

## 3-(4-Methylphenyl)-1-(2-naphthyl)prop-2-en-1-one

S. Sathiya Moorthi,<sup>a</sup>  
K. Chinnakali,<sup>b\*</sup> S. Nanjundan,<sup>c</sup>  
R. Balaji<sup>d</sup> and Hoong-Kun Fun<sup>e\*</sup><sup>a</sup>Department of Physics, Sri Muthukumaran Institute of Technology, Chikkarayapuram, Chennai 600 069, India, <sup>b</sup>Department of Physics, Anna University, Chennai 600 025, India, <sup>c</sup>Department of Chemistry, Anna University, Chennai 600 025, India, <sup>d</sup>German Wool Research Institute (DWI), Chair of Textile and Macromolecular Chemistry, University of Technology (RWTH - Aachen), Pauwelsstrasse 8.52074 Aachen, Germany, and <sup>e</sup>X-ray Crystallography Unit, School of Physics, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia

Correspondence e-mail: kali@annauniv.edu, hkfun@usm.my

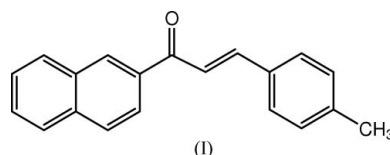
## Key indicators

Single-crystal X-ray study  
 $T = 273$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å  
Disorder in main residue  
 $R$  factor = 0.062  
 $wR$  factor = 0.212  
Data-to-parameter ratio = 33.0For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

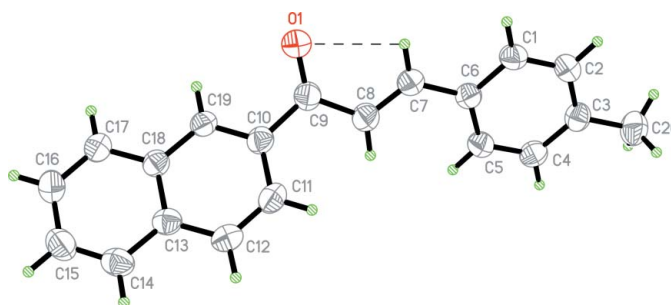
The title molecule,  $\text{C}_{20}\text{H}_{16}\text{O}$ , has an *s-cis* conformation for the ketone system. The dihedral angle between the two aromatic ring systems is  $50.3(1)^\circ$ . Centrosymmetrically related molecules are linked *via* weak  $\text{C}-\text{H} \cdots \pi$  interactions into a chain along  $[110]$ .

## Comment

Chalcone is a unique template that is associated with several biological activities. Chalcone and its analogues are relatively easily available, not only by isolation from natural products but also by classical and combinatorial synthesis. The cytotoxic, anticancer, antiviral, antiprotozoal, insecticidal, chemopreventative, mutagenic and enzyme-inhibitory properties of a number of chalcones have been reviewed by Dimmock *et al.* (1999) and Go *et al.* (2005). The antifungal and antibacterial activities of these compounds have also been reviewed (Opletalova & Sedivy, 1999; Opletalova, 2000). Chalcones and their analogues are also used as potential therapeutic agents in diseases of the cardiovascular system. The stabilizing action of chalcones on the vascular wall, vasodilating and antioxidative activity have been reported (Opletalova *et al.*, 2003). The crystal structure determination of the title compound, (I), was undertaken as part of our study of chalcones.



The molecule of (I) (Fig. 1) exhibits an *s-cis* conformation for the ketone system, defined by the torsion angle  $\text{O1}-\text{C9}-\text{C8}-\text{C7}$  of  $14.9(2)^\circ$ . A similar result was observed for 1-(2-

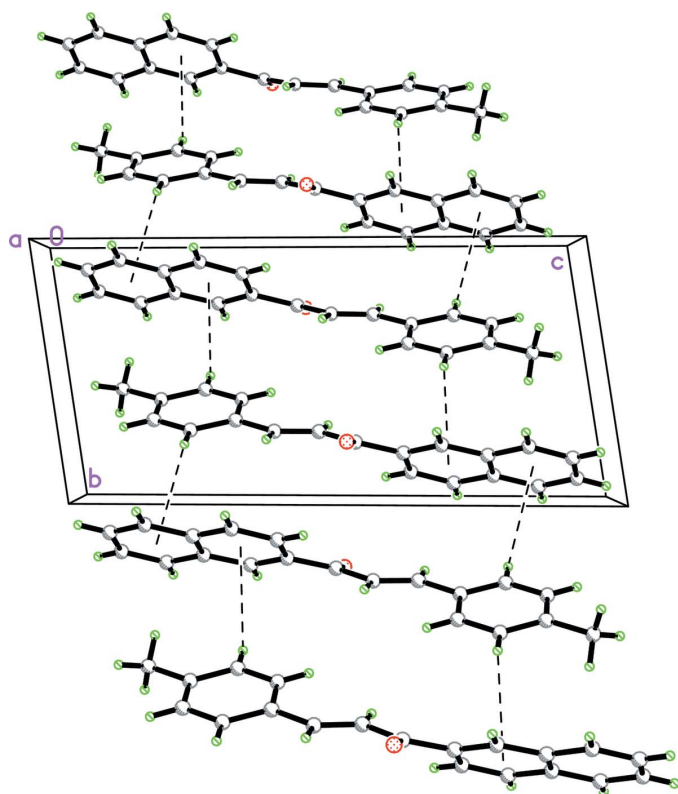
**Figure 1**

The structure of (I), showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. The dashed line indicates a hydrogen bond.

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**Figure 2**  
Part of a hydrogen-bonded (dashed lines) chain in (I).

naphthyl)-3-(4-nitrophenyl)prop-2-en-1-one [(II);  $-19.4(6)^\circ$ ; Shanmuga Sundara Raj *et al.*, 1996], 3-(2-chlorophenyl)-1-(2-naphthyl)prop-2-en-1-one [(III);  $-21.4(3)^\circ$ ; Kumaran *et al.*, 1996], 3-(4-chlorophenyl)-1-(2-naphthyl)prop-2-enone [(IV);  $-20.8(4)^\circ$ ; Shanmuga Sundara Raj *et al.*, 1997] and 1-(2-naphthalenyl)-3-(3-nitrophenyl)prop-2-en-1-one [(V);  $-14.9(3)^\circ$ ; Shanmuga Sundara Raj *et al.*, 1998]. The enone group of the molecule, containing atoms C7, C8, C9 and O1, is planar to within  $0.060(1) \text{ \AA}$ . The naphthalene ring system is planar, with atom C19 showing the largest out-of-plane displacement of  $0.018(1) \text{ \AA}$ . The mean plane through the enone group makes dihedral angles of  $22.8(1)$  and  $28.2(1)^\circ$ , respectively, with the benzene ring and naphthalene ring system. The dihedral angle between the two aromatic ring systems (C1–C6 and C10–C19) in (I) is  $50.3(1)^\circ$ , whereas those in (II), (III), (IV) and (V) are  $44.2(1)$ ,  $27.68(5)$ ,  $49.80(8)$  and  $2.2(1)^\circ$ , respectively.

Bond lengths and angles in (I) are comparable with those reported for (II), (III), (IV) and (V). The short  $\text{H5} \cdots \text{H8}$  ( $2.30 \text{ \AA}$ ) contact causes the bond angles  $\text{C5}–\text{C6}–\text{C7}$  [ $123.42(11)^\circ$ ] and  $\text{C6}–\text{C7}–\text{C8}$  [ $127.41(12)^\circ$ ] to deviate significantly from  $120^\circ$ . Also, the short  $\text{H8} \cdots \text{H11}$  ( $2.32 \text{ \AA}$ ) contact results in a slight widening of the  $\text{C9}–\text{C10}–\text{C11}$  angle to  $122.14(11)^\circ$ .

As seen in Fig. 2, centrosymmetrically related molecules are linked *via* weak  $\text{C}–\text{H} \cdots \pi$  interactions, involving the C13–C18 (centroid Cg1) and C10–C13/C18/C19 (centroid Cg2) benzene rings of the naphthalene ring system (Table 1), into a chain along [110].

## Experimental

Compound (I) was obtained by Claisen–Schmidt condensation of 2-acetonaphthone (1.70 g, 0.01 mol) and 4-methylbenzaldehyde (1.20 g, 0.01 mol) in ethanol (25 ml) in the presence of NaOH. The product was isolated by filtration and washed with dilute hydrochloric acid and then with water. The crude product was recrystallized from ethanol.

### Crystal data

$\text{C}_{20}\text{H}_{16}\text{O}$	$Z = 2$
$M_r = 272.33$	$D_x = 1.261 \text{ Mg m}^{-3}$
Triclinic, $P\bar{1}$	Mo $K\alpha$ radiation
$a = 5.9174(1) \text{ \AA}$	Cell parameters from 2939 reflections
$b = 7.7180(1) \text{ \AA}$	$\theta = 2.6–33.4^\circ$
$c = 15.9606(4) \text{ \AA}$	$\mu = 0.08 \text{ mm}^{-1}$
$\alpha = 81.239(2)^\circ$	$T = 273(2) \text{ K}$
$\beta = 84.617(2)^\circ$	Needle, colourless
$\gamma = 88.716(1)^\circ$	$0.67 \times 0.13 \times 0.07 \text{ mm}$
$V = 717.22(2) \text{ \AA}^3$	

### Data collection

Bruker SMART APEX2 CCD area-detector diffractometer	6301 independent reflections
$\omega$ scans	3154 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Bruker, 2005)	$R_{\text{int}} = 0.038$
$T_{\text{min}} = 0.948$ , $T_{\text{max}} = 0.995$	$\theta_{\text{max}} = 35.1^\circ$
21324 measured reflections	$h = -9 \rightarrow 9$
	$k = -12 \rightarrow 12$
	$l = -25 \rightarrow 25$

### Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.1034P)^2 + 0.0041P]$
$R[F^2 > 2\sigma(F^2)] = 0.062$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.212$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$S = 1.02$	$\Delta\rho_{\text{max}} = 0.24 \text{ e \AA}^{-3}$
6301 reflections	$\Delta\rho_{\text{min}} = -0.23 \text{ e \AA}^{-3}$
191 parameters	
H-atom parameters constrained	

**Table 1**

Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ).

$D–\text{H} \cdots A$	$D–\text{H}$	$\text{H} \cdots A$	$D \cdots A$	$D–\text{H} \cdots A$
$\text{C7}–\text{H7} \cdots \text{O1}$	0.93	2.49	2.8126 (16)	101
$\text{C1}–\text{H1} \cdots \text{Cg1}^i$	0.93	2.97	3.6189 (14)	128
$\text{C4}–\text{H4} \cdots \text{Cg2}^{ii}$	0.93	2.94	3.6189 (14)	131

Symmetry codes: (i)  $-x, -y, -z + 1$ ; (ii)  $-x + 1, -y + 1, -z + 1$ . Notes: Cg1 and Cg2 are the centroids of the C13–C18 and C10–C13/C18/C19 benzene rings, respectively.

H atoms were placed in calculated positions and constrained to ride on their parent atoms, with  $\text{C}–\text{H} = 0.93–0.96 \text{ \AA}$  and  $U_{\text{iso}}(\text{H}) = 1.2–1.5U_{\text{eq}}(\text{C})$ . The methyl group was found to be disordered over two positions rotated from each other by  $60^\circ$ . The occupation factors were fixed at 0.5.

Data collection: APEX2 (Bruker, 2005); cell refinement: APEX2; data reduction: SAINT (Bruker, 2005); program(s) used to solve structure: SHELXTL (Sheldrick, 1998); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL and PLATON (Spek, 2003).

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