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# 2-[1-(3,4-Dichlorophenyl)-3-oxo-3-phenylpropyl]-3,4-dihydro-2*H*-naphthalen-1-one

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**Key indicators**

Single-crystal X-ray study
*T* = 298 K
Mean σ(C–C) = 0.005 Å
*R* factor = 0.053
*wR* factor = 0.148
Data-to-parameter ratio = 10.7

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



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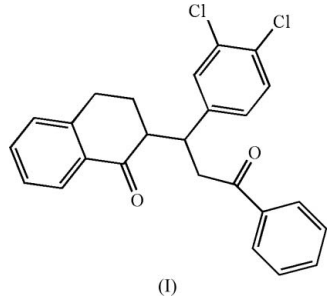
The title compound, $C_{25}H_{20}Cl_2O_2$, was synthesized by the reaction of 3,4-dihydronaphthalen-1(2*H*)-one with 3-(3,4-dichlorophenyl)-1-phenylprop-2-en-1-one under solvent-free conditions at room temperature. X-ray analysis reveals that the cyclohexanone ring adopts an envelope conformation

## Comment

1,5-Diketones are extremely important synthetic intermediates and are desirable starting materials for preparing many heterocyclic (Ariyan & Suschitiky, 1961) and polyfunctional compounds (Edwin & Alexanden, 1992; Gill *et al.*, 1952). The solvent-free reaction has attracted much attention in recent years (Tanaka & Toda, 2000) and has been proved to have many advantages: reduced pollution, low costs, and simplicity in process and handling. The solid-state Michael addition has performed well recently (Goud *et al.*, 1995; Annunziata *et al.*, 1997; Li *et al.*, 1999). We report here the crystal structure of the title compound, (I), which was synthesized by the solvent-free Michael addition reaction of 3,4-dihydronaphthalen-1(2*H*)-one and 3-(3,4-dichlorophenyl)-1-phenylprop-2-en-1-one at room temperature.




(I)

In (I), the fused cyclohexanone ring adopts an envelope conformation (Fig.1), with the atom C25 deviating from the C16/C17/C18/C23/C24 plane by 0.684 (4) Å. The C4–C9 and C10–C15 planes form dihedral angles of 85.6 (1) and 74.6 (1)°, respectively, with respect to the C16–C24 plane. The crystal packing is stablized by C—H$\cdots\pi$ interactions involving the C18–C23 benzene ring (Table 2).

## Experimental

Compound (I) was prepared by the reaction of 3,4-dihydronaphthalen-1(2*H*)-one (2 mmol) with 3-(3,4-dichlorophenyl)-1-phenylprop-2-en-1-one (2 mmol) catalysed by NaOH (0.2 g) under solvent-free conditions (m.p. 469–470 K). Single crystals suitable for X-ray diffraction were obtained by slow evaporation of an ethanol solution.

*Crystal data*

$C_{25}H_{20}Cl_2O_2$
$M_r$ = 423.31
Monoclinic, $P2_1/n$
$a$ = 9.9826 (19) Å
$b$ = 17.858 (3) Å
$c$ = 11.703 (2) Å
$\beta$ = 91.667 (3)°
$V$ = 2085.4 (6) Å$^3$
$Z$ = 4
$D_x$ = 1.348 Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 2344 reflections
$\theta$ = 2.3–21.1°
$\mu$ = 0.33 mm$^{-1}$
$T$ = 298 (2) K
Block, colourless
0.42 × 0.37 × 0.29 mm

*Data collection*

Bruker SMART CCD area-detector diffractometer
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.874, $T_{max}$ = 0.910
10745 measured reflections
3669 independent reflections
2008 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.038
$\theta_{max}$ = 25.0°
$h = -11 \rightarrow 11$
$k = -16 \rightarrow 21$
$l = -13 \rightarrow 13$

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.148
$S$ = 1.00
3669 reflections
342 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.074P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.46 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.58 e Å$^{-3}$

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| Cl1—C12 | 1.714 (3) | O1—C3 | 1.207 (3) |
| Cl2—C13 | 1.730 (3) | O2—C17 | 1.215 (3) |
| | | | |
| C10—C1—C16 | 110.1 (2) | C11—C10—C15 | 117.2 (3) |
| C3—C2—C1 | 114.0 (3) | C15—C10—C1 | 123.2 (3) |
| C5—C4—C9 | 117.9 (3) | C17—C16—C1 | 112.9 (2) |
| C5—C4—C3 | 123.1 (3) | C25—C16—C1 | 115.3 (2) |

**Table 2**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C11—H9···$Cg1^{i}$ | 0.91 (3) | 2.97 (3) | 3.855 (6) | 166 (3) |

Symmetry code: (i) $x-\frac{1}{2}, -y+\frac{3}{2}, z-\frac{1}{2}$. $Cg1$ is the centroid of the C18–C23 benzene ring.

H atoms were located in a difference map and refined isotropically. The C—H distances range from 0.89 (3) to 1.04 (3) Å.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1999); software used to prepare material for publication: *SHELXTL*.

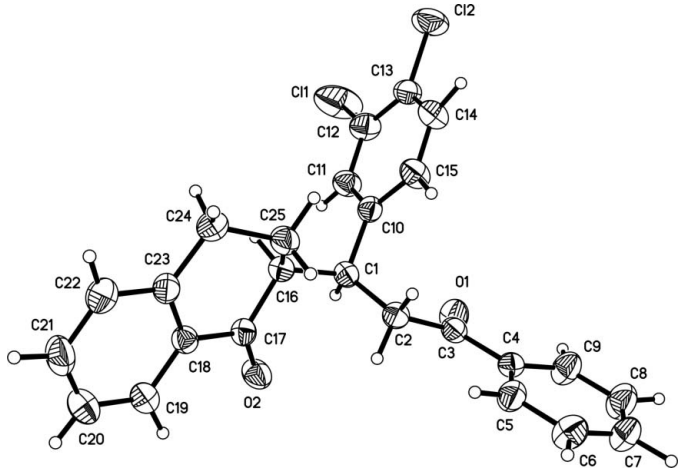



**Figure 1**
The structure of (I), showing 30% probability displacement ellipsoids.

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