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Key indicators

Single-crystal X-ray study $T=173~\mathrm{K}$ Mean $\sigma(\mathrm{C-C})=0.002~\mathrm{\mathring{A}}$ 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.

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

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)°.

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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).

$$CH_3$$
 (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

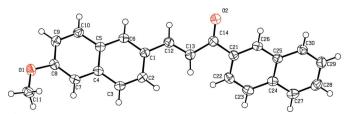


Figure 1View of (I) showing 50% displacement ellipsoids (arbitrary spheres for the H atoms).

© 2006 International Union of Crystallography All rights reserved purified by recrystallization from ethanol and crystals of (I) were grown by slow evaporation of an acetone–toluene (50:50 ν/ν) 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
$M_r = 338.38$	$D_x = 1.339 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
a = 7.5270 (8) Å	$\mu = 0.08 \text{ mm}^{-1}$
b = 5.9364 (4) Å	T = 173 (2) K
c = 37.576 (4) Å	Plate, light yellow
$\beta = 92.046 \ (8)^{\circ}$	$0.42 \times 0.37 \times 0.13 \text{ mm}$
$V = 1677.9 (3) \text{ Å}^3$	

Data collection

9309 measured reflections

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

Refinement

D C + D2	1/F 2/F 2) (0.0602 P)2
Refinement on F^2	$w = 1/[\sigma^2(F_0^2) + (0.0683P)^2]$
$R[F^2 > 2\sigma(F^2)] = 0.036$	+ 0.0701P
$wR(F^2) = 0.102$	where $P = (F_0^2 + 2F_c^2)/3$
S = 1.05	$(\Delta/\sigma)_{\rm max} = 0.001$
2940 reflections	$\Delta \rho_{\text{max}} = 0.21 \text{ e Å}^{-3}$
237 parameters	$\Delta \rho_{\min} = -0.15 \text{ e Å}^{-3}$
H-atom parameters constrained	Extinction correction: SHELXL97
	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 $U_{\rm iso}({\rm H})=1.2U_{\rm eq}({\rm C})$ or $U_{\rm iso}({\rm H})=1.5U_{\rm eq}({\rm C}_{\rm methyl})$. 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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