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7-Methoxy-3,4-dihydronaphthalen-1(2*H*)-one

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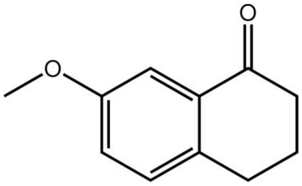
Key indicators: single-crystal X-ray study; T = 170 K; mean σ(C–C) = 0.002 Å; R factor = 0.044; wR factor = 0.125; data-to-parameter ratio = 19.5.

In the title compound, $C_{11}H_{12}O_2$, the six-membered ketone ring fused to the 7-methoxy benzene ring adopts a slightly distorted envelope configuration with the central methylene C atom being the flap. The crystal packing is stabilized by weak intermolecular C—H···O and C—H···π interactions, which lead to supramolecular layers in the *bc* plane.

Related literature

For the synthesis of steroid estrogens, see: Belov *et al.* (2007). For the manufacture of important antidepressant drugs, see: Shum *et al.* (2000). For multi-functional scaffolds of tetralone, see: Mahapatra *et al.* (2008). For related structures, see: Barcon *et al.* (2001); Haddad (1986); Orlov *et al.* (1996). For puckering parameters, see: Cremer & Pople (1975).



Experimental

Crystal data

$C_{11}H_{12}O_2$
M_r = 176.21
Monoclinic, $P2_1/c$
a = 7.4303 (4) Å
b = 7.4614 (4) Å
c = 16.4393 (8) Å
β = 90.976 (4)°
V = 911.27 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 170 K
0.35 × 0.25 × 0.10 mm

Data collection

Oxford Diffraction Xcalibur Eos Gemini diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2010)
T_{min} = 0.970, T_{max} = 0.991
8750 measured reflections
2345 independent reflections
1959 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.125
S = 1.04
2345 reflections
120 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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

*Cg*1 is the centroid of the C1–C3,C8–C10 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C11—H11*C*···O1^{i}	0.98	2.38	3.3095 (18)	157
C5—H5*A*···*Cg*1^{ii}	0.99	2.77	3.6730 (14)	152

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

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2010); 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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2750).

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supplementary materials

Acta Cryst. (2011). E**67**, o1646 [**doi:10.1107/S1600536811020174**]

7-Methoxy-3,4-dihydronaphthalen-1(2*H*)-one

J. P. Jasinski, J. A. Golen, S. Sekar, H. S. Yathirajan and **N. Naik**

Comment

The structural and therapeutic diversity of small heterocyclic molecules continue to attract the attention of organic and medicinal chemists. Tetralones are emerging prominently as pharmacologically important bioactive molecules. Tetralone is an important and common intermediate in organic synthesis and is a ketone derivative of tetralin. The title compound (Systematic name: 3 ,4-Dihydro-7-methoxy-2(1H)-naphthalenone), (I), $C_{11}H_{12}O_2$, is used in the preparation of agomelatine, which is an antidepressant. The importance of tetralone and its substituted derivatives as building blocks in the synthesis of steroid estrogens via isothiuronium salts is reported (Belov *et al.*, 2007). Tetralones are also important intermediates for the manufacturing of various serotonin inhibitor compounds having antidepressant activity, particularly sertraline, an important antidepressant drug (Shum *et al.*, 2000). Multi functional scaffolds of tetralone to generate further diversity with different functionalities is reported (Mahapatra *et al.*, 2008). The crystal structures of some related compounds, viz., 2,2-dibromo-3,4-dihydro-1(2H)-naphthalenone (Haddad *et al.*, 1986), 2-(4-nitrobenzylidene)-1-tetralone (Orlov *et al.*, 1996), (±)-1-tetralone-3-carboxylic acid and (±)-1-tetralone-2-acetic acid (Barcon *et al.*, 2001),have been reported. In view of the importance of tetralones, this paper reports the crystal structure of the title compound, (I).

In the title compound, $C_{11}H_{12}O_2$, the six-membered ketone ring fused to the benzene ring adopts a slightly distorted envelope configuration (Cremer & Pople, 1975) with puckering parameters Q, θ and φ of 0.4869 (14) Å, 56.33 (15) ° and 185.10 (18) °, respectively (Fig. 1). For an ideal envelope θ and φ have values of 54.7° and 180°. Crystal packing is stabilized by weak C—H···O and C—H···π (Table 1) intermolecular interactions.

Experimental

Anisole (4.3 ml, 0.040 mol) is acylated with succinic anhydride (4.2 g, 0.042 mol) in the presence of anhydrous aluminium chloride and nitrobenzene as solvent to give the intermediate keto acid. The keto group is reduced by hydrogenation with Pd/C as catalyst at 2-3 kgs pressure and 343-348 K for 2 -3 hours. Further work up, isolation and cyclization with poly phosphoric acid (PPA) gives 7-methoxy-1-tetralone (Fig. 1). X-ray quality crystals of (I) were obtained by slow evaporation from isopropyl alcohol (*M*.pt.: 333-336 K).

Refinement

All of the H atoms were placed in their calculated positions and then refined using the riding model with Atom—H lengths of 0.95 Å (CH), 0.99 Å (CH_2) or 0.98 Å (CH_3). Isotropic displacement parameters for these atoms were set to 1.19-1.20 (CH, CH_2) or 1.49 (CH_3) times U_{eq} of the parent atom.

Figures

Fig. 1. Reaction scheme for the title compound.

Fig. 2. Molecular structure of the title compound showing the atom labeling scheme and 50% probability displacement ellipsoids.

7-Methoxy-3,4-dihydronaphthalen-1(2*H*)-one

Crystal data

$C_{11}H_{12}O_2$

$M_r = 176.21$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 7.4303$ (4) Å

$b = 7.4614$ (4) Å

$c = 16.4393$ (8) Å

$\beta = 90.976$ (4)°

$V = 911.27$ (8) Å^3

$Z = 4$

$F(000) = 376$

$D_x = 1.284$ Mg m^{-3}

Mo *K*α radiation, $\lambda = 0.71073$ Å

Cell parameters from 4312 reflections

$\theta = 3.7$–32.3°

$\mu = 0.09$ mm^{-1}

$T = 170$ K

Block, colorless

0.35 × 0.25 × 0.10 mm

Data collection

Oxford Diffraction Xcalibur Eos Gemini diffractometer

Radiation source: Enhance (Mo) X-ray Source

graphite

Detector resolution: 16.1500 pixels mm^{-1}

ω scans

Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2010)

$T_{min} = 0.970$, $T_{max} = 0.991$

8750 measured reflections

2345 independent reflections

1959 reflections with $I > 2\sigma(I)$

$R_{int} = 0.023$

$\theta_{max} = 28.7°$, $\theta_{min} = 3.7°$

$h = -9 \rightarrow 10$

$k = -9 \rightarrow 10$

$l = -21 \rightarrow 22$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.044$

$wR(F^2) = 0.125$

$S = 1.04$

2345 reflections

120 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

$w = 1/[\sigma^2(F_o^2) + (0.0642P)^2 + 0.1602P]$
where $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{max} = 0.26$ e Å^{-3}

$\Delta\rho_{min} = -0.17$ e Å^{-3}

Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.053 (7)

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.

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 $F^2 > \sigma(F^2)$ 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}
O1	0.62487 (12)	0.84217 (13)	0.45326 (5)	0.0466 (3)
O2	0.87018 (12)	0.68273 (16)	0.72482 (6)	0.0553 (3)
C1	0.70272 (16)	0.66013 (17)	0.69096 (7)	0.0380 (3)
C2	0.67929 (14)	0.72639 (15)	0.61301 (6)	0.0335 (3)
H2A	0.7769	0.7829	0.5867	0.040*
C3	0.51381 (14)	0.71094 (14)	0.57282 (6)	0.0307 (2)
C4	0.49582 (15)	0.78093 (15)	0.48827 (7)	0.0336 (3)
C5	0.31401 (17)	0.77041 (18)	0.44739 (7)	0.0418 (3)
H5A	0.3094	0.6623	0.4125	0.050*
H5B	0.2977	0.8763	0.4117	0.050*
C6	0.15984 (16)	0.76306 (18)	0.50688 (8)	0.0447 (3)
H6A	0.1523	0.8781	0.5366	0.054*
H6B	0.0449	0.7447	0.4767	0.054*
C7	0.18949 (16)	0.61092 (18)	0.56688 (8)	0.0440 (3)
H7A	0.0917	0.6112	0.6070	0.053*
H7B	0.1850	0.4952	0.5375	0.053*
C8	0.36834 (15)	0.62853 (15)	0.61076 (7)	0.0355 (3)
C9	0.39581 (17)	0.56299 (18)	0.68908 (8)	0.0449 (3)
H9A	0.2986	0.5063	0.7157	0.054*
C10	0.55946 (18)	0.57744 (19)	0.72955 (7)	0.0457 (3)
H10A	0.5742	0.5315	0.7831	0.055*
C11	0.9071 (2)	0.6037 (3)	0.80161 (9)	0.0775 (6)
H11A	1.0326	0.6270	0.8176	0.116*
H11B	0.8871	0.4741	0.7982	0.116*
H11C	0.8271	0.6553	0.8422	0.116*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0447 (5)	0.0552 (6)	0.0401 (5)	−0.0057 (4)	0.0086 (4)	0.0067 (4)
O2	0.0402 (5)	0.0863 (8)	0.0392 (5)	0.0017 (5)	−0.0064 (4)	0.0004 (5)
C1	0.0357 (6)	0.0438 (6)	0.0344 (6)	0.0044 (5)	0.0005 (4)	−0.0048 (4)

C2	0.0312 (5)	0.0358 (6)	0.0338 (5)	−0.0018 (4)	0.0044 (4)	−0.0026 (4)
C3	0.0312 (5)	0.0288 (5)	0.0322 (5)	−0.0006 (4)	0.0033 (4)	−0.0018 (4)
C4	0.0368 (5)	0.0300 (5)	0.0341 (5)	0.0001 (4)	0.0032 (4)	−0.0031 (4)
C5	0.0452 (7)	0.0409 (6)	0.0390 (6)	−0.0030 (5)	−0.0065 (5)	−0.0005 (5)
C6	0.0332 (6)	0.0463 (7)	0.0542 (7)	−0.0003 (5)	−0.0063 (5)	−0.0041 (5)
C7	0.0320 (6)	0.0476 (7)	0.0524 (7)	−0.0083 (5)	0.0029 (5)	−0.0002 (5)
C8	0.0326 (6)	0.0342 (6)	0.0399 (6)	−0.0025 (4)	0.0052 (4)	−0.0010 (4)
C9	0.0423 (7)	0.0485 (7)	0.0442 (6)	−0.0052 (5)	0.0116 (5)	0.0080 (5)
C10	0.0506 (7)	0.0534 (8)	0.0332 (6)	0.0034 (6)	0.0060 (5)	0.0074 (5)
C11	0.0548 (9)	0.1375 (18)	0.0399 (7)	0.0233 (10)	−0.0073 (6)	0.0056 (9)

Geometric parameters (Å, °)

O1—C4	1.2159 (14)	C6—C7	1.5175 (19)
O2—C1	1.3649 (14)	C6—H6A	0.9900
O2—C11	1.4159 (19)	C6—H6B	0.9900
C1—C2	1.3818 (16)	C7—C8	1.5070 (16)
C1—C10	1.3925 (18)	C7—H7A	0.9900
C2—C3	1.3907 (15)	C7—H7B	0.9900
C2—H2A	0.9500	C8—C9	1.3891 (17)
C3—C8	1.3994 (15)	C9—C10	1.3804 (19)
C3—C4	1.4887 (15)	C9—H9A	0.9500
C4—C5	1.5006 (16)	C10—H10A	0.9500
C5—C6	1.5198 (18)	C11—H11A	0.9800
C5—H5A	0.9900	C11—H11B	0.9800
C5—H5B	0.9900	C11—H11C	0.9800
C1—O2—C11	118.26 (12)	C5—C6—H6B	109.7
O2—C1—C2	115.69 (10)	H6A—C6—H6B	108.2
O2—C1—C10	124.58 (11)	C8—C7—C6	111.28 (10)
C2—C1—C10	119.73 (11)	C8—C7—H7A	109.4
C1—C2—C3	120.49 (10)	C6—C7—H7A	109.4
C1—C2—H2A	119.8	C8—C7—H7B	109.4
C3—C2—H2A	119.8	C6—C7—H7B	109.4
C2—C3—C8	120.53 (10)	H7A—C7—H7B	108.0
C2—C3—C4	118.63 (9)	C9—C8—C3	117.73 (11)
C8—C3—C4	120.83 (10)	C9—C8—C7	121.83 (10)
O1—C4—C3	120.99 (10)	C3—C8—C7	120.43 (10)
O1—C4—C5	121.25 (10)	C10—C9—C8	122.25 (11)
C3—C4—C5	117.75 (10)	C10—C9—H9A	118.9
C4—C5—C6	113.35 (10)	C8—C9—H9A	118.9
C4—C5—H5A	108.9	C9—C10—C1	119.27 (11)
C6—C5—H5A	108.9	C9—C10—H10A	120.4
C4—C5—H5B	108.9	C1—C10—H10A	120.4
C6—C5—H5B	108.9	O2—C11—H11A	109.5
H5A—C5—H5B	107.7	O2—C11—H11B	109.5
C7—C6—C5	110.04 (10)	H11A—C11—H11B	109.5
C7—C6—H6A	109.7	O2—C11—H11C	109.5
C5—C6—H6A	109.7	H11A—C11—H11C	109.5
C7—C6—H6B	109.7	H11B—C11—H11C	109.5

C11—O2—C1—C2	−174.47 (13)	C5—C6—C7—C8	56.14 (14)
C11—O2—C1—C10	5.8 (2)	C2—C3—C8—C9	−0.25 (17)
O2—C1—C2—C3	−179.84 (10)	C4—C3—C8—C9	178.68 (10)
C10—C1—C2—C3	−0.07 (18)	C2—C3—C8—C7	−179.62 (10)
C1—C2—C3—C8	0.18 (17)	C4—C3—C8—C7	−0.69 (16)
C1—C2—C3—C4	−178.76 (10)	C6—C7—C8—C9	150.91 (12)
C2—C3—C4—O1	3.71 (16)	C6—C7—C8—C3	−29.74 (16)
C8—C3—C4—O1	−175.24 (11)	C3—C8—C9—C10	0.20 (19)
C2—C3—C4—C5	−177.30 (10)	C7—C8—C9—C10	179.56 (12)
C8—C3—C4—C5	3.75 (15)	C8—C9—C10—C1	−0.1 (2)
O1—C4—C5—C6	−156.85 (12)	O2—C1—C10—C9	179.77 (12)
C3—C4—C5—C6	24.16 (15)	C2—C1—C10—C9	0.02 (19)
C4—C5—C6—C7	−53.97 (14)		

Hydrogen-bond geometry (Å, °)

Cg1 is the centroid of the C1–C3,C8–C10 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C11—H11C···O1^{i}	0.98	2.38	3.3095 (18)	157
C5—H5A···Cg1^{ii}	0.99	2.77	3.6730 (14)	152

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

Fig. 1

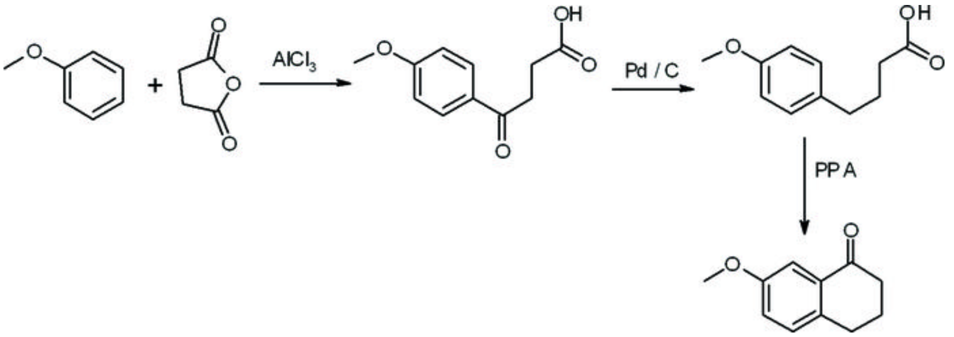

Fig. 2