The independent C—F bond lengths of 1·326 (3) and 1·335 (2) Å in this structure are normal (Krishnamurthy & Vijayan, 1979). All the atoms in the molecule except F(17) lie in one plane, the torsion angle C(3)—C(4)—C(15)—F(17) is −120·4 (2)°.

In the excited state, charge transfer occurs from the amino (donor) to carboxyl (acceptor) group (Masilamani, Chandrasekar, Sivaram, Sivasankar & Natarajan, 1986). The trifluoromethyl group, being a second electron-accepting moiety, is able to facilitate charge transfer from the donor site (Guo & Feng, 1987). As a consequence, twisted intramolecular charge transfer is probably enhanced in the excited state.

The packing of the molecules in the unit cell viewed down the *b* axis is shown in Fig. 2. Since the molecule as a whole lies on the mirror plane all the molecules in the unit cell are stacked along the *b* axis with a repeat distance of 3·44 Å. In the mirror plane, the molecules are linked by hydrogen bonds of the C—H···O type [C(13)···O(11)′ 3·319 (4); C(13)—H(C13) 0·93 (5); H(C13)···O(11)′ 2·41 (5) Å; C(13)—H(C13)···O(11)′ = 164 (4)°; symmetry code $x-\frac{1}{2}$, y, $\frac{1}{2}-z$] (Taylor & Kennard, 1982).

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2,3,6,7-1*H*,5*H*-Tetrahydro-10-methylquinolizino[1,9a,9-*gh*][1,4]benzoxazin[2]one

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Abstract. $C_{15}H_{16}N_2O_2$, $M_r = 256·3$, triclinic, $P\bar{1}$, $a = 8·238\,(1)$, $b = 8·358\,(1)$, $c = 10·890\,(2)$ Å, $\alpha = 77·26\,(1)$, $\beta = 74·09\,(2)$, $\gamma = 59·66\,(2)°$, $V = 619·2\,(2)$ Å^3, $Z = 2$, $D_m = 1·380$, $D_x = 1·374$ g cm^{-3}, $\lambda(\mathrm{Cu}\ K\alpha) = 1·5418$ Å, $\mu = 7·07$ cm^{-1}, $F(000) = 272$, $T = 297$ K. The final R value is 0·047 for 1931 observed $[F_o \geq 2\sigma(F_o)]$ reflections. The benzoxazine moiety is planar and the two piperidine rings adopt distorted sofa conformations. The crystal structure is stabilized by van der Waals interactions.

Introduction. Benzoxazine derivatives are found to give laser action in the 500–678 nm spectral range (Le Bris, Mugnier, Bourson & Valeur, 1984; Dupuy, Rulliere, Le Bris & Valeur, 1984). Some of these derivatives exhibit a wide tuning range compared to classical coumarin dyes. The title compound, a rigified laser dye, alone is found to give laser action in the range 480–630 nm in different solvents (Chandrasekar, Sastikumar, Nagarajan, Masilamani, Sivaram & Natarajan, 1986; Sastikumar, Chandrasekar, Bhaskaran, Masilamani, Natarajan & Sivaram, 1986). The structural study of this compound (Fig. 1) was performed to examine the conformational features of the fused piperidine ring system.

Experimental. Rectangular light brown crystals from methanol, D_m by flotation. Enraf–Nonius CAD-4 diffractometer, graphite-monochromated Cu $K\alpha$ radiation, crystal dimensions 0·3 × 0·3 × 0·5 mm, cell dimensions from 2θ angles of 25 reflections in the range $30 < \theta < 45°$; $\omega/2\theta$ scan technique, intensity variation of two standard reflections monitored every 100 reflections was <3%. Intensities were measured up to $2\theta = 140°$ for $h = 0$ to 10, $k = -10$ to 10 and $l = -13$ to 13, 2237 unique reflections were measured, 1931 were observed with $|F_o| \geq 2\sigma(|F_o|)$, intensity data were corrected for Lp but not for absorption. Structure solved by direct methods using *SHELXS*86 (Sheldrick, 1986), no correct solution in the space group $P\bar{1}$, attempts with $P1$ gave the correct solution with two centrosymmetrically related molecules. The origin shifted to that centre of symmetry, full-matrix least-squares refinement on F, using *SHELX*76 (Sheldrick, 1976), H atoms were from difference Fourier map, anisotropic thermal parameters for non-H and isotropic for H atoms, final $R = 0·047$, $wR = 0·054$, $w = 1·0/[\sigma^2(|F_o|) + 0·0073F_o^2]$, $S = 1·97$, $(\Delta/\sigma)_{max} = 0·04$, final difference map was featureless with max. and min. peak heights of 0·22 and $-0·28$ e Å^{-3}, no correction for secondary extinction, atomic scattering factors for all atoms were as in *SHELX*76 (Sheldrick, 1976), geometrical calculations were carried out using *PARST* (Nardelli, 1983).

Discussion. The final positional and equivalent isotropic thermal parameters for the non-H atoms are given in Table 1.* A perspective view, with atomic labelling, is shown in Fig. 1. Bond lengths and valence angles and endocyclic torsion angles for the rings in the quinolizine moiety are given in Table 2. The bond lengths and the valence angles in this structure are normal. The oxazine ($\chi^2 = 52·2$) and the benzene rings ($\chi^2 = 13·7$) are planar and the dihedral angle between them is 1·1°.

Table 1. *Positional parameters and equivalent isotropic thermal parameters*

$$B_{eq} = \tfrac{8}{3}\pi^2(U_{11} + U_{22} + U_{33}).$$

	x	y	z	B_{eq}(Å^2)
O(1)	−0·1942 (2)	0·2669 (1)	0·1746 (1)	3·71 (4)
C(2)	−0·1796 (2)	0·1549 (2)	0·2869 (1)	3·98 (6)
C(3)	−0·2059 (2)	−0·0081 (2)	0·2939 (1)	4·03 (6)
N(4)	−0·2370 (2)	−0·0495 (2)	0·1983 (1)	3·88 (5)
C(5)	−0·2840 (2)	0·0280 (2)	−0·0213 (1)	3·54 (6)
C(6)	−0·2999 (2)	0·1425 (2)	−0·1339 (1)	3·34 (5)
C(7)	−0·2804 (2)	0·3053 (2)	−0·1436 (1)	3·13 (5)
C(8)	−0·2436 (2)	0·3458 (2)	−0·0380 (1)	3·15 (5)
C(9)	−0·2283 (2)	0·2246 (2)	0·0713 (1)	3·11 (5)
C(10)	−0·2484 (2)	0·0651 (2)	0·0849 (1)	3·23 (5)
O(11)	−0·1473 (2)	0·1972 (2)	0·3729 (1)	5·58 (6)
C(12)	−0·1961 (3)	−0·1270 (3)	0·4196 (2)	5·55 (8)
C(13)	−0·3440 (3)	0·1071 (2)	−0·2474 (2)	4·24 (6)
C(14)	−0·4699 (3)	0·2917 (3)	−0·3154 (2)	4·68 (7)
C(15)	−0·3718 (3)	0·4097 (2)	−0·3573 (2)	4·63 (7)
N(16)	−0·2967 (2)	0·4215 (2)	−0·2546 (1)	4·01 (5)
C(17)	−0·2497 (3)	0·5724 (2)	−0·2765 (2)	4·67 (6)
C(18)	−0·1278 (2)	0·5504 (2)	−0·1868 (2)	4·36 (6)
C(19)	−0·2195 (2)	0·5157 (2)	−0·0506 (1)	3·97 (6)

Table 2. *Bond lengths* (Å), *bond angles* (°) *and selected torsion angles* (°) *for the quinolizine system*

O(1)—C(2)	1·359 (1)	C(7)—C(8)	1·413 (2)
O(1)—C(9)	1·385 (2)	C(7)—N(16)	1·364 (2)
C(2)—C(3)	1·467 (3)	C(8)—C(9)	1·371 (2)
C(2)—O(11)	1·204 (2)	C(8)—C(19)	1·503 (3)
C(3)—N(4)	1·290 (2)	C(9)—C(10)	1·396 (3)
C(3)—C(12)	1·499 (2)	C(13)—C(14)	1·518 (2)
N(4)—C(10)	1·379 (2)	C(14)—C(15)	1·496 (4)
C(5)—C(6)	1·371 (2)	C(15)—N(16)	1·460 (3)
C(5)—C(10)	1·398 (2)	N(16)—C(17)	1·452 (3)
C(6)—C(7)	1·427 (3)	C(17)—C(18)	1·506 (3)
C(6)—C(13)	1·504 (3)	C(18)—C(19)	1·507 (2)
C(2)—O(1)—C(9)	120·7 (1)	C(9)—C(8)—C(19)	123·1 (1)
O(1)—C(2)—O(11)	117·8 (1)	O(1)—C(9)—C(8)	117·2 (1)
O(1)—C(2)—C(3)	117·1 (1)	C(8)—C(9)—C(10)	124·1 (1)
C(3)—C(2)—O(11)	125·1 (1)	O(1)—C(9)—C(10)	118·7 (1)
C(2)—C(3)—C(12)	116·6 (1)	C(5)—C(10)—C(9)	116·9 (1)
C(2)—C(3)—N(4)	122·8 (1)	N(4)—C(10)—C(9)	121·8 (1)
N(4)—C(3)—C(12)	120·5 (2)	N(4)—C(10)—C(5)	121·3 (1)
C(3)—N(4)—C(10)	118·8 (2)	C(6)—C(13)—C(14)	109·4 (2)
C(6)—C(5)—C(10)	122·1 (1)	C(13)—C(14)—C(15)	110·2 (2)
C(5)—C(6)—C(13)	122·5 (1)	C(14)—C(15)—N(16)	112·6 (2)
C(5)—C(6)—C(7)	119·3 (1)	C(7)—N(16)—C(15)	122·7 (1)
C(7)—C(6)—C(13)	118·1 (1)	C(15)—N(16)—C(17)	114·9 (1)
C(6)—C(7)—N(16)	120·2 (1)	C(7)—N(16)—C(17)	122·3 (1)
C(6)—C(7)—C(8)	119·8 (1)	N(16)—C(17)—C(18)	112·8 (1)
C(8)—C(7)—N(16)	119·9 (1)	C(17)—C(18)—C(19)	109·3 (2)
C(7)—C(8)—C(19)	119·2 (1)	C(8)—C(19)—C(18)	109·4 (1)
C(7)—C(8)—C(9)	117·7 (1)		
C(7)—C(6)—C(13)—C(14)	−33·5 (2)	C(7)—C(8)—C(19)—C(18)	−32·8 (2)
C(13)—C(6)—C(7)—N(16)	−1·7 (2)	C(6)—C(13)—C(14)—C(15)	58·2 (2)
C(6)—C(7)—N(16)—C(17)	−170·4 (2)	C(13)—C(14)—C(15)—N(16)	−49·0 (3)
C(6)—C(7)—N(16)—C(15)	12·8 (3)	C(14)—C(15)—N(16)—C(7)	13·7 (3)
C(8)—C(7)—N(16)—C(17)	9·4 (3)	C(7)—N(16)—C(17)—C(18)	17·7 (3)
C(8)—C(7)—N(16)—C(15)	−167·4 (2)	N(16)—C(17)—C(18)—C(19)	−51·1 (2)
N(16)—C(7)—C(8)—C(19)	−1·0 (2)	C(17)—C(18)—C(19)—C(8)	57·5 (2)

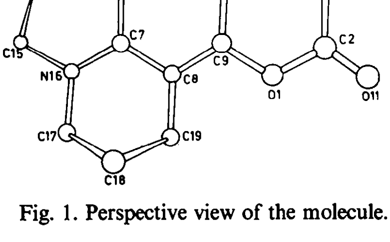

Fig. 1. Perspective view of the molecule.

Both piperidine rings adopt distorted sofa conformations with asymmetry parameters ΔC_s(C7) = 14·1 and ΔC_2(C7—N16) = 15·5° for ring A, ΔC_s(C7) = 10·6 and ΔC_2(C7—N16) = 8·5° for ring B (Duax,

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* Lists of structure factors, anisotropic thermal parameters, H-atom coordinates, 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 52508 (17 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

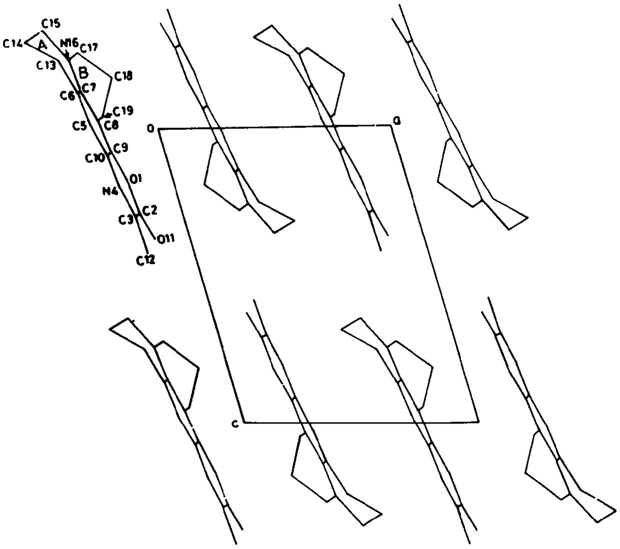

Fig. 2. Molecular packing of the title compound in the unit cell viewed down the *b* axis.

Weeks & Rohrer, 1976). In the piperidine ring *A*, the major puckering [0·818 (3) Å from the mean plane through C(6), C(7), C(13) and N(16)] occurs at C(14), while for ring *B* C(18) lies 0·787 (2) Å from the plane through C(7), C(8), N(16) and C(19), *i.e.* puckering of approximately the same magnitude but in the opposite direction. The means of the moduli of the endocyclic torsion angles in these rings are 28·2 and 28·3° respectively. In the quinolizine ring system as a whole the endocyclic torsion angles are related by almost exact twofold symmetry through C(7)—N(16).

The packing of the molecules down the *b* axis is shown in Fig. 2. The crystal structure is stabilized by van der Waals interactions.

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10-Cyano-1,2,5,6-tetrahydro-3*H*,7*H*,11*H*-[1]benzopyrano[6,7,8-*ij*]quinolizin-11-one

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Abstract. $C_{16}H_{14}N_2O_2$, $M_r = 266·30$, monoclinic, $P2_1/n$, $a = 7·224$ (1), $b = 11·856$ (1), $c = 15·255$ (2) Å, $\beta = 99·50$ (1)°, $V = 1288·6$ (3) Å^3, $Z = 4$, $D_x = 1·373$ g cm^{-3}, λ(Cu $K\alpha$) = 1·5418 Å, $\mu = 7·05$ cm^{-1}, $F(000) = 560$, $T = 297$ K. Final R value is 0·071 for 2255 observed [$F_o \geq 4\sigma(F_o)$] reflections. The coumarin moiety is planar and the cyano group is coplanar with it. One of the two fused piperidine rings (*A*) is disordered; the major (80%) conformer adopts a distorted sofa conformation while the minor conformer (20%) is a flattened half chair. Ring *B* is a perfect sofa. The crystal structure is stabilized by van der Waals interactions.

Introduction. The structural study of the title compound (Fig. 1), a rigified laser dye (Reynolds & Drexhage, 1975), is part of our investigations on the structural aspects of compounds of this type.

Experimental. The compound was from Exciton (USA), rectangular orange coloured crystals from a mixture of aqueous ethanol and chloroform, Enraf–Nonius CAD-4 diffractometer, graphite-monochromated Cu $K\alpha$ radiation, crystal size 0·33 × 0·35 × 0·38 mm, unit-cell dimensions from least-squares refinement of 2θ values of 25 reflections in the range $35 < \theta < 45°$, data collection range $2 < \theta < 75°$,