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Key indicators

Single-crystal X-ray study T = 173 KMean $\sigma(C-C) = 0.003 \text{ Å}$ 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.

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

The geometric parameters of the title compound, C₂₀H₁₆O₂, 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 $14.09 (8)^{\circ}$.

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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-(3nitrophenyl)-2-propen-1-one (Shanmuga Sundara Raj et al., 1998), 3-(6-methoxy-2-naphthyl)-1-(2-naphthyl)prop-2-en-1one (Yathirajan, Sarojini, Bindya et al., 2006) and 3-(6-methoxy-2-naphthyl)-1-(2-thienyl)prop-2-en-1-one 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) phenyllprop-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 $21.0 (3)^{\circ}$ 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 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

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lying along the b axis. In addition to these intermolecular interactions, intramolecular interactions C3-H3 \cdots 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

$C_{20}H_{16}O_2$	Z = 4
$M_r = 288.33$	$D_x = 1.286 \text{ Mg m}^{-3}$
Orthorhombic, Pca2 ₁	Mo $K\alpha$ radiation
a = 14.5275 (17) Å	$\mu = 0.08 \text{ mm}^{-1}$
b = 17.0930 (15) Å	T = 173 (2) K
c = 5.9950 (5) Å	Thick plate, light yellow
$V = 1488.7 (3) \text{ Å}^3$	$0.27 \times 0.24 \times 0.13 \text{ mm}$

Data collection

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

Refinement

•	
Refinement on F^2	$w = 1/[\sigma^2(F_0^2) + (0.0648P)^2]$
$R[F^2 > 2\sigma(F^2)] = 0.040$	where $P = (F_0^2 + 2F_c^2)/3$
$wR(F^2) = 0.097$	$(\Delta/\sigma)_{\rm max} < 0.001$
S = 1.03	$\Delta \rho_{\text{max}} = 0.21 \text{ e Å}^{-3}$
1535 reflections	$\Delta \rho_{\min} = -0.21 \text{ e Å}^{-3}$
201 parameters	Extinction correction: SHELXL97
H-atom parameters constrained	Extinction coefficient: 0.029 (5)

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

$D-H\cdots A$	D-H	$H \cdot \cdot \cdot A$	$D \cdot \cdot \cdot A$	D $ H$ $\cdot \cdot \cdot A$
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 $U_{\rm iso}({\rm H})$ = $1.2 U_{\rm eq}({\rm C})$ or with C–H = 0.98 Å and $U_{\rm iso}({\rm H})$ = $1.5 U_{\rm eq}({\rm C}_{\rm methyl})$. The methyl group was allowed to rotate but not to tip.

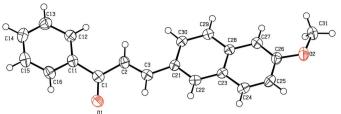


Figure 1

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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