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1-(3,4-Dimethoxyphenyl)ethanone

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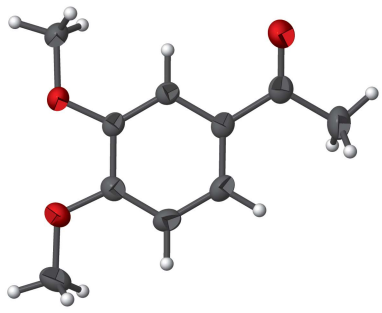
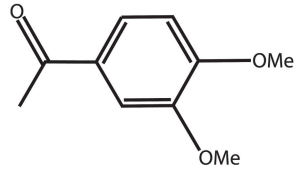
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $C_{10}H_{12}O_3$, has a single near planar molecule in the asymmetric unit, with the non-H atoms possessing a mean deviation from planarity of 0.132 Å. The molecules dimerize in the solid state through C—H···O interactions. These dimers are further linked through parallel slipped π–π interactions of the aryl rings [intercentroid distance = 3.5444 (11) Å, interplanar distance = 3.3998 (12) Å, slippage = 1.002 (2) Å].

3D view



Chemical scheme



Structure description

Herein, we report the crystal structure of 3,4-dimethoxyacetophenone (Fig. 1). The structure has a single near planar molecule in the asymmetric unit, with the non-hydrogen atoms possessing a mean deviation from planarity of 0.132 Å. A closer look reveals a planar dimethoxy aryl unit with a mean deviation from planarity of only 0.033 Å, and an acetyl group that is rotated 16.83 (7)^o from this plane. The structure exhibits bond distances and angles consistent with the structure of other 3,4-dimethoxy-substituted aryl compounds (de Ronde *et al.*, 2016; Mills-Robles *et al.*, 2015; Yang *et al.*, 2011).

In the crystal, the molecule dimerizes through C9—H9*A*···O3 interactions (Table 1). This interaction is also observed in the propionyl derivative of this compound (Fun *et al.*, 1997). These dimers are further linked through parallel slipped π–π interactions [intercentroid distance = 3.5444 (11) Å, interplanar distance = 3.3998 (12) Å, and slippage = 1.002 (2) Å]. These intermolecular interactions do not yield any infinite chains, sheets or networks in the structure. The packing of the title compound is shown in Fig. 2.

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

D—H···A	D—H	H···A	D···A	D—H···A
C9—H9A···O3^{i}	0.98	2.60	3.5418 (17)	162

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

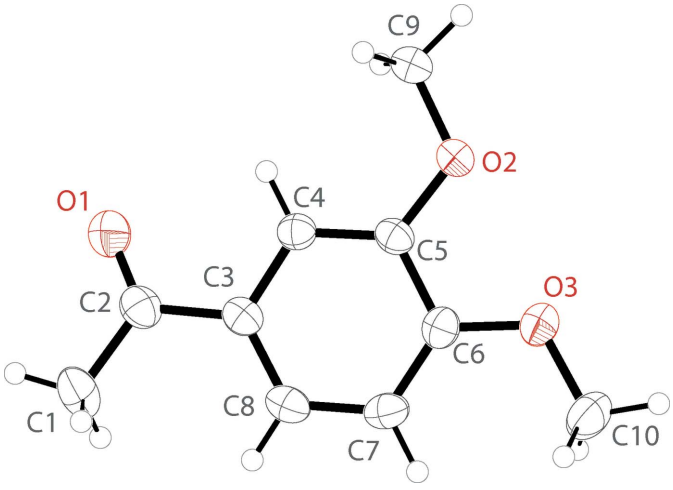


Figure 1
The molecular structure of the title compound, showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are drawn as spheres of arbitrary radius.

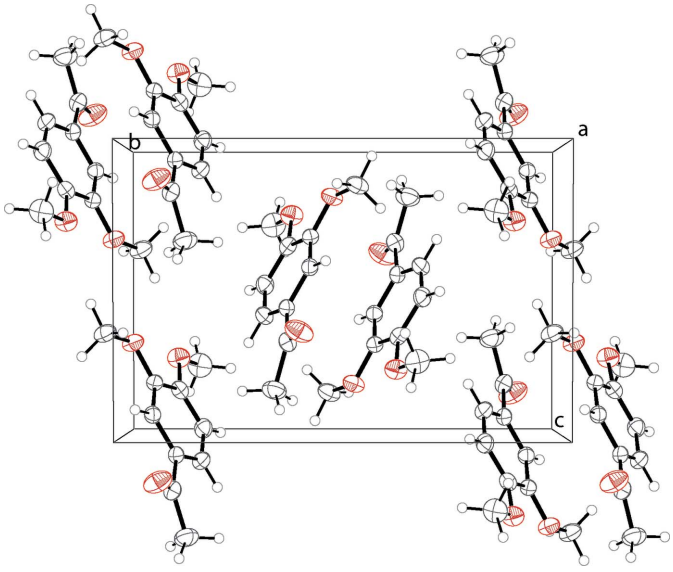


Figure 2
The molecular packing of the title compound, viewed along the *a* axis.

Synthesis and crystallization

A commercial sample (TCI) of 3,4-dimethoxyacetophenone was used for crystallization. A sample suitable for single-crystal X-ray analysis was grown from the slow evaporation of its methylene chloride solution.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{10}H_{12}O_3$
M_r	180.20
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	200
a, b, c (Å)	7.9543 (7), 13.3271 (11), 8.8107 (7)
β (°)	92.761 (3)
V (Å^3)	932.92 (13)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.09
Crystal size (mm)	0.18 × 0.1 × 0.05
Data collection	
Diffractometer	Bruker D8 Venture CMOS
Absorption correction	Multi-scan (*SADABS*; Bruker, 2014)
T_{min}, T_{max}	0.308, 0.331
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	22589, 1717, 1348
R_{int}	0.049
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.603
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.036, 0.096, 1.04
No. of reflections	1717
No. of parameters	122
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.17, −0.15

Computer programs: *APEX2* and *SAINT* (Bruker, 2014), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *OLEX2* (Dolomanov *et al.*, 2009) and *publCIF* (Westrip, 2010).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

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full crystallographic data

IUCrData (2016). **1**, x161794 [https://doi.org/10.1107/S2414314616017946]

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Crystal data

$C_{10}H_{12}O_3$
M_r = 180.20
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 7.9543 (7) Å
b = 13.3271 (11) Å
c = 8.8107 (7) Å
β = 92.761 (3)°
V = 932.92 (13) Å^3
Z = 4
$F(000)$ = 384
D_x = 1.283 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 6345 reflections
θ = 3.0–25.0°
μ = 0.09 mm^{-1}
T = 200 K
PLATE, colourless
0.18 × 0.1 × 0.05 mm

Data collection

Bruker D8 Venture CMOS diffractometer
Radiation source: Mo
TRIUMPH monochromator
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2014)
T_{min} = 0.308, T_{max} = 0.331
22589 measured reflections
1717 independent reflections
1348 reflections with $I > 2\sigma(I)$
R_{int} = 0.049
θ_{max} = 25.4°, θ_{min} = 3.0°
h = −9→9
k = −16→16
l = −10→10

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.096
S = 1.04
1717 reflections
122 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0459P)^2 + 0.2372P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}
Extinction correction: SHELXL2014 (Sheldrick, 2015), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.027 (5)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.96346 (14)	0.59482 (10)	0.63260 (13)	0.0553 (4)
O2	0.55355 (12)	0.52425 (8)	0.17851 (10)	0.0358 (3)
O3	0.28281 (12)	0.61821 (8)	0.23518 (11)	0.0390 (3)
C1	0.7983 (2)	0.65151 (14)	0.83175 (17)	0.0471 (4)
H1A	0.7053	0.6122	0.8703	0.071*
H1B	0.7707	0.7231	0.8360	0.071*
H1C	0.9011	0.6385	0.8944	0.071*
C2	0.82541 (19)	0.62201 (11)	0.67004 (16)	0.0346 (4)
C3	0.67942 (17)	0.62562 (10)	0.55786 (15)	0.0287 (3)
C4	0.69107 (17)	0.57335 (10)	0.41998 (14)	0.0277 (3)
H4	0.7914	0.5382	0.3995	0.033*
C5	0.55772 (17)	0.57306 (10)	0.31485 (14)	0.0275 (3)
C6	0.40893 (17)	0.62552 (10)	0.34497 (15)	0.0297 (3)
C7	0.39924 (18)	0.67871 (11)	0.47885 (16)	0.0342 (4)
H7	0.3006	0.7158	0.4982	0.041*
C8	0.53410 (18)	0.67777 (11)	0.58520 (16)	0.0339 (4)
H8	0.5261	0.7135	0.6779	0.041*
C9	0.69905 (19)	0.46789 (12)	0.14399 (16)	0.0393 (4)
H9A	0.6803	0.4353	0.0449	0.059*
H9B	0.7207	0.4167	0.2224	0.059*
H9C	0.7963	0.5129	0.1410	0.059*
C10	0.12522 (19)	0.66319 (14)	0.26553 (19)	0.0480 (4)
H10A	0.0433	0.6485	0.1818	0.072*
H10B	0.1395	0.7360	0.2752	0.072*
H10C	0.0846	0.6360	0.3604	0.072*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0393 (7)	0.0773 (9)	0.0483 (7)	0.0084 (6)	−0.0082 (5)	−0.0194 (6)
O2	0.0348 (6)	0.0445 (6)	0.0277 (5)	0.0075 (5)	−0.0018 (4)	−0.0078 (4)
O3	0.0308 (6)	0.0485 (6)	0.0374 (6)	0.0064 (5)	−0.0026 (4)	−0.0009 (5)
C1	0.0522 (10)	0.0559 (10)	0.0324 (8)	−0.0068 (8)	−0.0050 (7)	−0.0059 (8)
C2	0.0391 (9)	0.0297 (7)	0.0348 (8)	−0.0045 (6)	−0.0005 (6)	−0.0038 (6)
C3	0.0352 (8)	0.0234 (7)	0.0277 (7)	−0.0037 (6)	0.0029 (6)	−0.0003 (5)
C4	0.0292 (7)	0.0259 (7)	0.0284 (7)	0.0007 (5)	0.0035 (6)	0.0004 (5)
C5	0.0328 (7)	0.0257 (7)	0.0243 (7)	−0.0013 (6)	0.0040 (5)	0.0000 (5)
C6	0.0301 (7)	0.0280 (7)	0.0310 (7)	−0.0007 (6)	0.0005 (6)	0.0052 (6)
C7	0.0355 (8)	0.0302 (8)	0.0373 (8)	0.0067 (6)	0.0072 (6)	−0.0004 (6)
C8	0.0425 (9)	0.0296 (8)	0.0301 (7)	−0.0001 (6)	0.0062 (6)	−0.0052 (6)
C9	0.0392 (9)	0.0481 (9)	0.0306 (7)	0.0085 (7)	0.0017 (6)	−0.0097 (7)
C10	0.0315 (9)	0.0570 (10)	0.0553 (10)	0.0088 (7)	−0.0002 (7)	0.0018 (8)

Geometric parameters (Å, º)

O1—C2	1.2169 (18)	C4—C5	1.3742 (19)
O2—C5	1.3651 (16)	C5—C6	1.4107 (19)
O2—C9	1.4249 (17)	C6—C7	1.382 (2)
O3—C6	1.3631 (16)	C7—H7	0.9500
O3—C10	1.4263 (18)	C7—C8	1.390 (2)
C1—H1A	0.9800	C8—H8	0.9500
C1—H1B	0.9800	C9—H9A	0.9800
C1—H1C	0.9800	C9—H9B	0.9800
C1—C2	1.504 (2)	C9—H9C	0.9800
C2—C3	1.489 (2)	C10—H10A	0.9800
C3—C4	1.4073 (19)	C10—H10B	0.9800
C3—C8	1.380 (2)	C10—H10C	0.9800
C4—H4	0.9500		
C5—O2—C9	116.97 (10)	O3—C6—C7	124.97 (12)
C6—O3—C10	117.41 (11)	C7—C6—C5	119.78 (13)
H1A—C1—H1B	109.5	C6—C7—H7	120.1
H1A—C1—H1C	109.5	C6—C7—C8	119.86 (13)
H1B—C1—H1C	109.5	C8—C7—H7	120.1
C2—C1—H1A	109.5	C3—C8—C7	120.84 (13)
C2—C1—H1B	109.5	C3—C8—H8	119.6
C2—C1—H1C	109.5	C7—C8—H8	119.6
O1—C2—C1	120.49 (13)	O2—C9—H9A	109.5
O1—C2—C3	120.98 (13)	O2—C9—H9B	109.5
C3—C2—C1	118.53 (13)	O2—C9—H9C	109.5
C4—C3—C2	118.38 (12)	H9A—C9—H9B	109.5
C8—C3—C2	122.24 (12)	H9A—C9—H9C	109.5
C8—C3—C4	119.38 (13)	H9B—C9—H9C	109.5
C3—C4—H4	119.9	O3—C10—H10A	109.5
C5—C4—C3	120.16 (13)	O3—C10—H10B	109.5
C5—C4—H4	119.9	O3—C10—H10C	109.5
O2—C5—C4	125.43 (12)	H10A—C10—H10B	109.5
O2—C5—C6	114.62 (12)	H10A—C10—H10C	109.5
C4—C5—C6	119.94 (12)	H10B—C10—H10C	109.5
O3—C6—C5	115.25 (12)		
O1—C2—C3—C4	16.3 (2)	C4—C3—C8—C7	0.4 (2)
O1—C2—C3—C8	−164.02 (15)	C4—C5—C6—O3	−178.32 (12)
O2—C5—C6—O3	1.10 (17)	C4—C5—C6—C7	1.3 (2)
O2—C5—C6—C7	−179.26 (12)	C5—C6—C7—C8	−2.0 (2)
O3—C6—C7—C8	177.64 (13)	C6—C7—C8—C3	1.1 (2)
C1—C2—C3—C4	−162.91 (13)	C8—C3—C4—C5	−1.1 (2)
C1—C2—C3—C8	16.7 (2)	C9—O2—C5—C4	1.0 (2)
C2—C3—C4—C5	178.62 (12)	C9—O2—C5—C6	−178.43 (12)
C2—C3—C8—C7	−179.25 (13)	C10—O3—C6—C5	175.11 (13)
C3—C4—C5—O2	−179.16 (12)	C10—O3—C6—C7	−4.5 (2)

C3—C4—C5—C6	0.2 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C9—H9*A*···O3^{i}	0.98	2.60	3.5418 (17)	162

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