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Key indicators

Single-crystal X-ray study
 $T = 293\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.005\text{ \AA}$
 R factor = 0.069
 wR factor = 0.157
Data-to-parameter ratio = 12.3For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

Ethyl 2-phenyl-3-(pyridin-2-yl)acrylate

In the title compound, $\text{C}_{16}\text{H}_{15}\text{NO}_2$, the pyridine and benzene rings are nearly coplanar and form a π -conjugation system with the ethylcarboxylate substituent nearly perpendicular to the styrylpyridine plane. The molecular packing is stabilized by weak $\text{C}-\text{H}\cdots\pi$ interactions.

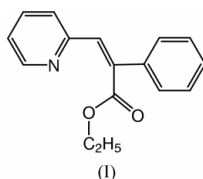
Received 24 March 2003

Accepted 3 April 2003

Online 9 April 2003

Comment

As part of our studies on photo-induced oxygenation reactions of indolizine derivatives (Tian *et al.*, 2001), we have recently carried out such a reaction on 2-phenyl-3-(4-chlorobenzoyl)-indolizine and obtained the title compound, (I), as one of the products. Here we report its crystal structure.



The bond lengths in the title structure are normal (Allen *et al.*, 1987) and show π -conjugation in the styrylpyridine moiety. The exocyclic angles $\text{C}6-\text{C}7-\text{C}8$ [$124.6(3)^\circ$] and $\text{C}7-\text{C}8-\text{C}9$ [$122.2(3)^\circ$] deviate from the normal value of 120° . This may be due to the repulsion between atoms $\text{H}6$ and $\text{H}9$ [$2.01(4)\text{ \AA}$]. The dihedral angle between the pyridine and benzene rings of $2.1(1)^\circ$ indicates planarity of the styrylpyridine moiety, resulting from the π -conjugation. The ethylcarboxylate substituent is also nearly planar, with $\text{C}14$ having a maximum deviation of $0.049(3)\text{ \AA}$ from the weighted least-squares plane. The ethylcarboxylate plane is nearly perpendicular to the styrylpyridine plane, making a dihedral angle of $81.5(1)^\circ$. In the crystal packing, symmetry-related molecules are interconnected by $\text{C}-\text{H}\cdots\pi$ interactions (Table 2) involving the pyridine and benzene rings to form a network. In

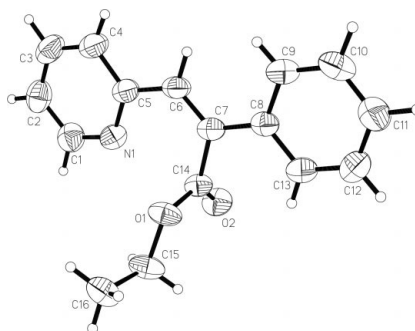


Figure 1

The structure of the title compound, showing 50% probability displacement ellipsoids and the atom-numbering scheme.

Table 2, $Cg1$ and $Cg2$ denote the centroids of the pyridine and benzene rings, respectively.

Experimental

The title compound was prepared by the photo-induced oxygenation reaction of 2-phenyl-3-(4-chlorobenzoyl)indolizine in ethanol with methylene blue as a sensitizer, and was isolated by column chromatography on silica gel with petroleum ether–ethyl acetate as eluents. Single crystals suitable for X-ray diffraction were obtained by slow evaporation of a petroleum ether–ethyl acetate solution.

Crystal data

$C_{16}H_{15}NO_2$	Mo $K\alpha$ radiation
$M_r = 253.29$	Cell parameters from 4380 reflections
Orthorhombic, $Pbca$	$\theta = 2.3\text{--}28.3^\circ$
$a = 11.0203$ (7) Å	$\mu = 0.08$ mm $^{-1}$
$b = 8.0642$ (5) Å	$T = 293$ (2) K
$c = 31.1269$ (18) Å	Block, colorless
$V = 2766.2$ (3) Å 3	$0.40 \times 0.24 \times 0.20$ mm
$Z = 8$	
$D_x = 1.216$ Mg m $^{-3}$	

Data collection

Siemens SMART CCD area-detector diffractometer	1920 reflections with $I > 2\sigma(I)$
ω scans	$R_{int} = 0.035$
Absorption correction: none	$\theta_{max} = 26.0^\circ$
13782 measured reflections	$h = -13 \rightarrow 10$
2709 independent reflections	$k = -9 \rightarrow 9$
	$l = -34 \rightarrow 38$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0455P)^2 + 1.7322P]$
$R[F^2 > 2\sigma(F^2)] = 0.069$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.157$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.16$	$\Delta\rho_{max} = 0.16$ e Å $^{-3}$
2709 reflections	$\Delta\rho_{min} = -0.18$ e Å $^{-3}$
221 parameters	
H atoms treated by a mixture of independent and constrained refinement	

Table 1

Selected geometric parameters (Å, °).

O1–C14	1.331 (3)	C5–C6	1.469 (4)
O1–C15	1.457 (3)	C6–C7	1.337 (4)
O2–C14	1.195 (3)	C7–C8	1.476 (4)
N1–C1	1.325 (4)	C7–C14	1.510 (3)
N1–C5	1.338 (3)		
C14–O1–C15	116.5 (2)	C8–C7–C14	115.4 (2)
C1–N1–C5	117.6 (3)	C13–C8–C9	116.2 (3)
N1–C1–C2	124.5 (4)	C9–C8–C7	122.2 (3)
C7–C6–C5	127.4 (3)	O2–C14–O1	125.3 (2)
C6–C7–C8	124.6 (3)	O1–C14–C7	110.0 (2)

Table 2

Hydrogen-bonding geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C1–H1 \cdots Cg1 ⁱ	0.99 (4)	2.95 (3)	3.793 (4)	144 (2)
C4–H4 \cdots Cg1 ⁱⁱ	0.91 (3)	2.97 (3)	3.661 (4)	135 (3)
C10–H10 \cdots Cg2 ⁱⁱ	0.95 (3)	2.91 (3)	3.682 (4)	140 (2)
C16–H16C \cdots Cg2 ⁱⁱⁱ	0.96	3.13	3.817 (4)	130

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

All H atoms, apart from the methyl H atoms, were located from a difference Fourier map and refined isotropically; the C–H distances range from 0.89 (4) to 0.99 (4) Å and U_{iso} values range from 0.063 (8) to 0.098 (12) Å 2 . The methyl H atoms were fixed geometrically and treated as riding on the parent C atom, with C–H = 0.96 Å and $U_{iso}(H) = 1.5 U_{eq}(C)$. Rotating-group refinement was used for the methyl group. As a result of the large fraction of weak data at higher angles, the 2θ maximum was limited to 52° .

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, 1990).

The authors thank the Malaysian Government and Universiti Sains Malaysia for research grant R&D No. 304/PFIZIK/670011. AU thanks Universiti Sains Malaysia for a Visiting Post-Doctoral Fellowship.

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