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(2*E*)-1-(2,4-Dichlorophenyl)-3-(6-methoxy-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 = 0.034
wR factor = 0.090
Data-to-parameter ratio = 14.4

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

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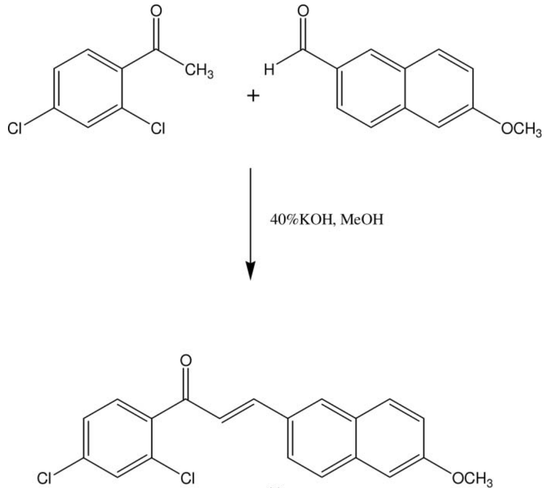
The geometric parameters of the title molecule, $C_{20}H_{14}Cl_2O_2$, are in the normal ranges. The central C═C double bond is *trans* configured and the two C atoms of this bond are slightly twisted out of the plane of the naphthyl group by 4.0 (3)°. The dihedral angle between the benzene ring and the naphthalene ring system is 44.94 (4)°. The crystal packing is stabilized by C—H···O and C—H···Cl contacts.

Comment

Reviews on the bioactivities of various chalcones have been reported (Dimmock *et al.*, 1999; 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-(3-nitrophenyl)-2-propen-1-one (Shanmuga Sundara Raj *et al.*, 1998), 3-(6-methoxy-2-naphthyl)-1-(2-naphthyl)prop-2-en-1-one (Yathirajan, Sarojini, Bindya *et al.*, 2006), 3-(6-methoxy-2-naphthyl)-1-(2-thienyl)prop-2-en-1-one (Yathirajan, Narayana *et al.*, 2006), 1-(2,4-dichloro-5-fluorophenyl)-3-(3,4-dimethoxyphenyl)prop-2-en-1-one (Yathirajan, Sarojini, Narayana *et al.*, 2006) and (2*E*)-1-(2,4-dichlorophenyl)-3-[4-(methylsulfanyl) phenyl]prop-2-en-1-one (Butcher *et al.*, 2007) have previously been reported. In continuation of our broad programme on chalcones, the present paper reports the crystal structure of a newly synthesized chalcone.



(I)

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The molecular structure of (I) is shown in Fig. 1. Bond lengths and angles can be regarded as normal (Allen *et al.*, 1987). The carbonyl group is twisted by 35.40 (19)° out of the plane of the dichlorophenyl ring. The torsion angle between the carbonyl group and the C atoms of the double bond is −10.9 (2)°. The torsion angle between the C atoms of the C=C double bond and the plane of the adjacent naphthyl group (C2—C3—C21—C22) is 4.0 (3)°. The two aromatic groups are not coplanar [dihedral angle = 44.94 (4)°]. The crystal packing is characterized by non-classical C—H···O and C—H···Cl hydrogen bonds (Table 1).

Experimental

To a thoroughly stirred solution of 2,4-dichloroacetophenone (1.89 g, 0.01 mol) and 6-methoxy-2-naphthaldehyde (1.86 g, 0.01 mol) in methanol (30 ml), 40% KOH solution (5 ml) was added (see scheme). The mixture was stirred overnight and filtered. The product obtained was recrytallized from an acetone–toluene (1:1) mixture (m.p. 429–431 K). Analysis for $C_{20}H_{14}Cl_2O_2$: found (calculated): C 67.20 (67.24), H 3.86 (3.95)%.

Crystal data

$C_{20}H_{14}Cl_2O_2$
$M_r = 357.21$
Monoclinic, $P2_1/c$
$a = 16.8724$ (7) Å
$b = 13.4610$ (7) Å
$c = 7.4932$ (3) Å
$\beta = 102.778$ (3)°
$V = 1659.70$ (13) Å^3
$Z = 4$
$D_x = 1.430$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.40$ mm^{-1}
$T = 173$ (2) K
Block, yellow
0.37 × 0.35 × 0.35 mm

Data collection

Stoe IPDS-II two-circle diffractometer
ω scans
Absorption correction: multi-scan (*MULABS*; Spek, 2003; Blessing, 1995)
$T_{\min} = 0.866$, $T_{\max} = 0.873$
28868 measured reflections
3143 independent reflections
2984 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.050$
$\theta_{\max} = 25.7°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.090$
$S = 1.08$
3143 reflections
219 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.041P)^2 + 0.8551P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.57$ e Å^{-3}
$\Delta\rho_{\min} = -0.21$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0156 (15)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···O1$^{\rm i}$	0.95	2.59	3.1367 (19)	117
C13—H13···O1$^{\rm ii}$	0.95	2.59	3.535 (2)	174
C16—H16···Cl1$^{\rm iii}$	0.95	2.83	3.5381 (16)	132

Symmetry codes: (i) $x, -y+\frac{1}{2}, z-\frac{1}{2}$; (ii) $-x, y+\frac{1}{2}, -z+\frac{1}{2}$; (iii) $-x, y-\frac{1}{2}, -z+\frac{1}{2}$.

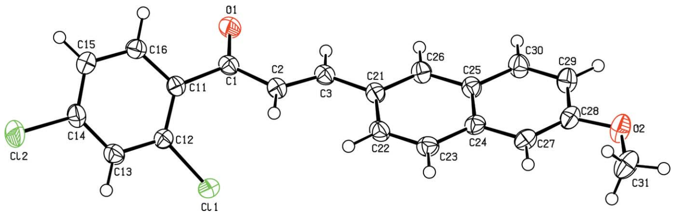

Figure 1
The molecular structure of (I), with displacement ellipsoids drawn at the 50% probability level.

H atoms were found in a difference map, but they were refined using a riding model with C—H = 0.95 Å for $C_{\rm aromatic}$ and C—H = 0.98 Å for $C_{\rm methyl}$. $U_{\rm iso}$(H) was set to 1.2$U_{\rm eq}$(C), or 1.5$U_{\rm eq}$($C_{\rm methyl}$). The methyl group was 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* and *PLATON*.

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