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1-(3,4-Dimethoxyphenyl)propan-1-one

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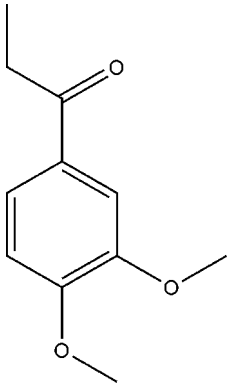
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.041; wR factor = 0.122; data-to-parameter ratio = 13.9.

The title compound, $C_{11}H_{14}O_3$, was isolated from the stems of *Trigonostemon xyphophylloides*, which belongs to *Trigonostemon* genus of Euphorbiaceae. The plants in this genus were used in folk medicine, such as for the treatment of diseases caused by viruses and fungi. The limited investigation of the chemistry of this plant prompted an examination of constituents of its twigs, from which the title compound was isolated. The molecule is approximately planar with an r.m.s. deviation of 0.1237Å. In the crystal, intermolecular C—H···O hydrogen bonds connect the molecules into a two-dimensional network structure with an $R_2^2(12)$ graph-set motif.

Related literature

For the medicinal and botanical background to the title compound, see: Zdero *et al.* (1990); Lopes *et al.* (1996). For weak hydrogen bonds, see: Steiner (1996).



Experimental

Crystal data

$C_{11}H_{14}O_3$
M_r = 194.22
Monoclinic, $P2_1/c$
a = 8.9308 (9) Å
b = 13.8582 (14) Å
c = 8.5692 (8) Å
β = 102.427 (1)°
V = 1035.72 (18) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 298 K
0.50 × 0.43 × 0.40 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.236, T_{max} = 0.965
5082 measured reflections
1827 independent reflections
1265 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.122
S = 1.04
1827 reflections
131 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C11—H11*C*···O2^{i}	0.96	2.66	3.607 (2)	171
C8—H8···O1^{ii}	0.93	2.50	3.419 (3)	171

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

Data collection: *APEX2* (Bruker, 2003); cell refinement: *SAINT-Plus* (Bruker, 2003); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; 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: NR2005).

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supporting information

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1-(3,4-Dimethoxyphenyl)propan-1-one

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S1. Comment

The title compound was isolated from plants such as *Pteronia camphorata* (Zdero *et al.*, 1990) and *Virola surinamensis* (Lopes *et al.*, 1996). In our ongoing studies of natural products with biological activity we isolated the compound from the 75% EtOH extract of the stems of *Trigonostemon xyphophylloides*, a plant used as a folk medicine which were collected from Jianfengling County, Hainan Province, P.R. China. We have undertaken the X-ray crystal structure analysis of the title compound in order to establish its molecular structure and relative stereochemistry.

The molecular structure of (I) is shown in Fig.1. All nonhydrogen atom are coplanar, the mean deviation is 0.1237Å and the largest deviation being -0.3235 (20)Å for atom O1.In the crystal, molecules are linked by intermolecular C–H···O hydrogen bonds into two dimensional network structure (Steiner, 1996) (Fig.2). There are two intermolecular C–H···O hydrogen bonds C8–H8···O1 and C11*c*–H11*c*···O2, each adjacent C11*c*–H11*c*···O2 form a ring of twelve atoms with with an $R^2_2(12)$ graphset motif.

S2. Experimental

Air-dried stems of *Trigonostemon xyphophylloides* (5.9 kg) were ground and percolated (3 × 2.5 h) with 75% EtOH at 60°C, which was suspended in 1.5 *L* water and then partitioned with petroleum ether, chloroform, ethyl acetate and n-BuOH, successively, yielding a petroleum ether extract, a chloroform extract, an ethyl acetate extract and a n-BuOH extract, respectively. The petroleum ether extract was subjected to a silica gel CC column using petroleum ether as first eluent and then increasing the polarity with EtOAc, to afford 20 fractions (A—T). Fraction D was further separated by column chromatography with a gradient of petroleum ether-EtOAc to give the title compound. The crude product was dissolved in small amount of ethyl acetate to obtain single crystals suitable for X-ray analysis by slow evaporation of ethyl acetate solution at 298 K.

S3. Refinement

H atoms were positioned geometrically and refined as riding groups, C—H = 0.93 Å for aromatic H, 0.96 Å for methyl H,0.97 Å for methylene H and constrained to ride on their parent atoms, with *U*iso(H)= *xU*eq(C), where *x* = 1.2 for aromatic H and methylene H, and *x* = 1.5 for other H.

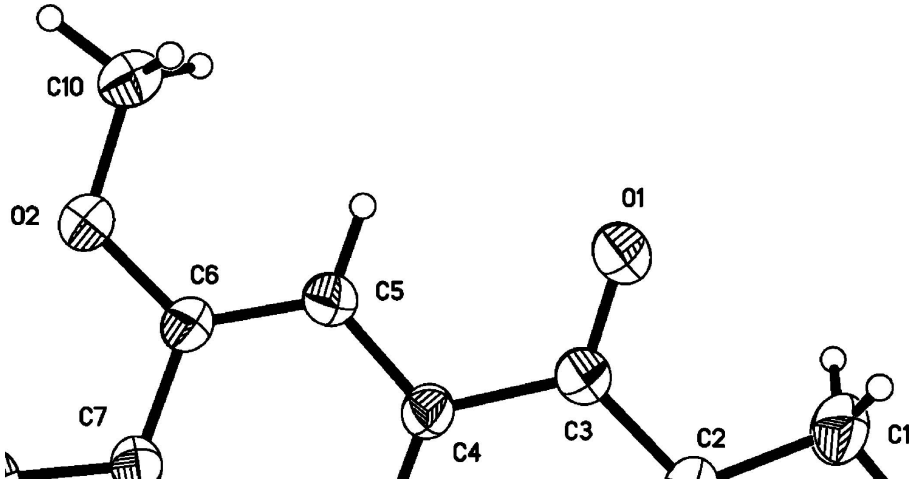

Figure 1

View of the title compound without the hydrogen atom-labeling scheme. Displacement ellipsoids are drawn at the 30% probability level.

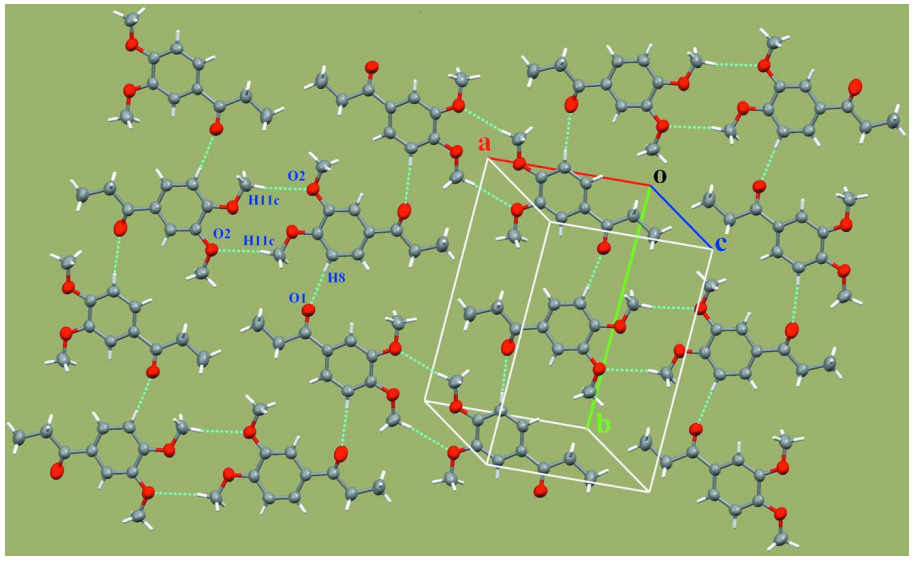

Figure 2

A view of the molecular packing.

1-(3,4-Dimethoxyphenyl)propan-1-one

Crystal data

$C_{11}H_{14}O_3$
$M_r = 194.22$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 8.9308\ (9)$ Å
$b = 13.8582\ (14)$ Å
$c = 8.5692\ (8)$ Å
$\beta = 102.427\ (1)°$
$V = 1035.72\ (18)$ Å^3
$Z = 4$

$F(000) = 416$
$D_x = 1.246$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1875 reflections
$\theta = 2.4–23.9°$
$\mu = 0.09$ mm^{-1}
$T = 298$ K
Block, colourless
0.50 × 0.43 × 0.40 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.236, T_{max} = 0.965
5082 measured reflections
1827 independent reflections
1265 reflections with $I > 2\sigma(I)$
R_{int} = 0.024
θ_{max} = 25.0°, θ_{min} = 2.3°
h = −10→9
k = −11→16
l = −9→10

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.122
S = 1.04
1827 reflections
131 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
$w = 1/[\sigma^2(F_o^2) + (0.0535P)^2 + 0.2478P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}
Extinction correction: *SHELXTL* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0080 (18)

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 $F^2 > 2$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	0.6568 (2)	0.70399 (12)	0.1437 (3)	0.1020 (7)
O2	0.21582 (15)	0.66963 (10)	0.42215 (18)	0.0649 (4)
O3	0.16048 (14)	0.48733 (10)	0.42736 (17)	0.0602 (4)
C1	0.9079 (2)	0.60873 (18)	0.0925 (3)	0.0775 (7)
H1A	0.9509	0.6544	0.1740	0.116*
H1B	0.8682	0.6422	−0.0058	0.116*
H1C	0.9859	0.5642	0.0773	0.116*
C2	0.7796 (2)	0.55404 (15)	0.1427 (3)	0.0578 (5)
H2A	0.7366	0.5081	0.0597	0.069*
H2B	0.8214	0.5179	0.2392	0.069*
C3	0.6546 (2)	0.61841 (15)	0.1727 (3)	0.0560 (5)
C4	0.52728 (19)	0.57857 (13)	0.2399 (2)	0.0463 (5)
C5	0.4315 (2)	0.64333 (13)	0.2967 (2)	0.0497 (5)
H5	0.4492	0.7093	0.2916	0.060*
C6	0.31209 (19)	0.61142 (13)	0.3597 (2)	0.0478 (5)

C7	0.28263 (19)	0.51162 (14)	0.3649 (2)	0.0478 (5)
C8	0.3772 (2)	0.44743 (13)	0.3093 (2)	0.0511 (5)
H8	0.3589	0.3815	0.3125	0.061*
C9	0.4994 (2)	0.48095 (13)	0.2487 (2)	0.0509 (5)
H9	0.5636	0.4370	0.2134	0.061*
C10	0.2320 (3)	0.77064 (14)	0.4052 (3)	0.0708 (7)
H10A	0.2190	0.7864	0.2940	0.106*
H10B	0.3322	0.7903	0.4614	0.106*
H10C	0.1557	0.8036	0.4487	0.106*
C11	0.1190 (3)	0.38787 (15)	0.4241 (3)	0.0670 (6)
H11A	0.2027	0.3511	0.4847	0.101*
H11B	0.0958	0.3654	0.3155	0.101*
H11C	0.0305	0.3801	0.4697	0.101*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0941 (13)	0.0551 (10)	0.182 (2)	0.0115 (8)	0.0862 (13)	0.0284 (11)
O2	0.0603 (8)	0.0511 (8)	0.0924 (11)	0.0016 (7)	0.0363 (8)	−0.0055 (7)
O3	0.0537 (8)	0.0536 (8)	0.0801 (10)	−0.0069 (6)	0.0291 (7)	0.0014 (7)
C1	0.0584 (13)	0.0816 (16)	0.1011 (19)	−0.0035 (12)	0.0364 (13)	−0.0103 (14)
C2	0.0530 (11)	0.0600 (12)	0.0648 (13)	0.0022 (9)	0.0220 (10)	−0.0019 (10)
C3	0.0530 (11)	0.0478 (12)	0.0714 (14)	0.0016 (9)	0.0226 (10)	0.0058 (10)
C4	0.0426 (10)	0.0462 (10)	0.0516 (11)	0.0049 (8)	0.0134 (8)	0.0046 (9)
C5	0.0467 (10)	0.0423 (10)	0.0612 (12)	0.0010 (8)	0.0144 (9)	0.0043 (9)
C6	0.0421 (10)	0.0477 (11)	0.0547 (12)	0.0044 (8)	0.0127 (8)	−0.0013 (9)
C7	0.0425 (10)	0.0509 (11)	0.0511 (11)	−0.0024 (8)	0.0126 (8)	0.0016 (9)
C8	0.0524 (11)	0.0408 (10)	0.0608 (12)	−0.0021 (9)	0.0135 (9)	0.0021 (9)
C9	0.0490 (10)	0.0446 (11)	0.0617 (12)	0.0059 (8)	0.0175 (9)	0.0000 (9)
C10	0.0690 (14)	0.0526 (13)	0.0963 (18)	0.0069 (10)	0.0303 (13)	−0.0095 (11)
C11	0.0650 (13)	0.0597 (13)	0.0828 (16)	−0.0167 (11)	0.0300 (11)	−0.0014 (12)

Geometric parameters (Å, º)

O1—C3	1.213 (2)	C4—C5	1.398 (2)
O2—C6	1.369 (2)	C5—C6	1.368 (2)
O2—C10	1.418 (2)	C5—H5	0.9300
O3—C7	1.357 (2)	C6—C7	1.410 (3)
O3—C11	1.426 (2)	C7—C8	1.381 (3)
C1—C2	1.511 (3)	C8—C9	1.385 (3)
C1—H1A	0.9600	C8—H8	0.9300
C1—H1B	0.9600	C9—H9	0.9300
C1—H1C	0.9600	C10—H10A	0.9600
C2—C3	1.494 (3)	C10—H10B	0.9600
C2—H2A	0.9700	C10—H10C	0.9600
C2—H2B	0.9700	C11—H11A	0.9600
C3—C4	1.487 (3)	C11—H11B	0.9600
C4—C9	1.381 (2)	C11—H11C	0.9600

C6—O2—C10	117.08 (15)	C5—C6—C7	119.73 (16)
C7—O3—C11	117.36 (15)	O2—C6—C7	115.37 (16)
C2—C1—H1A	109.5	O3—C7—C8	125.45 (17)
C2—C1—H1B	109.5	O3—C7—C6	115.27 (16)
H1A—C1—H1B	109.5	C8—C7—C6	119.27 (16)
C2—C1—H1C	109.5	C7—C8—C9	120.20 (17)
H1A—C1—H1C	109.5	C7—C8—H8	119.9
H1B—C1—H1C	109.5	C9—C8—H8	119.9
C3—C2—C1	112.94 (18)	C4—C9—C8	121.00 (17)
C3—C2—H2A	109.0	C4—C9—H9	119.5
C1—C2—H2A	109.0	C8—C9—H9	119.5
C3—C2—H2B	109.0	O2—C10—H10A	109.5
C1—C2—H2B	109.0	O2—C10—H10B	109.5
H2A—C2—H2B	107.8	H10A—C10—H10B	109.5
O1—C3—C4	119.34 (18)	O2—C10—H10C	109.5
O1—C3—C2	120.19 (18)	H10A—C10—H10C	109.5
C4—C3—C2	120.46 (17)	H10B—C10—H10C	109.5
C9—C4—C5	118.62 (16)	O3—C11—H11A	109.5
C9—C4—C3	123.16 (16)	O3—C11—H11B	109.5
C5—C4—C3	118.22 (16)	H11A—C11—H11B	109.5
C6—C5—C4	121.16 (17)	O3—C11—H11C	109.5
C6—C5—H5	119.4	H11A—C11—H11C	109.5
C4—C5—H5	119.4	H11B—C11—H11C	109.5
C5—C6—O2	124.90 (17)		

C1—C2—C3—O1	6.0 (3)	C11—O3—C7—C8	−5.2 (3)
C1—C2—C3—C4	−173.37 (19)	C11—O3—C7—C6	175.36 (16)
O1—C3—C4—C9	167.5 (2)	C5—C6—C7—O3	−179.08 (15)
C2—C3—C4—C9	−13.1 (3)	O2—C6—C7—O3	1.6 (2)
O1—C3—C4—C5	−12.5 (3)	C5—C6—C7—C8	1.4 (3)
C2—C3—C4—C5	166.88 (18)	O2—C6—C7—C8	−177.89 (16)
C9—C4—C5—C6	−0.1 (3)	O3—C7—C8—C9	−179.64 (17)
C3—C4—C5—C6	179.88 (18)	C6—C7—C8—C9	−0.2 (3)
C4—C5—C6—O2	177.98 (17)	C5—C4—C9—C8	1.4 (3)
C4—C5—C6—C7	−1.3 (3)	C3—C4—C9—C8	−178.62 (18)
C10—O2—C6—C5	6.7 (3)	C7—C8—C9—C4	−1.2 (3)
C10—O2—C6—C7	−174.01 (17)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C11—H11*C*···O2^{i}	0.96	2.66	3.607 (2)	171
C8—H8···O1^{ii}	0.93	2.50	3.419 (3)	171

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