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3-(6-Methoxy-2-naphthyl)-1-(2-naphthyl)prop-2-en-1-one

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Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.002 Å
R factor = 0.036
wR factor = 0.102
Data-to-parameter ratio = 12.4

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

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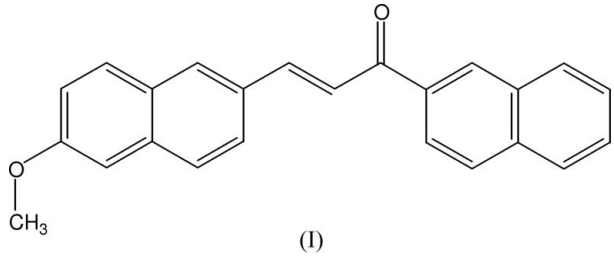
The title compound, $C_{24}H_{18}O_2$, is a chalcone derivative The torsion angle between the mean planes of the two naphthalene groups is 54.41 (2)°.

Comment

Substituted chalcones have many applications in medicine and physics. (see *e.g.* Xu *et al.*, 2005). The crystal structures of 1-(2-naphthyl)-3-(4-nitrophenyl)prop-2-en-1-one (Raj *et al.*, 1996) and 3-(4-methylphenyl)-1-(2-naphthyl)prop-2-en-1-one (Moorthi *et al.*, 2005) have been reported. In continuation of our work on chalcones (Yathirajan *et al.*, 2006*a*,*b*) the present work reports the crystal structure of the title compound, (I). (Fig. 1).



(I)

The bond lengths and angles in (I) can be regarded as normal (Cambridge Crystallographic Database, Version 5.27, November 2005 updated August 2006; *MOGUL* Version 1.1; Allen, 2002). The atoms of the C12/C13 double bond and the C14/O2 carbonyl group are almost coplanar with the C1–C10 naphthalene ring system (r.m.s. deviation from the mean plane = 0.173 Å), but the C21–C30 naphthalene ring system is twisted substantially with respect to C12–C14/O2: the dihedral angle between the two naphthalene system ring planes is 54.41 (2)°. There are no π–π stacking interactions in (I).

Experimental

Compound (I) was synthesized according to the method reported in the literature (Vogel, 1989) in a yield of 85%. The compound was

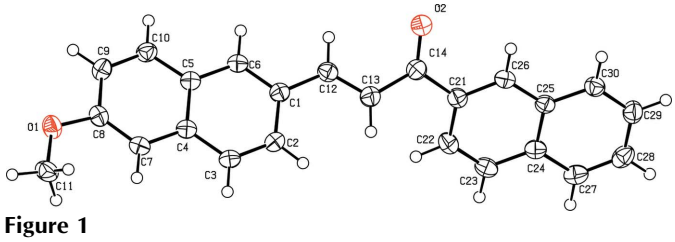


Figure 1
View of (I) showing 50% displacement ellipsoids (arbitrary spheres for the H atoms).

purified by recrystallization from ethanol and crystals of (I) were grown by slow evaporation of an acetone–toluene (50:50 *v*/*v*) solution (m.p. 448–450 K). Analysis found (calc.) (%) for $C_{24}H_{18}O_2$: C: 85.20 (85.18); H: 5.30 (5.36).

Crystal data

$C_{24}H_{18}O_2$	$Z = 4$
$M_r = 338.38$	$D_x = 1.339$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
$a = 7.5270$ (8) Å	$\mu = 0.08$ mm^{-1}
$b = 5.9364$ (4) Å	$T = 173$ (2) K
$c = 37.576$ (4) Å	Plate, light yellow
$\beta = 92.046$ (8)°	0.42 × 0.37 × 0.13 mm
$V = 1677.9$ (3) Å^3	

Data collection

STOE IPDS II two-circle diffractometer	2940 independent reflections
	2455 reflections with $I > 2\sigma(I)$
ω scans	$R_{int} = 0.035$
Absorption correction: none	$\theta_{max} = 25.0°$
9309 measured reflections	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0683P)^2 + 0.0701P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.036$	
$wR(F^2) = 0.102$	$(\Delta/\sigma)_{max} = 0.001$
$S = 1.05$	$\Delta\rho_{max} = 0.21$ e Å^{-3}
2940 reflections	$\Delta\rho_{min} = -0.15$ e Å^{-3}
237 parameters	Extinction correction: *SHELXL97*
H-atom parameters constrained	Extinction coefficient: 0.028 (3)

H atoms were found in a difference map, but were positioned geometrically and allowed to ride on their parent C atoms at distances of 0.95 and 0.98 Å for sp^2 and methyl groups, respectively, and with $U_{iso}(H) = 1.2U_{eq}(C)$ or $U_{iso}(H) = 1.5U_{eq}(C_{methyl})$. The methyl groups were allowed to rotate but not to tip.

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*.

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