

In the aqueous fraction remaining after the ethyl acetate extraction of the aqueous methanolic extract, 8-O-acetylharpagide, harpagide, and sucrose were detected on a column of polyamide identified by TLC and melting points in comparison with an authentic sample.

This is the first time that harpagide and 8-O-acetylharpagide have been isolated from oriental germander although harpagide has been detected in this plant previously by paper chromatography [9].

LITERATURE CITED

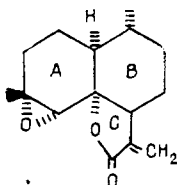
1. G. V. Lazur'evskii, I. V. Terent'eva, and A. A. Shamshurin, Practical Work on the Chemistry of Natural Compounds [in Russian], Moscow (1966), p. 166.
2. E. T. Oganesyanyan, A. V. Simonyan, and A. L. Shinkarenko, The Cyanidin Reaction in the Analysis of Flavonoids [in Russian], Pyatigorsk (1976), p. 3.
3. T. J. Mabry, K. R. Markham, and M. B. Thomas, The Systematic Identification of Flavonoids, Springer, New York (1970).
4. C. H. Brieskorn and W. Biechele, Tetrahedron Lett., 2603 (1969).
5. T. K. Chumbalov, V. I. Glyzin, and R. A. Zhubaeva, Khim. Prir. Soedin., 791 (1974).
6. A. R. Trim and R. Hill, Biochem. J., 50, 310 (1952).
7. M. L. Scarpati, M. Guiso, and L. Panizzi, Tetrahedron Lett., 3439 (1965).
8. H. Lichti and A. Wartburg, Helv. Chim. Acta, 49, 1552 (1966).
9. J. Ruhdorfer and H. Rimpler, Z. Naturforsch., 36c, 697 (1981).

MOLECULAR STRUCTURE OF THE SESQUITERPENE LACTONE ARTEANNUIN B

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On the basis of the results of NMR, IR, and CD spectroscopy, the following structure has been proposed for the sesquiterpene lactone arteannuin B isolated from *Artemisia annua* L.:



The results of an x-ray structural analysis of this compound that we have performed have confirmed the proposed structure and permitted the conformations of the three linked rings to be determined unambiguously. The spatial structure of the lactone arteannuin B (I) is shown in Fig. 1 in projection on the (010) plane, which shows the cis-linkage of rings A/B and the trans-linkage of B/C. The methyl groups at C(4) and C(10) have the β - and α -orientations, respectively. Ring A has the half-chair conformation: the C(3)...C(6) atoms are located in one plane, and C(1) and C(2) depart from this plane in opposite directions by 0.29 and 0.59 Å, respectively. The second six-membered ring, B, has the chair conformation. The lactone ring has the envelope conformation; the departure of the C(6) atom from the plane of the other four is determined with an accuracy of 0.08 Å and amounts to -0.60 Å. The values of the valence angles and of the bond lengths (see Table 1 and Fig. 1) agree, within the limits of error, with those given in [3] and with standards [4]. The errors in the determination of the bond lengths are not greater than 0.01 Å.

Crystals were obtained from a 1:4 mixture of hexane and benzene. The space group and the parameters of the elementary cell were determined by a photographic method and were refined on a Syntex P2₁ diffractometer: a = 9.045; b = 12.263; c = 12.275 Å; space group P2₁2₁2₁, z = 4. The calculations made use of 731 nonzero reflections. The structure was interpreted by

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TABLE 1. Valence angles (ω , deg)

Angle	ω	Angle	ω	Angle	ω
6-1-10	108,2 (5)	4-5-18	58,9 (3)	8-9-10	113,8 (5)
6-1-2	108,8 (4)	6-5-18	114,6 (5)	9-10-1	113,4 (5)
2-1-10	113,5 (4)	5-6-1	111,9 (4)	9-10-15	109,3 (5)
1-2-3	110,6 (5)	5-6-7	114,1 (4)	1-10-15	110,9 (5)
2-3-4	114,2 (5)	1-6-7	110,4 (4)	7-11-13	133,6 (5)
3-4-14	116,4 (5)	5-6-17	100,2 (4)	7-11-12	102,7 (4)
3-4-5	120,2 (5)	7-6-17	100,9 (4)	12-11-13	123,5 (5)
5-4-14	119,19 (6)	1-6-17	110,7 (4)	11-12-17	109,1 (5)
14-4-18	113,9 (5)	6-7-11	101,3 (4)	17-12-16	121,2 (6)
5-4-18	59,5 (3)	8-7-11	123,6 (4)	11-12-16	129,6 (6)
3-4-18	113,9 (5)	6-7-8	112,2 (4)	5-18-4	61,4 (3)
4-5-6	121,3 (5)	7-8-9	104,8 (4)	6-17-12	107,6 (4)

TABLE 2. Coordinates of the Atoms ($\times 10^4$, for H $\times 10^3$)

Atom	x/a	y/b	z/c	Atom	x/a	y/b	z/c
C(1)	1184 (6)	-0002 (5)	2152 (5)	H (1)	166	057	150
C(2)	0441 (7)	0624 (6)	3092 (6)	H (2)	142	-113	343
C(3)	-0202 (7)	-0174 (7)	3940 (5)	H (2')	-026	125	265
C(4)	0809 (6)	-1089 (6)	4234 (5)	H (3)	-037	029	483
C(5)	2157 (7)	-1303 (5)	3576 (4)	H (3')	-121	-056	357
C(6)	2540 (6)	-0607 (5)	2597 (5)	H (5)	248	-216	374
C(7)	3311 (6)	-1217 (4)	1696 (5)	H (7)	346	-058	106
C(8)	2384 (7)	-2146 (5)	1258 (5)	H (8)	307	-275	072
C(9)	0958 (7)	-1504 (6)	0754 (5)	H (8')	196	-278	205
C(10)	0156 (7)	-0845 (6)	1601 (5)	H (9)	161	-107	022
C(11)	4822 (6)	-13,5 (5)	2172 (5)	H (9')	042	-225	054
C(12)	5037 (7)	-0340 (6)	2808 (5)	H (10)	-048	-153	211
C(13)	5812 (7)	-2141 (5)	2111 (6)	H (13)	565	-288	167
C(14)	0136 (8)	-2013 (7)	4896 (7)	H (13')	661	-250	261
C(15)	-1122 (8)	-0288 (7)	1037 (6)	H (14)	085	-254	480
O(16)	6154 (5)	0057 (5)	3157 (5)	H (14')	-010	-159	571
O(17)	3707 (4)	0173 (3)	2923 (4)	H (15)	-199	047	152
O(18)	2247 (5)	-0738 (4)	4620 (3)	H (15')	-129	-063	029
				H (15'')	-099	0,50	090

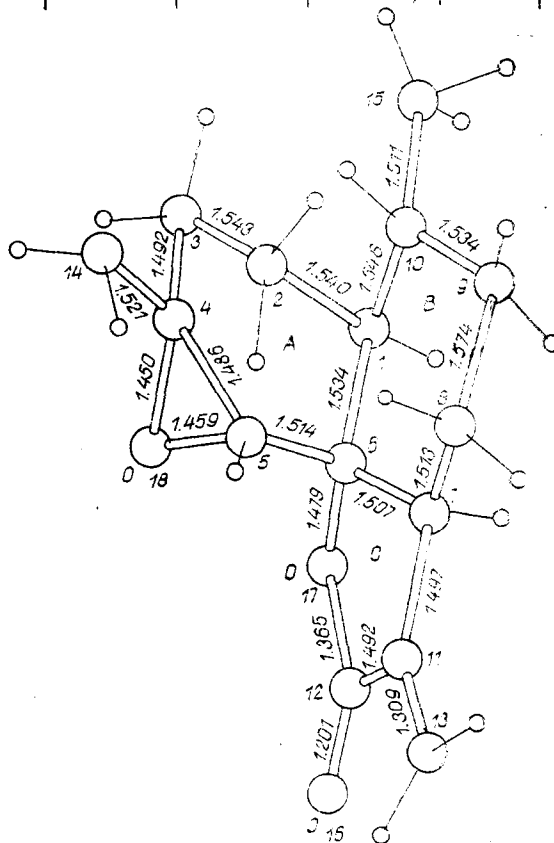


Fig. 1

the direct method using the Rentgen-75 program [5] in the automatic regime and was refined by the method of least squares (MLS) first in the isotropic approximation and then in the anisotropic approximation to $R = 0.064$. Difference series enabled all the hydrogen atoms (except for one H at C(14)) to be found. The coordinates of the atom are given in Table 2.

The experimental results were obtained on the Sintex P2, diffractometer with the participation of B. T. Ibragimov of the Institute of Bioorganic Chemistry, Academy of Sciences of the Uzbek SSR.

LITERATURE CITED

1. D. Jeremic, A. Jokic, A. Behbud, and M. Stefanovic, *Tetrahedron Lett.*, **32**, 3039-3042 (1973).
2. Tu You-you, Ni Mu-yun, Zhong Yu-rong, Li Lan-na, Cui Shu-lian, et al., *Plant. Med.*, **44**, 143-145 (1982).
3. G. Ruban and V. Zabel, *Acta Crystallogr.*, **4**, 34, 1163-1167 (1978).
4. *International Tables for X-ray Crystallography*, III. Kynoch Press, Birmingham (1962).
5. V. I. Ardrianov, Z. Sh. Safina, and B. L. Tarnopol'skii, *Zh. Strukt. Khim.*, **15**, 911 (1974).

COMPOSITION OF THE ESSENTIAL OIL OF THE MYCELIAL FUNGUS *Eremothecium ashbyi*

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The mycelial fungus *Eremothecium ashbyi* is used in industry as a producing agent of riboflavin [1]. The capacity of this microorganism also for synthesizing monoterpene alcohols — geraniol, nerol, and linalool — has been shown by TLC and GLC methods [2].

To investigate the prospects of the use of the aromatic material produced by *E. ashbyi* a more detailed investigation of its composition is necessary. In view of this, we have studied the essential oil of a number of strains of *E. ashbyi* — BKM-F 124, 1397, 1399, 1906, and 108 — after their cultivation for two days on a fermentation medium containing (g/liter): glucose, 10; peptone, 3; yeast extract, 0.5; sodium succinate, 1.5; K_2HPO_4 , 0.5; inositol, 140 mg/liter. The culture was grown in flasks on a shaking machine at 200 rpm and $28 \pm 2^\circ C$. The essential oil was isolated from the culture liquid by steam distillation [3]. Depending on the strain characteristics, its yield varied in the range of 53.2 ± 105.0 mg/liter [sic]. The product obtained was a mobile pale yellow liquid with n_D^{20} 1.4791-1.4840.

The essential oil was fractionated on a column of silica gel with the hexane-ethyl acetate (85:15) solvent system and was investigated by TLC and GLC (Chrom-4 chromatograph) using three columns with different polarities, by IR spectroscopy (Specord IR-75 instrument), and by chromat-mass spectrometry in the LKB GC-MS-2091 analytical system. The following main components of value for perfumery were identified in the essential oil: geraniol (41.3-54.9%), citronellol (1.9-3.8%), nerol (0.8-2.3%), linalool (0.1-0.4%), and β -phenylethanol (17.5-30.1%). The presence of citronellol and β -phenylethanol in the essential oil of *E. ashbyi* has not been reported previously. In addition, we detected minor components of the oil — geraniol, nerol, and esters of geraniol and citronellol (up to 1.2% in total).

The composition and ratio of the components given, and also the physicochemical and spectral indices of the essential oil of *E. ashbyi* are similar to those from the essential oil from fresh rose petals, containing mainly monoterpene alcohols and β -phenylethanol [4]. The interstrain differences in the composition and ratio of some components of the essential oil were insignificant.

LITERATURE CITED

1. M. G. Golysheva, E. V. Grishankova, V. É. Uspenskaya, M. I. Tsibul'skaya, L. Kh. Gofman, and T. A. Vasina, *Mikrobiologiya*, **34**, No. 4, 661 (1965).

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