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(*E*)-7-[(3-Chlorocinnamoyl)oxy]-4-methylcoumarin

Shu-Ping Yang,[a]* Li-Jun Han,[b] Da-Qi Wang[c] and Hai-Tao Xia[a]

[a]Department of Chemical Engineering, Huaihai Institute of Technology, Lianyungang 222005, People's Republic of China, [b]Department of Mathematics and Science, Huaihai Institute of Technology, Lianyungang 222005, People's Republic of China, and [c]College of Chemistry and Chemical Engineering, Liaocheng University, Shandong 252059, People's Republic of China

Correspondence e-mail: yangshuping@hhit.edu.cn

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In the title compound {systematic name: 4-methyl-2-oxo-2*H*-1-benzopyran-7-yl 3-(3-chlorophenyl)prop-2-enoate}, $C_{19}H_{13}ClO_4$, the molecules have an *E* configuration and the dihedral angle between the coumarin unit and the benzene ring of cinnamoyloxy is 49.0 (1)°. The molecules are linked by C—H···O and C—H···Cl hydrogen bonds into a [101] ribbon of alternating $R_2^2(14)$ rings. The molecules are linked by weak intermolecular C—H···O interactions into a $C_2^2(12)$ [001] chain and a $C_2^2(14)$ [$\bar{2}$01] chain. The combination of the [101] ribbons, the [001] chains and the [$\bar{2}$01] chains results in the formation of a three-dimensional network structure.

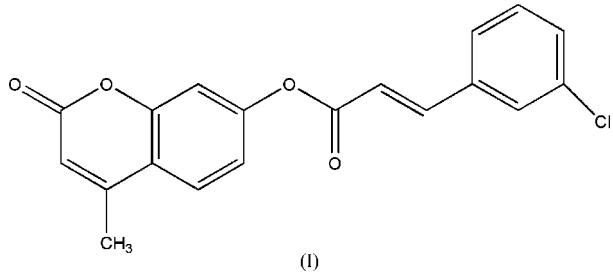
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.006 Å
R factor = 0.063
wR factor = 0.159
Data-to-parameter ratio = 12.9

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

Comment

Coumarin derivatives exhibit a wide variety of pharmacological activities including anti-HIV activity (Xie *et al., 2001*), antibacterial activity (Tanitame *et al., 2004*) and inhibition of acetylcholinesterase (AChE) (Brühlmann *et al., 2001*). We have recently reported the crystal structure of one coumarin derivative (Yang *et al.*, 2006). As part of our study of the crystal structures of coumarin derivatives with 7-cinnamoyloxy, we report here the crystal structure of a new coumarin derivative, (I).



(I)

As seen in Fig. 1, the molecules of (I) have an *E* configuration, with the coumarin unit and the benzene ring located

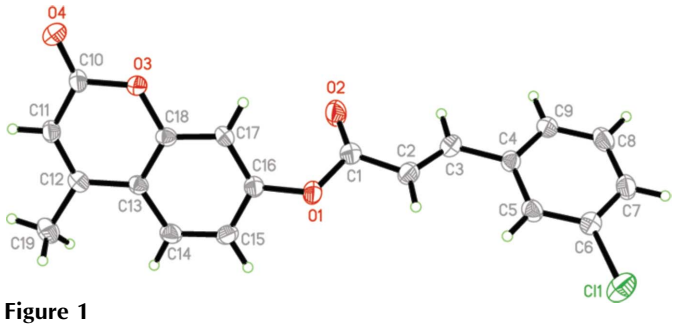


Figure 1
The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

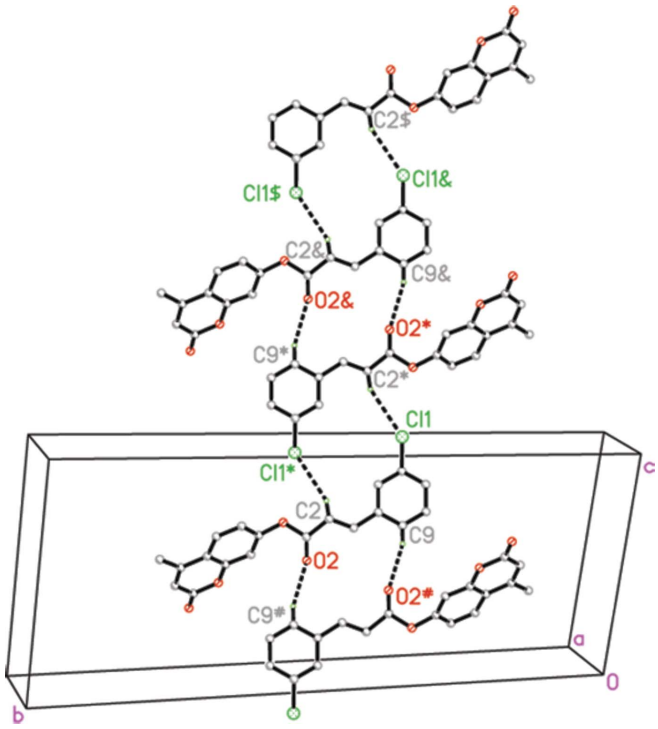


Figure 2
Part of the crystal structure of (I), showing the formation of a ribbon along [101]. For the sake of clarity, H atoms not involved in the motif shown have been omitted [symmetry codes: (*) $1-x, 1-y, 2-z$; (#) $-x, 1-y, 1-z$; (&) $1+x, y, 1+z$; ($) $2-x, 1-y, 3-z$]. Dashed lines indicate hydrogen bonds.

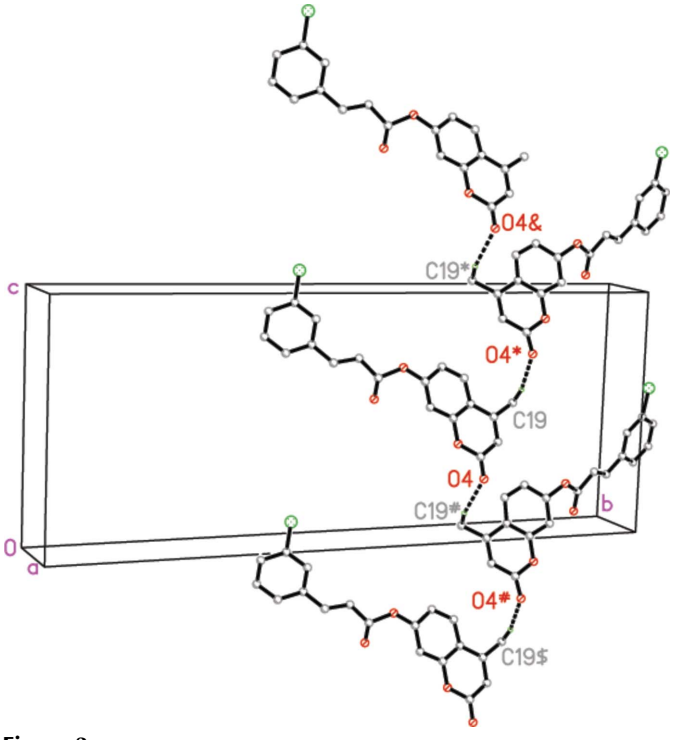


Figure 3
Part of the crystal structure of (I), showing the formation of a $C_2^2(12)$ chain of rings along the [001] direction. For the sake of clarity, H atoms not involved in the motif shown have been omitted [symmetry codes: (*) $x, \frac{3}{2}-y, \frac{1}{2}+z$; (#) $x, \frac{3}{2}-y, -\frac{1}{2}+z$; (&) $x, y, 1+z$; ($) $x, y, -1+z$]. Dashed lines indicate hydrogen bonds.

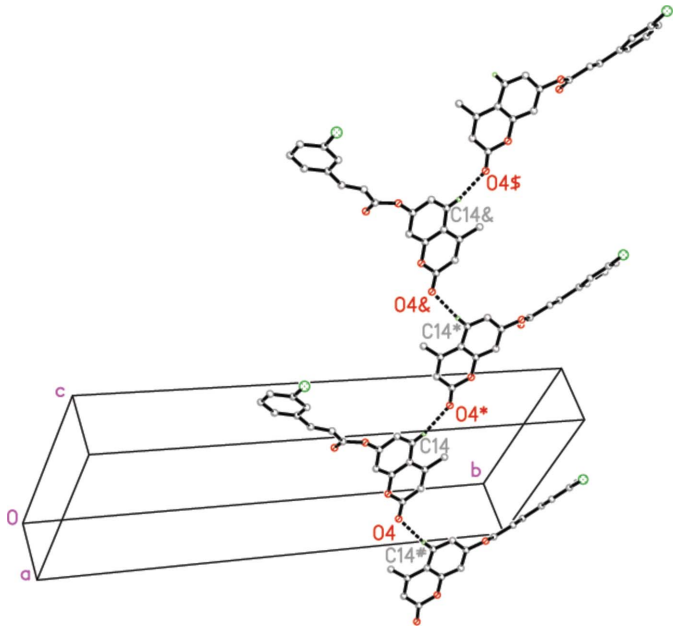


Figure 4
Part of the crystal structure of (I), showing the formation of a $C_2^2(7)$ chain of rings along the [$\bar{2}$01] direction. For the sake of clarity, H atoms not involved in the motif shown have been omitted [symmetry codes: (*) $-1+x, \frac{3}{2}-y, \frac{1}{2}+z$; (#) $1+x, \frac{3}{2}-y, -\frac{1}{2}+z$; (&) $-2+x, y, 1+z$; ($) $-3+x, \frac{3}{2}-y, \frac{3}{2}+z$]. Dashed lines indicate hydrogen bonds.

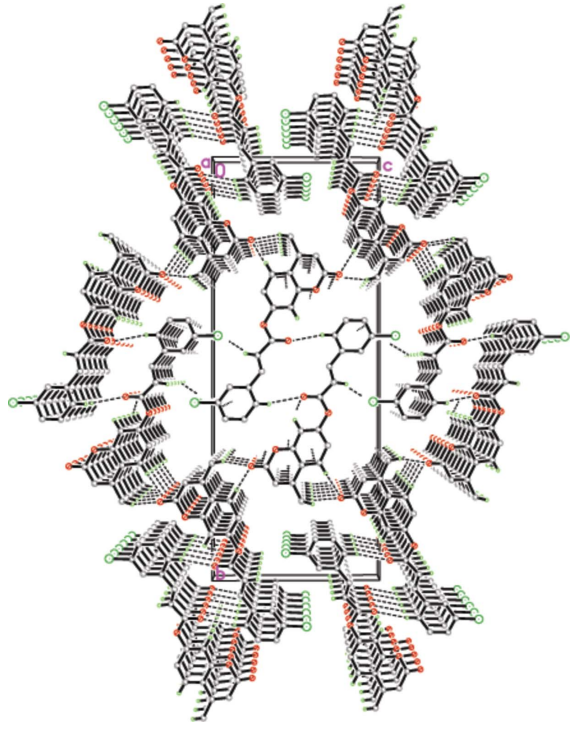


Figure 5
The packing of (I). Dashed lines indicate hydrogen bonds. H atoms not involved in hydrogen bonding have been omitted.

on opposite sides of the C=C bond. The coumarin unit and the benzene ring of the 7-cinnamoyloxy form a dihedral angle of 49.0 (1)°. The coumarin unit is almost planar, the dihedral angle between the pyrone and benzene rings being 1.6 (2)°. The geometric parameters for (I) are normal.

In the crystal structure of (I), the molecules are linked by a pair of C—H···O hydrogen bonds and a pair of C—H···Cl hydrogen bonds, so forming a [101] ribbon of alternating $R_2^2(14)$ rings (García-Báez *et al.*, 2002). Atoms C2 and C9 in the molecule at (x, y, z) both act as hydrogen-bond donors to, respectively, atom Cl1 in the molecule at $(1-x, 1-y, 2-z)$ and atom O2 in the molecule at $(-x, 1-y, 1-z)$. In a similar way, atoms Cl1 and O2 in the molecule at (x, y, z) both accept hydrogen bonds from atom C2 in the molecule at $(1-x, 1-y, 2-z)$ and atom C9 in the molecule at $(-x, 1-y, 1-z)$ (Fig. 2). The molecules are linked by intermolecular C—H···O weak interactions into a $C_2^2(12)$ chain (Bernstein *et al.*, 1995) along the [001] direction; atom C19 in the molecule at (x, y, z) acts as hydrogen-bond donor to atom O4 in the molecule at $(x, \frac{3}{2}-y, \frac{1}{2}+z)$ (Fig. 3). In the same way, a $C_2^2(14)$ chain is formed by weak intermolecular C—H···O interactions along the $[\bar{2}01]$ direction (Fig. 4 and Table 1). The combination of the [101] ribbon, the [001] chain and $[\bar{2}01]$ chain results in the formation of a three-dimensional network structure (Fig. 5).

Experimental

To a solution containing 4-methyl-7-hydroxycoumarin (1.76 g, 10 mmol) and anhydrous pyridine (10 ml), a solution of 3-chlorocinnamyl chloride (2.01 g, 10 mmol) and anhydrous acetone (10 ml) was slowly added at 278–283 K, with stirring for 30 min. The reaction mixture was stirred continuously for 24 h at room temperature (298–300 K) and then poured into ice–water (200 ml). The solid obtained was filtered off, washed with water and dried at room temperature. Colourless crystals of (I) suitable for X-ray structure analysis were obtained by recrystallizing the crude product from ethanol (m.p. 428–429 K).

Crystal data

$C_{19}H_{13}ClO_4$
$M_r = 340.74$
Monoclinic, $P2_1/c$
$a = 3.912\ (2)$ Å
$b = 32.035\ (16)$ Å
$c = 12.671\ (7)$ Å
$\beta = 91.442\ (8)^\circ$
$V = 1587.6\ (14)$ Å^3
$Z = 4$
$D_x = 1.426$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.26$ mm^{-1}
$T = 298\ (2)$ K
Column, colourless
0.35 × 0.17 × 0.09 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.914$, $T_{max} = 0.977$
8258 measured reflections
2811 independent reflections
1377 reflections with $I > 2\sigma(I)$
$R_{int} = 0.073$
$\theta_{max} = 25.0^\circ$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.063$
$wR(F^2) = 0.159$
$S = 1.03$
2811 reflections
218 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + 1.7481P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.23$ e Å^{-3}
$\Delta\rho_{min} = -0.22$ e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···Cl1^{i}	0.93	2.92	3.783 (5)	155
C9—H9···O2^{ii}	0.93	2.49	3.387 (6)	161
C14—H14···O4^{iii}	0.93	2.47	3.392 (6)	169
C19—H19*A*···O4^{iv}	0.96	2.51	3.444 (6)	163

Symmetry codes: (i) $-x+1, -y+1, -z+2$; (ii) $-x, -y+1, -z+1$; (iii) $x-1, -y+\frac{3}{2}, z+\frac{1}{2}$; (iv) $x, -y+\frac{3}{2}, z+\frac{1}{2}$.

All H atoms were positioned geometrically and refined as riding on their parent atoms, with C—H = 0.96 Å and U_{iso}(H) = $1.5U_{eq}$(methyl C), and C—H = 0.93 Å and U_{iso}(H) = $1.2U_{eq}$(C).

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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