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3-Acetyl-4-hydroxyphenyl acrylate

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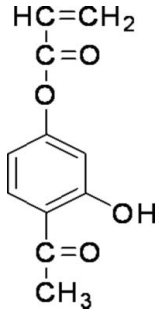
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.002 Å; R factor = 0.049; wR factor = 0.150; data-to-parameter ratio = 18.6.

In the title compound, $C_{11}H_{10}O_4$, the acetyl and acryloyloxy groups make dihedral angles of 3.93 (8) and 55.18 (6)°, respectively, with the benzene ring. The molecular structure is, in turn, stabilized by a medium-strength intramolecular O—H···O interaction, while the crystal packing is in turn stabilized by weak intermolecular C—H···O contacts.

Related literature

For related literature, see: Ren *et al.* (2006); Williams (1981); Xu *et al.* (2006). A similiar compound has been reported by Chakkaravarthi *et al.* (2007).



Experimental

Crystal data

$C_{11}H_{10}O_4$
M_r = 206.19
Monoclinic, $P2_1/n$
a = 12.3214 (16) Å
b = 6.1103 (8) Å
c = 14.1971 (19) Å
β = 104.527 (3)°
V = 1034.7 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 295 (2) K
0.30 × 0.20 × 0.20 mm

Data collection

Bruker Kappa APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.923, T_{max} = 0.980
11880 measured reflections
2561 independent reflections
1581 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.150
S = 1.04
2561 reflections
138 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 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	1.83	2.5467 (18)	145
C7—H7···O3^{i}	0.93	2.59	3.440 (2)	153
C10—H10···O2^{ii}	0.93	2.50	3.392 (2)	160

Symmetry codes: (i) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$; (ii) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2*; data reduction: *APEX2*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

The authors are grateful to the Sophisticated Analytical Instrument Facility, Indian Institute of Technology, Madras, for the data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BG2126).

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supplementary materials

Acta Cryst. (2007). E**63**, o4725 [**doi:10.1107/S1600536807057492**]

3-Acetyl-4-hydroxyphenyl acrylate

G. Chakkaravarthi, A. Anthonysamy, S. Balasubramanian and V. Manivannan

Comment

The acrylic derivatives have been used in clinical applications and biomaterials because of their excellent biocompatibility and long-term stability (Williams, 1981). The geometric parameters in the title compound (I) (Fig. 1) agree with the reported values of similar structures (Chakkaravarthi *et al.* (2007); Ren *et al.* (2006); Xu *et al.* (2006)).

The acetyl and acryloyloxy groups make dihedral angles of 3.93 (8)° and 55.18 (6)°, respectively, with the benzene ring. The O3—C9—C10—C11 and C1—C2—C3—C8 torsion angles [−177.46 (18)° and 176.94 (16)°, respectively] indicate anti-periplanar conformation of the respective groups. The molecular structure is stabilized by medium strength intramolecular O—H···O interaction while the crystal packing is in turn stabilized by weak intermolecular C—H···O contacts defining columns along [010]. (Table 1 and Fig. 2).

Experimental

2,4-Dihydroxyacetophenone(4.2 g, 27.60 mmol), triethylamine (3.85 ml, 27.67 mmol) and 150 ml of dry 2-butanone were taken in a 250 ml round bottom flask and the temperature was maintained at 273 K. Then the solution of acryloylchloride (2.3 ml, 28.30 mmol) in 30 ml of 2-butanone was added dropwise to the mixture with constant stirring for 30 minutes. After the addition was over, the reaction mixture was stirred for another 6 h. The salt formed during the reaction was filtered and the filtrate was washed with water and dried over anhydrous $MgSO_4$. The filtrate was concentrated under reduced pressure and the product was obtained. This was dissolved in the hexane and ethyl acetate solution (9:1). Crystals suitable for X-ray analysis were grown by slow evaporation of an ethyl acetate solution.

Refinement

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

Figures

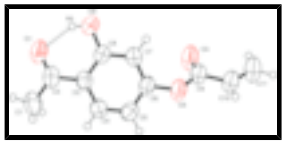


Fig. 1. The molecular structure of (I), with atom labels and 50% probability displacement ellipsoids for non-H atoms. Intramolecular hydrogen bond is shown as dashed line.

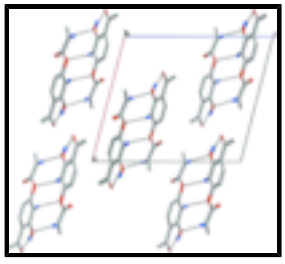


Fig. 2. The packing of (I), viewed down the columns direction, [010]. Hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted.

3-Acetyl-4-hydroxyphenyl acrylate

Crystal data

$C_{11}H_{10}O_4$	$F_{000} = 432$
$M_r = 206.19$	$D_x = 1.324$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2yn	Cell parameters from 2985 reflections
$a = 12.3214$ (16) Å	$\theta = 2.5$–24.6º
$b = 6.1103$ (8) Å	$\mu = 0.10$ mm^{-1}
$c = 14.1971$ (19) Å	$T = 295$ (2) K
$\beta = 104.527$ (3)º	Needle, colourless
$V = 1034.7$ (2) Å^3	0.30 × 0.20 × 0.20 mm
$Z = 4$	

Data collection

Bruker Kappa APEXII diffractometer	2561 independent reflections
Radiation source: fine-focus sealed tube	1581 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.022$
$T = 295$(2) K	$\theta_{max} = 28.3$º
ω and φ scan	$\theta_{min} = 2.0$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -16 \rightarrow 16$
$T_{min} = 0.923$, $T_{max} = 0.980$	$k = -8 \rightarrow 8$
11880 measured reflections	$l = -18 \rightarrow 18$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.049$	H-atom parameters constrained
$wR(F^2) = 0.150$	$w = 1/[\sigma^2(F_o^2) + (0.0614P)^2 + 0.1779P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{max} < 0.001$
2561 reflections	$\Delta\rho_{max} = 0.16$ e Å^{-3}

138 parameters	$\Delta\rho_{min} = -0.18$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	1.17657 (16)	0.2923 (4)	0.09037 (15)	0.0900 (6)
H1A	1.2553	0.2798	0.0945	0.135*
H1B	1.1630	0.4231	0.1231	0.135*
H1C	1.1358	0.2991	0.0233	0.135*
C2	1.13892 (14)	0.0991 (3)	0.13712 (12)	0.0686 (5)
C3	1.02051 (12)	0.0754 (3)	0.13889 (10)	0.0573 (4)
C4	0.94110 (14)	0.2365 (3)	0.10348 (13)	0.0718 (5)
H4	0.9633	0.3637	0.0775	0.086*
C5	0.83090 (14)	0.2133 (3)	0.10566 (14)	0.0742 (5)
H5	0.7790	0.3229	0.0817	0.089*
C6	0.79906 (12)	0.0249 (3)	0.14395 (11)	0.0595 (4)
C7	0.87330 (13)	−0.1366 (3)	0.18126 (13)	0.0681 (4)
H7	0.8499	−0.2616	0.2080	0.082*
C8	0.98466 (12)	−0.1117 (3)	0.17884 (12)	0.0647 (4)
C9	0.62307 (12)	−0.1612 (3)	0.11041 (12)	0.0630 (4)
C10	0.50996 (13)	−0.1397 (3)	0.12550 (13)	0.0733 (5)
H10	0.4923	−0.0143	0.1556	0.088*
C11	0.43508 (15)	−0.2867 (4)	0.09882 (16)	0.0927 (6)
H11A	0.4512	−0.4133	0.0686	0.111*
H11B	0.3643	−0.2674	0.1096	0.111*
O1	1.20776 (10)	−0.0411 (3)	0.17501 (11)	0.0960 (5)
O2	1.05545 (10)	−0.2747 (2)	0.21735 (13)	0.1046 (5)
H2	1.1177	−0.2487	0.2092	0.157*
O3	0.68743 (8)	0.01363 (19)	0.14911 (9)	0.0732 (4)
O4	0.65694 (10)	−0.3061 (2)	0.07039 (11)	0.0929 (5)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0714 (11)	0.1181 (16)	0.0850 (12)	−0.0226 (11)	0.0279 (10)	0.0082 (12)
C2	0.0542 (9)	0.0894 (12)	0.0628 (9)	−0.0094 (9)	0.0160 (7)	−0.0063 (9)
C3	0.0495 (8)	0.0684 (9)	0.0530 (8)	−0.0052 (7)	0.0108 (6)	−0.0020 (7)
C4	0.0593 (9)	0.0703 (10)	0.0822 (11)	−0.0062 (8)	0.0108 (8)	0.0139 (9)
C5	0.0560 (9)	0.0651 (10)	0.0944 (12)	0.0050 (8)	0.0054 (8)	0.0053 (9)
C6	0.0437 (7)	0.0659 (9)	0.0679 (9)	−0.0023 (7)	0.0122 (6)	−0.0101 (7)
C7	0.0524 (8)	0.0688 (10)	0.0826 (11)	−0.0050 (7)	0.0158 (8)	0.0106 (9)
C8	0.0471 (8)	0.0672 (10)	0.0767 (10)	0.0029 (7)	0.0098 (7)	0.0058 (8)
C9	0.0487 (8)	0.0726 (10)	0.0679 (9)	−0.0017 (7)	0.0148 (7)	−0.0072 (8)
C10	0.0493 (8)	0.0905 (12)	0.0814 (11)	−0.0011 (8)	0.0186 (8)	−0.0157 (10)
C11	0.0568 (10)	0.1180 (16)	0.1077 (15)	−0.0143 (11)	0.0289 (10)	−0.0223 (13)
O1	0.0515 (7)	0.1164 (11)	0.1217 (11)	0.0044 (7)	0.0248 (7)	0.0148 (9)

O2	0.0551 (7)	0.0884 (9)	0.1665 (15)	0.0122 (7)	0.0208 (8)	0.0429 (9)
O3	0.0468 (6)	0.0756 (8)	0.0988 (9)	−0.0033 (5)	0.0210 (5)	−0.0220 (6)
O4	0.0598 (7)	0.0952 (9)	0.1297 (11)	−0.0125 (6)	0.0352 (7)	−0.0440 (9)

Geometric parameters (Å, °)

C1—C2	1.485 (3)	C6—O3	1.3973 (17)
C1—H1A	0.9600	C7—C8	1.389 (2)
C1—H1B	0.9600	C7—H7	0.9300
C1—H1C	0.9600	C8—O2	1.3461 (19)
C2—O1	1.230 (2)	C9—O4	1.1831 (19)
C2—C3	1.473 (2)	C9—O3	1.3616 (19)
C3—C4	1.390 (2)	C9—C10	1.468 (2)
C3—C8	1.396 (2)	C10—C11	1.275 (2)
C4—C5	1.373 (2)	C10—H10	0.9300
C4—H4	0.9300	C11—H11A	0.9300
C5—C6	1.371 (2)	C11—H11B	0.9300
C5—H5	0.9300	O2—H2	0.8200
C6—C7	1.359 (2)		
C2—C1—H1A	109.5	C7—C6—O3	121.24 (15)
C2—C1—H1B	109.5	C5—C6—O3	116.45 (14)
H1A—C1—H1B	109.5	C6—C7—C8	118.89 (15)
C2—C1—H1C	109.5	C6—C7—H7	120.6
H1A—C1—H1C	109.5	C8—C7—H7	120.6
H1B—C1—H1C	109.5	O2—C8—C7	116.90 (15)
O1—C2—C3	120.09 (16)	O2—C8—C3	122.13 (14)
O1—C2—C1	119.40 (16)	C7—C8—C3	120.97 (14)
C3—C2—C1	120.51 (16)	O4—C9—O3	122.76 (14)
C4—C3—C8	117.45 (14)	O4—C9—C10	126.82 (15)
C4—C3—C2	122.33 (15)	O3—C9—C10	110.42 (14)
C8—C3—C2	120.21 (15)	C11—C10—C9	122.42 (17)
C5—C4—C3	121.95 (16)	C11—C10—H10	118.8
C5—C4—H4	119.0	C9—C10—H10	118.8
C3—C4—H4	119.0	C10—C11—H11A	120.0
C6—C5—C4	118.57 (16)	C10—C11—H11B	120.0
C6—C5—H5	120.7	H11A—C11—H11B	120.0
C4—C5—H5	120.7	C8—O2—H2	109.5
C7—C6—C5	122.15 (14)	C9—O3—C6	119.93 (12)
O1—C2—C3—C4	175.22 (16)	C6—C7—C8—C3	0.0 (3)
C1—C2—C3—C4	−4.4 (2)	C4—C3—C8—O2	−178.28 (16)
O1—C2—C3—C8	−3.5 (2)	C2—C3—C8—O2	0.5 (3)
C1—C2—C3—C8	176.94 (16)	C4—C3—C8—C7	1.1 (2)
C8—C3—C4—C5	−1.1 (3)	C2—C3—C8—C7	179.89 (15)
C2—C3—C4—C5	−179.82 (17)	O4—C9—C10—C11	2.9 (3)
C3—C4—C5—C6	−0.1 (3)	O3—C9—C10—C11	−177.46 (18)
C4—C5—C6—C7	1.3 (3)	O4—C9—O3—C6	−1.2 (3)
C4—C5—C6—O3	176.86 (15)	C10—C9—O3—C6	179.16 (14)
C5—C6—C7—C8	−1.2 (3)	C7—C6—O3—C9	−56.9 (2)
O3—C6—C7—C8	−176.60 (15)	C5—C6—O3—C9	127.46 (17)

C6—C7—C8—O2	179.42 (16)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O1	0.82	1.83	2.5467 (18)	145
C7—H7···O3^{i}	0.93	2.59	3.440 (2)	153
C10—H10···O2^{ii}	0.93	2.50	3.392 (2)	160

Symmetry codes: (i) −*x*+3/2, *y*−1/2, −*z*+1/2; (ii) −*x*+3/2, *y*+1/2, −*z*+1/2.

Fig. 1

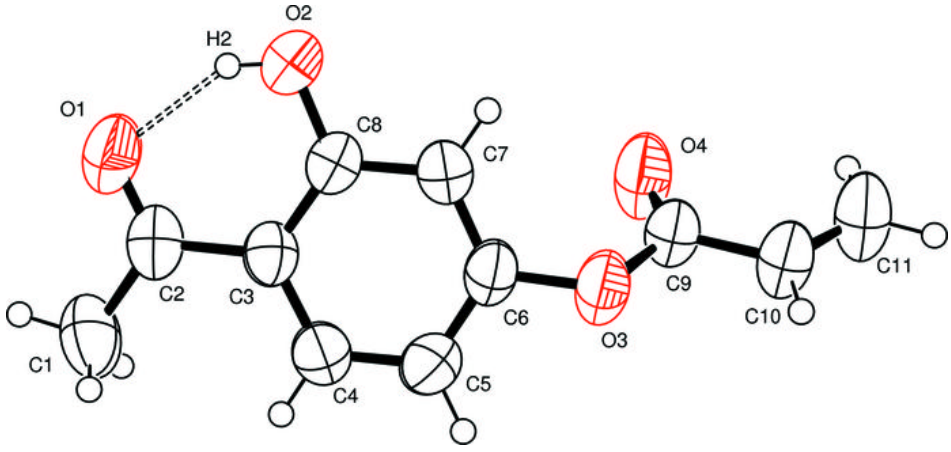
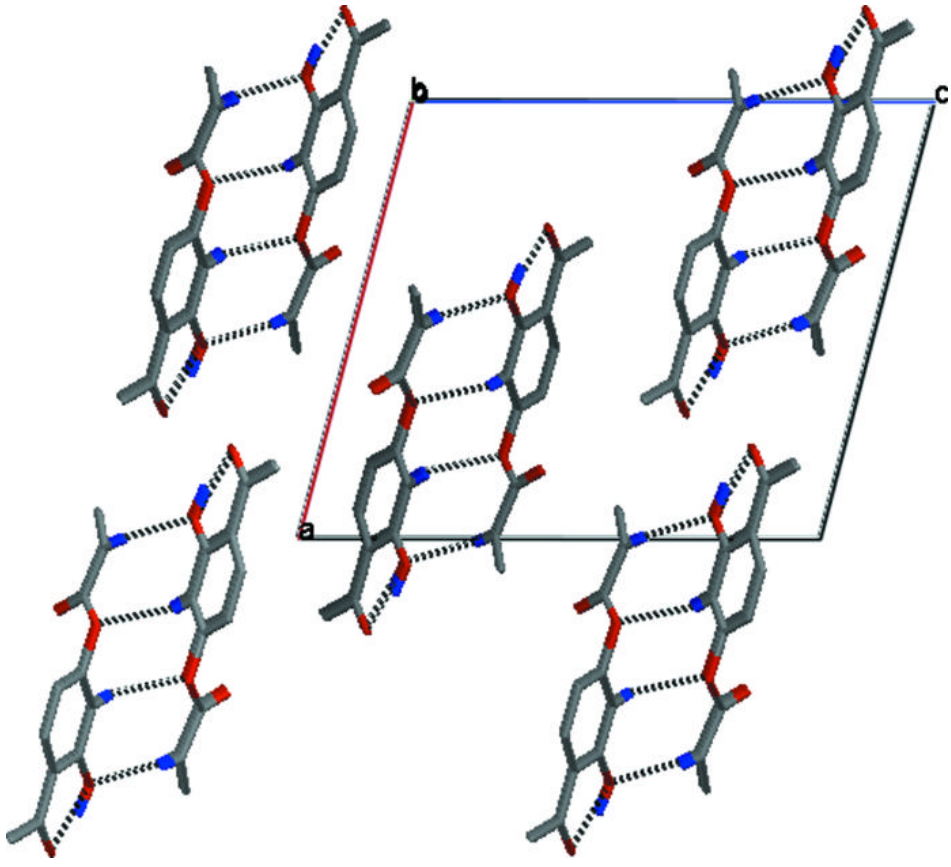


Fig. 2



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3-Acetyl-4-hydroxyphenyl acrylate. Corrigendum

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The chemical name in the title of the paper by Chakkaravarthi, Anthonysamy, Balasubramanian & Manivannan [*Acta Cryst.* (2007), E**63**, o4725] is corrected.

In the paper by Chakkaravarthi, Anthonysamy, Balasubramanian & Manivannan [*Acta Cryst.* (2007), E**63**, o4725], the chemical name in the title is incorrect. The correct title should be '4-Acetyl-3-hydroxyphenyl acrylate'.