

Alan J. Lough,<sup>a\*</sup> Karine  
Villeneuve<sup>b</sup> and William Tam<sup>b</sup><sup>a</sup>Department of Chemistry, University of  
Toronto, Toronto, Ontario, Canada M5S 3H6,  
and <sup>b</sup>Department of Chemistry, University of  
Guelph, Guelph, Ontario, Canada N1G 2W1Correspondence e-mail:  
alough@chem.utoronto.ca

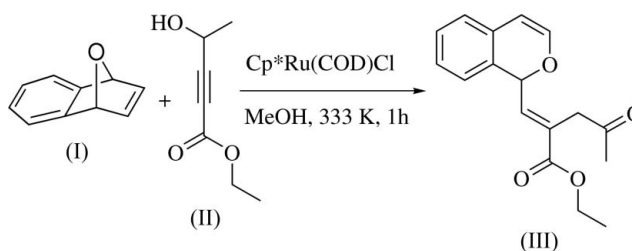
## Key indicators

Single-crystal X-ray study  
*T* = 150 K  
Mean  $\sigma(\text{C}-\text{C})$  = 0.004 Å  
Disorder in main residue  
*R* factor = 0.040  
*wR* factor = 0.099  
Data-to-parameter ratio = 8.8For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.Ethyl 2-acetyl-3-(1*H*-isochromen-1-yl)acrylateIn the title compound, C<sub>17</sub>H<sub>18</sub>O<sub>4</sub>, molecules related by the 2<sub>1</sub>  
screw axis are linked by weak intermolecular C—H···O  
hydrogen bonds, forming one-dimensional chains propagating  
along the *c* axis.

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## Comment

Recently, we have studied the ruthenium-catalysed [2 + 2]-  
cycloaddition reactions between bicyclic alkenes and  
propargyl alcohols (Villeneuve *et al.*, 2003). When 11-  
oxatricyclo[6.2.1.0<sup>2,7</sup>]undeca-2,4,6,9-tetraene, (I), was used as  
the bicyclic alkene component and ethyl 4-hydroxy-2-  
pentynoate, (II), was used as the alkyne component, the  
ruthenium-catalysed formation of a cyclopropane product was  
seen to be occurring (Villeneuve & Tam, 2006). However,  
when the solvent was changed from tetrahydrofuran to  
methanol, the title compound, (III), was formed instead.A view of the molecular structure of (III) is shown in Fig. 1.  
The conformation of the six-membered pyran ring is inter-  
mediate between a half-chair and a sofa. Atoms C1/C2/C3/C8  
form an approximate plane [maximum deviation =  
0.0488 (15) Å for C2], while C9 and O1 deviate from this plane  
by 0.434 (5) and −0.099 (5) Å, respectively. In the crystal  
structure, the molecules of (III) form one-dimensional chains  
along the polar *c*-axis direction *via* weak intermolecular C—  
H···O interactions (Table 1 and Fig. 2)

## Experimental

11-Oxatricyclo[6.2.1.0<sup>2,7</sup>]undeca-2,4,6,9-tetraene, (I) (204.9 mg,  
1.421 mmol), and ethyl 4-hydroxy-2-pentynoate, (II) (180.0 mg,  
1.266 mmol), were reacted in the presence of Cp\*RuCl(COD) (Cp\* =  
1,2,3,4,5-pentamethylcyclopentadiene and COD = 1,5-cycloocta-  
diene). The reaction mixture was stirred at 333 K for 1 h. The crude  
product was purified by column chromatography (gradient of ethyl  
acetate–hexanes = 1:19 to 1:4) to yield the isochromene (III) (yield:  
181.2 mg, 0.6330 mmol, 50%). Suitable crystals were grown from a  
solution of (III) in diethyl ether.

## Crystal data

$C_{17}H_{18}O_4$   
 $M_r = 286.31$   
 Orthorhombic,  $Pna2_1$   
 $a = 9.6237$  (7) Å  
 $b = 18.8830$  (12) Å  
 $c = 8.4729$  (4) Å  
 $V = 1539.73$  (17) Å<sup>3</sup>

$Z = 4$   
 $D_x = 1.235$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation  
 $\mu = 0.09$  mm<sup>-1</sup>  
 $T = 150$  (1) K  
 2.6, 27.5  
 $0.45 \times 0.22 \times 0.16$  mm

## Data collection

Bruker–Nonius KappaCCD  
 diffractometer  
 $\varphi$  scans and  $\omega$  scans with  $\kappa$  offsets  
 Absorption correction: multi-scan  
 (SORTAV; Blessing 1995)  
 $T_{\min} = 0.882$ ,  $T_{\max} = 0.986$

7737 measured reflections  
 1857 independent reflections  
 1567 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.042$   
 $\theta_{\text{max}} = 27.5^\circ$

## Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.040$   
 $wR(F^2) = 0.099$   
 $S = 1.07$   
 1857 reflections  
 211 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0434P)^2 + 0.2438P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.001$   
 $\Delta\rho_{\text{max}} = 0.20$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.15$  e Å<sup>-3</sup>  
 Extinction correction: *SHELXTL*  
 Extinction coefficient: 0.070 (9)

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$C9-H9A\cdots O4^i$	1.00	2.32	3.275 (3)	160
$C12-H12B\cdots O4^i$	0.99	2.57	3.442 (3)	147

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

In the absence of significant anomalous dispersion effects, Friedel pairs were merged. The two C atoms of the terminal ethyl group were modelled as disordered over two sites, the ratio of refined occupancies being 0.598 (10):0.402 (10) for C16/C17:C16A/C17A. The C16–C17 and C16–O3 bond lengths were restrained to be equal to the C16A–C17A and C16A–O3A bond lengths, respectively, with an effective standard deviation of 0.003 Å. H atoms were placed in calculated positions ( $C-H = 0.95-1.00$  Å) and refined as riding, with  $U_{\text{iso}}(H) = 1.2U_{\text{eq}}(C)$  or  $1.5U_{\text{eq}}(\text{methyl } C)$ .

Data collection: *COLLECT* (Nonius, 2002); cell refinement: *DENZO-SMN* (Otwinowski & Minor, 1997); data reduction: *DENZO-SMN*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXTL* (Sheldrick, 2001); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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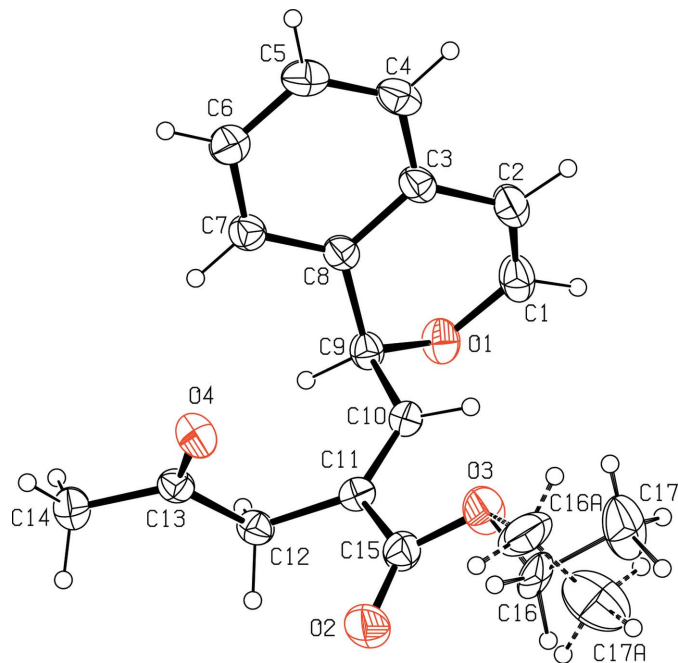


Figure 1

The molecular structure of (III), showing 30% probability displacement ellipsoids (arbitrary spheres for H atoms). The bonds of the minor disorder component are shown as dashed lines.

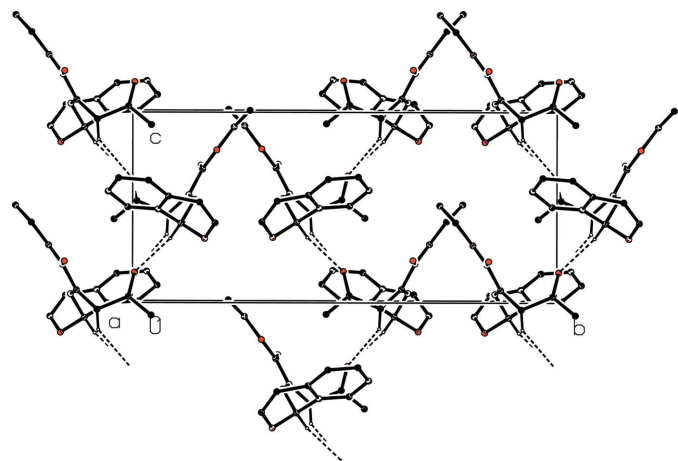


Figure 2

A partial packing plot of (III), showing hydrogen bonds as dashed lines. H atoms not involved in hydrogen bonding have been omitted. Only one disorder component is shown.

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