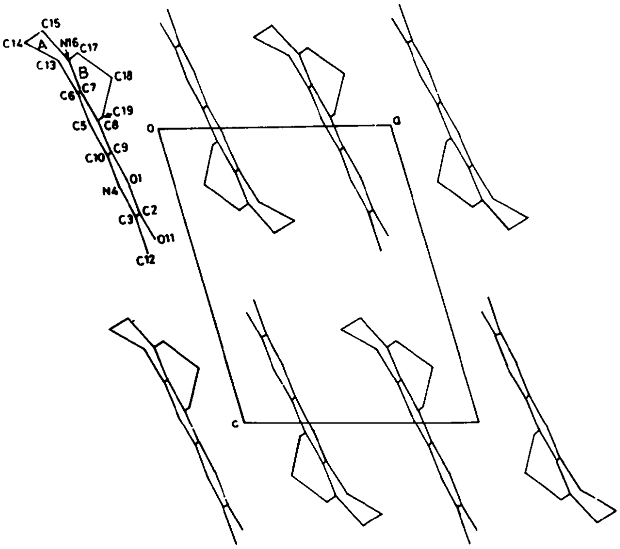

Fig. 2. Molecular packing of the title compound in the unit cell viewed down the b axis.

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

By K. Chinnakali, S. Selladurai, K. Sivakumar, K. Subramanian and S. Natarajan

Department of Physics, Anna University, Madras 600 025, *India*

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Abstract. $C_{16}H_{14}N_2O_2$, $M_r = 266{\cdot}30$, monoclinic, $P2_1/n$, $a = 7{\cdot}224$ (1), $b = 11{\cdot}856$ (1), $c = 15{\cdot}255$ (2) Å, $\beta = 99{\cdot}50$ (1)°, $V = 1288{\cdot}6$ (3) Å^3, $Z = 4$, $D_x = 1{\cdot}373$ g cm^{-3}, λ(Cu $K\alpha$) = 1·5418 Å, $\mu = 7{\cdot}05$ 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 $2 < \theta < 75°$,

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ω–2θ scan technique, *hkl* range: $h = 0$ to 9, $k = 0$ to 14 and $l = -19$ to 19, 2449 unique reflections were measured, 2255 were observed with $|F_o| \geq 4\sigma(|F_o|)$, correction for Lp and absorption (ψ scans, 92·03% minimum relative transmission), three standard reflections, 2% intensity variation. Structure solved by direct methods using *SHELXS*86 (Sheldrick, 1986), two ambiguous positions for C(15), that with the highest peak height was chosen, full-matrix least-squares refinement on F using *SHELX*76 (Sheldrick, 1976). The alternative position for C(15) was observed in a ΔF synthesis and site occupancies were refined, these were later fixed at 0·80 and 0·20, H-atom positions from difference Fourier map except for those of C(15) and C(15)′, isotropic refinement for H atoms and the disordered C(15), anisotropic temperature factors for all other non-H atoms, final $R = 0{\cdot}071$ (high R value is ascribed to the disorder in the structure), $wR = 0{\cdot}087$, $w = 1{\cdot}0/[\sigma^2(|F_o|) + 0{\cdot}0004F_o^2]$, $S = 1{\cdot}72$, $(\Delta/\sigma)_{\max} = 0{\cdot}002$, final difference map featureless with $\Delta\rho$ within $+0{\cdot}59$, $-0{\cdot}47$ e Å^{-3}. No correction for secondary extinction, atomic scattering factors for all the atoms were as in *SHELX*76 (Sheldrick, 1976), geometrical calculations using *PARST* (Nardelli, 1983).

Discussion. The positional and equivalent isotropic thermal parameters of the non-H atoms are given in Table 1;* Fig. 1 shows the atomic nomenclature used. Bond lengths and bond angles are listed in Table 2. Bond lengths and bond angles in the coumarin moiety are normal (Gnanaguru, Ramasubbu, Venkatesan & Ramamurthy, 1985; Chinnakali, Sivakumar & Natarajan, 1989).

The benzene ring in the coumarin moiety is planar ($\chi^2 = 8{\cdot}4$) and makes an angle of only 0·88 (7)° with the planar pyrone ring confirming the overall planarity of the coumarin ring system. The cyano group lies in the plane of the pyrone ring with

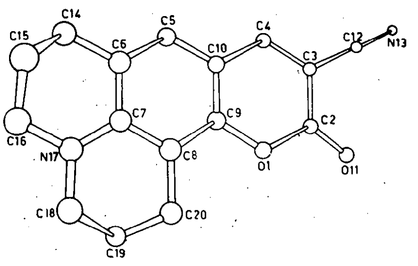

Fig. 1. Perspective view of the molecule.

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

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

	x	y	z	B_{eq} (Å^2)
O(1)	0·2413 (2)	0·1044 (1)	0·5644 (1)	4·01 (1)
C(2)	0·2286 (3)	0·1986 (2)	0·5109 (2)	3·94 (6)
C(3)	0·2233 (3)	0·1786 (2)	0·4165 (2)	4·03 (6)
C(4)	0·2331 (3)	0·0717 (2)	0·3843 (1)	4·00 (6)
C(5)	0·2616 (3)	−0·1351 (2)	0·4126 (2)	4·23 (6)
C(6)	0·2776 (4)	−0·2235 (2)	0·4705 (2)	4·16 (6)
C(7)	0·2778 (3)	−0·2019 (2)	0·5639 (1)	3·69 (5)
C(8)	0·2682 (3)	−0·0893 (2)	0·5943 (1)	3·62 (5)
C(9)	0·2511 (3)	−0·0039 (2)	0·5324 (1)	3·46 (6)
C(10)	0·2469 (3)	−0·0223 (2)	0·4406 (1)	3·66 (6)
O(11)	0·2255 (3)	0·2886 (1)	0·5468 (1)	5·32 (5)
C(12)	0·2132 (4)	0·2767 (2)	0·3623 (2)	4·71 (7)
N(13)	0·2047 (4)	0·3560 (2)	0·3184 (2)	6·30 (8)
C(14)	0·2969 (5)	−0·3435 (2)	0·4409 (2)	6·06 (9)
C(15)	0·2074 (5)	−0·4221 (4)	0·4947 (3)	5·70*
C(15)′	0·348 (1)	−0·423 (1)	0·510 (1)	4·14*
C(16)	0·2811 (5)	−0·4077 (2)	0·5945 (2)	5·70 (8)
N(17)	0·2913 (3)	−0·2891 (2)	0·6220 (1)	4·49 (5)
C(18)	0·3078 (4)	−0·2720 (2)	0·7175 (2)	5·29 (8)
C(19)	0·3874 (4)	−0·1587 (2)	0·7467 (2)	5·49 (8)
C(20)	0·2814 (4)	−0·0646 (2)	0·6919 (2)	4·66 (7)

* Isotropic refinement only.

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

O(1)—C(2)	1·377 (3)	C(8)—C(9)	1·376 (3)
O(1)—C(9)	1·379 (3)	C(8)—C(20)	1·505 (3)
C(2)—C(3)	1·453 (4)	C(9)—C(10)	1·413 (2)
C(2)—O(11)	1·201 (3)	C(12)—N(13)	1·150 (4)
C(3)—C(4)	1·365 (3)	C(14)—C(15)	1·461 (6)
C(4)—C(12)	1·422 (4)	C(15)—C(16)	1·537 (5)
C(4)—C(10)	1·400 (3)	C(16)—N(17)	1·465 (3)
C(5)—C(6)	1·363 (4)	N(17)—C(18)	1·456 (3)
C(5)—C(10)	1·413 (3)	C(18)—C(19)	1·499 (3)
C(6)—C(7)	1·447 (3)	C(19)—C(20)	1·523 (4)
C(6)—C(14)	1·506 (3)	C(14)—C(15)′	1·42 (1)
C(7)—C(8)	1·419 (3)	C(15)—C(15)′	1·00 (1)
C(7)—N(17)	1·355 (3)	C(16)—C(15)′	1·45 (1)

C(2)—O(1)—C(9)	123·2 (2)	O(1)—C(9)—C(10)	120·0 (2)
O(1)—C(2)—O(11)	117·0 (2)	C(5)—C(10)—C(9)	117·1 (2)
O(1)—C(2)—C(3)	116·3 (2)	C(4)—C(10)—C(9)	118·2 (2)
C(3)—C(2)—O(11)	126·7 (2)	C(4)—C(10)—C(5)	124·7 (2)
C(2)—C(3)—C(4)	120·9 (2)	C(3)—C(12)—N(13)	179·9 (3)
C(4)—C(3)—C(12)	115·7 (2)	C(6)—C(14)—C(15)	111·3 (3)
C(3)—C(4)—C(10)	121·4 (2)	C(14)—C(15)—C(16)	111·9 (3)
C(6)—C(5)—C(10)	122·3 (2)	C(15)—C(16)—N(17)	112·5 (3)
C(5)—C(6)—C(14)	122·3 (3)	C(7)—N(17)—C(16)	123·4 (2)
C(5)—C(6)—C(7)	119·2 (2)	C(16)—N(17)—C(18)	114·3 (2)
C(7)—C(6)—C(14)	118·5 (2)	C(7)—N(17)—C(18)	122·2 (2)
C(6)—C(7)—N(17)	119·8 (2)	N(17)—C(18)—C(19)	112·7 (2)
C(6)—C(7)—C(8)	119·7 (2)	C(18)—C(19)—C(20)	111·1 (2)
C(8)—C(7)—N(17)	120·4 (2)	C(8)—C(20)—C(19)	110·2 (2)
C(7)—C(8)—C(20)	120·5 (2)	C(2)—C(3)—C(12)	115·7 (2)
C(7)—C(8)—C(9)	118·1 (2)	C(6)—C(14)—C(15)′	115·5 (5)
C(9)—C(8)—C(20)	121·3 (2)	C(14)—C(15)′—C(16)	119·1 (8)
O(1)—C(9)—C(8)	116·5 (1)	C(15)′—C(16)—N(17)	111·5 (5)
C(8)—C(9)—C(10)	123·5 (2)		

C(7)—C(6)—C(14)—C(15)	33·3 (4)	C(18)—C(19)—C(20)—C(8)	−51·0 (3)
C(6)—C(14)—C(15)—C(16)	−54·4 (4)	C(19)—C(20)—C(8)—C(7)	25·1 (3)
C(14)—C(15)—C(16)—N(17)	45·6 (4)	C(20)—C(8)—C(7)—N(17)	2·7 (3)
C(15)—C(16)—N(17)—C(7)	−13·7 (4)	C(6)—C(7)—N(17)—C(18)	174·8 (2)
C(16)—N(17)—C(7)—C(6)	−8·4 (3)	C(8)—C(7)—N(17)—C(16)	173·1 (2)
N(17)—C(7)—C(6)—C(14)	−1·3 (3)	C(7)—C(6)—C(14)—C(15)′	−11·1 (6)
C(8)—C(7)—N(17)—C(18)	−3·7 (3)	C(6)—C(14)—C(15)′—C(16)	33·7 (9)
C(7)—N(17)—C(18)—C(19)	−24·1 (3)	C(14)—C(15)′—C(16)—C(17)	−41·4 (9)
N(17)—C(18)—C(19)—C(20)	51·4 (3)	C(7)—N(17)—C(16)—C(15)′	28·6 (6)

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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 52511 (18 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

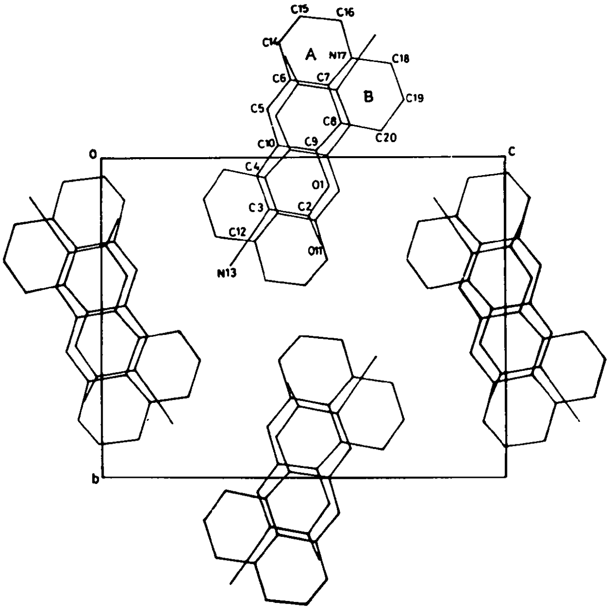

Fig. 2. Molecular packing of the title compound in the unit cell viewed down the *a* axis.

maximum deviations of −0·025 (3) and −0·046 (3) Å for C(12) and N(13) respectively.

In the quinolizine ring system, the major conformer of piperidine ring *A* [with C(15)] is a distorted sofa, [ΔC_2(C7—N17) = 12·34 and ΔC_s(C7) = 13·62°] while the minor conformer with C(15)′ is closer to a flattened half chair [ΔC_2(C6—C7) = 4·08 and ΔC_s(C7) = 11·79°]. The piperidine ring *B* adopts a perfect sofa conformation [ΔC_s(C7) = 0·86°] (Duax, Weeks & Rohrer, 1976). The endocyclic torsion angles defining the conformations of the fused piperidine ring system are given in Table 2. The mean value of the moduli of the torsion angles in each of these rings is 26°.

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

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Structure of Cerpegin, a New Alkaloid

By K. Sivakumar, S. Eswaramurthy, K. Subramanian and S. Natarajan

Department of Physics, Anna University, Madras 600 025, *India*

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Abstract. $C_{10}H_{11}NO_3$, M_r = 193·2, orthorhombic, *Pbca*, a = 13·731 (3), b = 12·264 (3), c = 11·318 (2) Å, V = 1905·9 (7) Å^3, Z = 8, D_x = 1·347 g cm^{-3}, λ(Cu $K\alpha$) = 1·5418 Å, μ = 7·95 cm^{-1}, F(000) = 816, T = 298 K, final R = 0·054 for 1472 observed reflections. Cerpegin consists of fused pyridinone and furanone systems in a planar arrangement, the ring planes making an angle of 1·02 (6)°. The crystal structure is stabilized by two intermolecular C—H···O contacts of 3·299 (3) and 3·409 (3) Å.

Introduction. The new alkaloid, cerpegin, has been isolated from the plant *Ceropegia Juncea*, which is used as a tranquillizer, anti-inflammatory and anti-ulcer agent in the Indian indigenous system of medicine. The structural study of this compound has been undertaken to verify the molecular structure proposed from the spectral data.

Experimental. Prismatic, transparent crystals from a mixture of acetone and hexane, crystal size 0·4 × 0·4 × 0·6 mm, preliminary cell parameters and space group from photographic methods, intensity data collected by multiple-film equi-inclination Weissenberg technique, nickel-filtered Cu $K\alpha$ radiation was used; intensities of 1068 reflections were visually

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