SUMMARY

We have isolated sulfated steroid alcohols from holothurians for the first time and have characterized them. It has been shown that these animals contain mainly sulfated saturated and Δ^5-monounsaturated sterols.

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MOLECULAR AND CRYSTAL STRUCTURE OF SOPHORIDINE N-OXIDE

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The spatial structure of natural sophoridine N-oxide has been studied by x-ray structural analysis. It has been shown that when sophoridine is oxidized, rings B and C, which have the boat form, are deformed in the direction of the twist form.

In the investigation of the spatial structures of the molecules of sparteine alkaloids and their N-oxides, it has been shown that the molecules of the alkaloids of this class tend to undergo a conformational transition on oxidation if they are labile or appreciably strained [1]. Sophoridine, which also has a labile molecule [2, 3], can radically change its conformation after oxidation. The results of a study by physicochemical methods of sophoridine N-oxide isolated from plants [4] and the N-oxide obtained by the synthetic oxidation of sophoridine show that the conformations of molecules of these compounds are not identical [5]. In order to elucidate the existence of a conformational transition on the oxidation of sophoridine and to determine the features of the molecules of the two modifications of the N-oxide, we have investigated the three-dimensional structure of natural sophoridine N-oxide and have proposed to perform a similar investigation of the synthetic N-oxide.

Sophoridine N-oxide crystallizes with two molecules (I and II) in the independent part of the elementary cell. The conformations and geometric parameters of molecules I and II are shown in Figs. 1 and 2.

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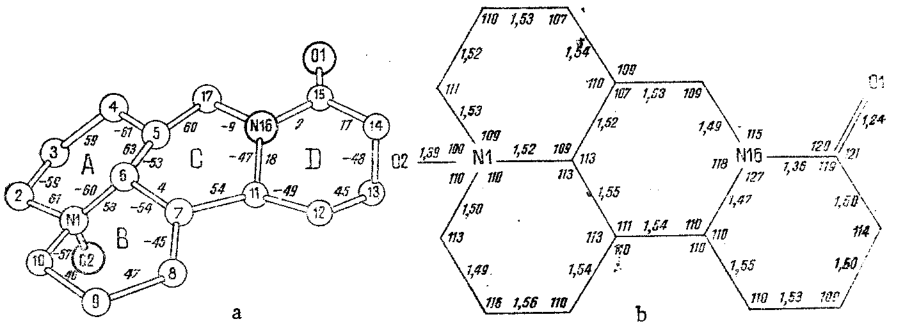

Fig. 1. Molecule I of sophoridine N-oxide: a) conformation in the crystal (the values of the torsional angles are given); b) bond lengths and values of the valence angles.

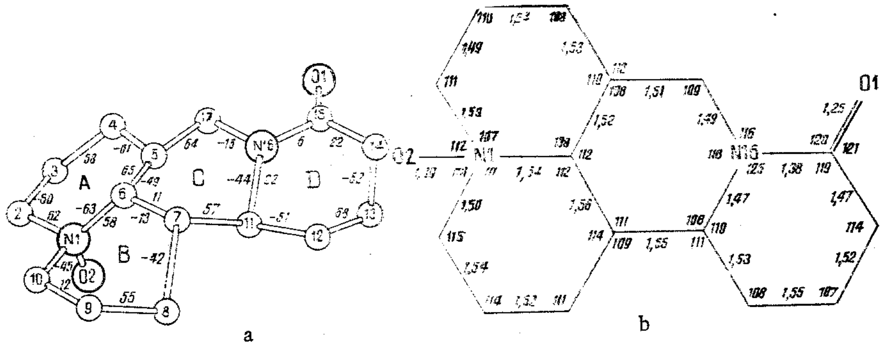

Fig. 2. Molecule II of sophoridine N-oxide: a) conformation in the crystal (the values of the torsional angles are given); b) bond lengths and values of the valence angles.

To evaluate the changes taking place on the oxidation of sophoridine and to compare the conformations of the two symmetrically independent molecules of the N-oxide we used the method for the quantitative comparison of the conformations on a computer proposed by P. M. Zorkii and A. E. Razumaeva [6, 7]. The method is based on a close matching of the molecules being compared by their centers of gravity, which is achieved at the minimum value of a special criterion — the integral characteristic of the geometric closeness of the molecule:

$$s=\left(\sum_{i=1}^{N} W_iR_i/\sum_{i=1}^{N} W_i\right)^{1/2},$$

where R_i represents the distances between atoms of the same type at the closest coincidence of the molecules; W_i represents weighting factors; and N is the number of atoms in the molecule (or fragment).

The discrepancies corresponding to the minimum of s give information on the relationship of the geometries of the molecules being compared. If for some of the atoms the weights are put equal to zero, then it is possible to compare the molecule by only some of its parts.

The quantitative comparison of the conformations I and II of sophoridine N-oxide has shown that the differences are localized mainly at the N(1), C(8), C(9), and C(10) atoms of ring B, corresponding to discrepancies of 0.10, 0.15, 0.11, and 0.22 Å (Table 1). The differences in the structures of rings C are comparatively smaller (the discrepancies of the C(5) and C(17) atoms amount to 0.10 Å). The geometric parameters (see Figs. 1 and 2), and also the maximum mean values of the absolute magnitudes of the deviations of the torsional angles of the rings of molecules I and II of N-oxide from the ideal values show small differences in the geometrics of rings B and C. The conformations of rings A and D in molecules I and II practically coincide. The conformation of ring A in molecule I is even closer to the ideal than its conformation in the molecule of the base.

TABLE 1. Quantitative Comparison of the Conformations of the Molecules of Sophoridine and Its N-Oxide on a Computer

Atom	Discrepancies R_i, Å		
	molecule I–molecule II of sophoridine N-oxide	sophoridine–molecule I of the N-oxide	sophoridine–molecule II of the N-oxide
N (1)	0,10	0,10	0,20
C (2)	0,09	0,06	0,16
C (3)	0,03	0,04	0,06
C (4)	0,06	0,06	0,14
C (5)	0,10	0,02	0,10
C (6)	0,06	0,04	0,02
C (7)	0,05	0,06	0,09
C (8)	0,15	0,20	0,32
C (9)	0,11	0,15	0,20
C (10)	0,22	0,06	0,30
C (11)	0,03	0,02	0,04
C (12)	0,03	0,05	0,02
C (13)	0,10	0,08	0,18
C (14)	0,05	0,10	0,13
C (15)	0,05	0,06	0,08
N (16)	0,04	0,05	0,02
C (17)	0,10	0,06	0,17
O	0,07	0,04	0,03
The criterion s, Å	0,09	0,08	0,15

The results of a quantitative comparison of the conformations of sophoridine and molecule I of its N-oxide show that the molecules compared are, on the whole, geometrically equal (s = 0.08 Å, Table 1). The greatest discrepancies of 0.20 and 0.15 Å correspond to the C(8) and C(9). On a background of small values of R_i for the other atoms of less than 0.10 Å, this shows the existence of local differences. One of such differences consists in the fact that, apparently, because of the interaction (repulsion) of the axial substituents at the "angular" N(1) and C(8) atoms of molecule I of the N-oxide — the oxide oxygen and a hydrogen atom — the boat of ring B is deformed. The N(1)...C(8) distance, equal in sophoridine to 2.65 Å, increases to 2.73 Å in molecule I of the N-oxide. The next difference — somewhat smaller than that of the boat of ring B — is the deformation of the boat of ring C in molecule I of the N-oxide. This comparatively small change is not shown clearly in the results of the quantitative comparison (Table 1).

As already mentioned, in the quantitative comparison of the molecules they are brought into close coincidence by their centers of gravity. Because of this, the method is insensitive to changes taking place close to the center of gravity of the molecule and shows changes at the peripheries of large molecules fairly clearly. In such cases, it is desirable to compare individual fragments of the molecule, using a suitable weighting scheme. The results of a comparison of only rings C of the molecules of sophoridine and the N-oxide I (s = 0.07 Å) showed that there are in fact differences in the geometries of these rings: The greatest discrepancies relate to the atoms C(6) (0.08 Å) and C(7) (0.10 Å).

The deformation arising in ring B when sophoridine is oxidized can apparently be transmitted through the angular C(7) atom to the neighboring ring C. As a result of the deformation of rings B and C their conformations in molecule I of the N-oxide change from the boat conformations in the direction of twist forms. In the course of the conformational rearrangement, the maximum change is undergone by the torsional angle C(6)C(7)C(8)C(9). As a result of the deformation of ring C of sophoridine on oxidation, the coplanarity of the "basis" atoms of this ring worsens (Table 2).

The "lactam fragment" — C(11), N(16), C(15), and C(14) — in molecule I of the N-oxide is more planar than in sophoridine, and the C(12) and C(13) atoms depart from the plane by 0.42 and 0.37 Å in opposite directions.

The criterion s for the pair sophoridine and molecule II of its N-oxide, which is 0.16 Å, shows that in molecule II of the N-oxide there are even greater changes in the conformation than in molecule I. In addition to the C(8) and C(9) atoms (0.32 and 0.20 Å), the N(1) and

TABLE 2. Coefficients of the Equations of the Planes and Deviations of the Atoms δ from These Planes in the Structure of Sophoridine N-Oxide (molecule I)

Plane	Atom	Coefficients of the equation of the plane				δ, Å
		A	*B*	*C*	*D*	
I (ring *A*)	N (1)	−4,30	10,78	4,08	2,26	0,010
	C (2)					−0,010
	C (4)					0,010
	C (5)					−0,010
	C (3)*					−0,704
	C (6)*					0,730
II (ring *B*)	C (6)	−3,61	11,27	2,83	2,77	0,005
	C (7)					−0,004
	C (9)					0,005
	C (10)					−0,005
	N (1)*					−0,674
	C (8)*					−0,581
III (ring *C*)	C (6)	−4,49	11,02	3,23	2,78	−0,046
	C (7)					0,047
	N (16)					−0,049
	C (17)					0,049
	C (5)*					−0,709
	C (11)*					−0,602
IV (ring *D*)	C (11)	−2,72	9,50	6,70	3,40	−0,003
	N (16)					0,007
	C (15)					−0,007
	C (14)					0,003
	C (13)*					−0,373
	C (12)*					0,419

*Atoms not included in the calculation of the equation of the plane.

C(10) atoms also have large deviations (0.20 and 0.31 Å). Consequently, on passing from the molecule of the base to the molecule I, and then to molecule II, of N-oxide the conformational changes gradually rise. For example, in molecule II of the N-oxide the deviations of the torsional angles in ring B from ±60°C amount to as much as 18° for the C(6)C(7)C(8)C(9) angle, i.e., the torsional angles in the formation of which the C(8) and C(9) atoms participate have changed appreciably. The deformation of ring C is smaller than that of ring B but greater than the deformation of the same ring C in molecule I of the N-oxide. The coplanarity of the "basis" atoms of rings B and C worsens still more than in the molecule I (Table 3).

In the half-chair ring D, the C(12) and C(13) atoms have the same deviation (0.41 Å) in opposite directions. The coplanarity of the atoms of the "lactam fragment" is of the same order as their coplanarity in sophoridine.

The lengths of the $C(sp^3)-C(sp^3)$ bonds in molecules I and II of the N-oxide range from 1.49 to 1.56 Å with a mean value of 1.53 Å. The greatest changes in the bond lengths as compared with the bond lengths in the base are observed in ring B for the C(8) — C(9) and C(9) — C(10) bonds (Figs. 1b and 2b). The mean value of the $N^+(1)-C(sp^3)$ bond lengths is 1.51 Å (molecule II, 1.52 Å), while the $N^+(1)-O(2)$ bond length is the same in the two molecules at 1.29 Å. These values agree well with the bond lengths of such bonds in other N-oxides of matrine alkaloids [8, 9] and in alkaloids of the sparteine series [4]. The N(16) — C(15) and C(15) — O(1) bond lengths are somewhat greater than the lengths of the corresponding bonds in the bases and N-oxides considered previously [3, 8-10].

The valence angles at the tetrahedral carbon atoms are close to the usual ones (Figs. 1b and 2b), with the exception of the angles at the C(9), C(10), and C(14) atoms. The increases in the angles at the C(9) and C(10) atoms in molecules (I and II) of the N-oxide are due to the deformation of ring B on oxidation that has been considered above. The values of the angles of the C(15) atom in molecules I and II of the N-oxide are the same and are distributed more uniformly than in unoxidized sophoridine [3], while at the N(16) atom the distribution of the angles remains practically unchanged.

In the crystal structure of sophoridine N-oxide (Fig. 3), the water molecules link the molecules I of the N-oxide by hydrogen bonds into helices about axis 2. The lengths of the

TABLE 3. Coefficients of the Equations of the Planes and the Deviations of the Atoms δ from These Planes in the Structure of Sophoridine N-Oxide (molecule II)

Plane	Atom	Coefficients of the equation of the plane				δ, Å
		A	*B*	*C*	*D*	
I (ring *A*)	C(4)	—2,33	7,37	9,36	7,67	0,000
	C(5)					—0,000
	N(1)					0 000
	C(2)					—0,000
	C(3)*					—0,703
	C(6)*					0,767
II (ring *B*)	C(6)	1,71	9,16	7,48	8,92	0,079
	C(7)					—0,078
	C(9)					0,079
	C(10)					—0,080
	N(1)*					—0,617
	C(8)*					—0,595
III (ring *C*)	C(6)	—3,44	8,10	8,52	8,50	—0,089
	C(7)					0,090
	N(16)					—0,094
	C(17)					0,093
	C(5)*					—0,683
	C(11)*					—0,634
IV (ring *D*)	C(11)	—1,05	5,30	10,80	7,27	—0,013
	N(16)					0,026
	C(15)					—0,025
	C(14)					0,012
	C(13)*					—0,416
	C(12)*					0,418

*Atoms not included in the calculation of the equation of the plane.

O(WI)...O(1) H-bond is 2.88 Å and of the O(WI)...O(2) bond 2.73 Å. The molecules II of the N-oxide are linked by O(W2)...O(1) and O(W2)...O(2) H-bonds, with lengths of 3.04 Å and 2.74 Å, respectively, into infinite chains parallel to [100]. The nonidentity of the conformations of the symmetrically independent molecules (I and II) of the N-oxide may be due to the different environments of these molecules in the crystal. A molecule of water of crystallization forms with the oxide atom O(2) of molecule I a hydrogen bond which, bringing itself closer to this molecule on the side of the C(8), C(9), and C(10) atoms of ring B, which have the boat form (C(9)...O(W1) and C(10)...O(W1) amount to 3.56 and 3.35 Å, respectively. Another molecule of water of crystallization forming a H-bond with the O(2) atom of molecule II of the N-oxide is located closer to the C(2), C(3), and C(4) atoms of ring A in the chair form (C(3)...O(W2) and C(2)...O(W2) amount to 3.56 and 3.36 Å, respectively).

EXPERIMENTAL

Prismatic crystals of sophoridine N-oxide were grown from a solution in a mixture of equal parts of ethanol and acetone. To determine the parameters of the elementary cell by a photographic method for the subsequent investigation in a diffractometer, these crystals were sealed into a thin-walled quartz capillary because of their extreme instability in the air. The parameters of the monoclinic elementary cell measured and refined on a Syntex $P2_1$ automatic diffractometer, and the other charcteristics of the crystal, were as follows: a = 10.666(2), b = 11.654(2), c = 12.127(3) Å; γ = 104.6(5)°; ρ_{calc} = 1.28 g/cm^3; space group $P2_1$; Z = 4.

A three-dimensional set of experimental reflections was obtained on the diffractometer mentioned by the θ/2θ-scanning method in monochromatic CuK_α radiation to θ = 58°. A total of 2864 independent refections was recorded, of which the 2133 with $1 \geqslant 2\sigma$ were used in the calculations. No corrections were introduced for absorption.

An attempt to interpret the structure of sophoridine N-oxide in the automatic regime by the direct multivariant methods using the tangent formula by means of the Rentgen-75 group of programs [11] was unsuccessful. Then a series of phase calculations was performed with different numbers of normalized amplitudes and ternary products, and a series of E-syntheses was constructed from the sets of phases obtained. However, the structure was not revealed

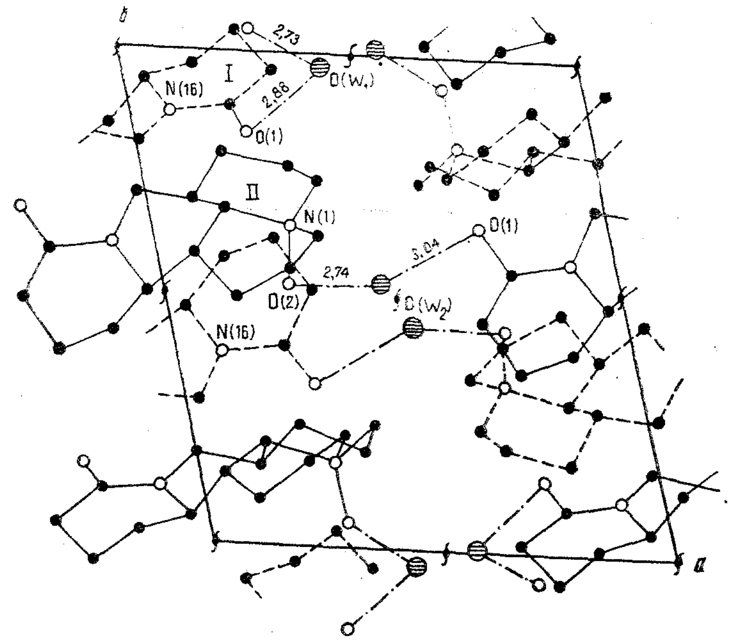

Fig. 3. Packing of the molecules of sophoridine N-oxide.

by this method, either. The screening of the reference reflections was performed with the retention unchanged of the coordinate reflections selected by the computer in the automatic regime. The E-synthesis of the first (according to the S estimates) variant with a minimum R factor of 0.35 and of the base reflections 3,4,2; 6,8,1; 8,4,5; 1,1,2; and 6,1,5 permitted the isolation of the overwhelming majority of the nonhydrogen atoms of the structure (25 out of 40).

The structure was refined by the method of least squares using the programs of the Kristall group [12] in the full-matrix variant. The coordinates of the nonhydrogen atoms obtained as the result of a series of least-square refinements in the isotropic (R = 0.162) and anisotropic (R = 0.123) approximations of the thermal vibrations were used to calculate

TABLE 4. Coordinates and Parameters of the Anisotropic Thermal Vibrations of the Nonhydrogen Atoms in the Structure of Sophoridine N-Oxide (molecule I) (all magnitudes multiplied by 10^4; the standard deviations are given in parentheses)

Atom	x/a	y/b	z/c	$B(11)$	$B(22)$	$B(33)$	$B(12)$	$B(23)$	$B(13)$
N (1)	2953 (4)	1867 (4)	3741 (5)	81 (5)	78 (4)	89 (5)	61 (7)	—42 (8)	—3 (8)
C (2)	3982 (6)	2560 (7)	2945 (7)	81 (7)	135 (8)	118 (8)	—27 (1)	—31 (11)	42 (12)
C (3)	3622 (7)	2222 (8)	1757 (7)	119 (9)	168 (10)	117 (8)	—41 (15)	0 (15)	106 (15)
C (4)	2315 (7)	2470 (7)	1473 (7)	125 (8)	128 (8)	85 (7)	—35 (12)	15 (2)	49 (12)
C (5)	1309 (6)	1744 (8)	2282 (7)	95 (10)	89 (3)	—59 (8)	—11 (11)	11 (10)	—10 (11)
C (6)	668 (6)	2127 (7)	3464 (7)	73 (8)	65 (4)	69 (9)	15 (13)	—25 (7)	—2 (8)
C (7)	589 (5)	1563 (7)	4299 (6)	84 (7)	73 (4)	58 (8)	117 (12)	—13 (11)	0 (7)
C (8)	1091 (3)	965 (6)	5281 (5)	100 (11)	123 (9)	65 (7)	36 (8)	15 (12)	—2 (11)
C (9)	2376 (5)	1784 (7)	5728 (4)	12 (6)	19 (4)	72 (7)	89 (11)	—54 (10)	-51 (12)
C (10)	3359 (6)	2304 (8)	4879 (3)	102 (3)	100 (8)	93 (10)	10 (9)	—54 (11)	—50 (9)
C (11)	—532 (4)	666 (3)	3726 (7)	97 (7)	68 (6)	54 (7)	22 (10)	14 (13)	—7 (7)
C (12)	—1660 (3)	19 (5)	4539 (6)	109 (12)	103 (7)	67 (6)	18 (11)	25 (7)	12 (10)
C (13)	—2846 (4)	—520 (6)	3911 (5)	92 (16)	95 (6)	107 (11)	—4 (7)	18 (9)	16 (11)
C (14)	—3308 (3)	303 (6)	3150 (2)	85 (7)	109 (11)	107 (10)	7 (9)	3 (10)	6 (9)
C (15)	—2256 (5)	1092 (7)	2473 (7)	110 (5)	77 (8)	90 (9)	40 (8)	7 (11)	—23 (10)
N (16)	—997 (4)	1235 (4)	2787 (5)	89 (5)	70 (4)	64 (5)	9 (7)	26 (8)	—4 (8)
C (17)	—11 (5)	1981 (3)	2044 (4)	108 (3)	90 (3)	71 (8)	26 (11)	22 (10)	—20 (9)
O (1)	—2512 (4)	1615 (4)	1645 (5)	132 (6)	115 (5)	122 (5)	43 (8)	34 (8)	94 (9)
O (2)	2879 (4)	659 (4)	3660 (4)	102 (5)	84 (4)	106 (4)	50 (7)	—46 (7)	0 (8)
O (W1)	4751 (5)	5442 (5)	1788 (5)	124 (6)	172 (7)	114 (6)	119 (10)	—49 (10)	25 (9)

mal Vibrations of the Nonhydrogen Atoms in the Structure of Sophoridine N-Oxide (molecule II) (all magnitudes are multiplied by 10^4; the standard deviations are given in parentheses)

Atom	x/a	y/b	z/c	B(11)	B(22)	B(33)	B(12)	B(23)	B(13)
N (1)	2963 (4)	6521 (4)	3797 (5)	63 (5)	99 (4)	102 (4)	35 (7)	—81 (7)	—26 (7)
C (2)	3809 (5)	7578 (3)	3174 (7)	69 (8)	124 (10)	114 (6)	—23 (10)	—54 (12)	0 (14)
C (3)	3194 (4)	7779 (6)	2112 (8)	106 (7)	119 (9)	106 (9)	—61 (11)	—22 (12)	42 (12)
C (4)	1867 (3)	8034 (7)	2333 (7)	96 (7)	89 (8)	105 (9)	—16 (10)	32 (11)	—5 (14)
C (5)	1041 (6)	6976 (6)	2960 (6)	73 (7)	91 (6)	63 (6)	20 (10)	0 (10)	—24 (10)
C (6)	1676 (6)	6832 (6)	4051 (6)	70 (7)	83 (7)	75 (6)	54 (11)	—30 (11)	19 (10)
C (7)	773 (7)	5883 (6)	4797 (6)	98 (8)	88 (7)	63 (6)	73 (12)	—10 (10)	—24 (11)
C (8)	1470 (8)	5006 (8	5339 (8)	143 (10)	128 (9)	105 (8)	102 (15)	33 (14)	—53 (15)
C (9)	2806 (10)	5658 (9)	5747 (9)	165 (13)	186 (12)	132 (10)	192 (20)	—3 (19)	—14 (20)
C (10)	3660 (8)	6383 (8)	4843 (9)	88 (9)	174 (10)	126 (9)	104 (16)	—62 (16)	—98 (15)
C (11)	—422 (6)	5166 (6)	4146 (6)	89 (7)	69 (6)	71 (6)	55 (10)	24 (10)	0 (10)
C (12)	—1340 (7)	4273 (7)	4894 (7)	107 (8)	84 (7)	96 (6)	43 (13)	33 (12)	16 (12)
C (13)	—2611 (7)	3751 (7)	4253 (7)	139 (9)	88 (7)	88 (7)	—17 (13)	33 (13)	10 (14)
C (14)	—3273 (7)	4748 (7)	4096 (7)	89 (9)	97 (7)	118 (7)	—4 (13)	—44 (12)	—14 (13)
C (15)	—2429 (6)	5833 (6)	3612 (6)	88 (8)	76 (6)	106 (6)	28 (11)	2 (11)	—16 (12)
N (16)	—1097 (4)	6016 (4)	3700 (5)	67 (5)	67 (5)	91 (5)	35 (7)	31 (19)	—14 (9)
C (17)	—305 (6)	7121 (6)	3180 (6)	79 (7)	77 (6)	96 (6)	24 (11)	17 (10)	—24 (12)
O (1)	—2890 (4)	6603 (4)	3168 (5)	78 (4)	100 (4)	153 (5)	49 (7)	29 (8)	—51 (8)
O (2)	2746 (4)	5480 (4)	3183 (4)	84 (4)	95 (4)	117 (5)	18 (7)	—96 (8)	19 (8)
O(W2)	4347 (4)	9808 (4)	5137 (5)	112 (6)	142 (6)	129 (6)	87 (9)	0 (9)	47 (10)

TABLE 6. Coordinates and Isotropic Thermal Parameters of the Hydrogen Atoms in the Structure of Sophoridine N-Oxide (molecule I) (the values of the coordinates have been multiplied by 10^3)

Atom	x/a	y/b	z/c	b_j	Atom	x/a	y/b	z/c	b_j
H_2 (1)	404	358	303	5,95	H_{10} (1)	360	331	489	6,74
H_2 (2)	491	242	315	5,95	H_{10} (2)	426	201	507	6,74
H_3 (1)	442	275	122	6,27	H_{11}	—20	—14	343	4,48
H_3 (2)	359	123	166	6,27					
H_4 (1)	237	349	154	5,54	H_{12} (1)	—139	—39	517	5,92
H_4 (2)	204	220	60	5,54	H_{12} (2)	—190	99	495	5,92
H_5	123	76	219	4,21	H_{13} (1)	—258	—125	344	6,23
H_6	192	314	350	4,21	H_{13} (2)	—360	—96	452	6,23
H_7	166	230	462	4,41	H_{14} (1)	—408	—28	262	6,64
H_8 (1)	36	76	594	6,41	H_{14} (2)	—380	90	365	6,64
H_8 (2)	128	8	500	6,41	H_{17} (1)	6	297	216	4,35
H_9 (1)	214	259	616	8,50					
H_9 (2)	279	127	634	8,50	H_{17} (2)	—27	174	118	4 35

TABLE 7. Coordinates and Isotropic Thermal Parameters of the Hydrogen Atoms in the Structure of Sophoridine N-Oxide (molecule II) (the values of the coordinates have been multiplied by 10^3)

Atom	x/a	y/b	z/c	b_j	Atom	x/a	y/b	z/c	b_j
H_2 (1)	397	842	366	6,53	H_{10} (1)	412	732	515	6.61
H_2 (2)	475	737	301	6,53	H_{10} (2)	442	591	465	6,61
H_3 (1)	389	849	162	7,65	H_{11}	—9	462	349	4,22
H_3 (2)	298	691	162	7,65					
H_4 (1)	202	904	234	5,88	H_{12} (1)	—91	359	521	5,48
H_4 (2)	139	839	155	5,88	H_{12} (2)	—160	480	560	5,48
H_5	97	618	243	4,04	H_{13} (1)	—222	346	342	6,60
H_6	195	771	448	4,59	H_{13} (2)	—310	291	465	6,60
H_7	40	639	543	4,31	H_{14} (1)	—415	438	356	6,12
H_8 (1)	87	457	606	6,32	H_{14} (2)	—366	490	496	6,12
H_8 (2)	154	428	477	6,32					
H_9 (1)	268	631	641	8,16	H_{17} (1)	—22	791	376	4,84
H_9 (2)	325	498	610	8,16	H_{17} (2)	—75	732	243	4,84

the position of the hydrogen atoms. The position and temperature parameters of the hydrogen atoms are refined. Here, as the initial B_j values we took the isotropic temperature parameters of the H atoms attached to carbon atoms. The final value of the R factor was 0.079. Tables 4 and 5 give the coordinates and the anisotropic thermal parameters of nonhydrogen atoms and Tables 6 and 7 the coordinates and anisotropic thermal parameters of the hydrogen atoms for molecules I and II of sophoridine N-oxide.

SUMMARY

Natural sophoridine N-oxide crystallizes with two molecules in the independent part of the elementary cell. The conformations of these symmetrically independent molecules are not identical: Rings B and C, which have the boat form in the molecule of the base, are deformed in the direction of the twist form, this deformation being greater in molecule II than molecule I.

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