Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(*E*)-4-(1,3-Benzodioxol-5-yl)but-3-en-2-one

S. Sarveswari,[a] V. Vijayakumar,[a] Priya Susan Mathew,[a] Rafael Mendoza-Meroño[b] and Santiago García-Granda[b]*

[a]Organic Chemistry Division, School of Advanced Sciences, VIT University, Vellore 632 014, India, and [b]Departamento de Química Física y Analítica, Facultad de Química, Universidad de Oviedo – CINN, C/ Julián Clavería 8, 33006 Oviedo, Asturias, Spain
Correspondence e-mail: sgg@uniovi.es

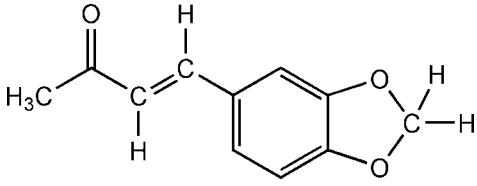
Received 23 January 2011; accepted 1 February 2011

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.036; wR factor = 0.094; data-to-parameter ratio = 10.4.

In the title compound, $C_{11}H_{10}O_3$, the benzodioxole ring adopts a flattened [puckering parameters: q_2 = 0.107 (2) Å, φ_2 = 160 (1)°] envelope conformation with the methylene C atom as the flap. The crystal packing features chains, parallel to the c axis, composed of dimers connected by weak C—H–O hydrogen bonds and extending in layers in the bc plane.

Related literature

For the synthesis of chalcones, see: Loh *et al.* (2010). For a related structure, see: Gao & Ng (2006).



Experimental

Crystal data

$C_{11}H_{10}O_3$
M_r = 190.19
Monoclinic, $P2_1/c$
a = 5.3469 (3) Å
b = 16.4849 (8) Å
c = 10.5475 (6) Å
β = 99.183 (5)°
V = 917.77 (9) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 0.83 mm^{-1}
T = 293 K
0.18 × 0.11 × 0.09 mm

Data collection

Oxford Diffraction Xcalibur Ruby Gemini diffractometer
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2009)
T_{min} = 0.950, T_{max} = 1.000
5375 measured reflections
1737 independent reflections
1121 reflections with $I > 2\sigma(I)$
R_{int} = 0.029

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.094
S = 0.92
1737 reflections
167 parameters
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.12 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C7—H7···O1^{i}	0.95 (2)	2.56 (2)	3.489 (2)	166 (1)
C9—H9···O1^{i}	0.93 (2)	2.60 (2)	3.517 (2)	171 (1)
C8—H8···O2^{ii}	0.93 (2)	2.90 (2)	3.819 (2)	177 (1)

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

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2009); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

VV is grateful to the DST-India for funding through the Young Scientist Scheme (Fast Track Proposal). Financial support was provided by the Agencia Española de Cooperación Internacional y Desarrollo (AECID), FEDER funding and the Spanish MICINN (MAT2006–01997, MAT2010–15095 and the Factoría de Cristalización Consolider Ingenio 2010).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG5110).

References

Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A., Burla, M. C., Polidori, G. & Camalli, M. (1994). *J. Appl. Cryst.* **27**, 435.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837-838.
Gao, S. & Ng, S. W. (2006). *Acta Cryst.* E**62**, o3517–o3518.
Loh, W.-S., Fun, H.-K., Sarveswari, S., Vijayakumar, V. & Reddy, B. P. (2010). *Acta Cryst.* E**66**, o353–o354.
Oxford Diffraction (2009). *CrysAlis PRO*. Oxford Diffraction Ltd, Yarnton, England.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supporting information

Acta Cryst. (2011). E**67**, o583 [doi:10.1107/S1600536811004077]

(*E*)-4-(1,3-Benzodioxol-5-yl)but-3-en-2-one

S. Sarveswari, V. Vijayakumar, Priya Susan Mathew, Rafael Mendoza-Meroño and Santiago García-Granda

S1. Comment

Chalcones and its heterocyclic analogs have been used as intermediates in organic synthesis and exhibit diverse biological activities such as antimicrobial and cytotoxic agents. From a chemistry point of view, an important feature of chalcones and their heteroanalogs is the ability to act as activated unsaturated systems in conjugated addition reactions of carbanions. In continuation with our interest in the synthesis of chalcones (Loh *et al.*, 2010) herein we report the structure of the title compound (I).

In the title compound (I) the spatial arrangement of the keto group C(10)═ O(3) and the olefinic double bond C(8)═C(9) with respect to the single bond C9—C10 is *trans*, as indicated the C(8)—C(9)—C(10)—O(3) torsion angle value(-176.10 (18)°). The C(8)═C(9) (1.325 (2))Å), C(9)—C(10) (1.459 (2) Å) and C10═O3 (1.225 (2) Å) distances values are similar of the structures previously reported (Gao and Ng, 2006).

Plane A is refered to C(8)/C(9)/C(10)/O(3) atoms (maximum desviation C(9) 0.0229 (17) Å). The dihedral angle between C(2)/C(7) benzene ring (maximum desviation C(4) -0.0040 (18) Å) and *plane A* is 7.25 (10)°. In benzodioxole ring C(1) is displaced from mean plane by 0.1351 (22) Å, forming a flattened envelope conformation with C(1) as the flap atom. The packing in the crystal structure is dominated by molecular chains made of dimers connected by C—H–O weak hydrogen bonds and extended along *bc* plane.

Insert scheme 1.

The asymmetric unit consists of a single molecule (I), shown in Figure 1.

S2. Experimental

A mixture of acetone (3.0 g 0.005*M*) and benzo[*d*][1,3]dioxole-5-carbaldehyde (1.5 g 0.01*M*) and a catalytic amount of KOH in distilled ethanol was stirred for about 12 h, the resulting mixture was concentrated to remove ethanol then poured on to ice and neutralized with dill acetic acid. The resultant solid was filtered, dried and purified by column chromatography using 1:1 mixture of ethyl acetate and petroleum ether. Recrystallized from acetone; Yield: 49% and m.pt: 412–414 K.

S3. Refinement

At the end of the refinement the highest peak in the electron density was 0.124 e Å $^{-3}$, while the deepest hole was -0.154 e Å $^{-3}$.

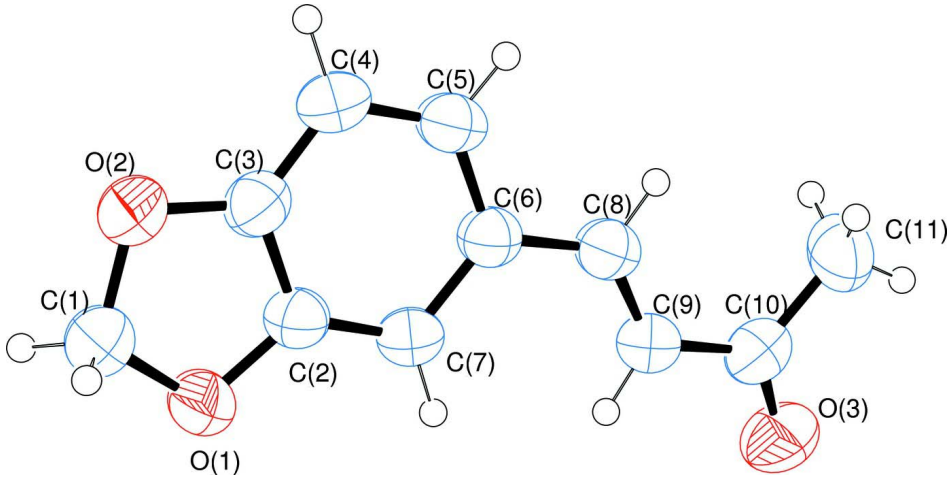


Figure 1

A view of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

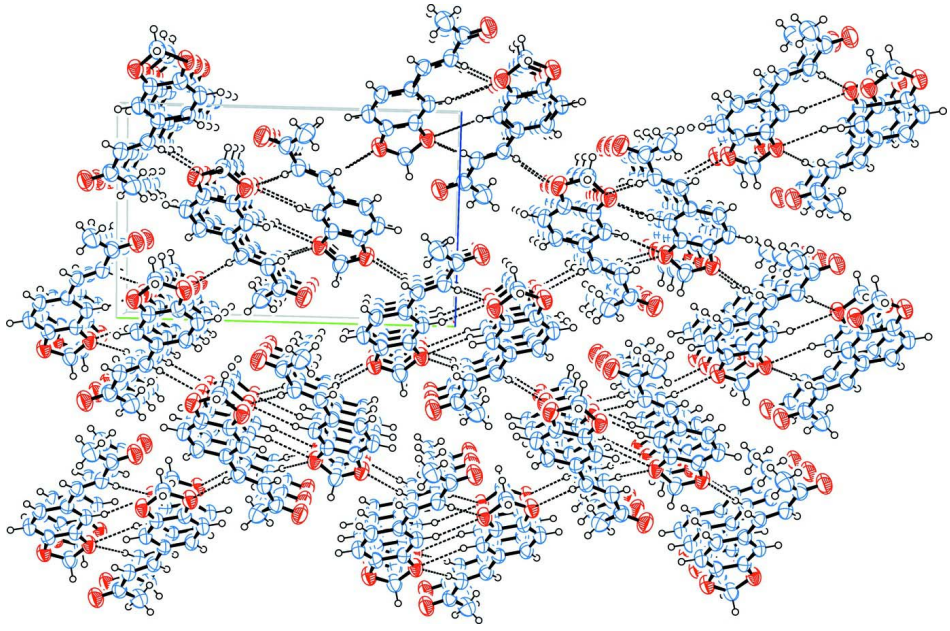


Figure 2

Packing diagram viewed parallel to the *bc* plane. Hydrogen bonds are indicated by dashed lines.

(*E*)-4-(1,3-Benzodioxol-5-yl)but-3-en-2-one

Crystal data

$C_{11}H_{10}O_3$
$M_r = 190.19$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 5.3469\ (3)$ Å
$b = 16.4849\ (8)$ Å
$c = 10.5475\ (6)$ Å
$\beta = 99.183\ (5)°$
$V = 917.77\ (9)$ Å^3
$Z = 4$
$F(000) = 400$
$D_x = 1.376$ Mg m^{-3}
Melting point: 413 K
Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å
Cell parameters from 1941 reflections
$\theta = 4.2–70.6°$

μ = 0.83 mm^{-1}
T = 293 K

Prismatic, yellow
0.18 × 0.11 × 0.09 mm

Data collection

Oxford Diffraction Xcalibur Ruby Gemini diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 10.2673 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2009)
T_{min} = 0.950, T_{max} = 1.000

5375 measured reflections
1737 independent reflections
1121 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 70.5°, θ_{min} = 5.0°
h = −5→6
k = −14→19
l = −12→11

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.094
S = 0.92
1737 reflections
167 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
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0547P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.12 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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}
O2	0.5552 (2)	0.23540 (7)	−0.17522 (12)	0.0686 (3)
O1	0.5790 (2)	0.09846 (7)	−0.13128 (11)	0.0669 (4)
C2	0.4130 (3)	0.13463 (9)	−0.06159 (15)	0.0528 (4)
C6	0.1246 (3)	0.14906 (9)	0.08521 (14)	0.0528 (4)
C5	0.1132 (3)	0.23186 (10)	0.05728 (16)	0.0597 (4)
C7	0.2809 (3)	0.09884 (10)	0.02303 (16)	0.0556 (4)
C3	0.3994 (3)	0.21645 (9)	−0.08768 (15)	0.0557 (4)
C8	−0.0220 (3)	0.11602 (10)	0.17895 (16)	0.0563 (4)
C4	0.2514 (3)	0.26731 (10)	−0.02911 (17)	0.0627 (4)
C9	−0.0146 (3)	0.04080 (10)	0.22361 (17)	0.0591 (4)
O3	−0.1186 (3)	−0.06111 (8)	0.35856 (14)	0.0857 (4)
C10	−0.1536 (3)	0.00895 (11)	0.32109 (16)	0.0632 (4)
C11	−0.3362 (5)	0.06204 (16)	0.3750 (3)	0.0802 (6)

C1	0.6491 (4)	0.16001 (11)	−0.2141 (2)	0.0683 (5)
H8	−0.129 (3)	0.1522 (10)	0.2107 (17)	0.065 (5)*
H7	0.295 (3)	0.0424 (10)	0.0405 (15)	0.058 (4)*
H4	0.242 (3)	0.3245 (11)	−0.0461 (17)	0.074 (5)*
H9	0.085 (3)	0.0018 (11)	0.1929 (15)	0.069 (5)*
H5	0.007 (3)	0.2651 (10)	0.0987 (15)	0.061 (4)*
H1A	0.567 (3)	0.1472 (11)	−0.304 (2)	0.079 (6)*
H1B	0.839 (4)	0.1638 (11)	−0.2067 (17)	0.078 (5)*
H11A	−0.415 (6)	0.0290 (19)	0.423 (3)	0.156 (12)*
H11C	−0.247 (5)	0.1005 (18)	0.433 (3)	0.148 (12)*
H11B	−0.442 (6)	0.0918 (19)	0.316 (3)	0.147 (12)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O2	0.0755 (7)	0.0532 (7)	0.0818 (8)	0.0007 (5)	0.0272 (6)	0.0100 (6)
O1	0.0752 (8)	0.0532 (7)	0.0789 (8)	0.0086 (5)	0.0323 (6)	0.0055 (6)
C2	0.0533 (8)	0.0466 (8)	0.0587 (9)	0.0033 (7)	0.0092 (7)	−0.0001 (7)
C6	0.0540 (8)	0.0482 (9)	0.0560 (9)	0.0025 (7)	0.0082 (7)	−0.0004 (7)
C5	0.0658 (10)	0.0485 (9)	0.0663 (10)	0.0081 (8)	0.0148 (8)	−0.0030 (8)
C7	0.0602 (9)	0.0430 (9)	0.0643 (10)	0.0042 (7)	0.0121 (7)	0.0024 (8)
C3	0.0569 (9)	0.0497 (9)	0.0605 (10)	−0.0023 (7)	0.0090 (7)	0.0046 (7)
C8	0.0565 (9)	0.0530 (10)	0.0594 (9)	0.0041 (7)	0.0094 (7)	−0.0033 (8)
C4	0.0719 (10)	0.0427 (9)	0.0745 (11)	0.0031 (8)	0.0144 (8)	0.0047 (8)
C9	0.0610 (9)	0.0497 (10)	0.0684 (10)	0.0019 (7)	0.0153 (8)	−0.0020 (8)
O3	0.1042 (10)	0.0586 (8)	0.0963 (10)	−0.0024 (7)	0.0216 (8)	0.0171 (7)
C10	0.0642 (10)	0.0564 (10)	0.0673 (10)	−0.0067 (8)	0.0048 (8)	0.0047 (8)
C11	0.0771 (13)	0.0829 (15)	0.0875 (16)	0.0063 (12)	0.0340 (12)	0.0146 (14)
C1	0.0753 (12)	0.0575 (10)	0.0766 (13)	0.0014 (9)	0.0260 (10)	0.0071 (9)

Geometric parameters (Å, º)

O2—C3	1.3746 (19)	C8—C9	1.325 (2)
O2—C1	1.425 (2)	C8—H8	0.926 (18)
O1—C2	1.3755 (18)	C4—H4	0.960 (18)
O1—C1	1.428 (2)	C9—C10	1.459 (2)
C2—C7	1.358 (2)	C9—H9	0.927 (18)
C2—C3	1.376 (2)	O3—C10	1.225 (2)
C6—C5	1.396 (2)	C10—C11	1.490 (3)
C6—C7	1.410 (2)	C11—H11A	0.90 (3)
C6—C8	1.462 (2)	C11—H11C	0.95 (3)
C5—C4	1.390 (2)	C11—H11B	0.92 (3)
C5—H5	0.944 (17)	C1—H1A	1.005 (19)
C7—H7	0.948 (17)	C1—H1B	1.009 (19)
C3—C4	1.366 (2)		
C3—O2—C1	105.93 (12)	C3—C4—H4	122.5 (11)
C2—O1—C1	105.90 (12)	C5—C4—H4	121.1 (11)

C7—C2—O1	127.63 (14)	C8—C9—C10	126.69 (16)
C7—C2—C3	122.73 (14)	C8—C9—H9	120.7 (11)
O1—C2—C3	109.63 (13)	C10—C9—H9	112.6 (11)
C5—C6—C7	119.01 (14)	O3—C10—C9	119.83 (17)
C5—C6—C8	119.81 (14)	O3—C10—C11	120.43 (17)
C7—C6—C8	121.17 (14)	C9—C10—C11	119.74 (17)
C4—C5—C6	122.66 (16)	C10—C11—H11A	105 (2)
C4—C5—H5	118.7 (10)	C10—C11—H11C	110.3 (18)
C6—C5—H5	118.6 (10)	H11A—C11—H11C	106 (2)
C2—C7—C6	117.36 (15)	C10—C11—H11B	115.3 (19)
C2—C7—H7	121.4 (9)	H11A—C11—H11B	115 (3)
C6—C7—H7	121.3 (9)	H11C—C11—H11B	106 (3)
C4—C3—O2	128.40 (14)	O2—C1—O1	107.73 (14)
C4—C3—C2	121.79 (15)	O2—C1—H1A	109.7 (11)
O2—C3—C2	109.80 (13)	O1—C1—H1A	108.3 (11)
C9—C8—C6	126.90 (16)	O2—C1—H1B	108.7 (10)
C9—C8—H8	117.3 (11)	O1—C1—H1B	110.9 (10)
C6—C8—H8	115.8 (11)	H1A—C1—H1B	111.5 (15)
C3—C4—C5	116.44 (16)		

C1—O1—C2—C7	174.79 (18)	C7—C2—C3—O2	179.18 (15)
C1—O1—C2—C3	−6.33 (18)	O1—C2—C3—O2	0.24 (18)
C7—C6—C5—C4	−0.4 (3)	C5—C6—C8—C9	−173.77 (17)
C8—C6—C5—C4	178.81 (16)	C7—C6—C8—C9	5.4 (3)
O1—C2—C7—C6	178.83 (15)	O2—C3—C4—C5	−179.36 (16)
C3—C2—C7—C6	0.1 (2)	C2—C3—C4—C5	−0.6 (3)
C5—C6—C7—C2	0.0 (2)	C6—C5—C4—C3	0.7 (3)
C8—C6—C7—C2	−179.22 (15)	C6—C8—C9—C10	177.30 (16)
C1—O2—C3—C4	−175.19 (18)	C8—C9—C10—O3	−176.10 (17)
C1—O2—C3—C2	5.96 (19)	C8—C9—C10—C11	3.5 (3)
C7—C2—C3—C4	0.3 (3)	C3—O2—C1—O1	−9.8 (2)
O1—C2—C3—C4	−178.69 (15)	C2—O1—C1—O2	9.91 (19)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7···O1^{i}	0.95 (2)	2.56 (2)	3.489 (2)	166 (1)
C9—H9···O1^{i}	0.93 (2)	2.60 (2)	3.517 (2)	171 (1)
C8—H8···O2^{ii}	0.93 (2)	2.90 (2)	3.819 (2)	177 (1)

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