Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

3-(4-Methoxyphenyl)-1-(2-nitrophenyl)-prop-2-en-1-one

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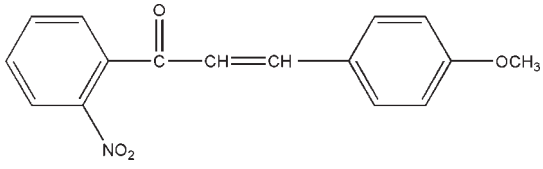
Received 8 October 2009; accepted 13 November 2009

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.041; wR factor = 0.124; data-to-parameter ratio = 16.4.

The title compound, $C_{16}H_{13}NO_4$, was prepared from 2-nitrylhypnone [systematic name: 1-(2-nitrophenyl)ethanone] and 4-methoxybenzophenone by a Claisen–Schmidt condensation. The dihedral angle formed by the two benzene rings is 80.73 (2). The crystal packing is stabilized by intermolecular C—H···O hydrogen bonds.

Related literature

For the biological activity of chalcones, see: Anto *et al.* (1994); De Vincenzo *et al.* (2000); Dimmock *et al.* (1998); Hsieh *et al.* (1998). For a related structure, see: Fun *et al.* (2008).



Experimental

Crystal data

$C_{16}H_{13}NO_4$
M_r = 283.27
Monoclinic, $P2_1/c$
a = 11.594 (2) Å
b = 7.7736 (16) Å
c = 15.174 (3) Å
β = 94.59 (3)°
V = 1363.1 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 293 K
0.21 × 0.18 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: none
12773 measured reflections
3107 independent reflections
2667 reflections with $I > 2\sigma(I)$
R_{int} = 0.018

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.124
S = 1.08
3107 reflections
190 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C16—H16A···O1^{i}	0.93	2.51	3.249 (1)	136
C14—H14A···O3^{ii}	0.93	2.59	3.259 (2)	129

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; 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*.

The authors would like to thank the National Natural Science Foundation of Shandong Province (Y2008B29) and the Yuandu Scholar Fund of Weifang City for support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FL2279).

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supporting information

Acta Cryst. (2009). E**65**, o3117 [doi:10.1107/S1600536809048120]

3-(4-Methoxyphenyl)-1-(2-nitrophenyl)prop-2-en-1-one

Huan-Mei Guo, Le-Qing Liu, Jie Yang and Fang-Fang Jian

S1. Comment

Among flavonoids, chalcones have been identified as interesting compounds having multiple biological actions which include antiinflammatory (Hsieh *et al.*,1998)and antioxidant (Anto *et al.*,1994). Of particular interest, the effectiveness of chalcones againest cancer has been investigated (De Vincenzo *et al.*, 2000; Dimmock *et al.*,1998). As part of our search for new biologically active compounds we synthesized the title compound(I) and report its crystal structure herein.

Scheme I

The molecule (I) (Fig. 1) is made up of two essentially planar segments. The atoms O1, C1,C2, C3, C4, C5, C6 and C7 make up one segment (largest deviation being 0.018Å for C6) with the nitro phenyl group being the second planar segment (largest deviation 0.0177Å for N1).The dihedral angel formed by the two planes is 81.07 (2)°. All of the bond lengths and bond angles are in normal ranges and comparable to those found in a related structure (Fun *et al.*, 2008). In the crystal structure, the molecules are stacked along the *b* axis and linked *via* C—H···O interactions (Fig. 2).

S2. Experimental

The title compound(I) was prepared by the process as following: A mixture of the 2-nitrylhypnone (0.02 mol), 4-methoxybenzophenone(0.02 mol) and 10%NaOH(10 ml) was stirred in ethanol(30 ml) for 3 h to afford the title compound(yield78%).Single crystals suitable for X-ray measurements were obtained by recrystallization from ethyl acetate at room temperature.

S3. Refinement

H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H distances of0.93–0.96 Å, and with U_{iso}(H) = 1.2U_{eq} of the parent atoms.

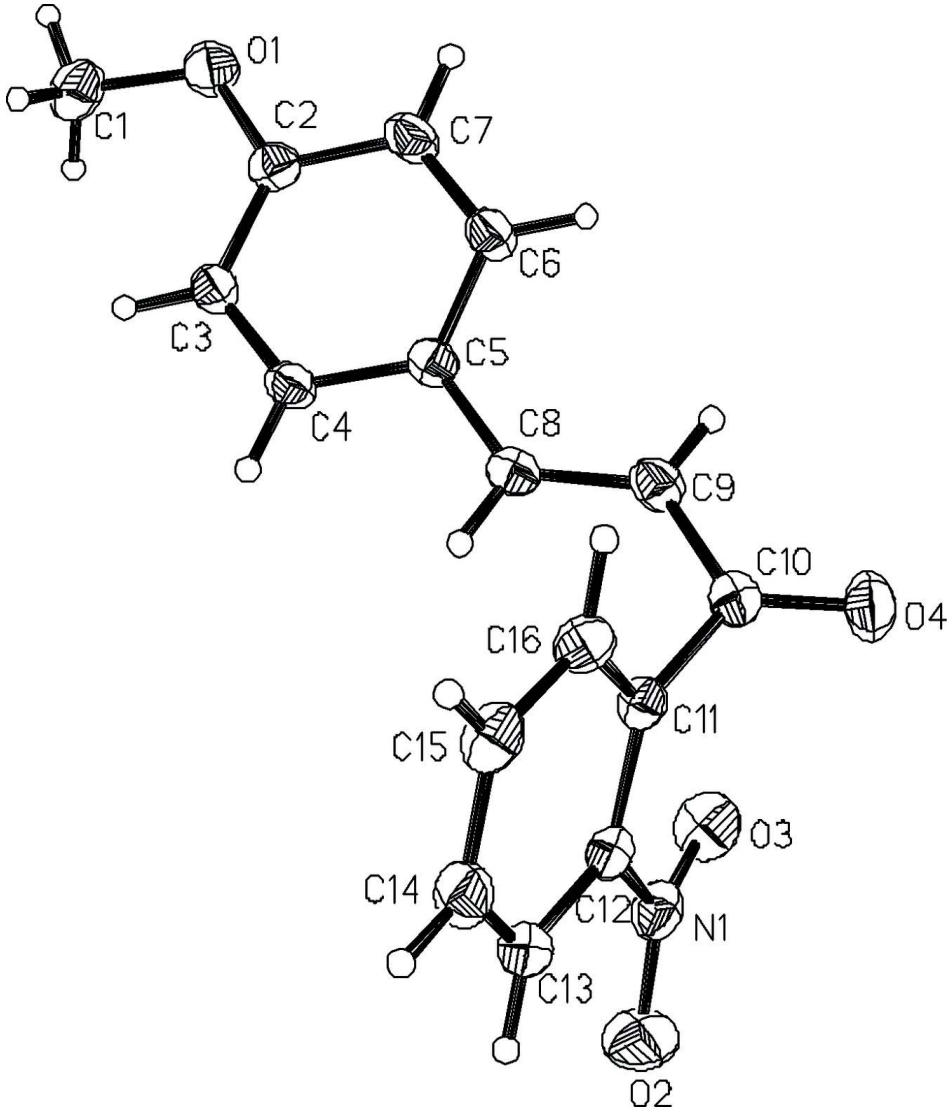

Figure 1

The molecular structure of the title compound with the atom-labeling scheme. Displacement ellipsoids are drawn at the 30% probability level.

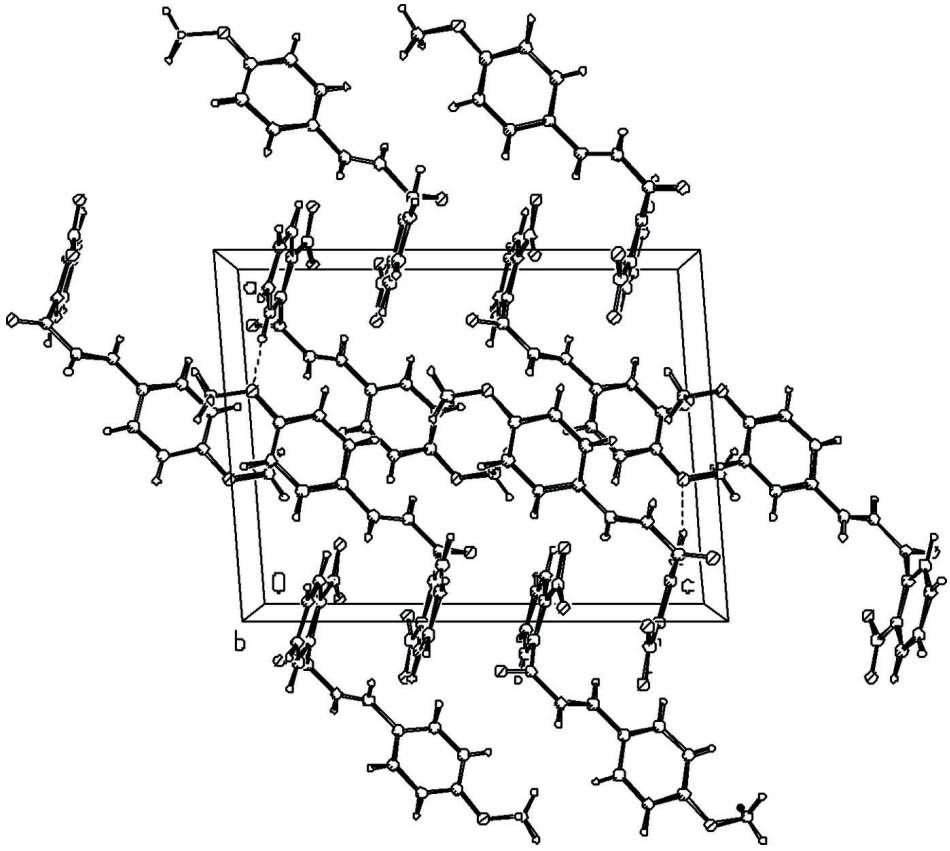

Figure 2

The crystal packing of the title compound,viewed along *a* axis.

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Crystal data

$C_{16}H_{13}NO_4$
$M_r = 283.27$
Monoclinic, $P2_1/c$
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$c = 15.174$ (3) Å
$\beta = 94.59$ (3)°
$V = 1363.1$ (5) Å^3
$Z = 4$
$F(000) = 592$
$D_x = 1.380$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2667 reflections
$\theta = 3.1$–27.5°
$\mu = 0.10$ mm^{-1}
$T = 293$ K
Bar, yellow
0.21 × 0.18 × 0.10 mm

Data collection

Bruker sMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
12773 measured reflections
3107 independent reflections
2667 reflections with $I > 2\sigma(I)$
$R_{int} = 0.018$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.1°$
$h = -15 \rightarrow 15$
$k = -10 \rightarrow 8$
$l = -19 \rightarrow 19$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.124$
$S = 1.08$
3107 reflections
190 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
$w = 1/[\sigma^2(F_o^2) + (0.0747P)^2 + 0.157P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.19$ e Å^{-3}
$\Delta\rho_{min} = -0.22$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C8	0.72395 (9)	0.18277 (14)	0.22201 (7)	0.0385 (2)
H8A	0.7810	0.2655	0.2340	0.046*
O4	0.82958 (9)	0.02414 (13)	0.02294 (6)	0.0603 (3)
C5	0.63411 (9)	0.17369 (13)	0.28408 (7)	0.0371 (2)
N1	1.07316 (9)	0.10395 (13)	0.16402 (6)	0.0447 (2)
C2	0.46388 (9)	0.17332 (14)	0.40548 (8)	0.0402 (3)
C7	0.44279 (10)	0.09466 (16)	0.32265 (8)	0.0482 (3)
H7A	0.3714	0.0436	0.3073	0.058*
O3	1.01265 (9)	−0.02297 (12)	0.16921 (7)	0.0611 (3)
C16	0.85299 (10)	0.42736 (15)	0.08146 (8)	0.0442 (3)
H16A	0.7755	0.4334	0.0604	0.053*
C11	0.90152 (9)	0.26829 (14)	0.10358 (7)	0.0359 (2)
C12	1.01784 (9)	0.26616 (13)	0.13472 (7)	0.0362 (2)
C6	0.52710 (10)	0.09263 (15)	0.26394 (8)	0.0445 (3)
H6A	0.5130	0.0366	0.2100	0.053*
C13	1.08378 (10)	0.41407 (16)	0.14300 (8)	0.0454 (3)
H13A	1.1615	0.4087	0.1636	0.054*
C9	0.73401 (10)	0.08635 (15)	0.15007 (8)	0.0435 (3)
H9A	0.6811	−0.0023	0.1384	0.052*
C14	1.03253 (12)	0.57038 (15)	0.12026 (9)	0.0514 (3)
H14A	1.0760	0.6710	0.1254	0.062*
C4	0.65192 (9)	0.25538 (14)	0.36590 (8)	0.0414 (3)
H4A	0.7213	0.3129	0.3799	0.050*
O2	1.17769 (9)	0.10328 (15)	0.18354 (8)	0.0719 (3)
C10	0.82364 (10)	0.11242 (15)	0.08857 (7)	0.0409 (3)

C15	0.91755 (12)	0.57743 (15)	0.09011 (9)	0.0493 (3)
H15A	0.8831	0.6828	0.0755	0.059*
C3	0.56915 (10)	0.25320 (14)	0.42687 (8)	0.0410 (3)
H3A	0.5842	0.3051	0.4818	0.049*
O1	0.37527 (8)	0.16582 (14)	0.45895 (6)	0.0582 (3)
C1	0.39013 (13)	0.24330 (19)	0.54405 (9)	0.0596 (4)
H1A	0.3210	0.2283	0.5740	0.089*
H1B	0.4054	0.3639	0.5378	0.089*
H1C	0.4540	0.1900	0.5778	0.089*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C8	0.0357 (5)	0.0373 (5)	0.0419 (5)	−0.0036 (4)	−0.0006 (4)	0.0031 (4)
O4	0.0715 (6)	0.0603 (6)	0.0498 (5)	−0.0125 (5)	0.0103 (4)	−0.0185 (4)
C5	0.0369 (5)	0.0338 (5)	0.0400 (5)	−0.0028 (4)	0.0002 (4)	0.0032 (4)
N1	0.0496 (5)	0.0450 (5)	0.0397 (5)	0.0120 (4)	0.0042 (4)	−0.0005 (4)
C2	0.0387 (5)	0.0357 (5)	0.0467 (6)	−0.0029 (4)	0.0060 (4)	0.0029 (4)
C7	0.0404 (6)	0.0522 (7)	0.0516 (7)	−0.0158 (5)	0.0010 (5)	−0.0042 (5)
O3	0.0728 (6)	0.0398 (5)	0.0711 (6)	0.0075 (4)	0.0090 (5)	0.0099 (4)
C16	0.0426 (6)	0.0422 (6)	0.0481 (6)	0.0065 (4)	0.0056 (5)	0.0045 (5)
C11	0.0386 (5)	0.0361 (5)	0.0338 (5)	0.0004 (4)	0.0068 (4)	−0.0003 (4)
C12	0.0396 (5)	0.0365 (5)	0.0330 (5)	0.0047 (4)	0.0061 (4)	−0.0024 (4)
C6	0.0438 (6)	0.0472 (6)	0.0419 (6)	−0.0112 (5)	−0.0004 (5)	−0.0041 (5)
C13	0.0394 (5)	0.0485 (7)	0.0487 (6)	−0.0032 (5)	0.0060 (5)	−0.0088 (5)
C9	0.0432 (6)	0.0406 (6)	0.0466 (6)	−0.0093 (4)	0.0018 (5)	−0.0011 (5)
C14	0.0590 (7)	0.0378 (6)	0.0590 (7)	−0.0104 (5)	0.0145 (6)	−0.0077 (5)
C4	0.0349 (5)	0.0418 (6)	0.0467 (6)	−0.0067 (4)	−0.0012 (4)	−0.0029 (5)
O2	0.0501 (6)	0.0756 (7)	0.0877 (8)	0.0208 (5)	−0.0089 (5)	0.0045 (6)
C10	0.0440 (6)	0.0387 (6)	0.0396 (5)	−0.0008 (4)	0.0007 (4)	−0.0014 (4)
C15	0.0618 (7)	0.0337 (6)	0.0537 (7)	0.0077 (5)	0.0134 (6)	0.0041 (5)
C3	0.0406 (6)	0.0400 (6)	0.0417 (5)	−0.0026 (4)	−0.0006 (4)	−0.0044 (4)
O1	0.0492 (5)	0.0682 (6)	0.0593 (5)	−0.0160 (4)	0.0177 (4)	−0.0100 (5)
C1	0.0642 (8)	0.0620 (8)	0.0548 (7)	0.0018 (6)	0.0188 (6)	−0.0020 (6)

Geometric parameters (Å, º)

C8—C9	1.3369 (17)	C11—C10	1.5174 (15)
C8—C5	1.4609 (16)	C12—C13	1.3809 (16)
C8—H8A	0.9300	C6—H6A	0.9300
O4—C10	1.2159 (15)	C13—C14	1.3841 (18)
C5—C4	1.3951 (16)	C13—H13A	0.9300
C5—C6	1.4031 (15)	C9—C10	1.4653 (17)
N1—O3	1.2168 (14)	C9—H9A	0.9300
N1—O2	1.2242 (15)	C14—C15	1.3753 (19)
N1—C12	1.4674 (14)	C14—H14A	0.9300
C2—O1	1.3604 (14)	C4—C3	1.3854 (17)
C2—C3	1.3846 (16)	C4—H4A	0.9300

C2—C7	1.4015 (17)	C15—H15A	0.9300
C7—C6	1.3743 (18)	C3—H3A	0.9300
C7—H7A	0.9300	O1—C1	1.4227 (17)
C16—C15	1.3866 (18)	C1—H1A	0.9600
C16—C11	1.3885 (15)	C1—H1B	0.9600
C16—H16A	0.9300	C1—H1C	0.9600
C11—C12	1.3929 (15)		

C9—C8—C5	127.78 (10)	C12—C13—H13A	120.5
C9—C8—H8A	116.1	C14—C13—H13A	120.5
C5—C8—H8A	116.1	C8—C9—C10	123.72 (10)
C4—C5—C6	117.62 (10)	C8—C9—H9A	118.1
C4—C5—C8	119.30 (9)	C10—C9—H9A	118.1
C6—C5—C8	123.02 (10)	C15—C14—C13	120.22 (11)
O3—N1—O2	123.06 (11)	C15—C14—H14A	119.9
O3—N1—C12	118.43 (10)	C13—C14—H14A	119.9
O2—N1—C12	118.50 (11)	C3—C4—C5	121.84 (10)
O1—C2—C3	124.96 (11)	C3—C4—H4A	119.1
O1—C2—C7	115.49 (10)	C5—C4—H4A	119.1
C3—C2—C7	119.55 (11)	O4—C10—C9	122.22 (11)
C6—C7—C2	120.28 (10)	O4—C10—C11	120.10 (11)
C6—C7—H7A	119.9	C9—C10—C11	117.30 (9)
C2—C7—H7A	119.9	C14—C15—C16	119.96 (11)
C15—C16—C11	121.41 (11)	C14—C15—H15A	120.0
C15—C16—H16A	119.3	C16—C15—H15A	120.0
C11—C16—H16A	119.3	C2—C3—C4	119.58 (10)
C16—C11—C12	117.07 (10)	C2—C3—H3A	120.2
C16—C11—C10	116.75 (10)	C4—C3—H3A	120.2
C12—C11—C10	126.14 (9)	C2—O1—C1	118.75 (10)
C13—C12—C11	122.33 (10)	O1—C1—H1A	109.5
C13—C12—N1	117.55 (10)	O1—C1—H1B	109.5
C11—C12—N1	120.05 (10)	H1A—C1—H1B	109.5
C7—C6—C5	121.06 (11)	O1—C1—H1C	109.5
C7—C6—H6A	119.5	H1A—C1—H1C	109.5
C5—C6—H6A	119.5	H1B—C1—H1C	109.5
C12—C13—C14	119.00 (11)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
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