Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

1-(5-Acetyl-2-hydroxyphenyl)ethanone

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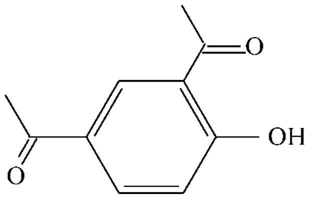
Received 4 May 2011; accepted 28 May 2011

Key indicators: single-crystal X-ray study; *T* = 153 K; mean σ(C–C) = 0.002 Å; disorder in main residue; *R* factor = 0.041; *wR* factor = 0.123; data-to-parameter ratio = 14.1.

The crystal structure of the title compound, $C_{10}H_{10}O_3$, is characterized by classical intramolecular hydrogen bonding. The hydroxy group is disordered over two positions (77 and 23%). The crystal structure is stabilized *via* π–π [3.5986 (1) Å] and weak nonclassical C—H···O interactions [3.2797 (15) Å].

Related literature

For hydrogen bonding, see: Desiraju & Steiner (1999). For π–π interactions, see: Janiak (2000). For the antifungal activity of the title compound, see: Prats *et al.* (2007).



Experimental

Crystal data

$C_{10}H_{10}O_3$
M_r = 178.18
Monoclinic, $P2_1/c$
a = 7.1134 (2) Å
b = 10.9260 (3) Å
c = 11.5291 (3) Å
β = 98.485 (2)°
V = 886.25 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 153 K
0.60 × 0.57 × 0.52 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
$T_{\min}$ = 0.659, $T_{\max}$ = 0.747
9182 measured reflections
1855 independent reflections
1577 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.018

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.123
S = 1.11
1855 reflections
132 parameters
H-atom parameters constrained
$\Delta\rho_{\max}$ = 0.30 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—H1O···O2	0.84	1.78	2.5240 (15)	147
O1*A*—H1O*A*···O3	0.84	1.58	2.369 (6)	156
C6—H6···O3$^{\rm i}$	0.95	2.55	3.2797 (15)	134

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; 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*.

This work was performed within the Cluster of Excellence ‘Structure Design of Novel High–Performance Materials *via* Atomic Design and Defect Engineering (ADDE)’, which is financially supported by the European Union (European Regional Development Fund) and by the Ministry of Science and Art of Saxony (SMWK). LI is gratefull to DFG for a travel grant.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RK2275).

References

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supplementary materials

Acta Cryst. (2011). E**67**, o1622   [**doi:10.1107/S1600536811020423**]

1-(5-Acetyl-2-hydroxyphenyl)ethanone

J. Hübscher, L. Izotova, S. Talipov, F. Eissmann and **E. Weber**

Comment

The title compound is known for its high antifungal activity (Prats *et al.*, 2007). In the molecule, the hydroxy–group is disordered over two positions [O1—H10 and O1A—H10A with occupancies of 0.769 (3) and 0.231 (3), respectively] related to each other *via* 180° rotation about the C3–C6 molecule axis. The molecule is almost planar with a maximum derivation from the mean plane of all non hydrogen atoms (RMS = 0.0458) of 0.1185 (14)Å for the methyl atom C8 (Fig. 1). The bond lengths and bond angles of the benzene ring are normal. The carbonyl and the disordered hydroxy–group of the molecule are involved in classical intramolecular H–bonds (O1—H1O···O2, 2.5240 (15)Å, 147.3°; O1A—H1OA···O3 2.369 (6)Å, 155.8°), while no conventional intermolecular hydrogen bond is found in the packing structure. The structure is stabilized *via* π–π–interactions (Janiak, 2000) involving the neighboring diacylphenol molecules in the stacks - Cg···Cg distance between consecutive molecules is 3.5986 (1)Å, which run in direction of the crystallographic *a*–axis (Fig. 2). Interaction between these stacks is realised *via* weak C—H···O interactions (Desiraju & Steiner, 1999) C6—H6···O3^{i} (3.2797 (15)Å). Symmetry code: (i) -*x*; *y*-1/2; -*z*-1/2.

Experimental

The title compound has been obtained as a by–product during attempted formation of a complex between 2–acetyl–4–ethynylphenol with Co(II) in *Me*OH solution due to hydrolysis. The prismatic shaped crystals are yellow colored and stable in the air.

Refinement

H atoms were positioned geometrically and allowed to ride on their respective parent atoms, with C—H = 0.98Å and U_{iso}(H) = 1.5U_{eq}(C) for methyl, C—H = 0.95Å and U_{iso}(H) = 1.2U_{eq}(C) for aryl and O—H = 0.84Å and U_{iso}(H) = 1.5U_{eq}(O) for hydroxy atoms.

Figures

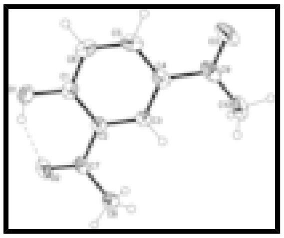

Fig. 1. Perspective view of the title compound with the atom numbring scheme. Displacement ellipsoids are drawn at 40% probability level. Dashed line represents intramolecular H–bond. Only major moiety of disordered hydroxy–group is presented.

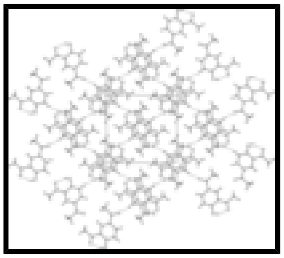

Fig. 2. Packing diagram of the title compound, viewed down the *a*–axis. The weak hydrogen bonds are shown as dashed lines.

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Crystal data

$C_{10}H_{10}O_3$

$M_r = 178.18$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 7.1134$ (2) Å

$b = 10.9260$ (3) Å

$c = 11.5291$ (3) Å

$\beta = 98.485$ (2)°

$V = 886.25$ (4) Å^3

$Z = 4$

$F(000) = 376$

$D_x = 1.335$ Mg m^{-3}

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 5377 reflections

$\theta = 2.6$–33.0°

$\mu = 0.10$ mm^{-1}

$T = 153$ K

Prism, yellow

0.60 × 0.57 × 0.52 mm

Data collection

Bruker Kappa APEXII CCD diffractometer

Radiation source: fine–focus sealed tube

graphite

φ and ω scans

Absorption correction: multi-scan (*SADABS*; Bruker, 2007)

$T_{min} = 0.659$, $T_{max} = 0.747$

9182 measured reflections

1855 independent reflections

1577 reflections with $I > 2\sigma(I)$

$R_{int} = 0.018$

$\theta_{max} = 26.6°$, $\theta_{min} = 2.6°$

$h = -8 \rightarrow 8$

$k = -13 \rightarrow 13$

$l = -14 \rightarrow 14$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.041$

$wR(F^2) = 0.123$

$S = 1.11$

1855 reflections

132 parameters

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

$w = 1/[\sigma^2(F_o^2) + (0.0664P)^2 + 0.1717P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.30$ e Å^{-3}

0 restraints	$\Delta\rho_{\text{min}} = -0.21$ e Å^{-3}

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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}	Occ. (<1)
O1	0.36987 (18)	0.74231 (10)	0.01694 (11)	0.0392 (4)	0.769 (3)
H1O	0.4139	0.7335	0.0881	0.059*	0.769 (3)
O1A	0.0897 (7)	1.0538 (5)	−0.2444 (3)	0.0555 (15)	0.231 (3)
H1OA	0.0636	1.1284	−0.2393	0.083*	0.231 (3)
O2	0.46630 (14)	0.80245 (8)	0.22874 (8)	0.0416 (3)	
O3	0.05289 (18)	1.25536 (12)	−0.17533 (10)	0.0643 (4)	
C1	0.30909 (15)	0.85929 (11)	−0.00259 (10)	0.0301 (3)	
H1A	0.3534	0.7780	0.0124	0.036*	0.231 (3)
C2	0.32180 (14)	0.94450 (10)	0.08990 (9)	0.0254 (3)	
C3	0.25975 (14)	1.06404 (10)	0.06490 (9)	0.0256 (3)	
H3	0.2690	1.1223	0.1267	0.031*	
C4	0.18496 (15)	1.09999 (11)	−0.04787 (10)	0.0301 (3)	
C5	0.17072 (16)	1.01185 (13)	−0.13782 (10)	0.0354 (3)	
H5	0.1177	1.0345	−0.2153	0.042*	0.769 (3)
C6	0.23194 (16)	0.89384 (13)	−0.11574 (10)	0.0361 (3)	
H6	0.2216	0.8358	−0.1777	0.043*	
C7	0.40012 (16)	0.90573 (11)	0.20988 (10)	0.0301 (3)	
C8	0.3997 (2)	0.99274 (13)	0.30966 (11)	0.0432 (3)	
H8A	0.4300	0.9484	0.3839	0.065*	
H8B	0.2738	1.0303	0.3053	0.065*	
H8C	0.4950	1.0567	0.3052	0.065*	
C9	0.11948 (17)	1.22703 (13)	−0.07529 (12)	0.0408 (3)	
C10	0.1355 (2)	1.31998 (13)	0.02060 (15)	0.0483 (4)	
H10A	0.0878	1.3989	−0.0117	0.073*	
H10B	0.2690	1.3285	0.0557	0.073*	
H10C	0.0603	1.2935	0.0807	0.073*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0458 (7)	0.0296 (6)	0.0432 (7)	0.0006 (5)	0.0100 (5)	−0.0058 (5)

O1A	0.056 (3)	0.080 (4)	0.028 (2)	−0.018 (3)	−0.0051 (18)	0.005 (2)
O2	0.0476 (6)	0.0300 (5)	0.0460 (5)	0.0046 (4)	0.0027 (4)	0.0099 (4)
O3	0.0627 (7)	0.0742 (8)	0.0516 (7)	0.0163 (6)	−0.0056 (5)	0.0302 (6)
C1	0.0222 (5)	0.0309 (6)	0.0383 (6)	−0.0045 (4)	0.0082 (4)	−0.0042 (5)
C2	0.0193 (5)	0.0284 (6)	0.0289 (6)	−0.0029 (4)	0.0046 (4)	0.0013 (4)
C3	0.0197 (5)	0.0283 (6)	0.0289 (6)	−0.0016 (4)	0.0034 (4)	0.0022 (4)
C4	0.0188 (5)	0.0392 (7)	0.0318 (6)	−0.0023 (5)	0.0022 (4)	0.0076 (5)
C5	0.0221 (6)	0.0562 (8)	0.0268 (6)	−0.0061 (5)	0.0002 (4)	0.0029 (5)
C6	0.0266 (6)	0.0491 (8)	0.0333 (6)	−0.0083 (5)	0.0062 (5)	−0.0102 (5)
C7	0.0271 (6)	0.0281 (6)	0.0352 (6)	−0.0018 (4)	0.0043 (4)	0.0065 (5)
C8	0.0586 (9)	0.0409 (7)	0.0285 (6)	0.0063 (6)	0.0012 (6)	0.0040 (5)
C9	0.0259 (6)	0.0486 (8)	0.0471 (7)	0.0029 (5)	0.0029 (5)	0.0203 (6)
C10	0.0455 (8)	0.0330 (7)	0.0667 (9)	0.0054 (6)	0.0090 (7)	0.0157 (6)

Geometric parameters (Å, °)

O1—C1	1.3573 (16)	C4—C5	1.4078 (18)
O1—H1O	0.8400	C4—C9	1.4833 (18)
O1A—C5	1.357 (4)	C5—C6	1.373 (2)
O1A—H1OA	0.8400	C5—H5	0.9500
O2—C7	1.2297 (15)	C6—H6	0.9500
O3—C9	1.2204 (17)	C7—C8	1.4926 (17)
C1—C6	1.3908 (17)	C8—H8A	0.9800
C1—C2	1.4083 (16)	C8—H8B	0.9800
C1—H1A	0.9500	C8—H8C	0.9800
C2—C3	1.3951 (16)	C9—C10	1.493 (2)
C2—C7	1.4751 (15)	C10—H10A	0.9800
C3—C4	1.3870 (15)	C10—H10B	0.9800
C3—H3	0.9500	C10—H10C	0.9800
C1—O1—H1O	109.5	C5—C6—C1	119.96 (11)
C5—O1A—H1OA	109.5	C5—C6—H6	120.0
O1—C1—C6	118.89 (11)	C1—C6—H6	120.0
O1—C1—C2	120.91 (11)	O2—C7—C2	120.74 (11)
C6—C1—C2	120.20 (11)	O2—C7—C8	119.50 (11)
C6—C1—H1A	119.9	C2—C7—C8	119.76 (10)
C2—C1—H1A	119.9	C7—C8—H8A	109.5
C3—C2—C1	118.66 (10)	C7—C8—H8B	109.5
C3—C2—C7	121.78 (10)	H8A—C8—H8B	109.5
C1—C2—C7	119.56 (10)	C7—C8—H8C	109.5
C4—C3—C2	121.65 (11)	H8A—C8—H8C	109.5
C4—C3—H3	119.2	H8B—C8—H8C	109.5
C2—C3—H3	119.2	O3—C9—C4	120.31 (15)
C3—C4—C5	118.21 (11)	O3—C9—C10	120.26 (13)
C3—C4—C9	121.99 (12)	C4—C9—C10	119.43 (11)
C5—C4—C9	119.80 (11)	C9—C10—H10A	109.5
O1A—C5—C6	124.4 (3)	C9—C10—H10B	109.5
O1A—C5—C4	114.2 (3)	H10A—C10—H10B	109.5
C6—C5—C4	121.30 (11)	C9—C10—H10C	109.5
C6—C5—H5	119.3	H10A—C10—H10C	109.5

C4—C5—H5	119.3	H10B—C10—H10C	109.5
O1—C1—C2—C3	179.13 (11)	O1A—C5—C6—C1	−178.5 (3)
C6—C1—C2—C3	−1.47 (16)	C4—C5—C6—C1	0.28 (17)
O1—C1—C2—C7	−0.74 (16)	O1—C1—C6—C5	−179.54 (11)
C6—C1—C2—C7	178.67 (10)	C2—C1—C6—C5	1.04 (17)
C1—C2—C3—C4	0.59 (16)	C3—C2—C7—O2	−174.85 (10)
C7—C2—C3—C4	−179.55 (10)	C1—C2—C7—O2	5.01 (17)
C2—C3—C4—C5	0.69 (16)	C3—C2—C7—C8	4.99 (17)
C2—C3—C4—C9	−179.72 (10)	C1—C2—C7—C8	−175.15 (11)
C3—C4—C5—O1A	177.7 (2)	C3—C4—C9—O3	−179.39 (12)
C9—C4—C5—O1A	−1.9 (3)	C5—C4—C9—O3	0.20 (19)
C3—C4—C5—C6	−1.14 (17)	C3—C4—C9—C10	0.55 (18)
C9—C4—C5—C6	179.26 (11)	C5—C4—C9—C10	−179.86 (11)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1O···O2	0.84	1.78	2.5240 (15)	147
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Fig. 1

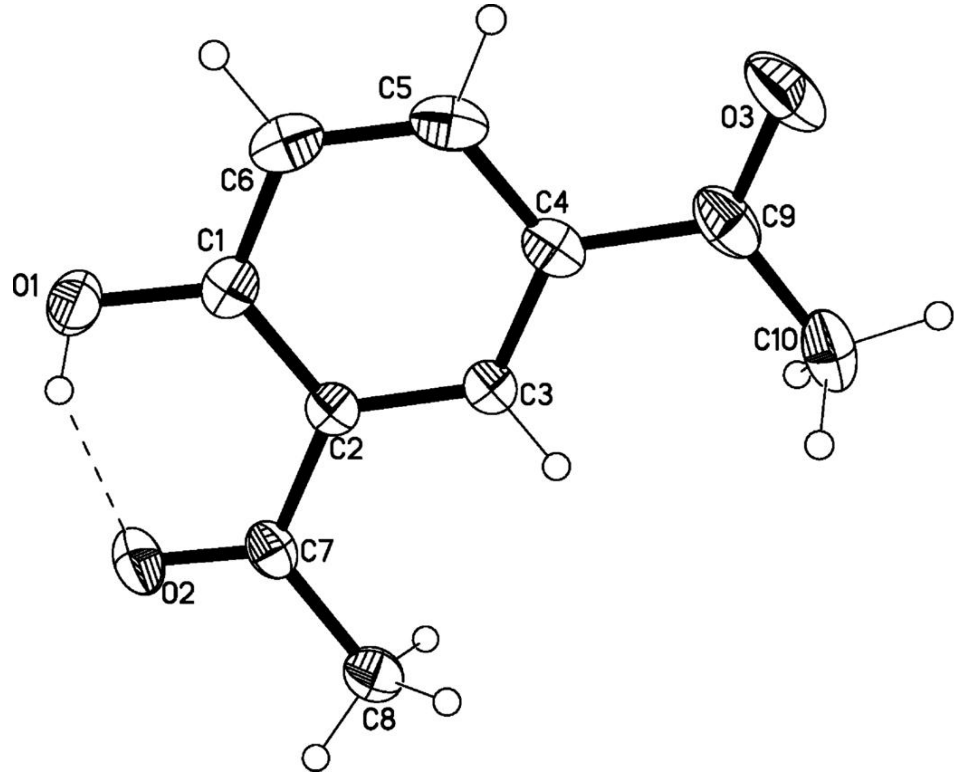

Fig. 2