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(2*E*)-3-(6-Methoxy-2-naphthyl)-1-phenylprop-2-en-1-one

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Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.003 Å
R factor = 0.040
wR factor = 0.097
Data-to-parameter ratio = 7.6

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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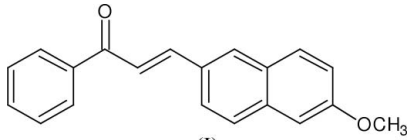
The geometric parameters of the title compound, $C_{20}H_{16}O_2$, are in the usual ranges. The central double bond is *trans* configured. Its two C atoms are slightly twisted out of the naphthyl plane. The dihedral angle between the aromatic groups is 14.09 (8)°.

Comment

Reviews on the bioactivities of varieties of chalcones are given by Dimmock *et al.* (1999) and Go *et al.* (2005). Recently, it has been noted that, among many organic compounds reported for their second harmonic generation, chalcone derivatives are known for their excellent blue light transmittance and good crystallizability (Fichou *et al.*, 1988; Goto *et al.*, 1991; Uchida *et al.*, 1998; Zhao *et al.*, 2000; Sarojini *et al.*, 2006). The crystal structures of 3-(4-chlorophenyl)-1-(2-naphthyl)prop-2-enone (Shanmuga Sundara Raj *et al.*, 1997), 1-(2-naphthalenyl)-3-(3-nitrophenyl)-2-propen-1-one (Shanmuga Sundara Raj *et al.*, 1998), 3-(6-methoxy-2-naphthyl)-1-(2-naphthyl)prop-2-en-1-one (Yathirajan, Sarojini, Bindya *et al.*, 2006) and 3-(6-methoxy-2-naphthyl)-1-(2-thienyl)prop-2-en-1-one (Yathirajan, Narayana *et al.*, 2006) have been reported. The crystal structures of 1-(2,4-dichloro-5-fluorophenyl)-3-(3,4-dimethoxyphenyl)prop-2-en-1-one (Yathirajan, Sarojini, Narayana *et al.*, 2006) and (2*E*)-1-(2,4-dichlorophenyl)-3-[4-(methylsulfanyl)phenyl]prop-2-en-1-one (Butcher *et al.*, 2007) have also been reported. In continuation of our broad programme on chalcones, the present paper reports the crystal structure of a newly synthesized chalcone.



(I)

A perspective view of the title compound, (I), is shown in Fig. 1. Bond lengths and angles can be regarded as normal [Cambridge Crystallographic Database, Version 5.28, November 2006 (Allen, 2002); *Mogul* Version 1.1 (Bruno *et al.*, 2004)]. The carbonyl group is twisted by 21.0 (3)° out of the plane of the phenyl ring. The torsion angle between the carbonyl group and the C atoms of the double bond is −15.9 (4)°. The torsion angle between the the C atoms of the double bond and the adjacent naphthyl residue (C2—C3—C21—C30) is −10.4 (3)°. The two aromatic residues are not coplanar [dihedral angle 14.9 (8)°].

There are non-conventional hydrogen bonds of the type C—H···O in the structure that link the molecules into chains

lying along the *b* axis. In addition to these intermolecular interactions, intramolecular interactions C3—H3···O1 are also present (Table 1).

Experimental

5 ml of 40% KOH solution was added to a thoroughly stirred solution of acetophenone (1.2 g, 0.01 mol) and 6-methoxy-2-napthaldehyde (1.86 g, 0.01 mol) in 25 ml of methanol. The mixture was stirred overnight and filtered. The solid obtained was recrystallized from acetone–toluene (1:1) mixture (m.p. 421–423 K). Analysis for $C_{20}H_{16}O_2$ found (calculated): C 83.18 (83.31), H 5.50 (5.59)%.

Crystal data

$C_{20}H_{16}O_2$
M_r = 288.33
Orthorhombic, $Pca2_1$
a = 14.5275 (17) Å
b = 17.0930 (15) Å
c = 5.9950 (5) Å
V = 1488.7 (3) Å^3
Z = 4
D_x = 1.286 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 173 (2) K
Thick plate, light yellow
0.27 × 0.24 × 0.13 mm

Data collection

Stoe IPDS II two-circle diffractometer
ω scans
Absorption correction: none
7578 measured reflections
1535 independent reflections
1367 reflections with $I > 2\sigma(I)$
R_{int} = 0.089
θ_{max} = 25.6°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.097
S = 1.03
1535 reflections
201 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0648P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.029 (5)

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

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···O1	0.95	2.44	2.798 (3)	102
C14—H14···O2^{i}	0.95	2.53	3.462 (3)	168

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

In the absence of significant anomalous scatterers Friedel pairs were merged. H atoms were found in a difference map, but they were refined using a riding model with C—H = 0.95 Å and U_{iso}(H) = 1.2U_{eq}(C) or with C—H = 0.98 Å and U_{iso}(H) = 1.5U_{eq}(C_{methyl}). The methyl group was allowed to rotate but not to tip.

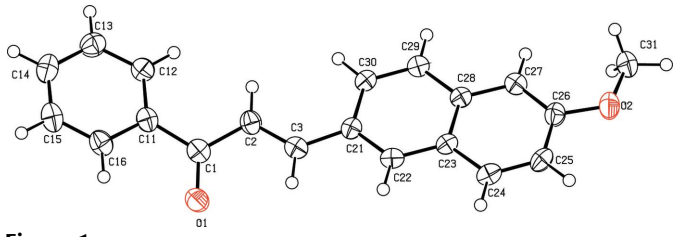


Figure 1
The molecular structure of the title compound with the atom numbering; displacement ellipsoids are at the 50% probability level.

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *PLATON*.

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