4)
C4—C5—C6—O1	179.0 (3)	C2—C3—C10—O3	−2.5 (6)

Hydrogen-bond geometry (Å, º)

Cg1 is the centroid of the C1–C6 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7*B*···*Cg*1^{i}	0.96	2.84	3.650 (5)	143
C8—H8*A*···*Cg*1^{ii}	0.97	2.97	3.731 (3)	136

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