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Key indicators

Single-crystal X-ray study
T = 173 K
Mean $\sigma(\text{C}-\text{C}) = 0.002 \text{ \AA}$
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>.

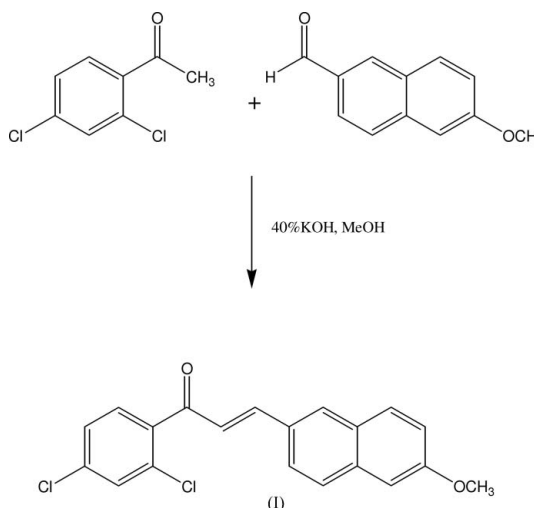
(2E)-1-(2,4-Dichlorophenyl)-3-(6-methoxy-2-naphthyl)prop-2-en-1-one

The geometric parameters of the title molecule, $\text{C}_{20}\text{H}_{14}\text{Cl}_2\text{O}_2$, are in the normal ranges. The central $\text{C}=\text{C}$ 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 $4.0 (3)^\circ$. The dihedral angle between the benzene ring and the naphthalene ring system is $44.94 (4)^\circ$. The crystal packing is stabilized by $\text{C}-\text{H} \cdots \text{O}$ and $\text{C}-\text{H} \cdots \text{Cl}$ contacts.

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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 (2E)-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.



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 $35.40(19)^\circ$ out of the plane of the dichlorophenyl ring. The torsion angle between the carbonyl group and the C atoms of the double bond is $-10.9(2)^\circ$. 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 $4.0(3)^\circ$. The two aromatic groups are not coplanar [dihedral angle = $44.94(4)^\circ$]. 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 recrystallized 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

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

Data collection

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

Refinement

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

Table 1

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C2–H2...O1 ⁱ	0.95	2.59	3.1367 (19)	117
C13–H13...O1 ⁱⁱ	0.95	2.59	3.535 (2)	174
C16–H16...Cl1 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) $-x, y - \frac{1}{2}, -z + \frac{1}{2}$.

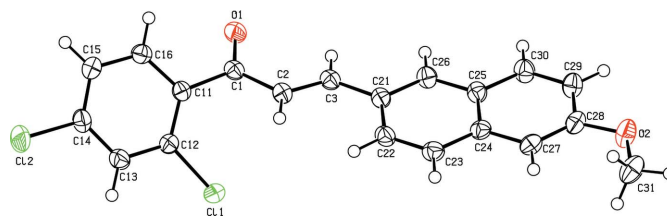


Figure 1

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 \AA for C_{aromatic} and C–H = 0.98 \AA for C_{methyl} . $U_{\text{iso}}(\text{H})$ was set to $1.2U_{\text{eq}}(\text{C})$, or $1.5U_{\text{eq}}(\text{C}_{\text{methyl}})$. 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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