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3-(3-Bromophenyl)-1-(2-naphthyl)prop-2-en-1-one

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Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.002 Å
R factor = 0.035
wR factor = 0.096
Data-to-parameter ratio = 32.7

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

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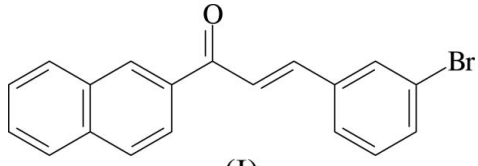
The title molecule, $C_{19}H_{13}BrO$, has an *s–cis* conformation for the ketone system. The dihedral angle between the benzene and naphthalene ring systems is 50.14 (3)°. C—H···Br interactions link the molecules into chains along the *c* axis, which are interlinked *via* C—H···π interactions.

Comment

Chalcones, 1,3-diphenyl-1-propan-3-one derivatives, have a wide range of biological properties, including anticancer (Achanta *et al.*, 2006; Kim, Choi *et al.*, 2006), antiproliferative (Hsu *et al.*, 2006), antimalarial (Wirasathien *et al.*, 2006), anti-inflammatory (Anuradha *et al.*, 2006), anti-allergic (Daikonya *et al.*, 2004) and antagonist (Kim, Kim *et al.*, 2006). Chalcones exhibit inhibitory activity against nitric oxide production (Han *et al.*, 2006), dengue 2 virus NS3 protease (Kiat *et al.*, 2006) and tyrosinase (Khatib *et al.*, 2005). Some chalcone derivatives exhibit nonlinear optical properties (Gao & Ng, 2006; Patil *et al.*, 2006*a*,*b*). As part of our studies of chalcone derivatives, the title compound, (I), has been synthesized and its crystal structure is reported here.



(I)

The molecule of (I) assumes an *s–cis* conformation for the ketone system, as evidenced by the torsion angle O1—C9—C8—C7 = 22.2 (2)° (Fig. 1). Similar values of −19.4 (6), −21.4 (3) and 14.9 (2)° were observed for 1-(2-naphthyl)-3-(4-nitrophenyl)prop-2-en-1-one, (II) (Raj *et al.*, 1996), 3-(2-chlorophenyl)-1-(2-naphthyl)prop-2-en-1-one, (III) (Kumaran *et al.*, 1996), and 3-(4-methylphenyl)-1-(2-naphthyl)prop-2-en-1-one, (IV) (Moorthi *et al.*, 2005), respectively. Atoms C7–C9 and O1 of the enone group are coplanar, with an r.m.s deviation of 0.071 Å. The mean plane through the enone group makes dihedral angles of 27.08 (5) and 23.06 (6)° with the benzene and naphthalene ring systems, respectively. The dihedral angle between the benzene and naphthalene ring systems is 50.14 (3)°.

Bond lengths and angles in (I) are comparable with those reported for (II), (III) and (IV). As observed in (IV), the short H5···H8 contact (2.27 Å) causes the bond angles C5—C6—C7 [122.94 (13)°] and C6—C7—C8 [126.53 (13)°] to deviate significantly from 120°, and the short H8···H11 contact

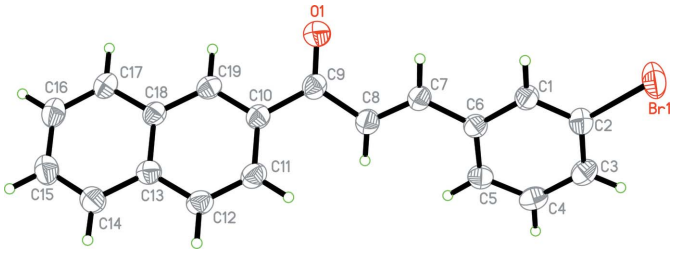


Figure 1
The molecular structure of (I), showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 80% probability level.

(2.25 Å) results in a slight widening of the C9—C10—C11 angle [121.68 (13)°].

In the crystal packing of (I), molecules related by translation along the *c* axis are linked to form a chain *via* C—H···Br interactions (Table 1). Centrosymmetrically related molecules in adjacent chains are interconnected through C—H···π interactions, involving the C13–C18 (centroid *Cg*1) and C1–C6 (centroid *Cg*2) benzene rings, into a three-dimensional framework (Fig. 2 and Table 1).

Experimental

The title compound was obtained by the Claisen–Schmidt condensation of 2′-acetonaphthone (5.10 g, 0.03 mol) and 3-bromobenzaldehyde (5.55 g, 0.03 mol) in ethanol (25 ml) in the presence of aqueous NaOH (10%). The product was isolated by filtration and washed with dilute hydrochloric acid to neutralize the alkali. It was then washed with distilled water and cold ethanol. The crude product was recrystallized from a solution in ethanol–chloroform (1:1 *v*/*v*).

Crystal data

$C_{19}H_{13}BrO$
M_r = 337.20
Triclinic, $P\overline{1}$
a = 5.8213 (1) Å
b = 7.3549 (1) Å
c = 16.7023 (3) Å
α = 88.199 (1)°
β = 84.947 (1)°
γ = 89.454 (1)°
V = 711.96 (2) Å^3
Z = 2
D_x = 1.573 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 2.88 mm^{-1}
T = 100.0 (1) K
Block, colourless
0.59 × 0.56 × 0.22 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.213, T_{max} = 0.530
19651 measured reflections
6221 independent reflections
5288 reflections with $I > 2\sigma(I)$
R_{int} = 0.026
θ_{max} = 35.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.096
S = 1.06
6221 reflections
190 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0464P)^2 + 0.4791P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.60 e Å^{-3}
$\Delta\rho_{min}$ = −0.66 e Å^{-3}

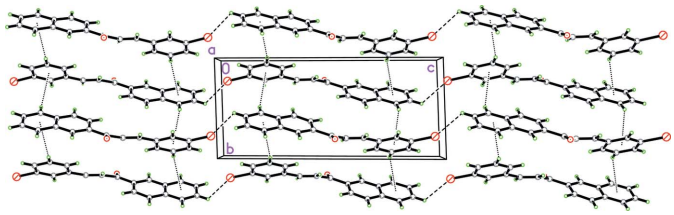


Figure 2
A packing diagram for (I), viewed down the *a* axis. Dashed and dotted lines represent C—H···Br and C—H···π interactions, respectively.

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

*Cg*1 is the centroid of the C13–C18 benzene ring and *Cg*2 is the centroid of the C1–C6 benzene ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C15—H15···Br1^{i}	0.95	2.93	3.5552 (16)	125
C1—H1···*Cg*1^{ii}	0.95	2.85	3.5236 (15)	129
C4—H4···*Cg*1^{iii}	0.95	2.84	3.5012 (15)	128
C14—H14···*Cg*2^{iv}	0.95	2.82	3.5274 (17)	132
C17—H17···*Cg*2^{v}	0.95	2.75	3.4772 (17)	134

Symmetry codes: (i) $x, y, z+1$; (ii) $-x, -y+1, -z+1$; (iii) $-x+1, -y, -z+1$; (iv) $-x+1, -y+1, -z+1$; (v) $-x, -y, -z+1$.

H atoms were positioned geometrically, with C—H = 0.95 Å, and treated as riding, with U_{iso}(H) = 1.2U_{eq}(C). The highest residual electron-density peak is located 0.71 Å from atom Br1.

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*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

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