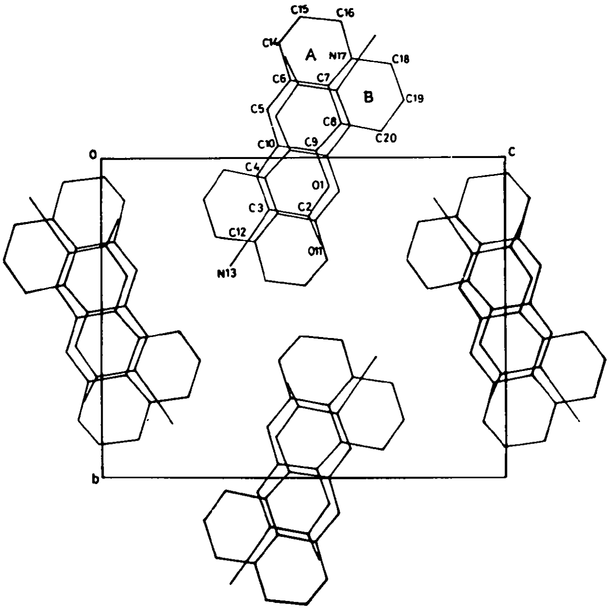

Fig. 2. Molecular packing of the title compound in the unit cell viewed down the *a* axis.

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

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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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Table 1. *Fractional atomic coordinates and equivalent isotropic temperature factors*

$B_{eq} = (8\pi^2/3)$ trace **U**.

	x	y	z	B_{eq}(Å^2)
C(1)	0·4965 (2)	0·6885 (2)	0·2680 (2)	3·45 (5)
O(2)	0·4662 (1)	0·8023 (1)	0·2632 (1)	4·28 (4)
C(3)	0·3922 (2)	0·8174 (2)	0·1850 (2)	3·69 (5)
C(4)	0·2959 (1)	0·6869 (2)	0·0486 (2)	3·29 (5)
N(5)	0·2925 (1)	0·5757 (1)	0·0205 (2)	3·45 (4)
C(6)	0·3504 (2)	0·5003 (2)	0·0717 (2)	3·93 (6)
C(7)	0·4192 (2)	0·5253 (3)	0·1518 (2)	3·82 (5)
C(8)	0·4271 (1)	0·6350 (2)	0·1840 (2)	3·07 (5)
C(9)	0·3680 (1)	0·7114 (3)	0·1353 (2)	3·12 (5)
O(10)	0·3588 (1)	0·9061 (1)	0·1680 (2)	5·21 (6)
O(11)	0·2410 (1)	0·7507 (1)	−0·0008 (2)	4·78 (5)
C(12)	0·2222 (2)	0·5421 (2)	−0·0685 (2)	4·72 (7)
C(13)	0·4847 (2)	0·6494 (2)	0·3939 (2)	4·65 (7)
C(14)	0·6010 (2)	0·6818 (2)	0·2265 (2)	5·99 (7)

Table 2. *Bond lengths* (Å) *and bond angles* (°), *involving non*-H *atoms*

C(1)—O(2)	1·457 (3)	C(4)—C(9)	1·426 (3)
C(1)—C(8)	1·497 (3)	C(4)—O(11)	1·222 (3)
C(1)—C(13)	1·512 (3)	N(5)—C(6)	1·350 (3)
C(1)—C(14)	1·512 (4)	N(5)—C(12)	1·455 (3)
O(2)—C(3)	1·360 (3)	C(6)—C(7)	1·345 (4)
C(3)—C(9)	1·455 (3)	C(7)—C(8)	1·398 (3)
C(3)—O(10)	1·196 (3)	C(8)—C(9)	1·357 (3)
C(4)—N(5)	1·401 (3)		

C(13)—C(1)—C(14)	112·2 (2)	N(5)—C(4)—C(9)	112·6 (2)
C(8)—C(1)—C(14)	112·5 (2)	C(4)—N(5)—C(12)	117·1 (1)
C(8)—C(1)—C(13)	113·0 (2)	C(4)—N(5)—C(6)	123·3 (2)
O(2)—C(1)—C(14)	108·1 (2)	C(6)—N(5)—C(12)	119·6 (2)
O(2)—C(1)—C(13)	107·9 (2)	N(5)—C(6)—C(7)	123·1 (2)
O(2)—C(1)—C(8)	102·4 (2)	C(6)—C(7)—C(8)	116·7 (2)
C(1)—O(2)—C(3)	111·6 (2)	C(1)—C(8)—C(7)	129·5 (2)
O(2)—C(3)—O(10)	121·0 (2)	C(7)—C(8)—C(9)	120·8 (2)
O(2)—C(3)—C(9)	107·5 (2)	C(1)—C(8)—C(9)	109·6 (2)
C(9)—C(3)—O(10)	131·5 (2)	C(4)—C(9)—C(8)	123·3 (2)
C(9)—C(4)—O(11)	127·5 (2)	C(3)—C(9)—C(8)	108·9 (2)
N(5)—C(4)—O(11)	119·9 (2)	C(3)—C(9)—C(4)	127·8 (2)

estimated using a calibrated chart. The structure was solved by direct methods using *MULTAN* (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980), refinement of the structure did not lower the R value below 0·128 due to the poor quality of the data. Hence the intensity data were recollected on an Enraf–Nonius CAD-4 diffractometer using the same crystal, graphite-monochromated Cu $K\alpha$ radiation was used, cell parameters from least-squares treatment of setting angles of 25 reflections with $25 < \theta < 40°$, $\omega/2\theta$ scan technique, the intensity variation of two standard reflections monitored at every 98 reflections was less than 3%, total number of reflections measured 1551 with $2\theta \leq 140°$, 1472 observed reflections with $I > 3\sigma(I)$, range of hkl: h 0 → 16, k 0 → 14 and l 0 → 13, Lp corrected but not absorption, structure solved by direct methods using *SHELXS*86 (Sheldrick, 1986), refinement on F by full-matrix least-squares method, H atoms from difference Fourier map, anisotropic thermal parameters for non-H and isotropic for H atoms, H-atom positions not refined, final $R = 0{\cdot}054$, $wR = 0{\cdot}062$, $w = 1/[\sigma^2(|F_o|) + 0{\cdot}00005F_o^2]$, $S = 1{\cdot}64$, $(\Delta/\sigma)_{max} = 0{\cdot}02$, max. and min. peak height in final difference map 0·27 and $-0{\cdot}21$ e Å^{-3}, no correction for secondary extinction, atomic scattering factors for all atoms as in *SHELX*76 (Sheldrick, 1976), other geometrical calculations using *PARST* (Nardelli, 1983), an IBM 360/44 computer was used.*

Discussion. Table 1 lists the final atomic coordinates and equivalent isotropic temperature factors of the non-H atoms. The numbering of atoms in the molecule is shown in Fig. 1. The bond lengths and angles are given in Table 2, and these are normal.

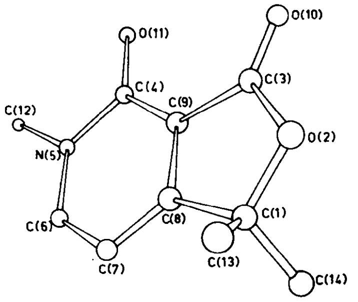

Fig. 1. Numbering of atoms in the molecule.

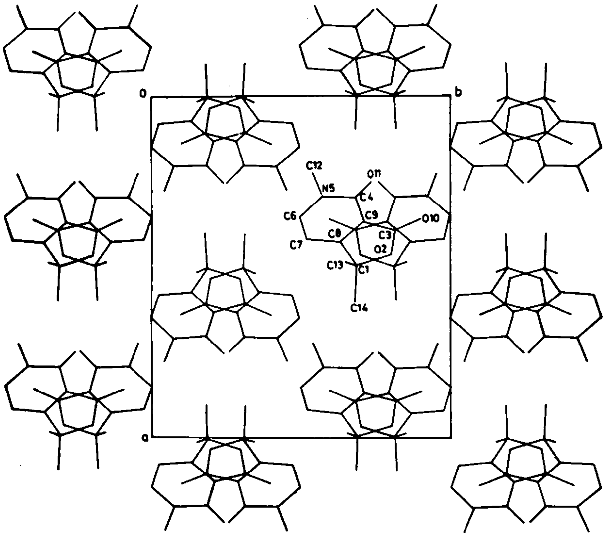

Fig. 2. Molecular packing of cerpegin in the unit cell viewed down the c axis.

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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 52531 (13 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

There is localization of the double bonds C(6)═C(7) and C(8)═C(9), confirmed by their respective lengths, 1·345 (4) and 1·357 (3) Å. The furanone ring is planar within experimental error, with a maximum deviation of 0·018 (2) Å from the mean plane for C(1); the keto oxygen O(10) lies in this plane. The pyridinone ring is also planar, the maximum deviation being −0·014 (2) Å for C(6); atoms O(11) and C(12) lie in the same plane. The dihedral angle between these two planes, 1·02 (6)°, means that the whole molecule, except the two methyl groups substituted at C(1), lie in a plane. These two methyl groups are on either side of this molecular plane with deviations of −1·188 (2) and 1·320 (2) Å for C(13) and C(14) respectively.

The packing of the molecules in the unit cell viewed down the *c* axis is shown in Fig. 2. There are two intermolecular hydrogen bonds of the C—H···O type observed in this structure. C(6)···O(11^{i}) = 3·409 (3), C(6)—H(6) = 1·04, H(6)···O(11^{i}) 2·41 Å, C(6)—H(6)···O(11^{i}) = 162°; C(7)···O(2^{ii}) = 3·299 (3), C(7)—H(7) = 0·98, H(7)···O(2^{ii}) = 2·35 Å, C(7)—H(7)··· O(2^{ii}) = 162° [symmetry code: (i) $-x+\frac{1}{2}, y-\frac{1}{2}, z$; (ii) $-x+1, y-\frac{1}{2}, z+\frac{1}{2}$]. These C—H···O hydrogen bonds are within the limits specified by Taylor & Kennard (1982).

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Structure of Gangetinin

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Abstract. $C_{26}H_{26}O_5$, $M_r = 418·5$, monoclinic, $P2_1$, $a = 7·315$ (1), $b = 10·774$ (1), $c = 14·760$ (2) Å, $\beta = 102·85$ (2)°, $V = 1134·1$ (4) Å^3, $Z = 2$, $D_x = 1·226$ g cm^{-3}, λ(Cu $K\alpha$) = 1·5418 Å, $\mu = 6·47$ cm^{-1}, $F(000) = 444$, $T = 297$ K, final R value is 0·035 for 1780 observed reflections. Gangetinin contains six fused rings *A–F*. The pyrone rings *A* and *F* adopt half-chair conformations while the pyrone ring *C* is a distorted sofa. There are two planar benzene rings *B* and *E* and a five-membered furan ring *D* in an envelope conformation. The ring junction *C*/*D* shows *cis* fusion which induces a large (*ca* 37°) bend in the hexacyclic framework.

Introduction. Gangetinin, a pterocarpanoid, has been isolated from the roots of the plant *Desmodium gangeticum* (Purushothaman, Chandrasekharan, Balakrishna & Connolly, 1975) along with the other pterocarpanoids gangetin and desmodin (Purushothaman, Kishore, Narayanaswami & Connolly, 1971). These pterocarpanoids show anti-implantation and anti-inflammatory activities (Pillai, Alam & Purushothaman, 1981).

Experimental. Crystals from methanol, Enraf–Nonius CAD-4 diffractometer, crystal size 0·3 × 0·3 × 0·5 mm, graphite-monochromated Cu $K\alpha$ radiation, cell parameters from least-squares treatment of the setting angles of 25 reflections in the range $30 < \theta < 45°$; $\omega/2\theta$ scan technique, intensity variation of two standard reflections monitored every 98 reflections showed no significant variation, total number of reflections measured 2157 with $2\theta \le 120°$, 1780 observed reflections with $I > 3\sigma(I)$, range of *hkl*: $h = -8$ to 8, $k = 0$ to 12, $l = 0$ to 17, intensity data corrected for Lp but not for absorption. Structure solved by direct methods using *MULTAN*80 (Main, Fiske, Hull, Lessinger, Germain, Declercq &

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