

difference electron density map were 0.30 and $-0.25 \text{ e } \text{Å}^{-3}$. The refinement was terminated when the parameter shifts fell below 0.09 of the corresponding e.s.d.'s and those for the solvent molecule below 0.4 e.s.d.'s. Atomic scattering factors were taken from *International Tables for X-ray Crystallography* (1974). Molecular geometry and interatomic distances were calculated by *PARST* (Nardelli, 1978). The fractional coordinates and the equivalent isotropic thermal parameters of all non-H atoms are listed in Table 1. The atomic numbering scheme with thermal ellipsoids for non-H atoms is drawn using *ORTEP* (Johnson, 1976) in Fig. 1. Interatomic distances and selected angles are listed in Table 2.*

* List of structure factors, H-atom positions and anisotropic thermal parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 54896 (22 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: LI9092]

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Structure of a Cyclopenta[*h*]indolizine

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Abstract. Ethyl 3,4-dihydrocyclopenta[*h*]indolizine-1-carboxylate, $\text{C}_{13}\text{H}_{13}\text{NO}_2$, $M_r = 215.25$, triclinic, $P\bar{1}$, $a = 8.239(1)$, $b = 9.750(1)$, $c = 7.856(1) \text{ Å}$, $\alpha = 105.67(1)^\circ$, $\beta = 118.14(1)^\circ$, $\gamma = 79.85(1)^\circ$, $V = 534.8(1) \text{ Å}^3$, $Z = 2$, $D_x = 1.336 \text{ g cm}^{-3}$, $\lambda(\text{Mo } K\alpha) = 0.71069 \text{ Å}$, $\mu = 0.85 \text{ cm}^{-1}$, $F(000) = 228$, $T = 297 \text{ K}$, final $R = 0.037$ for 1732 observed [$I > 3.00\sigma(I)$] reflections. The pyrrole and pyridine rings in the indolizine skeleton are planar with mean deviations 0.001 (1) and 0.004 (2) Å, respectively, and inclined to one another at 0.98° . The planar five-membered ring attached to the indolizine ring is slightly corrugated with larger mean deviation of 0.012 (2) Å, but this ring is also almost coplanar with the pyrrole ring with a dihedral angle of 1.49° . The delocalized ring system extends to the ester carbonyl group as indicated by the shortened $\text{C1}_{\text{ring}}-\text{C11}_{\text{ester}}$ bond of 1.442 (2) Å. The ester group at the 1-position is also coplanar with the indolizine ring with a dihedral angle of 1.61° .

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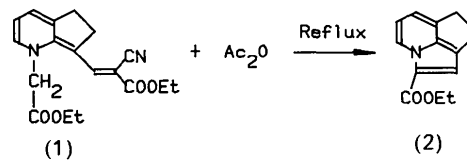
Related literature. The structure of the title compound was determined as part of a study on structures with possible photochromic properties (Vojtěchovský & Hašek, 1992, and references therein).

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Experimental. The reaction of ethyl 3-[2-cyano-2-(ethoxycarbonyl)vinyl]-1,2-dihydro-4*H*-cyclopenta[*b*]pyridine-4-acetate (1) (328 mg) with acetic anhydride ($3 \mu\text{m}^3$) under reflux for 12 h smoothly afforded the title compound, ethyl 3,4-dihydrocyclopenta[*h*]indolizine-1-carboxylate (2), in a 41% yield (Kakehi, Ito & Yotsuya, 1986).



Recrystallization from ethanol gave white prisms. D_m not determined. Crystal $0.24 \times 0.40 \times 0.48 \text{ mm}$. Rigaku AFC-5S diffractometer, graphite-monochromated $\text{Mo } K\alpha$ radiation. Cell constants from setting angles of 25 reflections ($39.31 < 2\theta < 39.90^\circ$). ω - 2θ scans. Correction for Lorentz-polarization effects. $2\theta_{\text{max}} = 55.0^\circ$ with $0 \leq h \leq 10$, $-12 \leq k \leq 12$,

Table 1. Fractional atomic coordinates and equivalent isotropic thermal parameters (Å²)
$$B_{eq} = (8\pi^2/3) \sum_{i=1}^3 \sum_{j=1}^3 U_{ij} a_i^* a_j^* a_i \cdot a_j$$

	x	y	z	B _{eq}
O1	-0.1818 (2)	0.2336 (1)	-0.6085 (2)	4.84 (5)
O2	-0.2602 (1)	0.0506 (1)	-0.5423 (1)	3.96 (5)
N1	0.0627 (2)	0.3175 (1)	-0.1950 (2)	3.11 (4)
C1	-0.0488 (2)	0.2018 (2)	-0.2809 (2)	3.19 (5)
C2	-0.0237 (2)	0.1379 (2)	-0.1282 (2)	3.30 (6)
C3	0.1032 (2)	0.2137 (2)	0.0505 (2)	3.19 (5)
C4	0.2045 (3)	0.2366 (2)	0.2738 (2)	3.82 (6)
C5	0.3237 (3)	0.3697 (2)	0.3395 (3)	4.09 (7)
C6	0.2735 (2)	0.4180 (2)	0.1507 (2)	3.47 (6)
C7	0.3129 (2)	0.5227 (2)	0.0924 (3)	4.31 (7)
C8	0.2244 (2)	0.5213 (2)	-0.1140 (3)	4.29 (7)
C9	0.1038 (2)	0.4239 (2)	-0.2539 (3)	3.78 (6)
C10	0.1505 (2)	0.3204 (1)	0.0017 (2)	3.11 (5)
C11	-0.1660 (2)	0.1668 (2)	-0.4908 (2)	3.41 (6)
C12	-0.3803 (2)	0.0039 (2)	-0.7515 (2)	3.87 (6)
C13	-0.4718 (3)	-0.1238 (2)	-0.7745 (3)	4.65 (8)

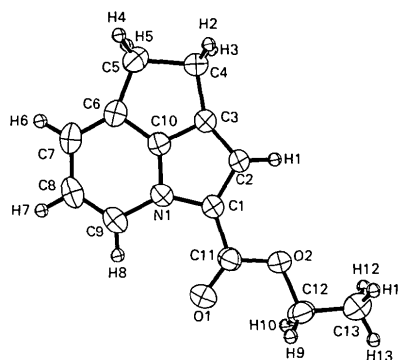
$-10 \leq l \leq 8$. Three standard reflections (002, 12 $\bar{2}$, 1 $\bar{1}$ 2) observed after every 150 reflections, average variation 1.3%. 2609 reflections measured, 2440 unique reflections ($R_{int} = 0.025$) and 1732 independent observed reflections [$I > 3.00\sigma(I)$]. Structure solved by direct methods with *MITHRIL* (Gilmore, 1984) utilizing the *TEXSAN* (Molecular Structure Corporation, 1985) system. Scattering factors and anomalous-dispersion corrections from *International Tables for X-ray Crystallography* (1974, Vol. IV, pp. 72, 99, 149). Azimuthal scans of several reflections indicated no need for an absorption correction. $\sum w(|F_o| - |F_c|)^2$ minimized, least-squares weights $4F_o^2/\sigma^2(F_o^2)$, 198 parameters varied. The H atoms were located from a difference Fourier map and refined isotropically. The full-matrix least-squares refinement with anisotropic thermal parameters for non-H atoms led to $R = 0.037$, $wR = 0.047$. Maximum shift/e.s.d. in final cycle, $\Delta/\sigma = 0.01$; goodness of fit indicator, $S = [\sum(|F_o| - |F_c|)/\sigma]/(n - m) = 1.71$; secondary-extinction value = 0.13282×10^{-4} ; maximum positive and negative electron density in the final difference map, $(\Delta\rho)_{max} = 0.17$ and $(\Delta\rho)_{min} = -0.18 \text{ e \AA}^{-3}$. Fractional coordinates and B_{eq} values are in Table 1,* the bond distances and angles in Table 2. Fig. 1 is an *ORTEPII* (Johnson, 1976) drawing showing the numbering system.

Related literature. The bond distances and angles for the indolizine skeleton are similar to those found in 1-acetoxy-2,3-diphenylindolizine (Wadsworth,

* Lists of structure factors, anisotropic thermal parameters, H-atom coordinates, bond distances and angles involving H atoms, torsion angles and least-squares planes have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 54941 (24 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: AL0510]

Table 2. Bond distances (Å) and angles (°)

O1—C11	1.216 (2)	C3—C4	1.516 (2)
O2—C11	1.347 (2)	C3—C10	1.372 (2)
O2—C12	1.452 (2)	C4—C5	1.589 (2)
N1—C1	1.394 (2)	C5—C6	1.523 (2)
N1—C9	1.391 (2)	C6—C7	1.367 (2)
N1—C10	1.356 (2)	C6—C10	1.386 (2)
C1—C2	1.412 (2)	C7—C8	1.428 (3)
C1—C11	1.442 (2)	C8—C9	1.355 (3)
C2—C3	1.392 (2)	C12—C13	1.494 (3)
C11—O2—C12	116.3 (1)	C5—C6—C7	139.5 (2)
C1—N1—C9	138.4 (1)	C5—C6—C10	104.4 (1)
C1—N1—C10	105.7 (1)	C7—C6—C10	116.1 (2)
C9—N1—C10	115.9 (1)	C6—C7—C8	117.4 (2)
N1—C1—C2	107.8 (1)	C7—C8—C9	124.1 (2)
N1—C1—C11	121.3 (1)	N1—C9—C8	118.7 (2)
C2—C1—C11	130.8 (1)	N1—C10—C3	113.1 (1)
C1—C2—C3	108.4 (1)	N1—C10—C6	127.8 (1)
C2—C3—C4	148.4 (1)	C3—C10—C6	119.1 (1)
C2—C3—C10	105.0 (1)	O1—C11—O2	123.4 (1)
C4—C3—C10	106.4 (1)	O1—C11—C1	125.1 (2)
C3—C4—C5	104.0 (1)	O2—C11—C1	111.5 (1)
C4—C5—C6	106.0 (1)	O2—C12—C13	107.3 (1)

Fig. 1. An *ORTEPII* (Johnson, 1976) illustration of the title compound.

Bender, Smith, Luss & Weidner, 1986). However, the distance for the N1—C10 bond [1.356 (2) Å] in the title compound is shorter than that [1.405 (3) Å] in 1-acetoxy-2,3-diphenylindolizine, whereas the bond angles 113.1 (1) and 127.8 (1)° for N1—C10—C3 and N1—C10—C6 in the former are larger than those of 106.5 (2) and 118.9 (2)° in the latter. This suggests that the annelation of the five-membered ring at the 1- and 8-positions of indolizine has a substantial effect on the configuration around C10.

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