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1-(4-Hydroxy-3,5-dimethoxyphenyl)-ethanone

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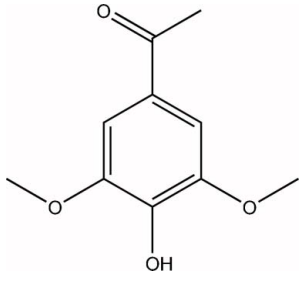
Key indicators: single-crystal X-ray study; T = 113 K; mean σ(C–C) = 0.002 Å; R factor = 0.028; wR factor = 0.077; data-to-parameter ratio = 8.9.

In the title molecule, $C_{10}H_{12}O_4$, the non-H atoms are essentially coplanar (r.m.s. deviation = 0.033 Å). In the crystal, molecules are linked into chains along [001] by O—H···O hydrogen bonds.

Related literature

For the use of the title compound to promote genetic transformation in plant tissue culture and genetic engineering, see: Mathews *et al.* (1990); Sheikholeslam & Weeks (1987).



Experimental

Crystal data

$C_{10}H_{12}O_4$ M_r = 196.20
Tetragonal, $I4_1cd$
a = 14.977 (2) Å
c = 17.142 (3) Å
V = 3845.5 (11) Å^3
Z = 16
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 113 K
0.32 × 0.26 × 0.21 mm

Data collection

Rigaku Saturn CCD area-detector diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.967, T_{max} = 0.978
14812 measured reflections
1178 independent reflections
1157 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.077
S = 1.16
1178 reflections
132 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O4^{i}	0.84	1.96	2.7210 (17)	151

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

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

The authors thank Mr Zhi-Hua Mao of Sichuan University for his help with the X-ray data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2962).

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supporting information

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1-(4-Hydroxy-3,5-dimethoxyphenyl)ethanone

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S1. Comment

The title compound is an important plant phenolic used in bioresearch. In plant tissue culture and genetic engineering, it is used to promote genetic transformation (Sheikholeslam & Weeks, 1987; Mathews *et al.*, 1990). We herein report its crystal structure.

All of the non-H atoms of the title molecule (Fig.1) are essentially coplanar. In the crystal structure, adjacent molecules are linked into chains along the [001] by O—H···.O hydrogen bonds.

S2. Experimental

Single crystals suitable for X-ray analysis were grown by slow evaporation at room temperature of an acetone solution of commerical 1-(4-hydroxy-3,5-dimethoxyphenyl)ethanone.

S3. Refinement

H atoms were placed in calculated positions and refined in the riding model approximation, with O-H = 0.84 Å, C-H = 0.95 (aromatic) and 0.98 Å (methyl), and with U_{iso}(H) = 1.2U_{eq}($C_{aromatic}$) and 1.5U_{eq}(C_{methyl},O). In the absence of significant anomalous scattering, Friedel pairs were merged prior to the final refinement.

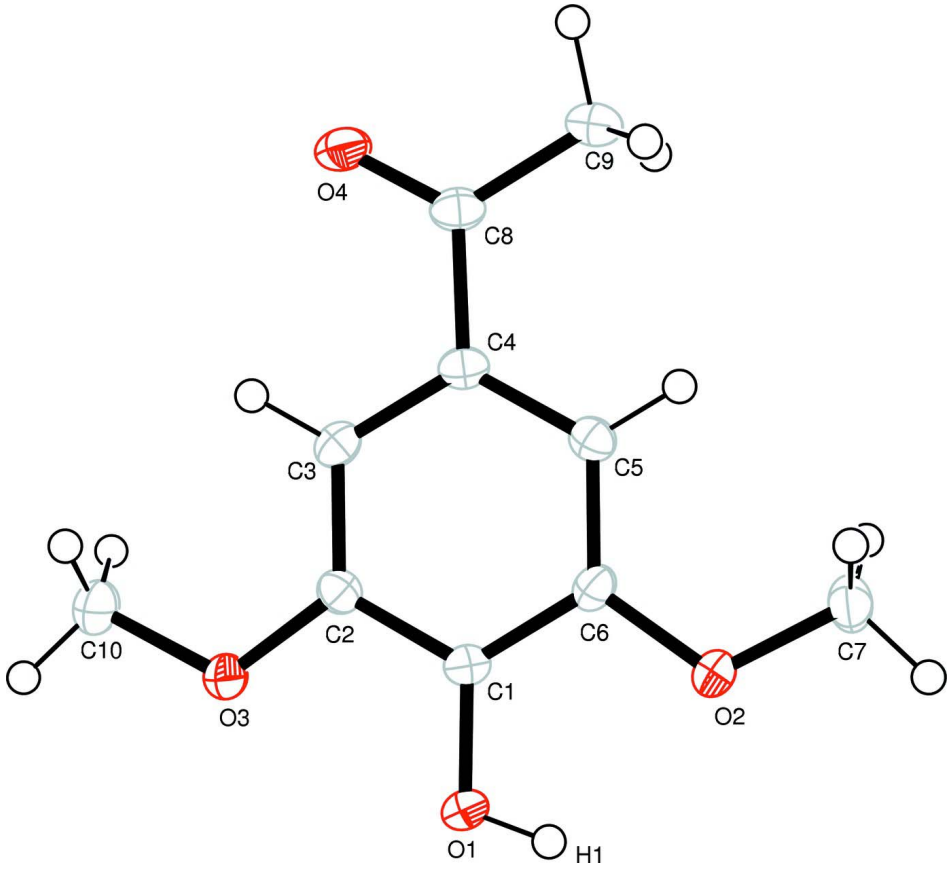

Figure 1

The molecular structure of the title compound, with displacement ellipsoids drawn at the 30% probability level.

1-(4-Hydroxy-3,5-dimethoxyphenyl)ethanone

Crystal data

$C_{10}H_{12}O_4$
$M_r = 196.20$
Tetragonal, $I4_1cd$
Hall symbol: I 4bw -2c
$a = 14.977\ (2)$ Å
$c = 17.142\ (3)$ Å
$V = 3845.5\ (11)$ Å^3
$Z = 16$
$F(000) = 1664$
$D_x = 1.356$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6429 reflections
$\theta = 3.0$–$27.9°$
$\mu = 0.11$ mm^{-1}
$T = 113$ K
Block, colourless
0.32 × 0.26 × 0.21 mm

Data collection

Rigaku Saturn CCD area-detector diffractometer
Radiation source: rotating anode
Confocal monochromator
Detector resolution: 7.31 pixels mm^{-1}
ω and φ scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
$T_{min} = 0.967$, $T_{max} = 0.978$
14812 measured reflections
1178 independent reflections
1157 reflections with $I > 2\sigma(I)$
$R_{int} = 0.031$
$\theta_{max} = 27.9°$, $\theta_{min} = 3.1°$
$h = -19\rightarrow19$
$k = -15\rightarrow19$
$l = -22\rightarrow22$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.028$
$wR(F^2) = 0.077$
$S = 1.16$
1178 reflections
132 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.0561P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.17$ e Å^{-3}
$\Delta\rho_{min} = -0.16$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0083 (13)

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O2	0.58678 (8)	0.08820 (8)	0.37342 (8)	0.0259 (3)
O1	0.42294 (7)	0.15165 (9)	0.39717 (6)	0.0245 (3)
H1	0.4621	0.1342	0.4288	0.037*
O3	0.31210 (7)	0.18800 (7)	0.28362 (6)	0.0231 (3)
C5	0.56661 (11)	0.09497 (10)	0.23142 (9)	0.0198 (3)
H5	0.6250	0.0733	0.2210	0.024*
O4	0.48863 (8)	0.12870 (8)	0.03437 (7)	0.0285 (3)
C3	0.42301 (10)	0.14750 (10)	0.18508 (9)	0.0199 (3)
H3	0.3842	0.1617	0.1430	0.024*
C4	0.50917 (11)	0.11554 (10)	0.17016 (9)	0.0193 (3)
C2	0.39445 (10)	0.15836 (10)	0.26140 (9)	0.0190 (3)
C6	0.53803 (10)	0.10625 (10)	0.30770 (9)	0.0195 (3)
C8	0.53803 (11)	0.10552 (10)	0.08750 (9)	0.0215 (3)
C1	0.45208 (11)	0.13863 (10)	0.32347 (9)	0.0190 (3)
C9	0.62896 (12)	0.06734 (13)	0.07049 (11)	0.0279 (4)
H9A	0.6386	0.0660	0.0140	0.042*
H9B	0.6327	0.0066	0.0914	0.042*
H9C	0.6748	0.1047	0.0951	0.042*
C7	0.67612 (11)	0.05852 (12)	0.36300 (10)	0.0267 (4)
H7A	0.6762	0.0026	0.3333	0.040*
H7B	0.7038	0.0485	0.4141	0.040*
H7C	0.7100	0.1040	0.3345	0.040*
C10	0.25044 (11)	0.20807 (13)	0.22248 (11)	0.0308 (4)

H10A	0.2760	0.2539	0.1883	0.046*
H10B	0.1945	0.2302	0.2451	0.046*
H10C	0.2385	0.1539	0.1921	0.046*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O2	0.0226 (6)	0.0370 (7)	0.0181 (5)	0.0070 (5)	−0.0037 (4)	−0.0010 (5)
O1	0.0238 (6)	0.0353 (7)	0.0143 (5)	0.0054 (5)	−0.0008 (5)	0.0001 (5)
O3	0.0180 (5)	0.0319 (6)	0.0194 (5)	0.0033 (4)	−0.0006 (4)	0.0006 (5)
C5	0.0195 (7)	0.0195 (7)	0.0204 (7)	−0.0004 (5)	0.0021 (6)	−0.0002 (6)
O4	0.0277 (6)	0.0412 (7)	0.0166 (5)	0.0004 (5)	0.0010 (5)	−0.0004 (5)
C3	0.0217 (7)	0.0200 (7)	0.0179 (7)	−0.0021 (5)	−0.0026 (6)	0.0005 (6)
C4	0.0224 (8)	0.0186 (7)	0.0169 (7)	−0.0032 (6)	0.0012 (6)	−0.0010 (6)
C2	0.0190 (7)	0.0185 (7)	0.0195 (7)	0.0000 (5)	0.0007 (6)	−0.0012 (6)
C6	0.0208 (8)	0.0205 (7)	0.0172 (7)	0.0004 (5)	−0.0038 (6)	−0.0001 (5)
C8	0.0244 (8)	0.0214 (7)	0.0187 (7)	−0.0053 (6)	0.0029 (6)	−0.0004 (6)
C1	0.0205 (7)	0.0202 (7)	0.0163 (7)	−0.0009 (6)	0.0006 (6)	−0.0003 (6)
C9	0.0279 (8)	0.0357 (9)	0.0201 (7)	0.0022 (7)	0.0058 (7)	−0.0009 (7)
C7	0.0206 (7)	0.0305 (8)	0.0290 (8)	0.0050 (6)	−0.0041 (7)	−0.0018 (7)
C10	0.0220 (8)	0.0439 (10)	0.0264 (8)	0.0054 (7)	−0.0049 (7)	0.0022 (8)

Geometric parameters (Å, º)

O2—C6	1.3695 (19)	C4—C8	1.489 (2)
O2—C7	1.421 (2)	C2—C1	1.402 (2)
O1—C1	1.3508 (19)	C6—C1	1.402 (2)
O1—H1	0.84	C8—C9	1.506 (2)
O3—C2	1.3650 (18)	C9—H9A	0.98
O3—C10	1.429 (2)	C9—H9B	0.98
C5—C6	1.386 (2)	C9—H9C	0.98
C5—C4	1.392 (2)	C7—H7A	0.98
C5—H5	0.95	C7—H7B	0.98
O4—C8	1.224 (2)	C7—H7C	0.98
C3—C2	1.386 (2)	C10—H10A	0.98
C3—C4	1.400 (2)	C10—H10B	0.98
C3—H3	0.95	C10—H10C	0.98
C6—O2—C7	117.41 (13)	O1—C1—C6	121.81 (13)
C1—O1—H1	109.5	O1—C1—C2	118.72 (13)
C2—O3—C10	116.60 (12)	C6—C1—C2	119.47 (14)
C6—C5—C4	119.59 (14)	C8—C9—H9A	109.5
C6—C5—H5	120.2	C8—C9—H9B	109.5
C4—C5—H5	120.2	H9A—C9—H9B	109.5
C2—C3—C4	119.80 (14)	C8—C9—H9C	109.5
C2—C3—H3	120.1	H9A—C9—H9C	109.5
C4—C3—H3	120.1	H9B—C9—H9C	109.5
C5—C4—C3	120.50 (14)	O2—C7—H7A	109.5

C5—C4—C8	121.08 (14)	O2—C7—H7B	109.5
C3—C4—C8	118.41 (14)	H7A—C7—H7B	109.5
O3—C2—C3	125.47 (13)	O2—C7—H7C	109.5
O3—C2—C1	114.41 (13)	H7A—C7—H7C	109.5
C3—C2—C1	120.12 (13)	H7B—C7—H7C	109.5
O2—C6—C5	125.96 (14)	O3—C10—H10A	109.5
O2—C6—C1	113.53 (13)	O3—C10—H10B	109.5
C5—C6—C1	120.51 (14)	H10A—C10—H10B	109.5
O4—C8—C4	120.27 (14)	O3—C10—H10C	109.5
O4—C8—C9	120.71 (15)	H10A—C10—H10C	109.5
C4—C8—C9	119.02 (15)	H10B—C10—H10C	109.5

C6—C5—C4—C3	0.0 (2)	C5—C4—C8—O4	−175.79 (15)
C6—C5—C4—C8	179.10 (14)	C3—C4—C8—O4	3.3 (2)
C2—C3—C4—C5	−0.3 (2)	C5—C4—C8—C9	3.6 (2)
C2—C3—C4—C8	−179.40 (14)	C3—C4—C8—C9	−177.28 (14)
C10—O3—C2—C3	0.9 (2)	O2—C6—C1—O1	1.2 (2)
C10—O3—C2—C1	−179.30 (13)	C5—C6—C1—O1	−178.92 (15)
C4—C3—C2—O3	−179.32 (14)	O2—C6—C1—C2	−178.90 (14)
C4—C3—C2—C1	0.9 (2)	C5—C6—C1—C2	1.0 (2)
C7—O2—C6—C5	2.7 (2)	O3—C2—C1—O1	−1.1 (2)
C7—O2—C6—C1	−177.48 (13)	C3—C2—C1—O1	178.65 (15)
C4—C5—C6—O2	179.47 (15)	O3—C2—C1—C6	178.98 (13)
C4—C5—C6—C1	−0.4 (2)	C3—C2—C1—C6	−1.2 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O4^{i}	0.84	1.96	2.7210 (17)	151

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