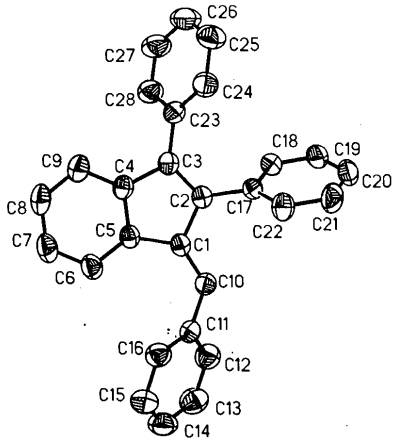

Fig. 1. *ORTEP* drawing (at 50% probability) of 1-benzylidene-2,3-diphenylindene showing the adopted labeling.

This compound was prepared under the auspices of the late Professor J. J. Zuckerman, formerly of the Department of Chemistry, University of Oklahoma, Norman, OK 73109.

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Ethyl 2,3-Bis(trifluoromethyl)-2,3-dihydroindolizine-1-carboxylate

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Abstract. $C_{13}H_{11}F_6NO_2$, $M_r = 327{\cdot}2$, monoclinic, $P2_1/c$, $a = 15{\cdot}144\ (2)$, $b = 14{\cdot}036\ (2)$, $c = 14{\cdot}101\ (2)$ Å, $\beta = 110{\cdot}99\ (1)°$, $V = 2798{\cdot}4$ Å^3, $Z = 8$, $D_x = 1{\cdot}55$ Mg m^{-3}, $F(000) = 1328$, λ(Mo $K\alpha$) $= 0{\cdot}71069$ Å, $\mu = 0{\cdot}110$ mm^{-1}, $T = 293$ K, $R = 0{\cdot}054$ for 2533 unique reflexions [$F \geq 3\sigma(F)$]. The asymmetric unit contains two molecules distinguished only by a minor disorder of one of the ethyl groups. With the exception of the disordered region, bond lengths agree within 1σ, bond angles within 2σ, and torsion angles within 3σ. A short C—C bond [1·421 (5), 1·425 (6) Å] links the carboxy and indolizine π systems, thereby forming a dipole, whose poles are situated at the ring N and carboxy O.

Experimental. The sample was prepared by 1,3-dipolar cycloaddition of *N*-2,2,2-trifluoroethylpyridinium-triflate to perfluorobut-2-yne in the presence of triethylamine and chloroform solvent. Purification by column chromatography followed by recrystallization from methylene chloride and methanol yielded crystals suitable for X-ray work.

Crystal dimensions 0·5 × 0·3 × 0·2 mm, Enraf–Nonius CAD-4 diffractometer, graphite-monochromated Mo $K\alpha$ radiation, unit-cell dimensions from setting angles of 25 accurately centred reflexions ($7{\cdot}5 \leq \theta \leq 8{\cdot}7°$), ω–2θ scan mode, ω scan width $0{\cdot}70 + 0{\cdot}35\tan\theta$ (°) and scan speed ranging from 0·6 to 5° min^{-1} according to the intensity gathered in a pre-scan, $-17 \leq h \leq 15$, $0 \leq k \leq 16$, $0 \leq l \leq 16$, $0 \leq \theta \leq 25°$, 5404 reflexions measured, 3691 unique ($R_{int} = 0{\cdot}011$), 2533 observed [$F \geq 3\sigma(F)$], intensity standards ($60\bar{2}$, $0\bar{5}3$, $\bar{1}1\bar{5}$) measured every 2·5 h, decay 12%, decay and Lp corrections applied but absorption ignored, *MULTAN*80 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980) used to solve the phase problem, all non-hydrogen atoms except minor component of disordered atom C(14*B*) [C(15*B*) 8 (2)% occupancy] found in Fourier map, remaining atoms, including H, from ΔF synthesis, full-matrix least-squares refinement based on F using *SHELX*76 (Sheldrick, 1976) with bond lengths C(13*B*)—C(15*B*) and C(13*B*)—C(14*B*) tied together, final $R = 0{\cdot}054$, $wR = 0{\cdot}045$, $w = 1{\cdot}9898/[\sigma^2(F) + 0{\cdot}0003F^2]$, anisotropic thermal parameters for heavier atoms, isotropic for H and C(15*B*). Maximum fluctuation in final ΔF map in range −0·22 to 0·24 e Å^{-3}, maximum Δ/σ 0·060 [x, H(131*B*)]. Scattering factors from *International Tables for X-ray Crystallography* (1974), computation carried out on the joint CDC7600/

0108-2701/89/050826-02$03.00

Table 1. *Fractional atomic coordinates* ($\times 10^4$) *and equivalent isotropic vibrational parameters* ($Å^2 \times 10^3$) *for non-hydrogen atoms*

	x	y	z	U/U_{eq}†
F(1A)	3527 (2)	6162 (2)	2150 (2)	93 (1)
F(2A)	3612 (1)	4685 (2)	2503 (2)	89 (1)
F(3A)	3572 (2)	5145 (2)	1048 (2)	100 (1)
F(4A)	5815 (2)	4737 (2)	940 (2)	118 (1)
F(5A)	6848 (2)	5049 (2)	2399 (2)	97 (1)
F(6A)	6564 (2)	3608 (2)	1910 (2)	109 (1)
O(1A)	5972 (2)	6657 (2)	4921 (2)	74 (1)
O(2A)	5255 (2)	7291 (2)	3372 (2)	87 (1)
C(1A)	5448 (2)	5635 (3)	3535 (3)	56 (1)
C(2A)	5000 (3)	5395 (3)	2424 (3)	56 (1)
C(3A)	5389 (3)	4404 (3)	2335 (3)	58 (1)
N(4A)	5755 (2)	4070 (2)	3391 (2)	55 (1)
C(5A)	5980 (3)	3149 (3)	3683 (3)	64 (1)
C(6A)	6322 (3)	2933 (3)	4670 (3)	66 (1)
C(7A)	6458 (3)	3663 (3)	5386 (3)	67 (1)
C(8A)	6227 (3)	4573 (3)	5101 (3)	61 (1)
C(9A)	5824 (2)	4814 (3)	4058 (3)	56 (1)
C(10A)	5532 (3)	6585 (3)	3904 (3)	65 (1)
C(11A)	3931 (3)	5351 (3)	2033 (3)	71 (1)
C(12A)	6158 (3)	4450 (3)	1902 (3)	77 (1)
C(13A)	6102 (4)	7603 (3)	5345 (4)	84 (1)
C(14A)	6679 (6)	7508 (5)	6455 (4)	116 (2)
F(1B)	11316 (2)	4526 (2)	3449 (2)	97 (1)
F(2B)	11277 (2)	4896 (2)	1965 (2)	117 (1)
F(3B)	11396 (2)	5981 (2)	3070 (2)	104 (1)
F(4B)	8962 (2)	4478 (2)	269 (2)	116 (1)
F(5B)	8003 (2)	4895 (2)	1002 (2)	100 (1)
F(6B)	8229 (2)	3421 (2)	789 (2)	116 (1)
O(1B)	9053 (2)	6631 (2)	4065 (2)	100 (1)
O(2B)	9744 (2)	7172 (2)	3000 (2)	105 (1)
C(1B)	9517 (3)	5528 (3)	3123 (3)	59 (1)
C(2B)	9907 (3)	5229 (3)	2330 (3)	58 (1)
C(3B)	9476 (3)	4238 (3)	2019 (3)	63 (1)
N(4B)	9157 (2)	3972 (2)	2848 (2)	60 (1)
C(5B)	8902 (3)	3073 (3)	3018 (4)	77 (1)
C(6B)	8581 (3)	2929 (4)	3775 (4)	89 (1)
C(7B)	8522 (3)	3696 (4)	4378 (4)	88 (1)
C(8B)	8785 (3)	4580 (4)	4223 (3)	69 (1)
C(9B)	9149 (2)	4750 (3)	3437 (3)	56 (1)
C(10B)	9468 (3)	6506 (3)	3372 (3)	78 (1)
C(11B)	10966 (3)	5156 (3)	2705 (3)	76 (1)
C(12B)	8655 (3)	4258 (4)	1020 (3)	83 (1)
C(13B)	8918 (6)	7617 (4)	4300 (6)	134 (2)
C(14B)	8407 (10)	7613 (7)	4994 (11)	201 (4)
C(15B)	7965 (18)	7925 (42)	4081 (47)	44 (26)

† $U_{eq} = \frac{1}{3}\sum_i\sum_j U_{ij}\mathbf{a}_i.\mathbf{a}_j a_i^* a_j^*$.

Table 2. *Selected bond lengths* (Å) *and angles* (°)

	Molecule *A*	Molecule *B*
F(1)–C(11)	1·331 (5)	1·328 (5)
F(2)–C(11)	1·332 (5)	1·340 (6)
F(3)–C(11)	1·330 (5)	1·337 (5)
F(4)–C(12)	1·329 (5)	1·336 (6)
F(5)–C(12)	1·328 (5)	1·326 (6)
F(6)–C(12)	1·330 (6)	1·324 (6)
O(1)–C(10)	1·351 (4)	1·350 (6)
O(1)–C(13)	1·441 (5)	1·455 (7)
O(2)–C(10)	1·223 (5)	1·216 (6)
C(1)–C(2)	1·505 (5)	1·499 (6)
C(1)–C(9)	1·377 (5)	1·370 (6)
C(1)–C(10)	1·421 (5)	1·425 (6)
C(2)–C(3)	1·533 (6)	1·533 (5)
C(2)–C(11)	1·514 (6)	1·503 (6)
C(3)–N(4)	1·467 (4)	1·465 (6)
C(3)–C(12)	1·498 (7)	1·508 (5)
N(4)–C(5)	1·362 (5)	1·365 (6)
N(4)–C(9)	1·384 (5)	1·375 (5)
C(5)–C(6)	1·336 (6)	1·339 (8)
C(6)–C(7)	1·400 (6)	1·394 (8)
C(7)–C(8)	1·347 (6)	1·344 (7)
C(8)–C(9)	1·416 (5)	1·423 (6)
C(13)–C(14)	1·500 (7)	1·448 (21)
		1·430 (34)
C(9)–C(1)–C(2)	108·5 (3)	109·4 (3)
C(3)–C(2)–C(1)	104·2 (3)	103·2 (4)
N(4)–C(3)–C(2)	102·9 (3)	103·3 (3)
C(5)–N(4)–C(3)	124·9 (3)	124·7 (4)
C(9)–N(4)–C(3)	111·0 (3)	110·9 (3)
C(9)–N(4)–C(5)	124·1 (3)	124·4 (4)
N(4)–C(9)–C(1)	110·5 (3)	110·2 (4)

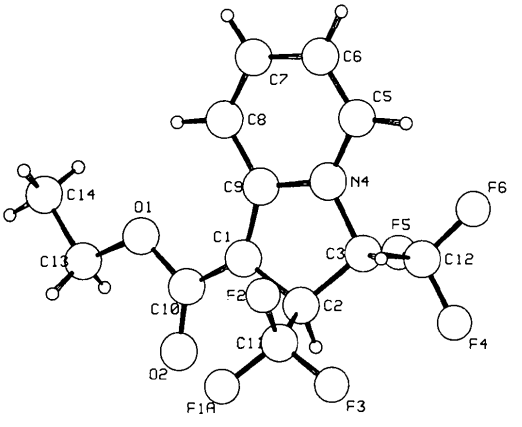

Fig. 1. The title molecule (*A*) drawn using *PLUTO* (Motherwell & Clegg, 1978). Each conformer shares a common atomic labelling scheme distinguished by the final character (*A* or *B*).

Amdahl 470 system of the University of Manchester Regional Computing Centre. Literature survey from the Cambridge Structural Database was performed using the Crystal Structure Search and Retrieval interactive system (CSSR, 1984). Fractional atomic coordinates and equivalent isotropic vibrational parameters for non-hydrogen atoms are presented in Table 1* and selected bond lengths and angles in Table 2. The title molecule, including atomic labelling, is displayed in Fig. 1.

Related literature. Ethyl 1-trifluoromethylindolizine-3-carboxylate (Pritchard, 1988).

The authors thank the SERC for financial support *via* an equipment grant.

* Lists of structure factors, H-atom coordinates, anisotropic vibrational parameters and full molecular geometry have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51594 (22 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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