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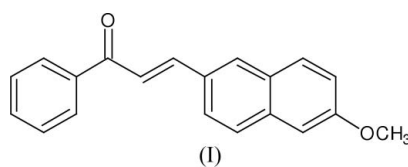
Key indicators

Single-crystal X-ray study
 $T = 173$ K
Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å
 R factor = 0.040
 wR factor = 0.097
Data-to-parameter ratio = 7.6For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

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

The geometric parameters of the title compound, $\text{C}_{20}\text{H}_{16}\text{O}_2$, 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 (2E)-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.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 $\text{C}-\text{H}\cdots\text{O}$ in the structure that link the molecules into chainsReceived 22 January 2007
Accepted 26 January 2007

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-naphthaldehyde (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 C₂₀H₁₆O₂ found (calculated): C 83.18 (83.31), H 5.50 (5.59)%.

Crystal data

C ₂₀ H ₁₆ O ₂	Z = 4
<i>M_r</i> = 288.33	<i>D_x</i> = 1.286 Mg m ⁻³
Orthorhombic, <i>Pca</i> 2 ₁	Mo <i>K</i> α radiation
<i>a</i> = 14.5275 (17) Å	<i>μ</i> = 0.08 mm ⁻¹
<i>b</i> = 17.0930 (15) Å	<i>T</i> = 173 (2) K
<i>c</i> = 5.9950 (5) Å	Thick plate, light yellow
<i>V</i> = 1488.7 (3) Å ³	0.27 × 0.24 × 0.13 mm

Data collection

Stoe IPDS II two-circle diffractometer	1535 independent reflections
<i>ω</i> scans	1367 reflections with <i>I</i> > 2σ(<i>I</i>)
Absorption correction: none	<i>R</i> _{int} = 0.089
7578 measured reflections	<i>θ</i> _{max} = 25.6°

Refinement

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

Table 1

Hydrogen-bond geometry (Å, °).

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
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) = 1.2*U*_{eq}(C) or with C—H = 0.98 Å and *U*_{iso}(H) = 1.5*U*_{eq}(C_{methyl}). The methyl group was allowed to rotate but not to tip.

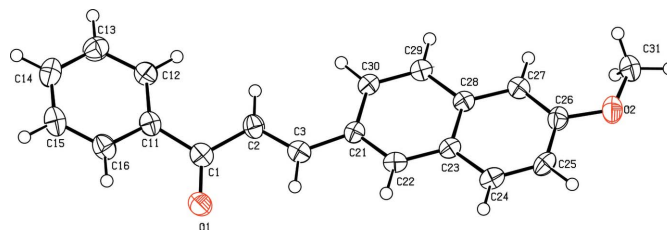


Figure 1

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*.

ANM thanks the University of Mysore for research facilities.

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