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2-Acetyl-4-methylphenyl methacrylate

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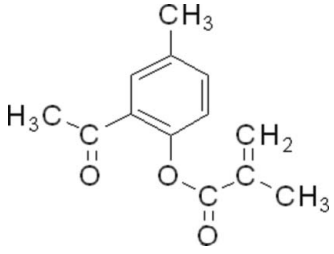
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.002 Å; R factor = 0.044; wR factor = 0.151; data-to-parameter ratio = 23.2.

The title compound, $C_{13}H_{14}O_3$, was synthesized by the reaction of 2-hydroxy-5-methylacetophenone with methacryloyl chloride. The molecular structure is stabilized by a weak C—H···O intramolecular interaction and the crystal packing is stabilized by a weak C—H···π interaction and a π–π interaction; the centroid–centroid separation and the interplanar distance are 5.048 (2) and 3.421 Å, respectively.

Related literature

For related literature, see: Gibson *et al.* (2006); Parker & Braden (1989); Ren *et al.* (2006). A similar acetophenone compound with methylbenzoyl has been reported (Kazak *et al.*, 2002).



Experimental

Crystal data

$C_{13}H_{14}O_3$
M_r = 218.24
Triclinic, $P\overline{1}$
a = 8.4619 (3) Å
b = 8.4810 (4) Å
c = 8.4929 (3) Å
α = 89.899 (2)°
β = 85.111 (3)°
γ = 76.090 (2)°
V = 589.36 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 295 (2) K
0.25 × 0.16 × 0.15 mm

Data collection

Bruker APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.922, T_{max} = 0.987
14784 measured reflections
3427 independent reflections
2434 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.151
S = 1.05
3427 reflections
148 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

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

Cg is the centroid of the benzene ring.

D—H···A	D—H	H···A	D···A	D—H···A
C12—H12B···O2	0.93	2.39	2.7147 (17)	101
C13—H13C···Cg^{i}	0.96	3.00	3.8415 (19)	148

Symmetry code: (i) $x-1, y, z$.

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: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

The authors acknowledge 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: IS2182).

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supplementary materials

Acta Cryst. (2007). E**63**, o3404 [**doi:10.1107/S1600536807031960**]

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

Comment

Methacrylate compounds have figured prominently in the development of soft-tissue-compatible materials, orthopedic and dental cements. Methacrylate activated vinyl esters are readily polymerized by free-radical polymerization to form linear, branched or network polymers (Parker & Braden, 1989).

The geometric parameters in the title compound, (I), are comparable with those observed in similar structures (Gibson *et al.*, 2006; Kazak *et al.*, 2002; Ren *et al.*, 2006). A similar acetophenone compound with methylbenzoyl moiety has been reported (Kazak *et al.*, 2002). The torsion angles O2—C10—C11—C12 and O3—C10—C11—C13 [18.37 (17)° and 18.45 (19)°, respectively] indicate *syn*-periplanar conformations and the torsion angle O2—C10—C11—C13 [−163.64 (13)°], shows anti-periplanar conformation. The molecule is stabilized by a weak C—H···O intramolecular interaction (Table 1) and the crystal packing is stabilized by a weak C—H···π interaction and a π-π interaction; the centroid-centroid separation, $Cg\cdots Cg^{i}$ [symmetry code: (i) $-x$, $1-y$, $-z$; *Cg* is the centroid of the benzene C2—C7 ring], is 5.048 (2) Å.

Experimental

2-Hydroxy-5-methylacetophenone (4.0 g, 26.65 mmol), K_2CO_3 (3.69 g, 26.69 mmol) and 100 ml of dry acetone were taken in a 250 ml round bottom flask and the temperature was maintained at 273 K. Then the solution of methacryloylchloride (2.7 ml, 27.63 mmol) in 20 ml of dry acetone was added dropwise to the mixture with constant stirring for 30 min. After the addition was over, the reaction mixture was stirred for 6 h. The salt formed during the reaction was filtered and the filtrate was washed with water and dried over anhydrous $MgSO_4$. The obtained compound was dissolved in hexane and ethyl acetate (9:1). Single crystals suitable for X-ray analysis were grown by slow evaporation of the solution.

Refinement

H atoms were positioned geometrically (C—H = 0.93 and 0.96 Å) and refined using riding model, with $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}$(methyl C).

Figures

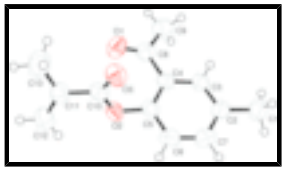

Fig. 1. The molecular structure of (I), with atom labels and 50% probability displacement ellipsoids for non-H atoms.

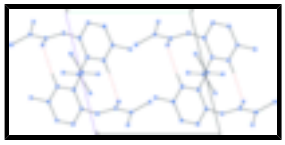

Fig. 2. The packing diagram of (I), viewed down the *c* axis. Hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted.

2-Acetyl-4-methylphenyl methacrylate

Crystal data

$C_{13}H_{14}O_3$	$Z = 2$
$M_r = 218.24$	$F_{000} = 232$
Triclinic, $P\overline{1}$	$D_x = 1.230$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 8.4619$ (3) Å	Cell parameters from 6575 reflections
$b = 8.4810$ (4) Å	$\theta = 2.5$–29.4º
$c = 8.4929$ (3) Å	$\mu = 0.09$ mm^{-1}
$\alpha = 89.899$ (2)º	$T = 295$ (2) K
$\beta = 85.111$ (3)º	Needle, colourless
$\gamma = 76.090$ (2)º	0.25 × 0.16 × 0.15 mm
$V = 589.36$ (4) Å^3	

Data collection

Bruker APEX II diffractometer	3427 independent reflections
Radiation source: fine-focus sealed tube	2434 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.022$
$T = 295$(2) K	$\theta_{max} = 30.1$º
φ and ω scans	$\theta_{min} = 2.4$º
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$h = -11 \rightarrow 11$
$T_{min} = 0.922$, $T_{max} = 0.987$	$k = -11 \rightarrow 11$
14784 measured reflections	$l = -11 \rightarrow 11$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.044$	H-atom parameters constrained
$wR(F^2) = 0.151$	$w = 1/[\sigma^2(F_o^2) + (0.0751P)^2 + 0.0589P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.05$	$(\Delta/\sigma)_{max} < 0.001$
3427 reflections	$\Delta\rho_{max} = 0.23$ e Å^{-3}
148 parameters	$\Delta\rho_{min} = -0.15$ 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	−0.44662 (18)	0.6979 (2)	1.13671 (19)	0.0725 (4)
H1A	−0.4721	0.5987	1.1055	0.109*
H1B	−0.5421	0.7859	1.1352	0.109*
H1C	−0.4113	0.6877	1.2415	0.109*
C2	−0.31230 (14)	0.73148 (16)	1.02360 (15)	0.0522 (3)
C3	−0.21210 (14)	0.60821 (14)	0.92885 (14)	0.0477 (3)
H3	−0.2296	0.5043	0.9373	0.057*
C4	−0.08662 (13)	0.63235 (13)	0.82175 (13)	0.0449 (3)
C5	−0.06243 (14)	0.78974 (14)	0.81322 (14)	0.0478 (3)
C6	−0.16081 (16)	0.91501 (15)	0.90530 (17)	0.0568 (3)
H6	−0.1440	1.0192	0.8973	0.068*
C7	−0.28434 (16)	0.88544 (16)	1.00941 (16)	0.0585 (3)
H7	−0.3501	0.9706	1.0712	0.070*
C8	0.01559 (15)	0.49421 (15)	0.72077 (14)	0.0516 (3)
C9	−0.0391 (2)	0.33884 (18)	0.7179 (2)	0.0766 (4)
H9A	0.0345	0.2624	0.6462	0.115*
H9B	−0.1473	0.3599	0.6837	0.115*
H9C	−0.0395	0.2947	0.8220	0.115*
C10	0.21145 (15)	0.78578 (13)	0.74115 (14)	0.0491 (3)
C11	0.32843 (16)	0.81776 (16)	0.61168 (15)	0.0559 (3)
C12	0.2755 (2)	0.9218 (2)	0.49656 (18)	0.0742 (4)
H12A	0.3497	0.9443	0.4177	0.089*
H12B	0.1647	0.9710	0.4960	0.089*
C13	0.4994 (2)	0.7343 (3)	0.6232 (2)	0.0878 (5)
H13A	0.5653	0.7611	0.5342	0.132*
H13B	0.5100	0.6190	0.6239	0.132*
H13C	0.5354	0.7679	0.7191	0.132*
O1	0.13873 (12)	0.50525 (13)	0.64342 (12)	0.0701 (3)
O2	0.05429 (10)	0.82955 (11)	0.70451 (11)	0.0565 (2)
O3	0.24860 (11)	0.73175 (12)	0.86701 (10)	0.0609 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0567 (8)	0.0888 (10)	0.0656 (9)	−0.0089 (7)	0.0051 (6)	0.0065 (7)
C2	0.0456 (6)	0.0597 (7)	0.0491 (6)	−0.0069 (5)	−0.0085 (5)	0.0057 (5)
C3	0.0475 (6)	0.0458 (6)	0.0509 (6)	−0.0114 (4)	−0.0102 (5)	0.0061 (5)
C4	0.0466 (6)	0.0435 (6)	0.0441 (6)	−0.0075 (4)	−0.0109 (4)	0.0044 (4)
C5	0.0473 (6)	0.0480 (6)	0.0488 (6)	−0.0110 (5)	−0.0104 (5)	0.0109 (5)
C6	0.0587 (7)	0.0417 (6)	0.0693 (8)	−0.0088 (5)	−0.0116 (6)	0.0035 (5)
C7	0.0541 (7)	0.0534 (7)	0.0623 (7)	−0.0009 (5)	−0.0073 (6)	−0.0059 (6)
C8	0.0542 (7)	0.0516 (6)	0.0469 (6)	−0.0071 (5)	−0.0097 (5)	−0.0008 (5)
C9	0.0955 (11)	0.0539 (8)	0.0798 (10)	−0.0197 (7)	0.0012 (8)	−0.0135 (7)

C10	0.0552 (7)	0.0428 (6)	0.0517 (6)	−0.0148 (5)	−0.0089 (5)	0.0032 (5)
C11	0.0593 (7)	0.0576 (7)	0.0531 (7)	−0.0195 (5)	−0.0027 (5)	−0.0004 (5)
C12	0.0772 (10)	0.0811 (10)	0.0633 (8)	−0.0207 (8)	0.0037 (7)	0.0166 (7)
C13	0.0616 (9)	0.1160 (14)	0.0836 (11)	−0.0185 (9)	−0.0028 (8)	0.0156 (10)
O1	0.0634 (6)	0.0728 (6)	0.0699 (6)	−0.0125 (5)	0.0063 (5)	−0.0137 (5)
O2	0.0539 (5)	0.0589 (5)	0.0584 (5)	−0.0158 (4)	−0.0088 (4)	0.0195 (4)
O3	0.0626 (5)	0.0705 (6)	0.0543 (5)	−0.0221 (4)	−0.0146 (4)	0.0115 (4)

Geometric parameters (Å, °)

C1—C2	1.5048 (19)	C8—O1	1.2067 (16)
C1—H1A	0.9600	C8—C9	1.4988 (19)
C1—H1B	0.9600	C9—H9A	0.9600
C1—H1C	0.9600	C9—H9B	0.9600
C2—C7	1.3851 (19)	C9—H9C	0.9600
C2—C3	1.3856 (17)	C10—O3	1.1990 (14)
C3—C4	1.3913 (16)	C10—O2	1.3550 (14)
C3—H3	0.9300	C10—C11	1.4849 (18)
C4—C5	1.3991 (16)	C11—C12	1.348 (2)
C4—C8	1.4986 (16)	C11—C13	1.462 (2)
C5—C6	1.3784 (18)	C12—H12A	0.9300
C5—O2	1.3948 (14)	C12—H12B	0.9300
C6—C7	1.3802 (19)	C13—H13A	0.9600
C6—H6	0.9300	C13—H13B	0.9600
C7—H7	0.9300	C13—H13C	0.9600
C2—C1—H1A	109.5	O1—C8—C9	120.02 (12)
C2—C1—H1B	109.5	C4—C8—C9	118.01 (12)
H1A—C1—H1B	109.5	C8—C9—H9A	109.5
C2—C1—H1C	109.5	C8—C9—H9B	109.5
H1A—C1—H1C	109.5	H9A—C9—H9B	109.5
H1B—C1—H1C	109.5	C8—C9—H9C	109.5
C7—C2—C3	117.54 (12)	H9A—C9—H9C	109.5
C7—C2—C1	121.73 (12)	H9B—C9—H9C	109.5
C3—C2—C1	120.73 (12)	O3—C10—O2	122.57 (11)
C2—C3—C4	123.21 (11)	O3—C10—C11	124.75 (11)
C2—C3—H3	118.4	O2—C10—C11	112.64 (10)
C4—C3—H3	118.4	C12—C11—C13	124.25 (13)
C3—C4—C5	116.97 (10)	C12—C11—C10	120.27 (13)
C3—C4—C8	120.52 (10)	C13—C11—C10	115.45 (12)
C5—C4—C8	122.51 (11)	C11—C12—H12A	120.0
C6—C5—O2	116.93 (10)	C11—C12—H12B	120.0
C6—C5—C4	121.12 (11)	H12A—C12—H12B	120.0
O2—C5—C4	121.82 (10)	C11—C13—H13A	109.5
C5—C6—C7	119.87 (11)	C11—C13—H13B	109.5
C5—C6—H6	120.1	H13A—C13—H13B	109.5
C7—C6—H6	120.1	C11—C13—H13C	109.5
C6—C7—C2	121.29 (11)	H13A—C13—H13C	109.5
C6—C7—H7	119.4	H13B—C13—H13C	109.5
C2—C7—H7	119.4	C10—O2—C5	116.49 (9)

O1—C8—C4	121.97 (11)		
C7—C2—C3—C4	−0.01 (18)	C3—C4—C8—O1	−169.44 (11)
C1—C2—C3—C4	179.70 (11)	C5—C4—C8—O1	10.93 (18)
C2—C3—C4—C5	0.67 (17)	C3—C4—C8—C9	10.45 (17)
C2—C3—C4—C8	−178.98 (10)	C5—C4—C8—C9	−169.18 (12)
C3—C4—C5—C6	−1.06 (17)	O3—C10—C11—C12	−159.54 (14)
C8—C4—C5—C6	178.59 (10)	O2—C10—C11—C12	18.37 (17)
C3—C4—C5—O2	−176.70 (9)	O3—C10—C11—C13	18.45 (19)
C8—C4—C5—O2	2.94 (17)	O2—C10—C11—C13	−163.65 (13)
O2—C5—C6—C7	176.65 (11)	O3—C10—O2—C5	−7.91 (17)
C4—C5—C6—C7	0.80 (19)	C11—C10—O2—C5	174.13 (10)
C5—C6—C7—C2	−0.10 (19)	C6—C5—O2—C10	105.59 (12)
C3—C2—C7—C6	−0.29 (19)	C4—C5—O2—C10	−78.59 (14)
C1—C2—C7—C6	180.00 (12)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C12—H12B···O2	0.93	2.39	2.7147 (17)	101
C13—H13C···Cg^{i}	0.96	3.00	3.8415 (19)	148

Symmetry codes: (i) *x*−1, *y*, *z*.

Fig. 1

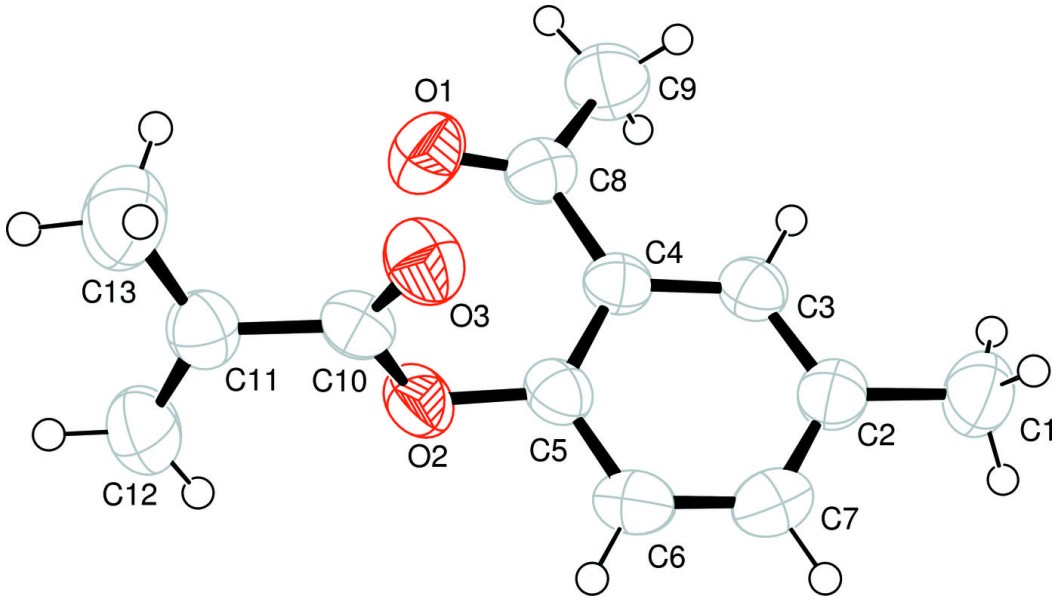

Fig. 2