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#### Key indicators

Single-crystal X-ray study  
 $T = 293$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å  
 $R$  factor = 0.034  
 $wR$  factor = 0.104  
Data-to-parameter ratio = 9.9

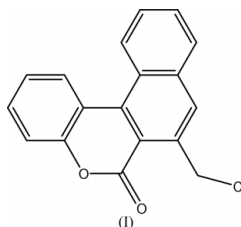
For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

## 7-Chloromethylbenzo[*b*]naphtho[1,2-*d*]pyran-6-one

In the title compound,  $\text{C}_{18}\text{H}_{11}\text{ClO}_2$ , the pyranone ring adopts a boat conformation. There is one intramolecular  $\text{C}-\text{H}\cdots\text{O}$  interaction, forming a six-membered ring. The crystal structure is stabilized by intermolecular  $\text{C}-\text{H}\cdots\text{O}$  interactions and van der Waals forces.

#### Comment

Recently, we have carried out photo-induced reactions of coumarins with phenylethenes (Usman *et al.*, 2002). In our continuing studies of these reactions, the title compound, (I), was unexpectedly obtained in the photo-induced reaction of 3,4-dichlorocoumarin with phenylpropadiene in benzene. An X-ray crystallographic analysis was undertaken to find the stereochemistry of (I).



The bond lengths and angles in (I) are within normal ranges (Allen *et al.*, 1987). All the  $\text{C}-\text{C}$  bond distances in the benzene and naphthalene rings have typical  $\text{Csp}^2-\text{Csp}^2$  values. The average  $\text{C}-\text{C}$  bond distances within these two rings are 1.387 (4) and 1.402 (8) Å. The dihedral angle between the  $\text{C}1-\text{C}6$  and  $\text{C}10-\text{C}15$  benzene rings is 31.50 (8)°.

The two benzene rings in the naphthalene moiety make a dihedral angle of 11.06 (7)° with each other. The pyranone ring adopts a boat conformation, with atoms  $\text{O}1$  and  $\text{C}7$  deviating by 0.122 (5) and 0.157 (6) Å, respectively, from the mean plane through the other four atoms. The  $\text{C}1-\text{C}6$  benzene ring makes a dihedral angle of 26.34 (7)° with the naphthalene

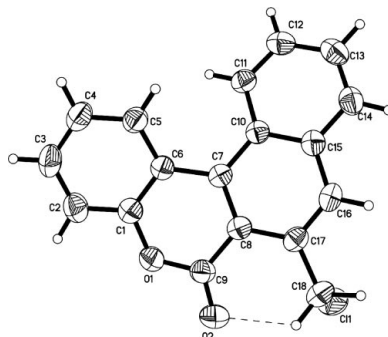


Figure 1

View of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme.

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mean plane. Atom C18 of the chloromethyl group, attached to the naphthalene ring moiety at C17, is almost coplanar with the C7/C8/C10/C15–C17 benzene ring, deviating from it by 0.191 (3) Å.

In the title structure, there is one intramolecular C18–H18B···O2 hydrogen-bond interaction (Fig. 1), forming a closed six-membered ring O2–C9–C8–C17–C18–H18B.

In the crystal structure, the molecules are linked, by a weak intermolecular C–H···O interaction (Table 2), into the chains which are stacked parallel to the *b* axis (Fig. 2). The packing is stabilized by this interaction and by van der Waals forces.

## Experimental

The title compound was prepared by the photolysis of a benzene solution of 3,4-dichlorocoumarin in the presence of an excess of phenylpropadiene, followed by chromatographic separation of the reaction mixture on a silica-gel column with petroleum ether–ethyl acetate (b.p. 333–363 K) as eluants. A single crystal suitable for X-ray crystallographic analysis was prepared by slow evaporation of a dichloromethane–acetone solution.

### Crystal data

C <sub>18</sub> H <sub>11</sub> ClO <sub>2</sub>	$D_x = 1.482 \text{ Mg m}^{-3}$
$M_r = 294.72$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 5237 reflections
$a = 9.9771 (5) \text{ \AA}$	$\theta = 2.4\text{--}28.3^\circ$
$b = 16.1368 (8) \text{ \AA}$	$\mu = 0.29 \text{ mm}^{-1}$
$c = 8.2899 (4) \text{ \AA}$	$T = 293 (2) \text{ K}$
$\beta = 98.129 (1)^\circ$	Block, colourless
$V = 1321.3 (1) \text{ \AA}^3$	$0.50 \times 0.44 \times 0.42 \text{ mm}$
$Z = 4$	

### Data collection

Siemens SMART CCD area-detector diffractometer	2312 independent reflections
$\omega$ scans	2111 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$R_{\text{int}} = 0.015$
$T_{\text{min}} = 0.869$ , $T_{\text{max}} = 0.888$	$\theta_{\text{max}} = 25.0^\circ$
6465 measured reflections	$h = -11 \rightarrow 11$
	$k = -19 \rightarrow 16$
	$l = -9 \rightarrow 9$

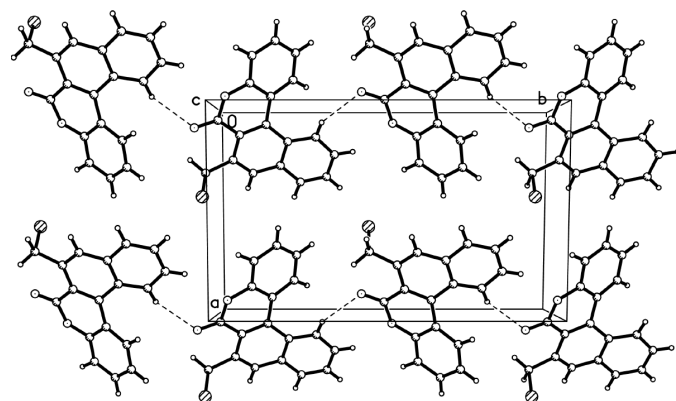
### Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.0586P)^2 + 0.4109P]$
$R[F^2 > 2\sigma(F^2)] = 0.034$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.104$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.05$	$\Delta\rho_{\text{max}} = 0.29 \text{ e \AA}^{-3}$
2312 reflections	$\Delta\rho_{\text{min}} = -0.29 \text{ e \AA}^{-3}$
234 parameters	
All H-atom parameters refined	

**Table 1**

Selected geometric parameters (Å, °).

O1–C9	1.358 (2)	C8–C9	1.477 (2)
O1–C1	1.376 (2)	C17–C18	1.501 (2)
C6–C7	1.467 (2)		
C5–C6–C7	125.46 (15)	C17–C8–C9	119.43 (14)
C10–C7–C6	122.84 (14)	C8–C17–C18	124.62 (15)



**Figure 2**

Packing diagram of (I), viewed down the *c* axis, showing extended chains in the *b* direction. Dashed lines denote C–H···O intermolecular interactions.

**Table 2**

C–H···O interactions (Å, °).

$D\text{--}H\cdots A$	$D\text{--}H$	$H\cdots A$	$D\cdots A$	$D\text{--}H\cdots A$
C11–H11···O2 <sup>i</sup>	0.95 (2)	2.54 (2)	3.371 (2)	147 (2)
C18–H18B···O2	1.00 (2)	2.17 (2)	2.768 (3)	117 (2)

Symmetry code: (i)  $2 - x, y - \frac{1}{2}, \frac{3}{2} - z$ .

All H atoms were located in difference Fourier maps and were refined isotropically. Owing to a large fraction of weak data at higher angles, the  $2\theta$  maximum was limited to  $50^\circ$ .

Data collection: SMART (Siemens, 1996); cell refinement: SAINT (Siemens, 1996); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Sheldrick, 1997); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL, PARST (Nardelli, 1995) and PLATON (Spek, 2003).

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