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## Key indicators

Single-crystal X-ray study

T = 100 K

Mean  $\sigma(C-C) = 0.002 \text{ \AA}$ 

R factor = 0.043

wR factor = 0.118

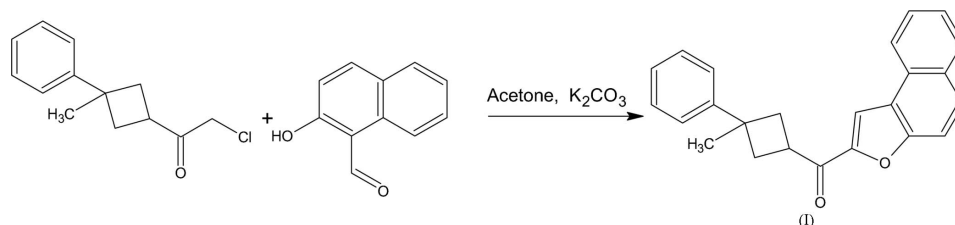
Data-to-parameter ratio = 13.3

For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.(3-Methyl-3-phenylcyclobutyl)(naphtho[2,1-*b*]-  
furan-2-yl)methanoneIn the title compound,  $C_{24}H_{20}O_2$ , C—H $\cdots$ O, C—H $\cdots\pi$  and  $\pi$ — $\pi$  interactions result in a three-dimensional supramolecular network.

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## Comment

The naphthofuran skeleton is present in many natural products of biological importance and its synthetic derivatives display diverse biological activity. Nevertheless, little is known about their fluorescence properties and potential utility as suitable fluorescent markers. Arene ring-fused furans have attracted widespread interest in view of their presence in natural products and their biological and pharmacological activities (Piloto *et al.*, 2005).Compared with benzofurans, reports on the synthesis of naphthofurans and benzodifurans are rather limited, though many of the extended arenofurans exhibit interesting biological properties and have potential applications as fluorescent dyes and probes, and as photosensitizers. The title compound, (I), was synthesized by the base-catalyzed cyclization reaction of the corresponding *o*-alkoxybenzoylarene derivative (Park & Jeong, 2005).The naphtho[2,1-*b*]furan-2-yl part of (I) is composed of three rings, *A* (O2/C13–C15/C24), *B* (C15/C16/C21–C24) and *C* (C16–C21). In the cyclobutane ring, the C9/C7/C10 plane forms a dihedral angle of 28.90 (1)° with the C10/C11/C9 plane. This is larger than previously reported angles of 23.82 (3)° (Kırılmış *et al.*, 2005) and 23.5 (4)° (Swenson *et al.*, 1997). The dihedral angle between the C1–C6 plane and the plane through rings *A*, *B*, *C* and atoms C12 and O1 is 78.65 (6)°.C—H $\cdots$ O, C—H $\cdots\pi$  and  $\pi$ — $\pi$  interactions have been reported as important in the generation of supramolecular architectures (Yilmaz *et al.*, 2005). There are three intermolecular C—H $\cdots$ O hydrogen-bonding interactions in the crystal structure (Table 1 and Fig. 2). These interactions lead to close packing between neighbouring molecules. There are also two C—H $\cdots\pi$  interactions: C9—H9B $\cdots$ Cg1<sup>i</sup> = 2.78 Å and C11—H11 $\cdots$ Cg2<sup>i</sup> = 2.82 Å, where Cg1 and Cg2 are the centroids of rings *A* and *B*, respectively [symmetry code: (i) 1

+ *x*, *y*, *z*]. In (I), the packing of the molecules is additionally reinforced by a  $\pi$ - $\pi$  stacking interaction between rings *A* and *C*, with a  $Cg1 \cdots Cg3^i$  distance of 3.5278 (1) Å, where *Cg3* is the centroid of ring *C*.

### Experimental

2-Hydroxy-1-naphthaldehyde (1.89 g, 11 mmol), potassium carbonate (2.07 g, 15 mmol) and acetonitrile (150 ml) were placed in a 500 ml two-necked flask with a reflux condenser. The mixture was stirred for 2 h at room temperature. 1-Phenyl-1-methyl-3-(2-chloro-1-oxoethyl)cyclobutane (2.225 g, 10 mmol) in acetonitrile (25 ml) was then added dropwise over a period of about 30 min and refluxed for 8 h. The course of the reaction was monitored by IR spectroscopy. The solvent was then removed under reduced pressure, the residue was extracted with diethyl ether and the ether phase dried over magnesium sulfate. After filtration and removal of the solvent under reduced pressure, compound (I) was crystallized from acetone (yield %76, m.p. 453–454 K).

#### Crystal data

$C_{24}H_{20}O_2$	$V = 885.23 (12) \text{ \AA}^3$
$M_r = 340.40$	$Z = 2$
Triclinic, $P\bar{1}$	$D_x = 1.277 \text{ Mg m}^{-3}$
$a = 5.9316 (4) \text{ \AA}$	Mo $K\alpha$ radiation
$b = 11.969 (1) \text{ \AA}$	$\mu = 0.08 \text{ mm}^{-1}$
$c = 13.760 (1) \text{ \AA}$	$T = 100 (2) \text{ K}$
$\alpha = 112.064 (5)^\circ$	Block, colorless
$\beta = 97.270 (6)^\circ$	$0.35 \times 0.14 \times 0.10 \text{ mm}$
$\gamma = 96.165 (6)^\circ$	

#### Data collection

Nonius KappaCCD diffractometer	16640 measured reflections
$\omega$ scans	3929 independent reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 2002)	2986 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.987$ , $T_{\max} = 0.999$	$R_{\text{int}} = 0.045$
	$\theta_{\text{max}} = 27.1^\circ$

#### Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.0631P)^2 + 0.2126P]$
$R[F^2 > 2\sigma(F^2)] = 0.044$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.118$	$(\Delta\rho)_{\text{max}} < 0.001$
$S = 1.05$	$\Delta\rho_{\text{max}} = 0.30 \text{ e \AA}^{-3}$
3929 reflections	$\Delta\rho_{\text{min}} = -0.24 \text{ e \AA}^{-3}$
295 parameters	
Only H-atom coordinates refined	

**Table 1**

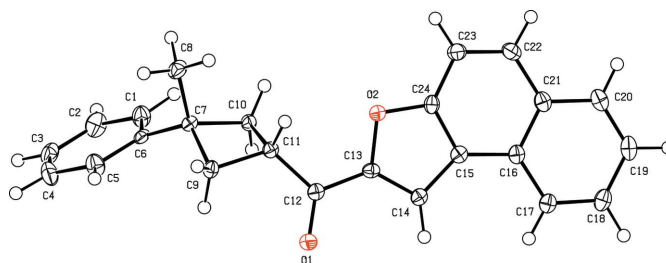
Hydrogen-bond geometry (Å, °).

<i>D</i> — <i>H</i> ⋯ <i>A</i>	<i>D</i> — <i>H</i>	<i>H</i> ⋯ <i>A</i>	<i>D</i> ⋯ <i>A</i>	<i>D</i> — <i>H</i> ⋯ <i>A</i>
C3—H3⋯O1 <sup>i</sup>	0.97 (2)	2.53 (2)	3.482 (2)	165 (2)
C14—H14⋯O1 <sup>ii</sup>	0.97 (2)	2.49 (2)	3.341 (2)	146 (2)
C17—H17⋯O1 <sup>ii</sup>	0.97 (2)	2.49 (2)	3.381 (2)	153 (2)

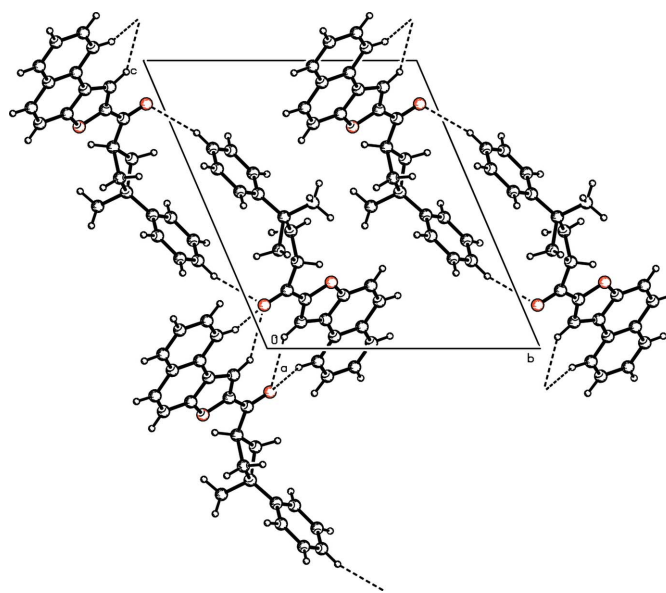
Symmetry codes: (i)  $-x + 1, -y + 2, -z + 1$ ; (ii)  $-x + 2, -y + 2, -z + 2$ .

H atoms were located in difference maps and their coordinates refined freely [ $C-H = 0.96 (2)$ – $1.03 (2) \text{ \AA}$ ].  $U_{\text{iso}}(\text{H})$  values were set at  $0.04 \text{ \AA}^2$ .

Data collection: *COLLECT* (Bruker–Nonius, 2002); cell refinement: *EVALCCD* (Bruker–Nonius, 2002); data reduction: *EVALCCD*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2001); program(s) used to refine structure: *SHELXTL*; mole-



**Figure 1**  
Plot of the title compound, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are shown as small circles of arbitrary radii.



**Figure 2**  
A view of the unit-cell contents. Dashed lines indicate hydrogen bonds.

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

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