TABLE 1

| Birch species, site and time of collection | Unsaponifiable part of the ethereal extract | Compound | Total amount of triterpenoids |
|---|---|---|---|
| | % on the weight of the air-dry leaves | | |
| Betula krylovii K r y l., collection of the botanical garden of the Ukrainian Division, USSR AS, July, 1985 | 1,83 | I (0,18), II (0,002), III (0,01), IV (0,01), V (0,009), VI (0,02), VII (0,08), VIII (0,01) | 0,32 |
| B. kirghisorum S a v.-R v c z., collection of the botanical garden of the Ukrainian Division, USSR AS, July, 1984 | 1,50 | IX (0,08), X (0,1), XI (0,08), XII (0,1) | 0,36 |
| B. nana L., Sverdlovsk province, July, 1984 | 4,9 | II (0,02), XIII (0,38), XIV (0,02), XV (0,03) | 0,45 |
| B. microphylla B u n g e*., collection of the botanical garden of the Ukrainian Division, USSR AS, July, 1985 | 1,04 | IX (0,28), X (0,06), XI (0,04), XII (0,03), XIII (0,01), XIV (0,02), XVII (0,02) | 0,46 |
| B. kelleriana S u k.*, collection of the botanical garden of the Ukrainian Division, USSR AS, July, 1985 | 1,96 | IX (1,38), X (0,05), XIV (0,04), XVII (0,05) | 1,52 |
| B. rotundifolia S p a c h., Gorno Altai AO, July, 1986 | 1,91 | II (0,25), XIII (0,04), XVI (0,13) | 0,42 |

*Population cultures, Gorno-Altai AO [Autonomous Province].

## LITERATURE CITED


1. N. D. Pokhilo, V. A. Denisenko, V. V. Makhan'kov, and N. I. Uvarova, Khim. Prir. Soedin., No. 2, 179 (1986).
2. N. D. Pokhilo and N. I. Uvarova, Khim. Prir. Soedin., No. 3, 325 (1988).
3. S. A. Mamaev and A. K. Makhnev, Population Genetics [in Russian], Nauka, Moscow (1980), p. 140.

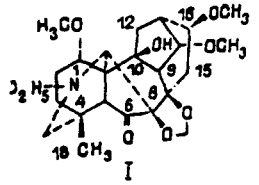

# STRUCTURE OF THE PRODUCT OF THE REACTION OF 6-DEHYDROELDELIDINE WITH SODIUM IN LIQUID AMMONIA


I. M. Yusopova, B. Tashkhodzhaev, A. S. Narzullaev, S. S. Sabirov, and B. T. Ibragimov

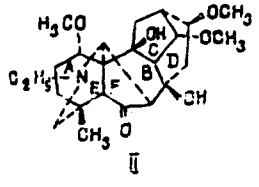


UDC 547.944/945+548.737


In a study of the reaction of dehydroeldelidine (I) with sodium in liquid ammonia a product was obtained with the composition $C_{24}H_{37}NO_6$, mp 163-166°C (ether) for which structure (II) was suggested on the basis of spectral characteristics [1].




I




II


Institute of the Chemistry of Plant Substances, Uzbek SSR Academy of Sciences, Tashkent. Abu Ali ibn Sina [Avicenna] Tashkent State Medical Institute, Dushanbe.


Translated from Khimiya Prirodnykh Soedinenii, No. 2, pp. 279-281, March-April, 1990. Original article submitted April 10, 1989.




0009-3130/90/2602-0230$12.50

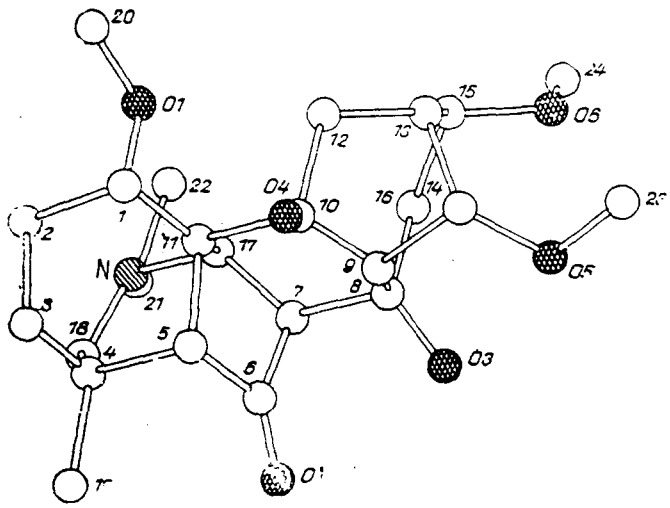


Fig. 1

TABLE 1. Coordinates (×10⁴) of the Nonhydrogen Atoms of the Molecule (II)

| Atom | x | y | z | Atom | x | y | z |
|---|---|---|---|---|---|---|---|
| C1 | 1612 (6) | 3653 (5) | 2638 (3) | C17 | 3780 (6) | 3229 (4) | 3446 (2) |
| C2 | 1905 (8) | 4815 (5) | 2395 (3) | C18 | 4016 (7) | 5260 (4) | 3516 (3) |
| C3 | 1601 ( ) | 5623 (5) | 2969 (3) | C19 | 2149 (8) | 6283 (4) | 4150 (3) |
| C4 | 24[illegible]6 (7) | 5339 (4) | 3619 (3) | C20 | 1345 (10) | 2819 (7) | 1538 (3) |
| C5 | 1846 (6) | 4235 (4) | 3901 (3) | C21 | 6038 (6) | 4169 (5) | 3214 (3) |
| C6 | 2811 (6) | 3903 (4) | 4509 (2) | C22 | 6665 (7) | 3223 (7) | 2808 (3) |
| C7 | 3906 (5) | 3090 (4) | 4247 (2) | C23 | 1302 (8) | —0998 (5) | 4974 (3) |
| C8 | 3424 (6) | 1939 (4) | 4475 (3) | C24 | 533[illegible] (7) | —1345 (5) | 3992 (4) |
| C9 | 1845 (6) | 1833 (4) | 4307 (2) | O1 | 2154 (4) | 2879 (3) | 2149 (2) |
| C10 | 1449 (5) | 2230 (4) | 3577 (2) | O2 | 2745 (4) | 4260 (3) | 5077 (2) |
| C11 | 2155 (5) | 3318 (4) | 3357 (2) | O3 | 3584 (4) | 1904 (3) | 5208 (2) |
| C12 | 1846 (6) | 1196 (4) | 3127 (3) | O4 | —0059 (3) | 2343 (3) | 3530 (2) |
| C13 | 2122 (6) | 0243 (4) | 3635 (3) | O5 | 1805 (4) | 0137 (3) | 4919 (2) |
| C14 | 1382 (6) | 0619 (4) | 4295 (3) | O6 | 3912 (4) | —0927 (3) | 4054 (2) |
| C15 | 3714 (6) | 1115 (4) | 3729 (3) | N | 4490 (5) | 4212 (4) | 3177 (2) |
| C16 | 4397 (6) | 1035 (5) | 4151 (4) | | | | |

A comparison of the structures of (I) and (II) has shown that hydrogenolysis of the methylenedioxy group has taken place and a new hydroxy group has been formed at C8. In order to confirm the structure suggested previously, an x-ray structural investigation has been made of 8-hydroxy-7,8-demethylenedioxy-6-dehydroeldelidine, and Fig. 1 shows its structure in projection of the (100) crystallographic plane. The molecule consists of six rings the numbering of which is given in conformity with that of diterpene alkaloids of the aconitine type. The conformations of the rings are as follows: the cyclohexane rings A, D, and E — chair; the cyclopentane ring B — boat; and the cyclopentane rings C and F — slightly distorted envelope. The linkage of rings A/B is trans and those of rings B/C and B/D cis.

Thus, compound (II) is 8β, 10β-dihydroxy-1α, 14α, 16β-trimethoxy-4β-methyl-6-dehydroaconitine.

The lengths of the ordinary C–C bonds range between 1.51 and 1.56 Å (the error of the experiment was not more than 0.01 Å), which agrees with the standard values [2]. No anomalous deviations are observed in the values of the valence angles (error not more than 0.5°). The space group and the parameters of the elementary cell were established by the photographic method and were refined on a diffractometer using $CuK_\alpha$ radiation a = 9.458(3), b = 12.226 (3), c = 19.433(2) Å; space group $P2_12_12_1$; Z = 4. The calculations made use of 1760 reflections. The structure was interpreted by the direct method using the Rentgen-75 program [3] in the automatic regime and was refined by the method of least squares in the anisotropic approximation to R = 0.089. The coordinates of the basis atoms are given in Table 1.

## LITERATURE CITED


1. A. S. Narzullaev, M. S. Yunusov, E. G. Sirotenko, Ya. V. Rashkes, and S. S. Sabirov, Khim. Prir. Soedin., 527 (1989).
2. International Tables for X-ray Crystallography, Kynoch Press, Birmingham, Vol. IV (1962).
3. V. I. Andrianov, Z. I. Safina, and B. L. Tarnopol'skii, Zh. Strukt. Khim., 15, 911 (1974).