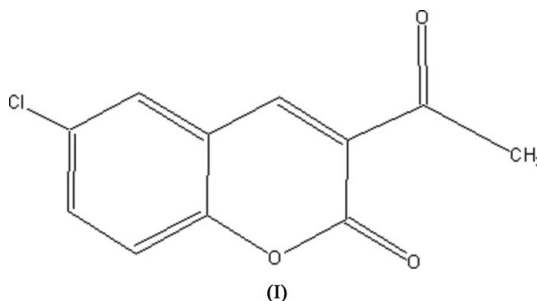
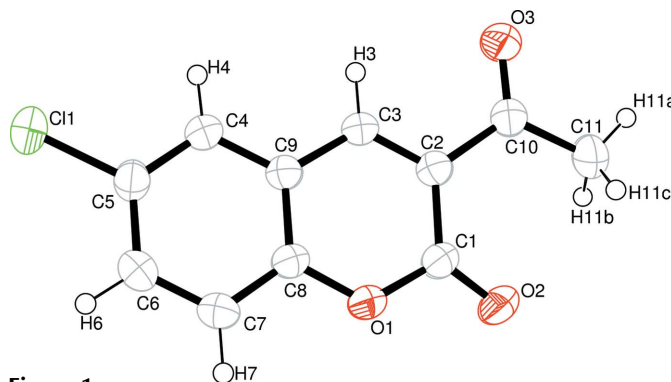


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deepak@sscu.iisc.ernet.in**Key indicators**Single-crystal X-ray study
 $T = 290$ K
Mean $\sigma(\text{C}-\text{C}) = 0.002$ Å
 R factor = 0.032
 wR factor = 0.090
Data-to-parameter ratio = 11.5For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.**3-Acetyl-6-chloro-2H-chromen-2-one**In the title compound, $\text{C}_{11}\text{H}_7\text{ClO}_3$, the coumarin system is planar and makes a dihedral angle of $6.6(1)^\circ$ with the acetyl group. The crystal structure is stabilized by $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds and aromatic $\pi-\pi$ interactions.Received 2 May 2006
Accepted 8 May 2006**Comment**Coumarins are an important class of organic compounds and have been extensively studied. As they exhibit vast structural diversity, they find useful applications in several areas of synthetic chemistry, medicinal chemistry and photochemistry (Vishnumurthy *et al.*, 1996, 1997, 1999). The formation of [2 + 2]-cycloaddition products upon irradiation (Vishnumurthy *et al.*, 2001) of coumarin and its derivatives has demonstrated the importance of pre-organization of molecules in the crystalline solid state. We report here the structure of the title compound, (I), a chloro coumarin derivative (Table 1 and Fig. 1); the crystal structure of the bromo analogue has been reported previously (Kokila *et al.*, 1996).The coumarin ring system is planar, with a maximum deviation of $0.042(2)$ Å from the weighted least-squares plane for atom C1. A short $\text{Cl1}\cdots\text{O2}(x, y - 1, z)$ contact [$3.190(2)$ Å] is present in the crystal structure. In addition,**Figure 1**
View of the title compound, drawn with 50% probability ellipsoids.

C—H···O hydrogen-bonding interactions form dimers and generate rings that can be described as having graph sets (Bernstein *et al.*, 1995) $R_2^2(10)$ and $R_2^2(14)$ to O3, and $R_2^2(12)$ to O2 (Table 2). These dimers generate planar sheets parallel to the *bc* plane (Fig. 2). The structure is further stabilized by aromatic π – π interactions, with distances between the centroids of the benzene (*Cg1*) and pyranone rings [*Cg2* at (*x* + 1, *y*, *z*)] of 3.998 (3) Å (Fig. 3).

Experimental

The title compound was synthesized according to the method of Venugopala *et al.* (2004). Single crystals of (I) were grown from a glacial acetic acid solution.

Crystal data

$C_{11}H_7ClO_3$	$V = 478.5 (5) \text{ \AA}^3$
$M_r = 222.62$	$Z = 2$
Triclinic, $P\bar{1}$	$D_x = 1.545 \text{ Mg m}^{-3}$
$a = 3.988 (2) \text{ \AA}$	Mo $K\alpha$ radiation
$b = 11.010 (7) \text{ \AA}$	$\mu = 0.38 \text{ mm}^{-1}$
$c = 11.156 (7) \text{ \AA}$	$T = 290 (2) \text{ K}$
$\alpha = 97.078 (9)^\circ$	Block, yellow
$\beta = 90.238 (10)^\circ$	$0.39 \times 0.39 \times 0.21 \text{ mm}$
$\gamma = 100.049 (10)^\circ$	

Data collection

Bruker SMART CCD area-detector diffractometer	3726 measured reflections
φ and ω scans	1890 independent reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	1875 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.866$, $T_{\max} = 0.928$	$R_{\text{int}} = 0.013$
	$\theta_{\text{max}} = 26.4^\circ$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0553P)^2 + 0.0809P]$
$R[F^2 > 2\sigma(F^2)] = 0.032$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.090$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.08$	$\Delta\rho_{\text{max}} = 0.19 \text{ e \AA}^{-3}$
1890 reflections	$\Delta\rho_{\text{min}} = -0.21 \text{ e \AA}^{-3}$
164 parameters	
All H-atom parameters refined	

Table 1

Selected geometric parameters (Å, °).

C11—C5	1.7357 (18)	O1—C1	1.3842 (19)
O1—C8	1.367 (2)	O2—C1	1.1961 (19)
C3—C2—C10—C11	−177.73 (14)		

Table 2

Hydrogen-bond geometry (Å, °).

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
C3—H3···O3 ⁱ	0.92 (2)	2.51 (2)	3.346 (3)	152 (2)
C4—H4···O3 ⁱ	0.92 (2)	2.60 (2)	3.392 (2)	144 (2)

Symmetry code: (i) $-x + 2, -y + 1, -z + 1$.

All H atoms were located in a difference Fourier map and refined isotropically [C—H = 0.91 (2)–1.04 (3) Å].

Data collection: SMART (Bruker, 2000); cell refinement: SAINT (Bruker, 2000); data reduction: SAINT; program(s) used to solve

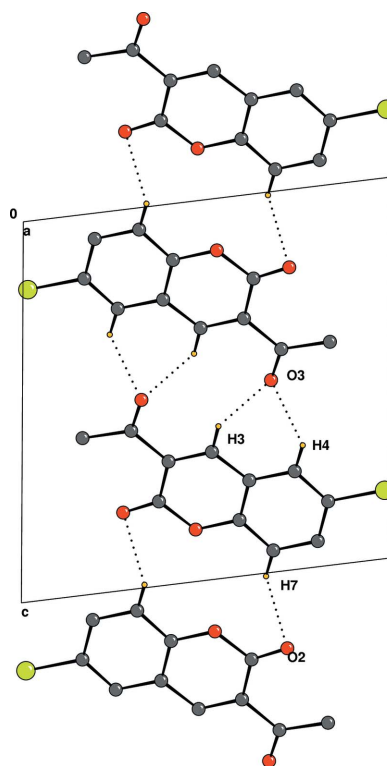


Figure 2
Packing diagram of (I), highlighting the C—H···O dimers. Hydrogen bonds are drawn as dotted lines.

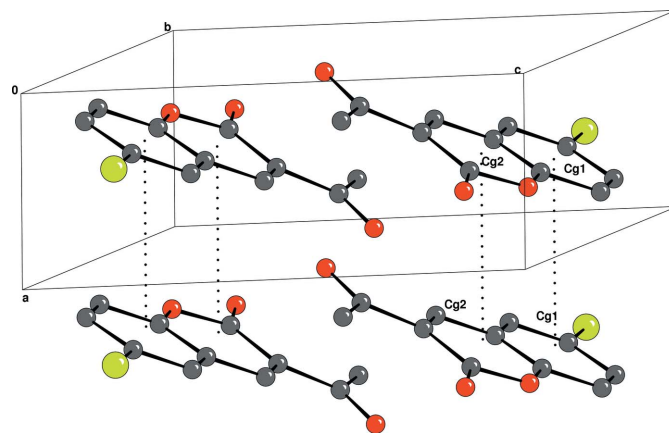


Figure 3

View of the π – π interactions in the title compound; benzene-ring (*Cg1*) and pyranone-ring centroids (*Cg2*) are joined by dotted lines.

structure: SIR92 (Altomare *et al.*, 1993); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEP-3 for Windows (Farrugia, 1997) and CAMERON (Watkin *et al.*, 1993); software used to prepare material for publication: PLATON (Spek, 2003).

We thank DST for data collection on the CCD facility under the IRHPA–DST scheme. DC thanks CSIR, India, for a Junior Research Fellowship.

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