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(Acetoxy)(2-methylphenyl)methyl acetate

J. Kanchanadevi,[a] G. Anbalagan,[b] V. Saravanan,[c] A. K. Mohanakrishnan[c] and V. Manivannan[d]*

[a]Department of Physics, Velammal Institute of Technology, Panchetty, Chennai 601204, India, [b]Department of Physics, Presidency College (Autonomous), Chennai 600 005, India, [c]Department of Organic Chemistry, University of Madras, Guindy Campus, Chennai 600 025, India, and [d]Department of Research and Development, PRIST University, Vallam, Thanjavur 613 403, Tamil Nadu, India
Correspondence e-mail: crystallography2010@gmail.com, phdguna@gmail.com

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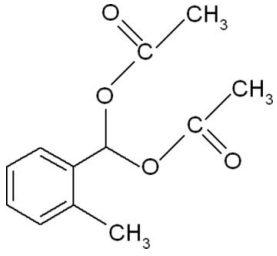
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.003 Å; R factor = 0.041; wR factor = 0.125; data-to-parameter ratio = 16.2.

In the title compound, $C_{12}H_{14}O_4$, the two acetoxy groups are inclined by 57.92 (5)° and 62.71 (6)° to the benzene ring. An intermolecular C—H···O interaction involving the two acetoxy groups generates a centrosymmetric dimer *via* an $R_2^2(16)$ ring motif.

Related literature

For the structure of the 4-methyl isomer, see: Rajnikant *et al.* (2009). For graph-set notation, see: Bernstein *et al.* (1995)



Experimental

Crystal data

$C_{12}H_{14}O_4$
M_r = 222.23
Monoclinic, $C2/c$
a = 15.757 (5) Å
b = 7.564 (5) Å
c = 19.886 (5) Å
β = 99.17 (5)°
V = 2339.8 (18) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 295 K
0.25 × 0.20 × 0.15 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.950, T_{max} = 0.975
12571 measured reflections
2414 independent reflections
1856 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.125
S = 1.05
2414 reflections
149 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C9—H9A···O4^{i}	0.96	2.50	3.425 (3)	161

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GK2393).

References

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supporting information

Acta Cryst. (2011). E**67**, o2111 [doi:10.1107/S1600536811028625]

(Acetoxy)(2-methylphenyl)methyl acetate

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S1. Comment

The geometric parameters of the title molecule (Fig. 1) agree well with similar structure (Rajnikant *et al.*, 2009). Intermolecular C—H···O interaction involving the two acetoxy groups generates a centrosymmetric dimer *via* $R^2_2(16)$ ring motif, Fig. 2 (Bernstein *et al.*, 1995).

S2. Experimental

To a solution of 2-methylbenzaldehyde (5 g, 41.61 mmol) in dry acetic anhydride (25 ml) anhydrous indium bromide (0.147 g, 0.416 mmol) was added. It was then stirred at room temperature for 4 h under nitrogen atmosphere. The reaction mixture was then poured over crushed ice (300 g). The solid obtained was filtered and washed thoroughly with water and the product was recrystallized from methanol to give pure product as a colorless solid with a yield of 82% and melting point 333 K.

S3. Refinement

H atoms were positioned geometrically and refined using riding model with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C) for aromatic C—H, C—H = 0.98 Å and U_{iso}(H) = 1.2U_{eq}(C) for methine C—H, C—H = 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C) for methyl group.

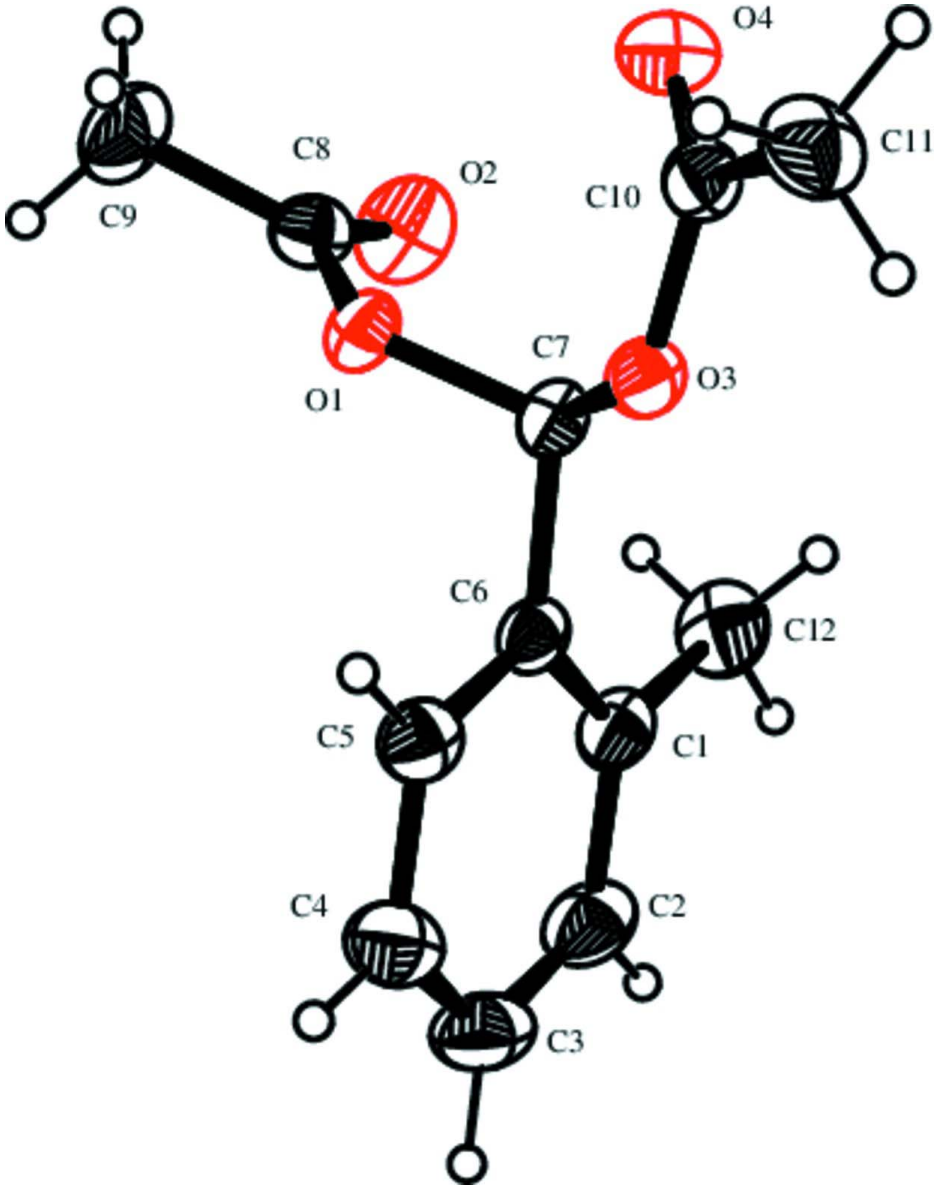

Figure 1

The molecular structure of the title compound, with atom labels and 30% probability displacement ellipsoids for non-H atoms.

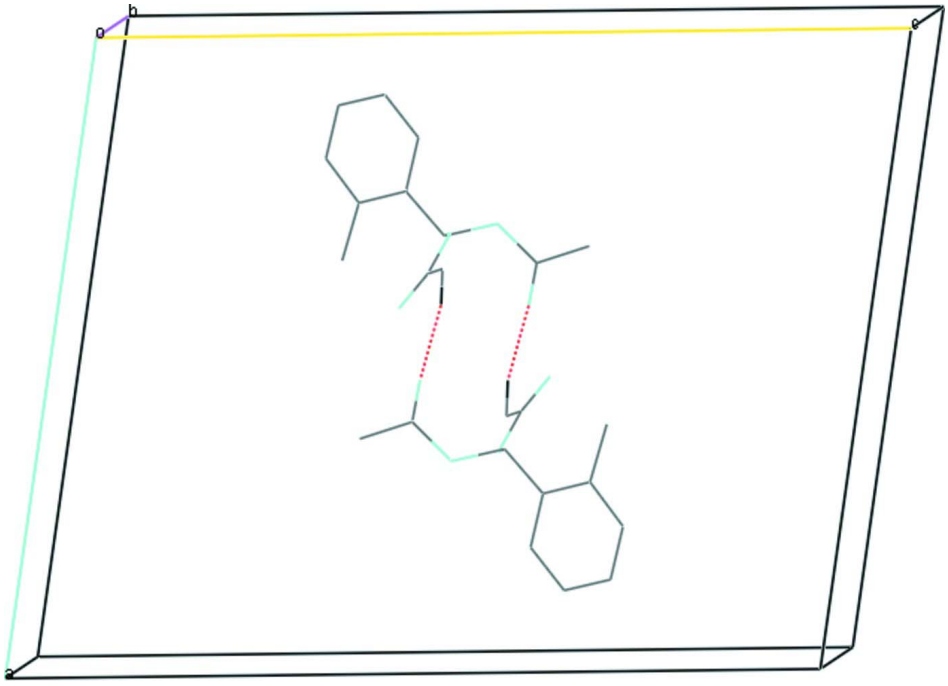

Figure 2

The $R^2_2(16)$ ring set motif of the title compound, viewed down the *b* axis. Hydrogen bonds are shown as dashed lines (hydrogen atoms have been omitted).

(Acetoxy)(2-methylphenyl)methyl acetate

Crystal data

$C_{12}H_{14}O_4$
$M_r = 222.23$
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
$a = 15.757\ (5)$ Å
$b = 7.564\ (5)$ Å
$c = 19.886\ (5)$ Å
$\beta = 99.17\ (5)°$
$V = 2339.8\ (18)$ Å^3
$Z = 8$
$F(000) = 944$
$D_x = 1.262$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 7598 reflections
$\theta = 2.1–26.5°$
$\mu = 0.10$ mm^{-1}
$T = 295$ K
Block, colourless
0.25 × 0.20 × 0.15 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.950$, $T_{max} = 0.975$
12571 measured reflections
2414 independent reflections
1856 reflections with $I > 2\sigma(I)$
$R_{int} = 0.027$
$\theta_{max} = 26.5°$, $\theta_{min} = 2.1°$
$h = -13\rightarrow19$
$k = -9\rightarrow8$
$l = -24\rightarrow24$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.125$
$S = 1.05$
2414 reflections
149 parameters
0 restraints
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
$w = 1/[\sigma^2(F_o^2) + (0.0609P)^2 + 0.9232P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.20$ e Å^{-3}
$\Delta\rho_{min} = -0.19$ e Å^{-3}
Extinction correction: *SHELXL*, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0066 (8)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.70247 (11)	−0.0332 (2)	0.68559 (8)	0.0539 (4)
C2	0.77083 (15)	−0.0812 (3)	0.73557 (9)	0.0703 (6)
H2	0.7592	−0.1354	0.7751	0.084*
C3	0.85476 (14)	−0.0510 (3)	0.72841 (10)	0.0744 (6)
H3	0.8990	−0.0842	0.7628	0.089*
C4	0.87350 (12)	0.0281 (3)	0.67050 (10)	0.0670 (5)
H4	0.9303	0.0492	0.6654	0.080*
C5	0.80723 (10)	0.0760 (2)	0.61999 (9)	0.0530 (4)
H5	0.8196	0.1295	0.5806	0.064*
C6	0.72234 (10)	0.04578 (19)	0.62698 (7)	0.0447 (4)
C7	0.65391 (10)	0.10316 (19)	0.56986 (7)	0.0434 (4)
H7	0.5963	0.0783	0.5802	0.052*
C8	0.60492 (10)	0.3993 (2)	0.57295 (8)	0.0513 (4)
C9	0.61840 (14)	0.5811 (2)	0.54922 (12)	0.0794 (6)
H9A	0.5646	0.6435	0.5424	0.119*
H9B	0.6407	0.5762	0.5071	0.119*
H9C	0.6586	0.6416	0.5828	0.119*
C10	0.60738 (10)	0.0292 (2)	0.45432 (8)	0.0494 (4)
C11	0.62941 (13)	−0.0747 (3)	0.39646 (10)	0.0717 (5)
H11A	0.5777	−0.1068	0.3666	0.108*
H11B	0.6598	−0.1798	0.4133	0.108*
H11C	0.6651	−0.0050	0.3719	0.108*
C12	0.61143 (13)	−0.0643 (3)	0.69723 (10)	0.0740 (6)
H12A	0.6119	−0.1331	0.7379	0.111*
H12B	0.5804	−0.1269	0.6591	0.111*
H12C	0.5840	0.0472	0.7022	0.111*
O1	0.66431 (6)	0.28750 (13)	0.55632 (5)	0.0477 (3)
O2	0.54980 (9)	0.35382 (19)	0.60388 (8)	0.0794 (4)
O3	0.66880 (7)	0.01209 (13)	0.51011 (5)	0.0469 (3)
O4	0.54496 (8)	0.11891 (18)	0.45344 (6)	0.0649 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0757 (11)	0.0441 (9)	0.0415 (9)	0.0013 (8)	0.0083 (8)	0.0000 (7)
C2	0.1023 (16)	0.0611 (11)	0.0444 (10)	0.0105 (11)	0.0019 (9)	0.0072 (8)
C3	0.0860 (14)	0.0725 (13)	0.0567 (12)	0.0227 (11)	−0.0132 (10)	−0.0030 (10)
C4	0.0614 (10)	0.0700 (12)	0.0659 (12)	0.0116 (9)	−0.0017 (9)	−0.0120 (10)
C5	0.0596 (10)	0.0499 (9)	0.0496 (9)	0.0049 (7)	0.0089 (7)	−0.0031 (7)
C6	0.0590 (9)	0.0351 (7)	0.0394 (8)	0.0033 (6)	0.0060 (6)	−0.0028 (6)
C7	0.0533 (8)	0.0358 (8)	0.0423 (8)	0.0010 (6)	0.0119 (6)	0.0014 (6)
C8	0.0531 (9)	0.0507 (9)	0.0482 (9)	0.0113 (7)	0.0023 (7)	−0.0071 (7)
C9	0.0886 (14)	0.0432 (10)	0.1066 (17)	0.0173 (10)	0.0163 (12)	0.0014 (10)
C10	0.0558 (9)	0.0470 (9)	0.0445 (9)	−0.0060 (7)	0.0055 (7)	0.0033 (7)
C11	0.0824 (13)	0.0797 (13)	0.0508 (10)	−0.0020 (10)	0.0039 (9)	−0.0145 (9)
C12	0.0912 (14)	0.0805 (13)	0.0538 (11)	−0.0122 (11)	0.0222 (10)	0.0127 (10)
O1	0.0520 (6)	0.0355 (6)	0.0573 (7)	0.0054 (4)	0.0135 (5)	0.0036 (5)
O2	0.0832 (9)	0.0732 (9)	0.0908 (10)	0.0161 (7)	0.0418 (8)	−0.0052 (8)
O3	0.0573 (6)	0.0417 (6)	0.0407 (6)	0.0042 (4)	0.0053 (5)	−0.0033 (4)
O4	0.0595 (7)	0.0741 (9)	0.0586 (7)	0.0104 (6)	0.0021 (6)	0.0037 (6)

Geometric parameters (Å, º)

C1—C6	1.389 (2)	C8—O2	1.192 (2)
C1—C2	1.392 (3)	C8—O1	1.3413 (19)
C1—C12	1.508 (3)	C8—C9	1.480 (3)
C2—C3	1.372 (3)	C9—H9A	0.9600
C2—H2	0.9300	C9—H9B	0.9600
C3—C4	1.371 (3)	C9—H9C	0.9600
C3—H3	0.9300	C10—O4	1.1929 (19)
C4—C5	1.377 (2)	C10—O3	1.3572 (19)
C4—H4	0.9300	C10—C11	1.480 (3)
C5—C6	1.386 (2)	C11—H11A	0.9600
C5—H5	0.9300	C11—H11B	0.9600
C6—C7	1.500 (2)	C11—H11C	0.9600
C7—O3	1.4248 (18)	C12—H12A	0.9600
C7—O1	1.434 (2)	C12—H12B	0.9600
C7—H7	0.9800	C12—H12C	0.9600
C6—C1—C2	117.32 (17)	O2—C8—C9	125.89 (16)
C6—C1—C12	122.91 (15)	O1—C8—C9	111.48 (16)
C2—C1—C12	119.76 (17)	C8—C9—H9A	109.5
C3—C2—C1	122.11 (18)	C8—C9—H9B	109.5
C3—C2—H2	118.9	H9A—C9—H9B	109.5
C1—C2—H2	118.9	C8—C9—H9C	109.5
C4—C3—C2	120.01 (17)	H9A—C9—H9C	109.5
C4—C3—H3	120.0	H9B—C9—H9C	109.5
C2—C3—H3	120.0	O4—C10—O3	123.03 (15)
C3—C4—C5	119.19 (19)	O4—C10—C11	125.86 (16)

C3—C4—H4	120.4	O3—C10—C11	111.10 (15)
C5—C4—H4	120.4	C10—C11—H11A	109.5
C4—C5—C6	121.02 (17)	C10—C11—H11B	109.5
C4—C5—H5	119.5	H11A—C11—H11B	109.5
C6—C5—H5	119.5	C10—C11—H11C	109.5
C5—C6—C1	120.36 (15)	H11A—C11—H11C	109.5
C5—C6—C7	117.72 (14)	H11B—C11—H11C	109.5
C1—C6—C7	121.92 (14)	C1—C12—H12A	109.5
O3—C7—O1	105.94 (11)	C1—C12—H12B	109.5
O3—C7—C6	107.31 (12)	H12A—C12—H12B	109.5
O1—C7—C6	109.49 (12)	C1—C12—H12C	109.5
O3—C7—H7	111.3	H12A—C12—H12C	109.5
O1—C7—H7	111.3	H12B—C12—H12C	109.5
C6—C7—H7	111.3	C8—O1—C7	117.51 (13)
O2—C8—O1	122.63 (16)	C10—O3—C7	116.42 (12)

C6—C1—C2—C3	0.7 (3)	C1—C6—C7—O3	−121.51 (15)
C12—C1—C2—C3	−178.03 (19)	C5—C6—C7—O1	−55.29 (17)
C1—C2—C3—C4	−0.3 (3)	C1—C6—C7—O1	123.95 (15)
C2—C3—C4—C5	−0.1 (3)	O2—C8—O1—C7	7.3 (2)
C3—C4—C5—C6	0.1 (3)	C9—C8—O1—C7	−173.66 (14)
C4—C5—C6—C1	0.3 (2)	O3—C7—O1—C8	134.50 (12)
C4—C5—C6—C7	179.53 (15)	C6—C7—O1—C8	−110.08 (14)
C2—C1—C6—C5	−0.7 (2)	O4—C10—O3—C7	2.1 (2)
C12—C1—C6—C5	177.99 (17)	C11—C10—O3—C7	−178.64 (14)
C2—C1—C6—C7	−179.89 (15)	O1—C7—O3—C10	−71.00 (15)
C12—C1—C6—C7	−1.2 (2)	C6—C7—O3—C10	172.10 (12)
C5—C6—C7—O3	59.25 (17)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C9—H9*A*···O4^{i}	0.96	2.50	3.425 (3)	161

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