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Funding for this project was supplied by the Robert A. Welch Foundation (F-652) and the National Institutes of Health (GM 31077) to SFM.

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Acta Cryst. (1989). C**45**, 2020–2022

Structure of Eugenine, an Alkaloid from *Narcissus eugeniae*

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(*Received* 16 *December* 1988; *accepted* 3 *July* 1989)

Abstract. (5*R**,6a*S**,11a*R**,11b*R**)-5-Ethoxy-6a,7,-11a,11b-tetrahydro-2-methoxy-*N*-methyl-5*H*-[2]benzopyran[3,4-*g*]indolin-3-ol, $C_{19}H_{25}NO_4$, $M_r = 331{\cdot}4$, orthorhombic, $P2_12_12_1$, $a = 8{\cdot}585\ (5)$, $b = 13{\cdot}527\ (2)$, $c = 15{\cdot}429\ (8)$ Å, $V = 1791\ (3)$ Å^3, $Z = 4$, $D_x = 1{\cdot}229$ Mg m^{-3}, Mo $K\alpha$ radiation, $\lambda = 0{\cdot}71069$ Å, $\mu = 0{\cdot}90$ cm^{-1}, $F(000) = 712$, room temperature. The structure was solved by direct methods and refined to a final R value of 0·045 ($wR = 0{\cdot}042$) for 950 observed reflections. In the structure there is one weak intermolecular hydrogen bond C(10)—H(10*a*)···O(*m*) = 2·34 (8) Å forming an infinite chain along the twofold axis. The molecule is far from planar and the assignment of an ethyl radical in position C(5) has been confirmed in the X-ray analysis. Only the benzene ring is planar and the C—C bond distances and C—C—C bond angles have average values of 1·383 (19) Å and 119·9 (1)° respectively. Distances and angles elsewhere in the molecule are not unusual.

Experimental. Platy white crystals of eugenine, crystallized from acetone, 0·11 × 0·07 × 0·06 mm. Enraf–Nonius CAD–4 computer-controlled single-crystal diffractometer, graphite-monochromated Mo $K\alpha$ radiation, ω–2θ scan. Cell parameters from setting angles of 25 reflections having $1 \le \theta \le 25°$. Data collection at 293 K: index range $-10 \le h \le 10$, $0 \le k \le 16$, $0 \le l \le 18$ with $2\theta \le 50°$, three standard reflections (444, $\bar{4}44$, $4\bar{4}4$) measured every 60 min showed only random deviations from mean intensity, 1810 unique measured reflections of which 950 observed with $I(hkl) \ge 2\sigma(I)$.

Structure solved by *MULTAN*80 (Main *et al.*, 1980). The least-squares refinement used *SHELX*76 (Sheldrick, 1976). $\sum w(|F_o| - |F_c|)^2$ minimized where $w = 1{\cdot}355/|\sigma^2(F) + 0{\cdot}001125\ (F)^2|$. 317 parameters refined: atom coordinates, anisotropic temperature factors for all non-H atoms, positions of H atoms calculated; $R = 0{\cdot}045$, $wR = 0{\cdot}042$, $(\Delta/\sigma)_{max} = 0{\cdot}86$, max and min. in final $\Delta\rho$ map 0·20 and $-0{\cdot}21$ e Å^{-3}.

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Table 1. *Fractional atomic coordinates* ($\times 10^4$) *and equivalent isotropic temperature coefficients* ($Å^2$)

$B_{eq} = (8\pi^2/3)\sum_i\sum_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$

	x	y	z	B_{eq}
C(10)	8219 (13)	−2217 (6)	883 (7)	5·36 (2)
C(9)	7676 (14)	−2393 (8)	−29 (7)	6·21 (2)
C(8a)	6923 (11)	−1425 (6)	−291 (6)	4·43 (1)
C(11a)	6991 (10)	−754 (5)	478 (5)	3·75 (1)
C(8)	6271 (12)	−1198 (7)	−1026 (7)	4·81 (2)
C(7)	5381 (15)	−282 (8)	−1139 (7)	5·54 (2)
C(6a)	5429 (10)	429 (5)	−380 (5)	3·837 (6)
C(11b)	5560 (11)	−71 (5)	497 (5)	3·59 (1)
C(5)	6859 (11)	1867 (6)	61 (5)	3·635 (7)
C(4a)	6197 (9)	1657 (5)	943 (5)	3·48 (1)
C(11c)	5596 (9)	739 (5)	1167 (5)	3·366 (7)
C(1)	4978 (10)	610 (6)	1993 (5)	3·73 (1)
C(2)	4976 (11)	1361 (6)	2583 (6)	4·33 (1)
C(3)	5559 (9)	2282 (5)	2369 (5)	3·77 (1)
C(4)	6164 (10)	2426 (6)	1554 (6)	4·07 (1)
Ce(2)	4383 (16)	318 (7)	3777 (7)	5·40 (2)
Cm(1)	6636 (15)	3071 (8)	−1047 (7)	5·78 (1)
Ce(1)	7850 (15)	−1003 (7)	1989 (7)	5·76 (2)
Cm(2)	5683 (19)	3890 (12)	−1361 (10)	10·23 (2)
N(11)	7177 (8)	−1443 (5)	1217 (4)	4·15 (1)
O(6)	6796 (6)	1032 (3)	−494 (3)	4·26 (1)
O(*h*)	5577 (8)	3064 (3)	2959 (4)	4·90 (2)
O*e*(2)	4411 (8)	1275 (3)	3423 (4)	5·47 (4)
O(*m*)	5960 (6)	2644 (4)	−286 (3)	4·408 (5)

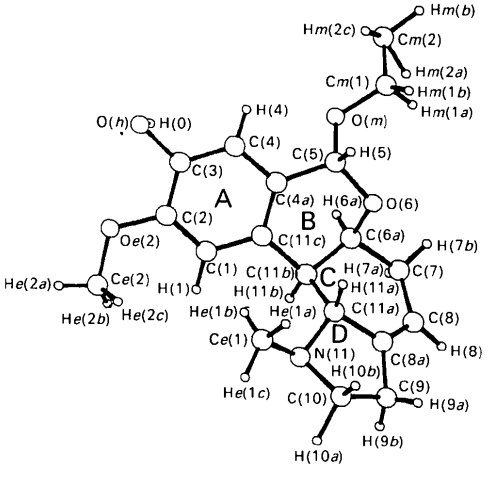

Fig. 1. Molecular structure of $C_{19}H_{25}NO_4$ showing the atom numbering.

Table 2. *Selected bond distances* (Å) *and angles* (°) *of the title compound*

Ring *A*			
C(11c)—C(1)	1·391 (11)	C(3)—O(*h*)	1·396 (9)
C(2)—C(1)	1·364 (12)	C(4)—C(3)	1·374 (12)
C(2)—O*e*(2)	1·389 (11)	C(4a)—C(4)	1·404 (11)
O*e*(2)—C*e*(2)	1·405 (11)	C(4a)—C(11c)	1·388 (10)
C(3)—C(2)	1·383 (11)		
Ring *B*			
C(6a)—C(11b)	1·517 (11)	O(*m*)—C*m*(1)	1·431 (12)
C(11c)—C(11b)	1·507 (10)	C*m*(1)—C*m*(2)	1·456 (20)
C(5)—C(4a)	1·502 (11)	C(5)—O(6)	1·418 (9)
C(5)—O(*m*)	1·409 (10)	C(6a)—O(6)	1·440 (9)
Rings *C* and *D*			
N(11)—C(10)	1·470 (12)	N(11)—C*e*(1)	1·451 (13)
C(10)—C(9)	1·501 (15)	C(11c)—C(11b)	1·537 (12)
C(9)—C(8a)	1·515 (14)	C(7)—C(6a)	1·516 (13)
C(8a)—C(11a)	1·495 (12)	C(8)—C(7)	1·466 (15)
N(11)—C(11a)	1·481 (9)	C(8a)—C(8)	1·301 (14)
Ring *A*			
C(11c)—C(1)—C(2)	121·2 (8)	C(3)—C(4)—C(4a)	121·1 (7)
C(1)—C(2)—C(3)	120·7 (8)	C(4)—C(4a)—C(11c)	119·2 (7)
C(2)—C(3)—C(4)	118·9 (7)	C(4a)—C(11c)—C(1)	118·8 (7)
Ring *B*			
C(6a)—C(11b)—C(11c)	106·8 (6)	C(4a)—C(5)—O(6)	112·4 (6)
C(4a)—C(11c)—C(11b)	119·2 (7)	O(6)—C(6a)—C(11b)	107·5 (6)
C(5)—C(4a)—C(11c)	122·4 (7)		
Ring *C*			
C(11b)—C(11a)—C(8a)	110·4 (7)	C(8)—C(7)—C(6a)	115·5 (9)
C(11a)—C(8a)—C(8)	124·4 (8)	C(11b)—C(6a)—C(7)	114·1 (6)
C(8a)—C(8)—C(7)	121·8 (9)	C(6a)—C(11b)—C(11a)	108·1 (7)
Ring *D*			
C(8a)—C(9)—C(10)	104·2 (8)	N(11)—C(11a)—C(8a)	103·5 (6)
C(9)—C(10)—N(11)	104·6 (8)	C(11a)—C(8a)—C(9)	107·2 (8)
C(10)—N(11)—C(11a)	104·1 (6)		

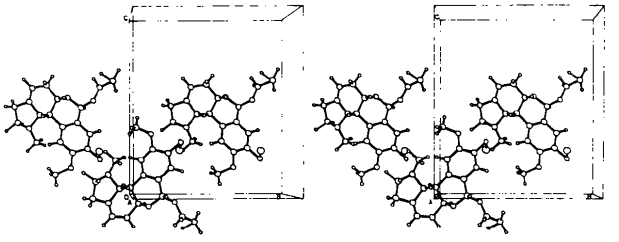

Fig. 2. A stereoscopic view of the unit-cell packing.

Atomic scattering factors from *International Tables for X-ray Crystallography* (1974). Drawings made with *PLUTO* (Motherwell & Clegg, 1978).*

Table 1 gives the final atomic coordinates. Bond lengths and angles are in Table 2; these are in good agreement with the results obtained for similar molecules (Clardy, Chan & Wildman, 1972). The structure of the compound is shown in Fig. 1 together with the atomic numbering. Fig. 2 shows a stereo-

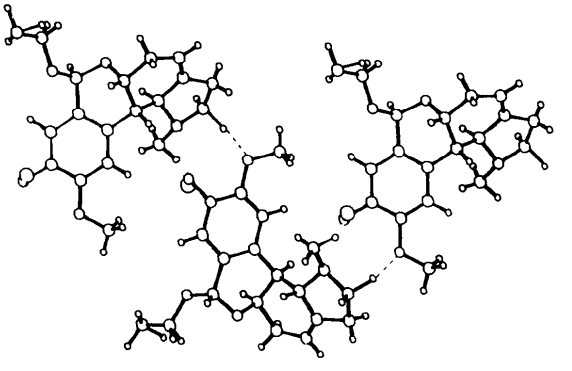

Fig. 3. Hydrogen-bond-like interaction making a chain along the *b* axis.

* Lists of structure factors, anisotropic thermal parameters, H-atom coordinates and all bond distances and angles have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52086 (8 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

view of the packing of the molecules in the cell. Fig. 3 shows the hydrogen-bond-like interaction C(10)—H(10*a*)···O(*m*)($\frac{1}{2}-x$, $\frac{1}{4}+y$, $\frac{1}{4}-z$).

Related literature. Alkaloids of the Amaryllidaceae plant family are currently being studied for their pharmacological properties. Members of the genus *Narcissus* L. are very widely distributed in the Iberian Peninsula. The title compound is an alkaloid isolated from *Narcissus eugeniae* (Bastida, Viladomat, Llabrés, Falco, Codina & Rubiralta, 1989). This plant was found to contain four alkaloids: galanthamine, homolycorine as the major alkaloid, lycorenine, and a new alkaloid, for which the name eugenine was proposed (Bastida *et al.*, 1989).

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Acta Cryst. (1989). C**45**, 2022–2023

Trimethyl(phenyl)ammonium-chlorid

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(*Eingegangen am* 21. *Juni* 1989; *angenommen am* 24. *Juli* 1989)

Abstract. $[N(CH_3)_3(C_6H_5)]Cl$, $M_r = 171{\cdot}67$, orthorhombic, $P2_12_12_1$, $a = 13{\cdot}307\ (2)$, $b = 10{\cdot}635\ (2)$, $c = 6{\cdot}742\ (1)$ Å, $V = 954{\cdot}1$ Å^3, $Z = 4$, $D_x = 1{\cdot}20$ g cm^{-3}, Mo $K\alpha$, $\lambda = 0{\cdot}7107$ Å, $\mu = 2{\cdot}95$ cm^{-1}, $F(000) = 368$, $T = 294$ K. $R = 0{\cdot}035$ for 735 unique observed reflections. The cations have N—C bond lengths of 1·50 to 1·52 Å. The Cl^- ion is nested in the three methyl groups of a neighboring cation and has Cl···H contacts to three phenyl H atoms of three other cations.

Experimentelles. Handelsübliches $[N(CH_3)_3(C_6H_5)]Cl$ wurde in CH_2Cl_2 gelöst und durch Zusatz von CCl_4 zur Kristallisation gebracht. Kristallgröße 0,14 × 0,15 × 0,27 mm. Vierkreisdiffraktometer Enraf–Nonius CAD-4. Gitterparameterbestimmung mit 12 Reflexen, $15 < \theta < 23°$. ω-scan, $\Delta\omega = 0{,}80° + 0{,}35° \tan\theta$, Meßgeschwindigkeit jeweils auf 2% statistischen Zählfehler abgestimmt, Meßbereich $\theta < 24°$, 0

Tabelle 1. *Atomkoordinaten und Parameter* $U_{äq}$ (Å^2) *für den äquivalenten isotropen Temperaturfaktor*

$U_{äq} = \frac{1}{3}(U_{11} + U_{22} + U_{33})$.

	x	*y*	*z*	$U_{äq}$
Cl	0,45615 (8)	0,4708 (1)	0,0869 (2)	0,0509 (7)
N	0,3692 (3)	0,6635 (3)	0,5972 (6)	0,050 (3)
C(1)	0,3246 (3)	0,7459 (4)	0,7547 (6)	0,035 (2)
C(2)	0,2204 (4)	0,7528 (5)	0,7670 (7)	0,047 (3)
C(3)	0,1774 (4)	0,8347 (5)	0,9026 (9)	0,055 (3)
C(4)	0,2365 (4)	0,9076 (5)	1,0239 (7)	0,057 (3)
C(5)	0,3396 (4)	0,8983 (4)	1,0139 (7)	0,053 (3)
C(6)	0,3842 (3)	0,8178 (5)	0,8782 (8)	0,048 (3)
C(7)	0,3289 (3)	0,5303 (4)	0,6141 (8)	0,051 (3)
C(8)	0,4815 (3)	0,6543 (5)	0,6070 (9)	0,056 (4)
C(9)	0,3415 (4)	0,7180 (5)	0,3966 (8)	0,057 (4)

Tabelle 2. *Bindungsabstände* (Å), Cl···H-*Kontaktabstände unter* 3,1 Å *und Bindungswinkel* (°)

Bezeichnung symmetrieäquivalenter Positionen: (i) $0{,}5-x$, $1-y$, $-0{,}5+z$; (ii) $1-x$, $-0{,}5+y$, $1{,}5-z$; (iii) $0{,}5+x$, $1{,}5-y$, $1-z$. Phenyl-H-Atome haben die gleichen Nummern wie die zugehörigen C-Atome; bei Methyl-H-Atomen bezeichnet die erste Ziffer die Nummer des C-Atoms.

N—C(1)	1,499 (5)	C(1)—N—C(7)	110,6 (4)
N—C(7)	1,519 (5)	C(1)—N—C(8)	113,7 (4)
N—C(8)	1,499 (5)	C(1)—N—C(9)	108,2 (3)
N—C(9)	1,516 (6)	C(7)—N—C(8)	106,7 (3)
C(1)—C(2)	1,391 (6)	C(7)—N—C(9)	109,8 (4)
C(2)—C(3)	1,386 (7)	C(8)—N—C(9)	107,8 (4)
C(3)—C(4)	1,374 (7)	N—C(1)—C(2)	117,9 (4)
C(4)—C(5)	1,377 (7)	N—C(1)—C(6)	121,6 (4)
C(5)—C(6)	1,386 (7)	C(6)—C(1)—C(2)	120,5 (4)
C(6)—C(1)	1,381 (6)	C(1)—C(2)—C(3)	118,9 (5)
		C(2)—C(3)—C(4)	120,7 (5)
Cl···H(2^i)	2,52	C(3)—C(4)—C(5)	120,0 (5)
Cl···H(3^{ii})	2,98	C(4)—C(5)—C(6)	120,2 (5)
Cl···H(4^{iii})	2,78	C(5)—C(6)—C(1)	119,6 (4)
Cl···H(73)	3,05		
Cl···H(82)	3,06		
Cl···H(91)	2,66		

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