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3,4-Dihydroxyphenethyl acetate

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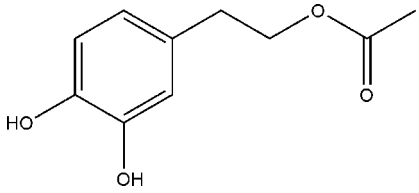
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.046; wR factor = 0.146; data-to-parameter ratio = 14.1.

In the title compound, $C_{10}H_{12}O_4$, the dihedral angle between the acetate group and the aromatic ring is 20.47 (10)°. In the crystal, molecules are linked by O—H···O hydrogen bonds, forming [001] chains. Weak C—H···O interactions consolidate the packing.

Related literature

For the synthesis, see: Bovicelli *et al.* (2007).



Experimental

Crystal data

$C_{10}H_{12}O_4$
M_r = 196.20
Monoclinic, $P2_1/n$
a = 11.088 (2) Å
b = 7.7100 (15) Å
c = 12.687 (3) Å
β = 114.50 (3)°
V = 986.9 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 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} = 0.970, T_{max} = 0.990
3672 measured reflections
1819 independent reflections
1439 reflections with $I > 2\sigma(I)$
R_{int} = 0.025
3 standard reflections every 200 reflections
intensity decay: 1%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.146
S = 1.01
1819 reflections
129 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.28 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
O1—H1A···O2^{i}	0.82	2.11	2.827 (2)	145
O2—H2A···O4^{ii}	0.82	1.89	2.7138 (19)	179
C10—H10A···O1^{iii}	0.96	2.36	3.316 (3)	177

Symmetry codes: (i) $-x+2, -y, -z$; (ii) $-x+2, -y, -z+1$; (iii) $x, y, z+1$.

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; 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: *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5912).

References

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supplementary materials

Acta Cryst. (2011). E**67**, o1996 [**doi:10.1107/S1600536811026730**]

3,4-Dihydroxyphenethyl acetate

F. Shen, J. Zhu, L. Wang, K. Wang and W. Yang

Experimental

The title compound was prepared by the literature method (Bovicelli *et al.* 2007). Colourless blocks of (I) were obtained by slow evaporation of an ethanol solution.

Refinement

H atoms were positioned geometrically with C—H = 0.93, 0.98 and 0.97 Å for aromatic, methine and methylene H atoms, respectively, and constrained to ride on their parent atoms, with U_{iso}(H) = 1.2 (or 1.5 for methyl groups) times U_{eq}(C).

Figures

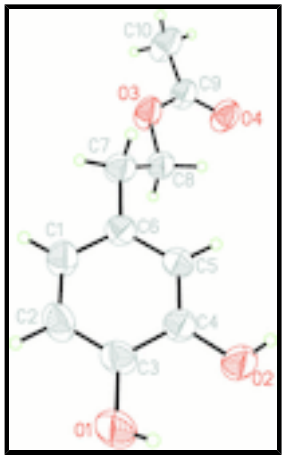

Fig. 1. The molecular structure of (I) with displacement ellipsoids drawn at 30% probability levels.

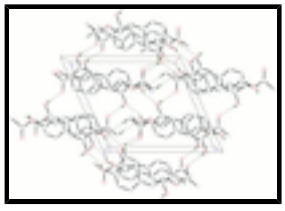

Fig. 2. A practical packing diagram of the title compound. Hydron bonds are shown as dashed lines.

3,4-Dihydroxyphenethyl acetate

Crystal data

$C_{10}H_{12}O_4$	F(000) = 416
M_r = 196.20	D_x = 1.320 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, λ = 0.71073 Å
a = 11.088 (2) Å	Cell parameters from 25 reflections

b = 7.7100 (15) Å	θ = 9–13°
c = 12.687 (3) Å	μ = 0.10 mm^{-1}
β = 114.50 (3)°	T = 293 K
V = 986.9 (3) Å^3	Block, colorless
Z = 4	0.30 × 0.20 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer	1439 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.025
graphite	θ_{max} = 25.4°, θ_{min} = 2.1°
ω/2θ scans	h = 0→13
Absorption correction: ψ scan (North *et al.*, 1968)	k = −9→9
T_{min} = 0.970, T_{max} = 0.990	l = −15→13
3672 measured reflections	3 standard reflections every 200 reflections
1819 independent reflections	intensity decay: 1%

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.046	H-atom parameters constrained
$wR(F^2)$ = 0.146	$w = 1/[\sigma^2(F_o^2) + (0.1P)^2 + 0.110P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.01	$(\Delta/\sigma)_{max} < 0.001$
1819 reflections	$\Delta\rho_{max}$ = 0.28 e Å^{-3}
129 parameters	$\Delta\rho_{min}$ = −0.21 e Å^{-3}
0 restraints	Extinction correction: *SHELXS97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.113 (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}
O1	0.82657 (16)	0.1555 (2)	−0.06613 (11)	0.0744 (5)
H1A	0.8814	0.0814	−0.0619	0.112*
C1	0.61846 (18)	0.1594 (2)	0.09171 (14)	0.0500 (5)
H1B	0.5326	0.1915	0.0787	0.060*
O2	0.99568 (12)	0.0172 (2)	0.13823 (10)	0.0600 (4)
H2A	1.0401	−0.0162	0.2045	0.090*
C2	0.6604 (2)	0.1768 (3)	0.00363 (14)	0.0551 (5)
H2B	0.6023	0.2195	−0.0681	0.066*
O3	0.67398 (12)	0.1071 (2)	0.48254 (10)	0.0591 (4)
C3	0.78691 (19)	0.1315 (2)	0.02105 (14)	0.0493 (5)
O4	0.85894 (13)	0.0936 (2)	0.64219 (11)	0.0667 (5)
C4	0.87258 (17)	0.0653 (2)	0.12809 (14)	0.0444 (4)
C5	0.83054 (17)	0.0485 (2)	0.21595 (13)	0.0435 (4)
H5A	0.8886	0.0053	0.2875	0.052*
C6	0.70253 (17)	0.0951 (2)	0.19887 (14)	0.0425 (4)
C7	0.65213 (17)	0.0689 (3)	0.29153 (14)	0.0498 (5)
H7A	0.5705	0.1339	0.2703	0.060*
H7B	0.6312	−0.0529	0.2934	0.060*
C8	0.74690 (17)	0.1231 (2)	0.41116 (15)	0.0490 (5)
H8A	0.8242	0.0483	0.4398	0.059*
H8B	0.7757	0.2418	0.4109	0.059*
C9	0.73987 (17)	0.0917 (2)	0.59542 (15)	0.0497 (5)
C10	0.6508 (2)	0.0698 (4)	0.65552 (17)	0.0706 (7)
H10A	0.6997	0.0906	0.7369	0.106*
H10B	0.6163	−0.0463	0.6439	0.106*
H10C	0.5788	0.1508	0.6246	0.106*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0785 (10)	0.1125 (13)	0.0404 (7)	0.0258 (9)	0.0327 (7)	0.0154 (7)
C1	0.0448 (9)	0.0593 (11)	0.0435 (9)	0.0051 (8)	0.0162 (8)	−0.0028 (7)
O2	0.0493 (7)	0.0940 (11)	0.0420 (7)	0.0130 (7)	0.0241 (6)	0.0090 (6)
C2	0.0565 (11)	0.0675 (12)	0.0346 (9)	0.0115 (9)	0.0122 (8)	0.0035 (8)
O3	0.0406 (7)	0.1006 (11)	0.0383 (7)	0.0101 (6)	0.0185 (5)	0.0056 (6)
C3	0.0586 (11)	0.0581 (11)	0.0337 (8)	0.0033 (8)	0.0217 (8)	−0.0002 (7)
O4	0.0414 (8)	0.1125 (12)	0.0430 (7)	0.0016 (7)	0.0144 (6)	0.0054 (7)
C4	0.0455 (9)	0.0515 (10)	0.0373 (8)	0.0000 (7)	0.0184 (7)	−0.0019 (7)
C5	0.0462 (9)	0.0501 (9)	0.0344 (8)	0.0020 (7)	0.0169 (7)	0.0041 (7)
C6	0.0436 (9)	0.0458 (9)	0.0386 (9)	−0.0013 (7)	0.0176 (7)	−0.0026 (7)
C7	0.0469 (10)	0.0627 (11)	0.0443 (10)	0.0003 (8)	0.0235 (8)	0.0026 (8)
C8	0.0439 (9)	0.0641 (11)	0.0438 (9)	0.0065 (8)	0.0231 (8)	0.0074 (8)
C9	0.0414 (10)	0.0702 (12)	0.0380 (9)	0.0037 (8)	0.0170 (7)	−0.0026 (8)
C10	0.0529 (12)	0.1190 (19)	0.0459 (11)	−0.0016 (12)	0.0264 (9)	−0.0075 (11)

Geometric parameters (Å, °)

O1—C3	1.362 (2)	C4—C5	1.381 (2)
O1—H1A	0.8200	C5—C6	1.391 (2)
C1—C6	1.383 (2)	C5—H5A	0.9300
C1—C2	1.384 (2)	C6—C7	1.510 (2)
C1—H1B	0.9300	C7—C8	1.503 (3)
O2—C4	1.368 (2)	C7—H7A	0.9700
O2—H2A	0.8200	C7—H7B	0.9700
C2—C3	1.371 (3)	C8—H8A	0.9700
C2—H2B	0.9300	C8—H8B	0.9700
O3—C9	1.316 (2)	C9—C10	1.487 (2)
O3—C8	1.448 (2)	C10—H10A	0.9600
C3—C4	1.392 (2)	C10—H10B	0.9600
O4—C9	1.202 (2)	C10—H10C	0.9600
C3—O1—H1A	109.5	C8—C7—C6	114.80 (14)
C6—C1—C2	120.88 (16)	C8—C7—H7A	108.6
C6—C1—H1B	119.6	C6—C7—H7A	108.6
C2—C1—H1B	119.6	C8—C7—H7B	108.6
C4—O2—H2A	109.5	C6—C7—H7B	108.6
C3—C2—C1	120.62 (16)	H7A—C7—H7B	107.5
C3—C2—H2B	119.7	O3—C8—C7	105.67 (13)
C1—C2—H2B	119.7	O3—C8—H8A	110.6
C9—O3—C8	119.11 (13)	C7—C8—H8A	110.6
O1—C3—C2	119.20 (16)	O3—C8—H8B	110.6
O1—C3—C4	121.50 (17)	C7—C8—H8B	110.6
C2—C3—C4	119.29 (16)	H8A—C8—H8B	108.7
O2—C4—C5	123.78 (16)	O4—C9—O3	122.44 (17)
O2—C4—C3	116.22 (15)	O4—C9—C10	125.14 (16)
C5—C4—C3	119.99 (16)	O3—C9—C10	112.42 (15)
C4—C5—C6	120.92 (16)	C9—C10—H10A	109.5
C4—C5—H5A	119.5	C9—C10—H10B	109.5
C6—C5—H5A	119.5	H10A—C10—H10B	109.5
C1—C6—C5	118.30 (15)	C9—C10—H10C	109.5
C1—C6—C7	119.81 (15)	H10A—C10—H10C	109.5
C5—C6—C7	121.82 (15)	H10B—C10—H10C	109.5
C6—C1—C2—C3	−0.5 (3)	C2—C1—C6—C7	−176.88 (17)
C1—C2—C3—O1	−177.86 (17)	C4—C5—C6—C1	−0.2 (3)
C1—C2—C3—C4	0.9 (3)	C4—C5—C6—C7	176.70 (15)
O1—C3—C4—O2	−3.4 (3)	C1—C6—C7—C8	−138.32 (18)
C2—C3—C4—O2	177.79 (17)	C5—C6—C7—C8	44.8 (2)
O1—C3—C4—C5	177.72 (17)	C9—O3—C8—C7	158.48 (17)
C2—C3—C4—C5	−1.0 (3)	C6—C7—C8—O3	173.27 (15)
O2—C4—C5—C6	−178.03 (16)	C8—O3—C9—O4	1.5 (3)
C3—C4—C5—C6	0.7 (3)	C8—O3—C9—C10	−177.75 (18)
C2—C1—C6—C5	0.1 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1A···O2^{i}	0.82	2.11	2.827 (2)	145
O2—H2A···O4^{ii}	0.82	1.89	2.7138 (19)	179
C10—H10A···O1^{iii}	0.96	2.36	3.316 (3)	177

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

Fig. 1

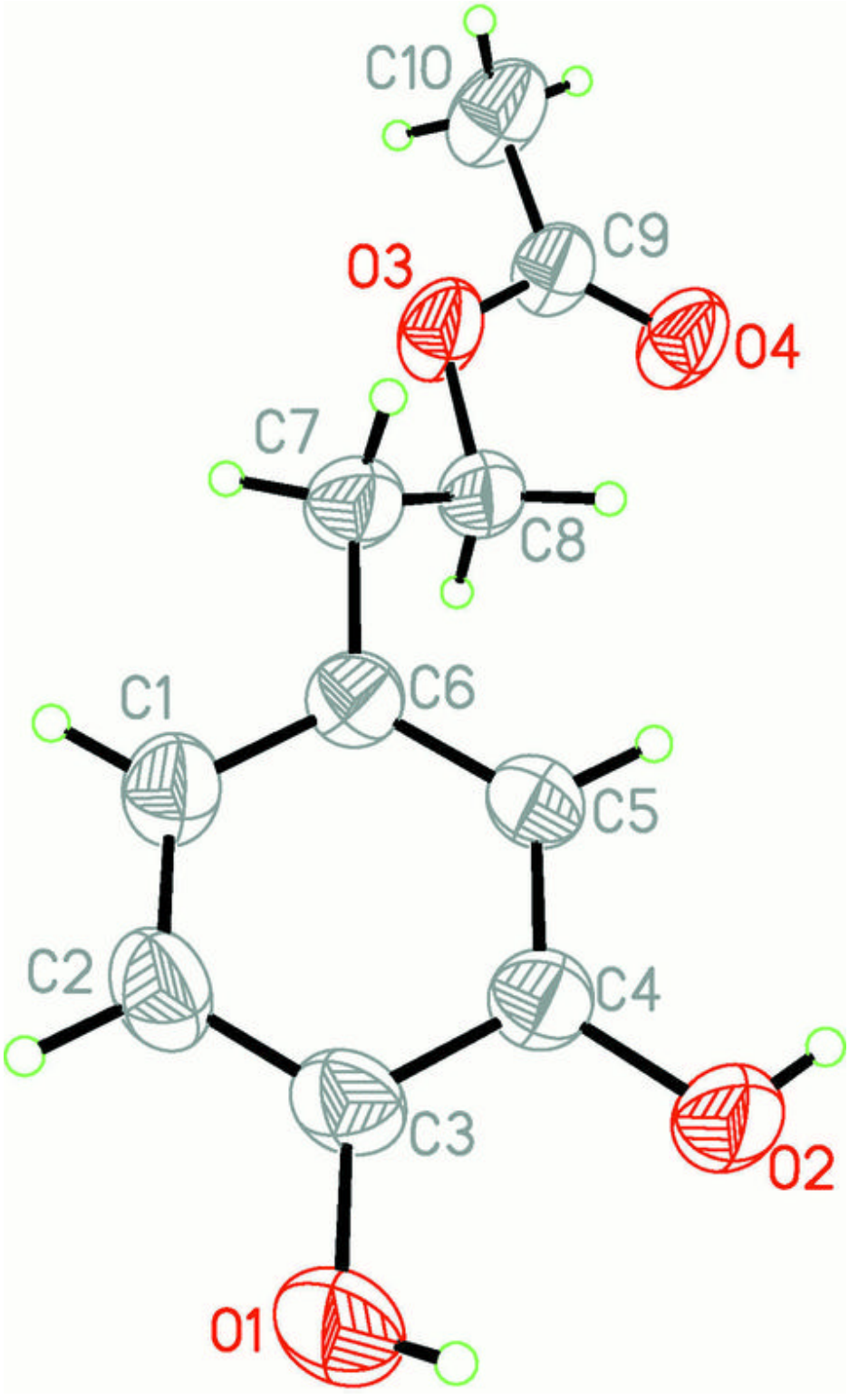

Fig. 2