S—C4—N3	127.0 (2)	126.3 (2)
N2—C4—N3	110.5 (2)	110.1 (2)
N2—C5—N4	110.2 (2)	109.9 (2)
N2—C5—C16	121.2 (2)	124.4 (2)
N4—C5—C16	128.6 (2)	125.7 (2)
O2—C16—C5	107.7 (2)	108.4 (2)
C16—O2—C17	116.6 (2)	117.5 (2)
O2—C17—C18	115.6 (2)	124.4 (2)
O2—C17—C22	124.3 (2)	115.5 (2)
C18—C17—C22	120.1 (2)	120.0 (3)
C17—C18—C19	120.1 (3)	118.4 (3)
C18—C19—C20	119.5 (3)	122.5 (3)
C19—C20—C21	120.8 (3)	117.3 (3)
C20—C21—C22	119.7 (2)	121.9 (3)
C17—C22—C21	119.7 (3)	119.8 (3)
C19—C20—C23	–	121.0 (3)
N1—C3—C10	115.2 (2)	114.9 (2)
C2—C3—C10	116.2 (2)	115.8 (2)
C3—C10—C11	120.5 (2)	119.7 (2)
C3—C10—C15	120.8 (2)	120.6 (2)
C11—C10—C15	118.8 (2)	119.7 (2)
C10—C11—C12	120.2 (3)	120.5 (2)
C11—C12—C13	120.3 (2)	119.4 (3)
C12—C13—C14	119.9 (3)	120.5 (3)
C13—C14—C15	120.7 (3)	120.7 (3)
C10—C15—C14	120.1 (2)	119.1 (3)
S—C1—C6	115.2 (1)	114.6 (2)
C2—C1—C6	123.6 (2)	123.2 (2)
O1—C6—C1	117.8 (2)	116.5 (2)
O1—C6—C7	109.8 (2)	109.8 (2)
C6—O1—C9	105.2 (2)	105.0 (2)
C1—C6—C7	132.3 (3)	133.7 (2)
C6—C7—C8	106.7 (3)	107.3 (2)
C7—C8—C9	105.8 (2)	105.3 (2)
O1—C9—C8	112.4 (3)	112.6 (2)
O1—C9—N5	117.1 (2)	116.2 (2)
N5—C9—C8	130.4 (3)	131.2 (2)
O3—N5—O4	124.8 (3)	124.3 (2)
O3—N5—C9	119.0 (3)	116.7 (2)
O4—N5—C9	116.3 (3)	119.0 (2)
C1—C20—C19	120.4 (2)	–
C1—C20—C21	118.8 (2)	–
C21—C20—C23	–	121.7 (3)
N2—C5—C16—O2	−179.0 (2)	80.9 (3)
N4—C5—C16—O2	−0.8 (4)	−102.9 (3)
C5—C16—O2—C17	178.7 (2)	178.0 (2)
C16—O2—C17—C18	−174.1 (2)	−9.5 (4)
C16—O2—C17—C22	5.2 (4)	172.7 (2)
S—C1—C6—O1	177.9 (2)	160.9 (2)
C2—C1—C6—O1	−1.0 (4)	−16.8 (3)
S—C1—C6—C7	−3.4 (4)	−19.6 (4)
C2—C1—C6—C7	177.7 (3)	162.7 (3)
O1—C9—N5—O3	−5.1 (4)	−176.6 (2)
O1—C9—N5—O4	175.9 (3)	3.8 (3)
C8—C9—N5—O3	170.5 (3)	2.5 (4)
C8—C9—N5—O4	−8.5 (5)	−177.1 (3)
C2—C3—C10—C11	33.2 (4)	36.9 (3)
C2—C3—C10—C15	−146.9 (3)	−143.0 (2)
N1—C3—C10—C11	−152.7 (3)	−146.4 (2)
N1—C3—C10—C15	27.2 (4)	33.7 (3)

The structures were solved by direct methods using *MULTAN*11/82 (Main *et al.*, 1982). All calculations were performed on a MicroVAX II using the *SDP/VAX* structure determination package (Frenz, 1983).

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates, least-squares-planes data and complete geometry have been deposited with the IUCr (Reference: CR1075). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Tuberostemonine L-G

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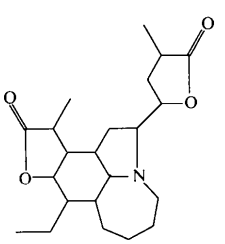
Abstract

The tuberostemonine molecule, $C_{22}H_{33}NO_4$, consists of a pyrrolidine, a cyclohexane, an azepine and two furan rings. Each furan ring adopts the envelope conformation while the pyrrolidine ring takes that of a twist-chair. The cyclohexane and the azepine rings have chair conformations. In the title compound, the vicinal rings are *cis*-fused, whereas in a previously investigated tuberostemonine (m.p. 359–361 K) a

trans-fusion of the pyrrolidine and the cyclohexane rings was found.

Comment

Tuberostemonine is an alkaloid which is used for the treatment of common coughs and, in particular, whooping cough. Previously it has been isolated either from *Stemona tuberosa Lour* (Lobstein & Grumbach, 1932; Suzuki, 1934) or from *Stemona sessilifolia* (Schild, 1936). The tuberostemonine isolated from *Stemona sessilifolia* (m.p. 391–393 K), designated tuberostemonine A, was investigated by spectroscopic methods by Edwards, Feniak & Handa (1962). However, from *Stemona tuberosa Lour*, tuberostemonine can be isolated in two crystal forms. The first one, obtained by Suzuki (1934), melts at 359–361 K. It was investigated by spectroscopic methods (Götz, Bögri & Gray, 1961) and then, to determine the absolute configuration, by X-ray diffraction (Harada, Irie, Masaki, Osaki & Uyeo, 1967). The second one, obtained for the first time by Lobstein & Grumbach (1932) from the root of the Bach-bo plant (a Vietnamese *Stemona tuberosa Lour*), melts at 433–434 K. It was studied by spectroscopic methods (Thanh Ky, Ngoc Kim & Xuan Dung, 1991) and designated tuberostemonine L-G, (1). Since the spectroscopic data did not give sufficient information on the molecular structure and conformation, the crystal structure was determined by X-ray diffraction and compared with the structure of the tuberostemonine reported by Harada, Irie, Masaki, Osaki & Uyeo (1967).



(1)

The average values of the C—C, C—N, C—O and C=O bond lengths are 1.520 (6), 1.465 (5), 1.411 (5) and 1.200 (6) Å, respectively. Fig. 1 shows a *SCHAKAL*88 (Keller, 1988) stereoview of the title compound. The conformations of the five- and six-membered rings are characterized according to Cremer & Pople (1975). The two furan rings, (I) and (II), have similar envelope conformations with pseudorotational phase angles of 110.6 (6) and 68.9 (8)°, respectively. The group of atoms O(2), C(1), C(2) and C(5), and that of O(3), C(14), C(16) and C(18) are planar with maximum deviations of 0.016 (4) and 0.017 (4) Å; the deviation of atoms C(4) and C(15) from the least-squares planes of these groups are −0.607(4) and 0.474(5) Å, respectively. The pyrrolidine ring fused to the six- and seven-membered rings has a twist conformation. A C_2 axis lies approximately on the N atom and the midpoint of the C(11)—C(12) bond. The deviations of the atoms C(11) and C(12) from the plane defined by C(10), N and C(13) are −0.326 (7) and 0.313 (7) Å, respectively. All three five-membered rings have their puckering amplitudes between 0.29 and 0.39 Å. The cyclohexane ring has a slightly distorted chair conformation with puckering parameters (Cremer & Pople, 1975) $Q = 0.461$ (3) Å, $\Theta = 169.2$ (4) and $\Phi = 174$ (2)°. For the azepine ring, the atoms C(9), C(22), C(19) and C(20) form a plane with a maximum deviation of 0.003 (5) Å. The deviation of the atoms C(10), N and C(21) from this plane are 1.062 (4), 1.022 (4) and −0.665 (5) Å, respectively. In addition, the torsion angles (Table 2) of the azepine ring are similar to the theoretical values calculated for the chair conformation of cycloheptane and 1,3-dioxepane (Bocian & Strauss, 1977). According to Stoddart (1971), the seven-membered ring also has a chair conformation. The cyclohexane and pyrrolidine rings are *cis*-fused to the seven-membered ring. Similarly, the furan ring (I) and the pyrrolidine ring are also *cis*-fused to the cyclohexane ring. The H—C(13)—C(14)—H unit has a *trans* conformation (Fig. 2*a*). The absolute configuration of the title compound was not determined, but was chosen (see Fig. 1) to have the same configuration at C(10) as in the structure studied by Harada *et al.* (1967).

The structure of tuberostemonine was originally determined by spectroscopic methods (Götz, Bögri & Gray, 1961; Edwards, Feniak & Handa, 1962); Götz, Bögri, Gray & Strunz (1968) concluded that the X-ray structure determined by Harada, Irie, Masaki, Osaki & Uyeo (1967) (Fig. 2*b*) gave a correct and general representation of tuberostemonine. However, a comparison of the molecular configuration of tuberostemonine L-G with that of the tuberostemonine studied by Harada, Irie, Masaki, Osaki & Uyeo (1967) shows that they are diastereomers. The difference between these configurations is at the ring

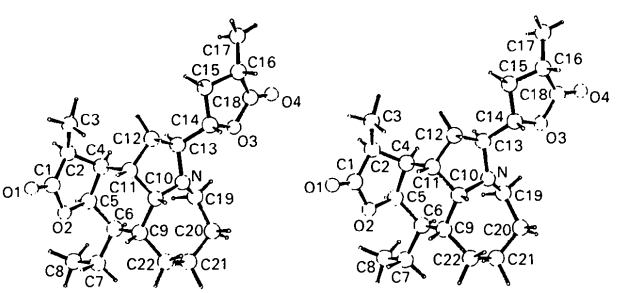


Fig. 1. Stereoview (*SCHAKAL*88; Keller, 1988) of the molecule of tuberostemonine L-G, showing the atomic numbering.

junction between the pyrrolidine and cyclohexane rings. In tuberostemonine L-G the rings are *cis*-fused, while in the molecule reported by Harada, Irie, Masaki, Osaki & Uyeo (1967) they are *trans*-fused (Figs. 2*a* and 2*b*).

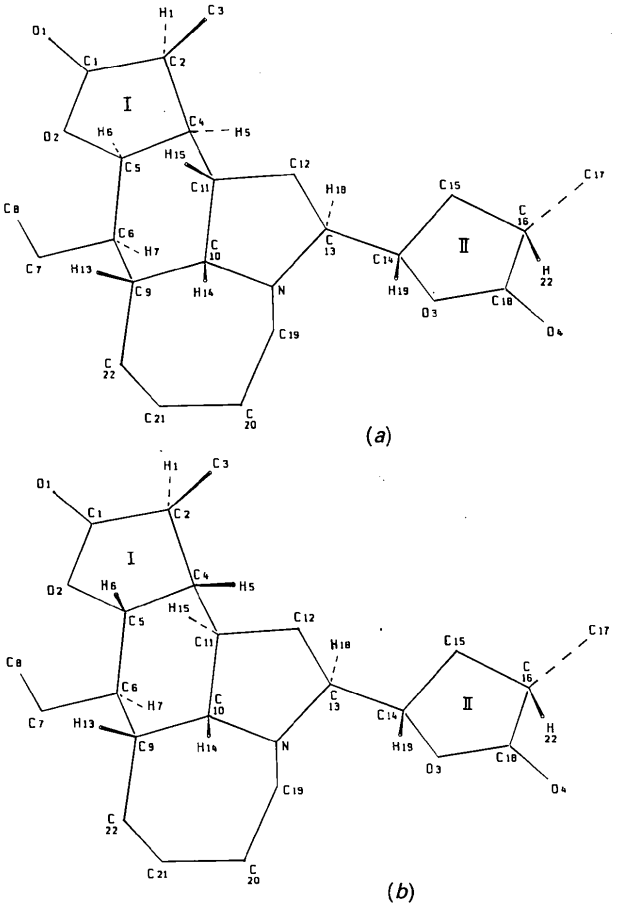


Fig. 2. Schematic representation of the title compound (*a*) compared with the structure of the tuberostemonine molecule (*b*) determined by Harada, Irie, Masaki, Osaki & Uyeo (1967).

Experimental

Tuberostemonine was recrystallized from a mixture of alkaloids isolated from the root of the Bach-bo plant in the Pharmaceutical Laboratory of Hanoi University. Crystals were obtained from ethanol with a melting point of 433–434 K.

Crystal data

$C_{22}H_{33}NO_4$	Cu $K\alpha$ radiation
M_r = 375.6	λ = 1.5418 Å
Orthorhombic	Cell parameters from 48 reflections
$P2_12_12_1$	θ = 35–37.5°
a = 6.432 (1) Å	μ = 0.61 mm^{-1}
b = 14.237 (2) Å	T = 291 K
c = 23.034 (2) Å	Prismatic
V = 2109.3 (5) Å^3	0.57 × 0.50 × 0.36 mm
Z = 4	Colourless
D_x = 1.182 Mg m^{-3}	

Data collection

Stoe diffractometer	θ_{max} = 64°
$\omega/2\theta$ scans	$h = 0 \rightarrow 7$
Absorption correction: none	$k = 0 \rightarrow 16$
2121 measured reflections	$l = 0 \rightarrow 26$
2121 independent reflections	3 standard reflections
2016 observed reflections [$F_o > 2\sigma(F_o)$]	frequency: 90 min
	intensity variation: 4%

Refinement

Refinement on F	$(\Delta/\sigma)_{max}$ = 0.19
R = 0.038	$\Delta\rho_{max}$ = 0.2 e Å^{-3}
wR = 0.032	$\Delta\rho_{min}$ = −0.2 e Å^{-3}
S = 5.11	Extinction correction: none
1956 reflections	Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)
376 parameters	
H-atom parameters not refined	
$w = 1/\sigma^2(F_o)$	

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2)

$$U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	U_{eq}
O(1)	−0.2941 (4)	0.5519 (2)	0.6284 (1)	0.092 (1)
O(2)	−0.0004 (3)	0.4831 (1)	0.5993 (1)	0.070 (1)
O(3)	0.6516 (3)	0.2587 (1)	0.8340 (1)	0.068 (1)
O(4)	0.9021 (4)	0.2442 (2)	0.8995 (1)	0.099 (1)
N	0.3850 (3)	0.2772 (2)	0.7246 (1)	0.054 (1)
C(1)	−0.1159 (5)	0.5319 (2)	0.6380 (1)	0.071 (1)
C(2)	0.0110 (5)	0.5524 (2)	0.6918 (1)	0.063 (1)
C(3)	−0.1223 (6)	0.5623 (3)	0.7456 (2)	0.079 (1)
C(4)	0.1786 (5)	0.4761 (2)	0.6882 (1)	0.053 (1)
C(5)	0.2108 (5)	0.4708 (2)	0.6227 (1)	0.061 (1)
C(6)	0.3070 (5)	0.3831 (2)	0.5980 (1)	0.064 (1)
C(7)	0.3026 (7)	0.3838 (3)	0.5312 (1)	0.086 (1)
C(8)	0.4062 (9)	0.4666 (4)	0.5038 (2)	0.115 (2)
C(9)	0.2054 (5)	0.2948 (2)	0.6235 (1)	0.060 (1)
C(10)	0.1953 (4)	0.2950 (2)	0.6900 (1)	0.051 (1)
C(11)	0.1011 (4)	0.3839 (2)	0.7151 (1)	0.050 (1)
C(12)	0.1611 (5)	0.3760 (2)	0.7789 (1)	0.055 (1)
C(13)	0.3827 (4)	0.3371 (2)	0.7765 (1)	0.051 (1)
C(14)	0.4310 (4)	0.2858 (2)	0.8325 (1)	0.057 (1)
C(15)	0.4037 (6)	0.3431 (3)	0.8875 (1)	0.066 (1)
C(16)	0.5605 (5)	0.3020 (3)	0.9290 (1)	0.072 (1)
C(17)	0.6410 (9)	0.3664 (5)	0.9757 (2)	0.123 (2)
C(18)	0.7258 (5)	0.2653 (2)	0.8886 (1)	0.070 (1)
C(19)	0.5868 (5)	0.2610 (3)	0.6988 (1)	0.069 (1)
C(20)	0.5998 (6)	0.1719 (3)	0.6626 (2)	0.086 (1)
C(21)	0.5102 (7)	0.1808 (3)	0.6018 (1)	0.085 (1)
C(22)	0.2795 (6)	0.2005 (3)	0.5988 (1)	0.076 (1)

Table 2. *Selected geometric parameters* (Å, °)

O(1)—C(1)	1.201 (4)	O(2)—C(1)	1.353 (4)
O(2)—C(5)	1.472 (4)	O(3)—C(14)	1.470 (3)
O(3)—C(18)	1.350 (3)	O(4)—C(18)	1.199 (4)
N—C(10)	1.479 (3)	N—C(13)	1.468 (3)
N—C(19)	1.447 (4)	C(1)—C(2)	1.513 (4)
C(2)—C(3)	1.513 (5)	C(2)—C(4)	1.532 (4)
C(4)—C(5)	1.526 (4)	C(4)—C(11)	1.536 (4)
C(5)—C(6)	1.504 (4)	C(6)—C(7)	1.539 (4)
C(6)—C(9)	1.534 (4)	C(7)—C(8)	1.495 (7)
C(9)—C(10)	1.535 (3)	C(9)—C(22)	1.534 (5)
C(10)—C(11)	1.518 (4)	C(11)—C(12)	1.521 (3)
C(12)—C(13)	1.530 (4)	C(13)—C(14)	1.516 (4)
C(14)—C(15)	1.518 (4)	C(15)—C(16)	1.507 (4)

C(16)—C(17)	1.505 (7)	C(16)—C(18)	1.505 (4)
C(19)—C(20)	1.521 (5)	C(20)—C(21)	1.520 (5)
C(21)—C(22)	1.511 (6)		
C(1)—O(2)—C(5)	109.1 (2)	C(14)—O(3)—C(18)	110.1 (2)
C(10)—N—C(13)	109.3 (2)	C(10)—N—C(19)	123.1 (2)
C(13—N—C(19)	115.9 (2)	O(1)—C(1)—O(2)	121.6 (3)
O(1)—C(1)—C(2)	128.3 (3)	O(2)—C(1)—C(2)	110.1 (3)
C(1)—C(2)—C(3)	112.5 (3)	C(1)—C(2)—C(4)	101.4 (2)
C(3)—C(2)—C(4)	120.6 (2)	C(2)—C(4)—C(5)	100.7 (2)
C(2)—C(4)—C(11)	110.9 (2)	C(5)—C(4)—C(11)	113.7 (2)
O(2)—C(5)—C(4)	103.3 (2)	O(2)—C(5)—C(6)	109.9 (2)
C(4)—C(5)—C(6)	118.1 (2)	C(5)—C(6)—C(7)	111.4 (3)
C(5)—C(6)—C(9)	111.1 (2)	C(7)—C(6)—C(9)	112.3 (3)
C(6)—C(7)—C(8)	114.8 (3)	C(6)—C(9)—C(10)	113.5 (2)
C(6)—C(9)—C(22)	116.4 (3)	C(10)—C(9)—C(22)	112.6 (2)
N—C(10)—C(9)	120.2 (2)	N—C(10)—C(11)	105.4 (2)
C(9)—C(10)—C(11)	113.5 (2)	C(4)—C(11)—C(10)	115.5 (2)
C(4)—C(11)—C(12)	111.8 (2)	C(10)—C(11)—C(12)	101.8 (2)
C(11)—C(12)—C(13)	103.2 (2)	N—C(13)—C(12)	104.4 (2)
N—C(13)—C(14)	114.3 (2)	C(12)—C(13)—C(14)	109.6 (2)
O(3)—C(14)—C(13)	110.1 (2)	O(3)—C(14)—C(15)	103.5 (2)
C(13)—C(14)—C(15)	115.3 (2)	C(14)—C(15)—C(16)	104.0 (3)
C(15)—C(16)—C(17)	116.5 (4)	C(15)—C(16)—C(18)	102.5 (2)
C(17)—C(16)—C(18)	114.2 (3)	O(3)—C(18)—O(4)	120.7 (3)
O(3)—C(18)—C(16)	110.5 (3)	O(4)—C(18)—C(16)	128.8 (3)
N—C(19)—C(20)	114.1 (3)	C(19)—C(20)—C(21)	114.5 (3)
C(20)—C(21)—C(22)	115.4 (3)	C(9)—C(22)—C(21)	116.8 (3)

C(10)—N—C(19)—C(20)	64.4 (5)
C(19)—C(20)—C(21)—C(22)	63.8 (6)
C(21)—C(22)—C(9)—C(10)	77.7 (5)
C(9)—C(10)—N—C(19)	−1.3 (5)
N—C(19)—C(20)—C(21)	−80.1 (5)
C(20)—C(21)—C(22)—C(9)	−64.7 (5)
C(22)—C(9)—C(10)—N	−60.1 (5)

The structure was solved by direct methods using *SHELXS*86 (Sheldrick, 1985). H atoms were located in a difference Fourier synthesis using *Xtal* (Stewart & Hall, 1983).

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Lists of structure factors, anisotropic displacement parameters and H-atom coordinates have been deposited with the IUCr (Reference: KA1019). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Interactions Between Sulfonated Azo Dyes and Biomolecules: Orange G/Adenine and Orange G/Cytosine Salts

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Abstract

The disulfonated azo dye Orange G [the disodium salt of 7-hydroxy-8-(phenylazo)-1,3-naphthalenedisulfonic acid] forms salts with adenine and cytosine on co-crystallization from aqueous HCl. The 1:2 dye:adenine crystal, $2C_5H_6N_5^+.C_{16}H_{10}N_2O_7S_2^{2-}.5H_2O$, is a pentahydrate and the 1:2 dye:cytosine crystal, $2C_4H_6N_3O^+.C_{16}H_{10}N_2O_7S_2^{2-}.H_2O$, is a monohydrate. In the solid state the dye is found to exist predominantly as the hydrazo, rather than the azo, tautomer. In both structures, one of the protonated nucleotide bases approaches close to a sulfonate group of the dye in an 'edge-on' fashion. Molecules in the Orange G/adenine structure lie in segregated layers, but molecules in the Orange G/cytosine structure lie in mixed stacks.

Comment

Interactions between biomolecules containing sulfate groups and biomolecules (such as proteins) capable of recognizing these groups are currently the object of intensive biomedical study. Although the focus of