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2-Hydroxy-3-methoxymethyl-5-methylbenzaldehyde

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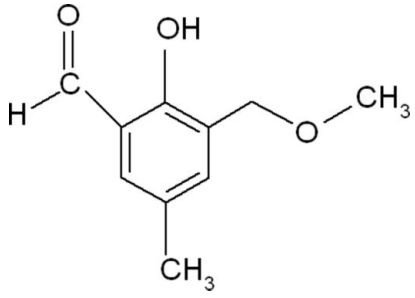
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.003 Å; R factor = 0.054; wR factor = 0.181; data-to-parameter ratio = 19.2.

In the title molecule, $C_{10}H_{12}O_3$, all non-H atoms lie in a common plane (r.m.s deviation = 0.010 Å). The molecular conformation is stabilized by an intramolecular O—H···O hydrogen bond.

Related literature

For the biological activity of methylbenzene derivatives, see: Anbarasan *et al.* (2011); Chan & Daniels (2007). For related structures see: Wang *et al.* (2011); Kılıç *et al.* (2009); For graph-set notation of hydrogen bonds, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$C_{10}H_{12}O_3$
M_r = 180.20
Monoclinic, $P2_1/c$
a = 13.899 (3) Å
b = 8.9184 (19) Å
c = 7.5043 (16) Å
β = 94.098 (6)°
V = 927.8 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 295 K
0.30 × 0.24 × 0.20 mm

Data collection

Bruker Kappa APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.972, T_{max} = 0.981
10089 measured reflections
2329 independent reflections
1213 reflections with $I > 2\sigma(I)$
R_{int} = 0.050

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.181
S = 1.03
2329 reflections
121 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···O1	0.82	1.91	2.628 (3)	146

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT* (Bruker, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT6886).

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2-Hydroxy-3-methoxymethyl-5-methylbenzaldehyde

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S1. Comment

In recent days methylbenzene (toluene) and substituted methylbenzene have become very important on account of their wide range of applications in medicine and industry (Anbarasan *et al.*, 2011). For example 3-chloro-2-methylbenzene-1-sulfonylchloride shows the biological activity of hydroxysteriod dehydrogenase inhibitors (Chan & Daniels, 2007).

The geometric parameters of the compound (I), (Fig. 1) agree well with those of a reported similar structure (Wang *et al.*, 2011; Kılıç *et al.*, 2009) The molecular structure is stabilized by an intramolecular O-H..O interaction generating a six-membered ring S(6) graph-set motif (Bernstein *et al.*, 1995).

S2. Experimental

To a methanolic solution of 2-hydroxy-5-methyl-1,3-benzenedicarboxaldehyde (1g, 6mmol) decarborane (0.37, 3 mmol) was added slowly with constant stirring at room temperature in nitrogen atmosphere for 24 hours. A pale yellow solution formed after 24h and was concentrated to get the crude product. The crude product was washed well with methanol and dried in vacuum. The product was recrystallized in chloroform to get pale yellow coloured crystals suitable for single crystal XRD. yield 0.96g, 80% .

S3. Refinement

H atoms were positioned geometrically and refined using riding model with C-H = 0.93Å and U_{iso}(H) = 1.2Ueq(C) for aromatic C-H, C-H = 0.97Å and U_{iso}(H) = 1.2Ueq(C) for CH_2, C-H = 0.96Å and U_{iso}(H) = 1.5Ueq(C) for CH_3 and O-H = 0.82Å and U_{iso}(H) = 1.2Ueq(C) for OH.

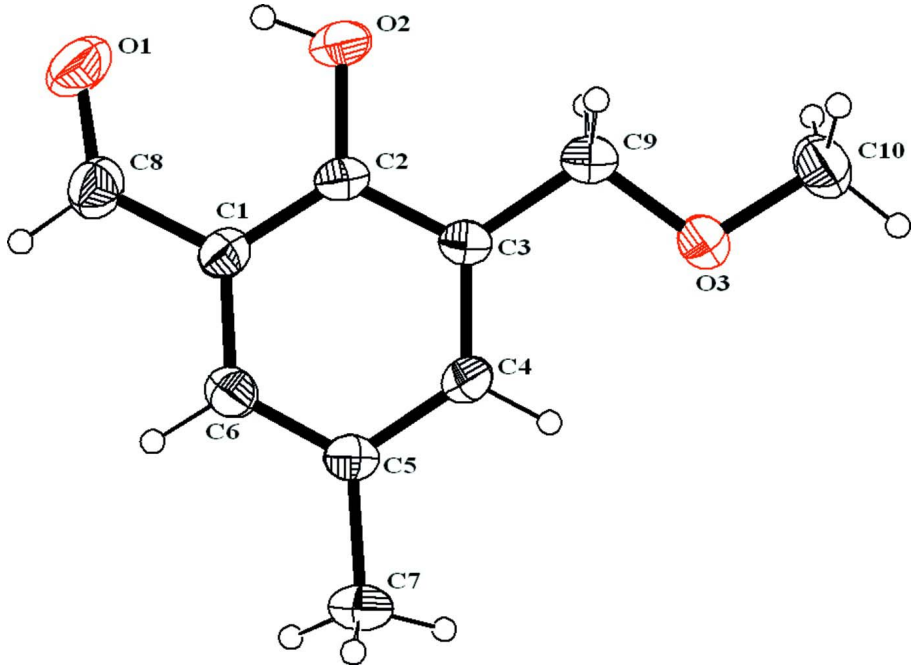

Figure 1

The molecular structure of (I), with atom labels and 30% probability displacement ellipsoids for non-H atoms.

2-Hydroxy-3-methoxymethyl-5-methylbenzaldehyde

Crystal data

$C_{10}H_{12}O_3$
$M_r = 180.20$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 13.899$ (3) Å
$b = 8.9184$ (19) Å
$c = 7.5043$ (16) Å
$\beta = 94.098$ (6)°
$V = 927.8$ (3) Å^3
$Z = 4$
$F(000) = 384$
$D_x = 1.290$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3221 reflections
$\theta = 2.7$–24.8°
$\mu = 0.10$ mm^{-1}
$T = 295$ K
Block, yellow
0.30 × 0.24 × 0.20 mm

Data collection

Bruker Kappa APEXII diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.972$, $T_{max} = 0.981$
10089 measured reflections
2329 independent reflections
1213 reflections with $I > 2\sigma(I)$
$R_{int} = 0.050$
$\theta_{max} = 28.7°$, $\theta_{min} = 2.7°$
$h = -18\rightarrow18$
$k = -11\rightarrow12$
$l = -9\rightarrow9$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.054$
$wR(F^2) = 0.181$
$S = 1.03$
2329 reflections
121 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
$w = 1/[\sigma^2(F_o^2) + (0.0625P)^2 + 0.4641P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.24$ e Å^{-3}
$\Delta\rho_{min} = -0.22$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C8	0.92734 (18)	1.0908 (3)	0.1482 (4)	0.0617 (7)
H8	0.9842	1.1345	0.1959	0.074*
C1	0.85176 (16)	1.1898 (2)	0.0792 (3)	0.0459 (6)
C6	0.86550 (16)	1.3446 (3)	0.0868 (3)	0.0497 (6)
H6	0.9241	1.3825	0.1349	0.060*
C5	0.79476 (17)	1.4420 (2)	0.0250 (3)	0.0479 (6)
C4	0.70806 (16)	1.3801 (2)	−0.0467 (3)	0.0457 (6)
H4	0.6595	1.4449	−0.0906	0.055*
C3	0.69089 (16)	1.2288 (2)	−0.0558 (3)	0.0426 (5)
C2	0.76424 (16)	1.1324 (2)	0.0081 (3)	0.0438 (5)
C9	0.59741 (17)	1.1631 (3)	−0.1290 (3)	0.0536 (6)
H9A	0.6088	1.0965	−0.2275	0.064*
H9B	0.5690	1.1049	−0.0370	0.064*
C10	0.4451 (2)	1.2195 (3)	−0.2637 (4)	0.0741 (9)
H10A	0.4569	1.1579	−0.3648	0.111*
H10B	0.4030	1.3006	−0.3012	0.111*
H10C	0.4155	1.1602	−0.1759	0.111*
C7	0.8079 (2)	1.6091 (3)	0.0330 (4)	0.0687 (8)
H7A	0.7929	1.6451	0.1483	0.103*
H7B	0.7657	1.6556	−0.0576	0.103*
H7C	0.8736	1.6336	0.0132	0.103*
O1	0.92264 (14)	0.9535 (2)	0.1490 (3)	0.0772 (6)
O2	0.74664 (13)	0.98329 (17)	0.0006 (3)	0.0618 (5)
H2	0.7946	0.9376	0.0410	0.093*
O3	0.53348 (12)	1.27783 (19)	−0.1888 (3)	0.0638 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C8	0.0507 (15)	0.0628 (17)	0.0718 (19)	0.0088 (12)	0.0061 (12)	0.0047 (13)
C1	0.0469 (13)	0.0412 (12)	0.0500 (14)	0.0053 (10)	0.0060 (10)	0.0027 (9)
C6	0.0463 (13)	0.0475 (14)	0.0549 (15)	−0.0047 (10)	0.0020 (10)	−0.0034 (11)
C5	0.0530 (14)	0.0374 (11)	0.0532 (14)	−0.0033 (10)	0.0039 (10)	−0.0027 (10)
C4	0.0475 (13)	0.0361 (11)	0.0535 (14)	0.0042 (9)	0.0028 (10)	0.0029 (10)
C3	0.0475 (12)	0.0357 (11)	0.0449 (13)	−0.0051 (9)	0.0059 (9)	0.0007 (9)
C2	0.0515 (13)	0.0319 (11)	0.0487 (13)	−0.0005 (9)	0.0086 (10)	0.0017 (9)
C9	0.0560 (14)	0.0406 (12)	0.0638 (16)	−0.0052 (11)	0.0027 (12)	0.0040 (11)
C10	0.0586 (17)	0.0758 (19)	0.085 (2)	−0.0147 (14)	−0.0139 (14)	0.0095 (16)
C7	0.0728 (18)	0.0374 (13)	0.095 (2)	−0.0071 (12)	−0.0003 (15)	−0.0078 (13)

O1	0.0704 (13)	0.0538 (12)	0.1080 (18)	0.0216 (9)	0.0109 (11)	0.0142 (11)
O2	0.0665 (12)	0.0333 (9)	0.0858 (14)	0.0009 (7)	0.0063 (10)	0.0045 (8)
O3	0.0500 (10)	0.0528 (10)	0.0858 (13)	−0.0075 (8)	−0.0136 (9)	0.0087 (9)

Geometric parameters (Å, º)

C8—O1	1.227 (3)	C2—O2	1.352 (2)
C8—C1	1.440 (3)	C9—O3	1.407 (3)
C8—H8	0.9300	C9—H9A	0.9700
C1—C2	1.391 (3)	C9—H9B	0.9700
C1—C6	1.394 (3)	C10—O3	1.413 (3)
C6—C5	1.368 (3)	C10—H10A	0.9600
C6—H6	0.9300	C10—H10B	0.9600
C5—C4	1.398 (3)	C10—H10C	0.9600
C5—C7	1.503 (3)	C7—H7A	0.9600
C4—C3	1.372 (3)	C7—H7B	0.9600
C4—H4	0.9300	C7—H7C	0.9600
C3—C2	1.392 (3)	O2—H2	0.8200
C3—C9	1.494 (3)		
O1—C8—C1	125.2 (3)	O3—C9—C3	110.18 (18)
O1—C8—H8	117.4	O3—C9—H9A	109.6
C1—C8—H8	117.4	C3—C9—H9A	109.6
C2—C1—C6	119.6 (2)	O3—C9—H9B	109.6
C2—C1—C8	120.5 (2)	C3—C9—H9B	109.6
C6—C1—C8	119.9 (2)	H9A—C9—H9B	108.1
C5—C6—C1	121.5 (2)	O3—C10—H10A	109.5
C5—C6—H6	119.3	O3—C10—H10B	109.5
C1—C6—H6	119.3	H10A—C10—H10B	109.5
C6—C5—C4	117.3 (2)	O3—C10—H10C	109.5
C6—C5—C7	122.3 (2)	H10A—C10—H10C	109.5
C4—C5—C7	120.4 (2)	H10B—C10—H10C	109.5
C3—C4—C5	123.3 (2)	C5—C7—H7A	109.5
C3—C4—H4	118.3	C5—C7—H7B	109.5
C5—C4—H4	118.3	H7A—C7—H7B	109.5
C4—C3—C2	118.0 (2)	C5—C7—H7C	109.5
C4—C3—C9	123.2 (2)	H7A—C7—H7C	109.5
C2—C3—C9	118.74 (19)	H7B—C7—H7C	109.5
O2—C2—C1	121.9 (2)	C2—O2—H2	109.5
O2—C2—C3	117.8 (2)	C9—O3—C10	111.7 (2)
C1—C2—C3	120.25 (19)		
O1—C8—C1—C2	0.9 (4)	C8—C1—C2—O2	−0.1 (3)
O1—C8—C1—C6	179.6 (2)	C6—C1—C2—C3	0.2 (3)
C2—C1—C6—C5	−0.3 (3)	C8—C1—C2—C3	179.0 (2)
C8—C1—C6—C5	−179.0 (2)	C4—C3—C2—O2	179.3 (2)
C1—C6—C5—C4	−0.2 (3)	C9—C3—C2—O2	−0.1 (3)
C1—C6—C5—C7	179.6 (2)	C4—C3—C2—C1	0.2 (3)

C6—C5—C4—C3	0.7 (3)	C9—C3—C2—C1	−179.2 (2)
C7—C5—C4—C3	−179.1 (2)	C4—C3—C9—O3	1.4 (3)
C5—C4—C3—C2	−0.8 (3)	C2—C3—C9—O3	−179.2 (2)
C5—C4—C3—C9	178.7 (2)	C3—C9—O3—C10	178.3 (2)
C6—C1—C2—O2	−178.8 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O1	0.82	1.91	2.628 (3)	146
C4—H4···O3	0.93	2.38	2.736 (3)	103