14. L. A. Gribov and V. A. Dement'ev, Methods and Algorithms for Calculations in the Theory of the Vibrational Spectra of Molecules [in Russian], Nauka, Moscow (1981).
15. É. Lukevits, N. P. Erchak, Yu. Yu. Popelis, and I. V. Dipan, Zh. Obshch. Khim., 47, 802 (1977).

2,2-DIMETHYL-5-(5-R-FURFURYLIDENE)-1,3-DIOXANE-4,6-DIONES. 3.* SELECTIVE HYDROGENATION OF THE EXOCYCLIC DOUBLE BOND AND THREE-DIMENSIONAL STRUCTURES OF THE REACTION PRODUCTS

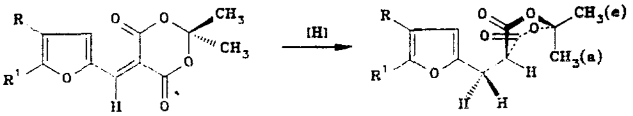
G. D. Krapivin, V. E. Zavodnik,
N. I. Val'ter, V. K. Bel'skii,
and V. G. Kul'nevich

UDC 547.841'727:548.
737:542.942.3

The reaction of 2,2-dimethyl-5-(5-R-furfurylidene)-1,3-dioxane-4,6-diones with sodium borohydride in alcohol leads exclusively to products of hydrogenation of the exocyclic double bond. The three-dimensional structure of one of them – 2,2-dimethyl-5-(5-methyl-furfuryl)-1,3-dioxane-4,6-dioxane – was investigated by x-ray diffraction analysis (XDA).

In [2] on the basis of an analysis of the PMR spectra of substituted 5-benzyl-2,2-dimethyl-1,3-dioxane-4,6-diones it was concluded that the molecules of these compounds are folded into a "sandwich" in which the benzene ring is situated almost parallel to the planar dioxanedione ring. However, recent x-ray diffraction studies of Meldrum's acid and its 5-ethyl and 5-phenyl derivatives [3, 4] have shown that in the crystal the dioxanedione ring has a boat conformation, while the substituent in the 5 position is equatorially oriented. These data cast doubt on the possibility of the formation of the "sandwich" structures proposed in [2].

The present research was carried out to shed some light on the problem of the three-dimensional structures of compounds that are, in principle, capable of forming intramolecular complexes of this type. We selected furfuryldioxanediones as the subjects of our investigation. These compounds are of interest, first, from the point of view of the study of the chemical properties of furfurylidenedioxanediones [5] – particularly the possibility of the selective hydrogenation of the exocyclic C=C bond of the latter – and, second, for a comparison of the three-dimensional structures of the molecules before and after hydrogenation of the ylidene bond.



I a-f II a-f

I, II a-e R=H, f R=Br; a R^1=H, b R^1=Me, c R^1=C≡CPh, d R^1=Br, e,f R^1=I

Various methods exist for the hydrogenation of alkylidene and benzylidene derivatives of Meldrum's acid on both a heterogeneous catalyst [6] and under homogeneous conditions (lithium aluminum hydride [7], sodium borohydride [8], the borane–dimethylamine complex [9]). Our investigations showed that the catalytic hydrogenation of furfurylidenedioxanediones I on Raney nickel and on palladium on carbon at increased and atmospheric pressure leads to complex and difficult-to-separate mixtures of products. Hydrogenation on inactivated (with water and then with dilute acetic acid until the pyrophoric character in the dry state vanishes) Raney nickel in a stream of hydrogen at atmospheric pressure and room temperature makes it possible to ob-

---

*See [1] for Communication 2.

Krasnodar Polytechnical Institute, Krasnodar 350670. L. Ya. Karpov Scientific-Research Institute of Phyhsical Chemistry, Moscow 107120. Translated from Khimiya Geterotsiklicheskikh Soedinenii, No. 9, pp. 1201-1207, September, 1989. Original article submitted April 13, 1987; revision submitted December 13, 1988.

0009-3122/89/2509-1005$12.50

TABLE 1. Characteristics of the Synthesized Compounds

Compound	Empirical formula	mp, °C	ν_{CO}, cm^{-1}		λ_{max}, nm (lg ε)	Yield, %
			ν_s	ν_{as}		
IIa	$C_{11}H_{12}O_5$	92...93	1801	1765	218 (4,34)	96 (92*)
IIb	$C_{12}H_{14}O_5$	67...68	1795	1750	224 (4,25)	95 (90*)
IIc	$C_{19}H_{16}O_5$	118...119	1800	1760	222 (4,30)	95
IId	$C_{11}H_{11}BrO_5$	104...105	1803	1765	222 (4,21)	86
IIe	$C_{11}H_{11}IO_5$	119...121	1802	1765	230 (4,14)	87
IIf	$C_{11}H_{10}BrIO_5$	126...127	1800	1760	233 (4,19)	94

*Method A.

TABLE 2. PMR Spectra of the Synthesized Compounds (δ, ppm; J, Hz)

Compound	3-H	4-H	$J_{3,4}$	CH*	CH_2*	CH_3 (e)	CH_3 (a)	Other signals
IIa	6,08	6,18	3,0	3,78	3,42	1,72	1,60	7,20 (1H, dd , 5-H); $J_{4,5}=1,8$; $J_{3,5}=0,8$
IIb	5,92	5,78	3,0	3,80	3,33	1,72	1,58	2,16 (3H, d, Me); $J_{4\text{-H—Me}}=0,6$
IIc	6,13	6,48	3,5	3,88	3,41	1,70	1,62	7,28 (5H, s, Ph)
IId	6,10	6,10	—	3,82	3,37	1,73	1,63	—
IIe	6,37	6,07	3,5	3,82	3,40	1,75	1,65	—
IIf	6,22	—	—	3,80	3,42	1,75	1,67	—

*In the $CHCH_2$ group ^3J = 5.0 Hz (5.3 Hz for IIb).

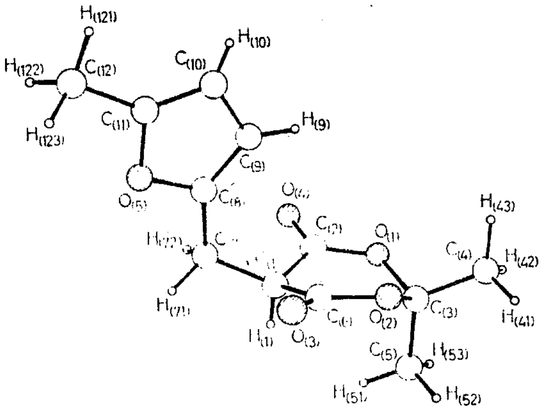


Fig. 1. Structure of the IIb molecule (B_1 conformer).

tain only IIa,b in high yields (Table 1, method A). Phenylacetylenic derivative Ic is not hydrogenated under these conditions, and halo derivatives Ie-f undergo resinification.

The reaction with lithium aluminum hydride in methanol leads to complex mixtures of products and is accompanied by resinification. The yields of II reach quantitative levels with sodium borohydride (Table 1). The method is simple to carry out and makes it possible to use compounds with diverse substituents in the furan ring; 95% ethanol can be used successfully as the solvent.

Furfuryldioxanediones IIa-f (Tables 1 and 2) are colorless crystalline substances; monohalo-substituted IId,e are unstable when they are stored in light.

Only one intense absorption band at 218-232 nm, which corresponds to a π → π* transition in the substituted furan ring, is observed in the electronic spectra of II in hexane. Phenyl furylacetylene IIc, in the spectrum of which several absorption bands are observed, constitutes an exception; the longest-wave band with a well-expressed vibrational structure has a maximum at 298 nm.

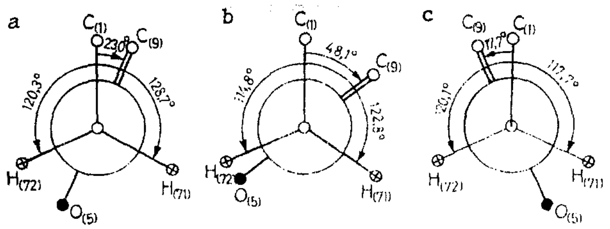


Fig. 2. Newman projection along the $C_{(7)}-C_{(8)}$ bond: a) A conformer; b) B conformer; c) B_1 conformer.

As in the spectra of furfurylidenedioxanediones I [5], in the IR spectra of furfuryldioxanediones II (Table 1) there are two characteristic bands of symmetrical and asymmetrical stretching vibrations of carbonyl groups; the ν_{as} band is approximately twice as intense as the ν_s band. However, in the case of furfuryl derivatives II these bands are shifted 40-50 cm^{-1} to the high-frequency side as compared with the corresponding bands of furfurylidene compounds I [5].

The PMR spectra of II (Table 2) contain singlet signals of two chemically unequivalent methyl groups of the dioxanedione ring, a set of lines of an A_2B spin system (A_2X at 250 MHz) of the protons of the CH_2CH grouping, and signals of protons of the furan ring (and the substituents in them).

To carry out the x-ray diffraction studies we used IIb, which forms crystals of the same syngony but different structural classes from different solvents. In the monoclinic crystals grown from toluene–hexane (2:1) there is only one type of A molecule. In the unit cell of the monoclinic crystal obtained from solution in ethyl acetate there are two pairs of symmetrically independent conformers B and B_1.

The Newman projections (Fig. 2) show characteristic differences among the A, B, and B_1 conformers, the coordinates of the atoms, the bond lengths, and some bond angles of which are presented in Tables 3-5.

The furan ring in the A, B, and B_1 molecules is planar within the limits 0.005 Å. The $C_{(7)}$ and $C_{(12)}$ atoms lie in the plane of the furan ring, and their maximum deviation from the plane does not exceed 0.005 Å.

A quantitative comparison of the geometry of the dioxanedione fragment, including the $C_{(7)}$ atom, of all three type of molecules led to low values of the s criterion (0.070, 0.060, and 0.045 A for the B/B_1, B/A, and B_1/A pairs of molecules, respectively). In accordance with the classification in [10, 11] the values of the s criterion found fall into the first group, i.e., the dioxanedione fragments of all three conformers are geometrically equal, which makes it possible to use any of the independent molecules in the subsequent examination of the structure of the dioxanedione ring.

The six-membered ring has a boat conformation; the $C_{(1)}$ and $C_{(3)}$ atoms deviate from the plane of the remaining four atoms of the "bottom of the boat" by 0.33 and 0.41 Å, respectively. The $O_{(1)}O_{(2)}C_{(3)}$ and $C_{(1)}C_{(2)}C_{(6)}$ dihedral angles between the planes of the "bottom of the boat" and the "walls of the boat" are equal to 36.2° and 26.8°, respectively.

The tendency of the CC(=O)OC fragments to adopt a planar orientation leads to deviation of the $O_{(3)}$ and $O_{(4)}$ atoms from the plane of the "bottom of the boat" by 0.25 Å. The $C_{(4)}$ atom of the equatorial group deviates from this plane by approximately the same distance.

The A, B, and B_1 molecules differ not only with respect to the angles of rotation of the plane of the furan ring relative to the plane of symmetry of the dioxanedione ring [the $C_{(1)}$-$C_{(3)}C_{(4)}C_{(5)}C_{(7)}$ plane, the deviation of the atoms from the plane does not exceed 0.03 Å] but also with respect to the mutual orientation of the "bottom of the boat" and the furan ring.

In the B and B_1 molecules the planes of the "bottom of the boat" and the furan rings are virtually mutually perpendicular (the angles between the planes are 92.6° and 89.6°, respectively). The angle between these planes in the A molecule is 101.9°.

TABLE 3. Coordinates of the Atoms of the Independent A, B, and B_1 Molecules ($\cdot 10^4$ for the O and C atoms; $\cdot 10^3$ for the H atoms)*

Atom	Molecule A			Molecule B			Molecule B_1		
	x	*y*	*z*	*x*	*y*	*z*	*x*	*y*	*z*
$O_{(1)}$	7176(3)	1334(2)	0000(0)	714(8)	6606(2)	5000(0)	6403(6)	−270(2)	952(2)
$O_{(2)}$	8400(2)	2594(1)	2980(5)	4147(8)	7539(3)	4468(3)	9501(7)	−1006(2)	1755(2)
$O_{(3)}$	6994(2)	3119(2)	5928(5)	4484(10)	7632(3)	3071(3)	9916(8)	−788(3)	3158(3)
$O_{(4)}$	4554(4)	825(2)	−200(9)	−1705(10)	5761(3)	4162(3)	3867(7)	628(2)	1579(3)
$O_{(5)}$	2715(4)	3248(3)	4728(11)	3237(10)	6010(3)	1611(3)	6368(7)	1821(2)	3745(2)
$C_{(1)}$	5639(3)	1606(2)	3655(6)	635(9)	7020(3)	3507(3)	6022(10)	−336(3)	2521(3)
$C_{(2)}$	5724(3)	1232(2)	1028(6)	−238(11)	6403(4)	4232(3)	5313(10)	57(3)	1663(3)
$C_{(3)}$	8638(7)	1764(5)	1418(14)	2304(14)	7409(4)	5178(4)	7876(8)	−1036(3)	986(3)
$C_{(4)}$	9879(7)	2246(5)	−441(13)	3903(14)	7246(4)	5958(4)	9704(13)	−948(5)	239(4)
$C_{(5)}$	9044(6)	898(4)	2969(14)	713(16)	8221(5)	5252(5)	6108(13)	−1871(4)	996(4)
$C_{(6)}$	7041(3)	2506(2)	4324(6)	3228(13)	7421(4)	3645(4)	8624(10)	−719(3)	2524(3)
$C_{(7)}$	4016(5)	1832(3)	4368(12)	200(12)	6604(4)	2610(4)	5625(11)	295(3)	327(3)
$C_{(8)}$	3736(3)	2815(2)	3317(6)	2050(13)	5913(4)	2398(4)	7247(10)	1153(3)	3233(3)
$C_{(9)}$	4281(4)	3441(3)	1375(8)	2917(13)	5202(3)	2802(3)	9344(10)	1456(3)	2803(3)
$C_{(10)}$	3569(4)	4324(3)	1575(8)	4732(14)	4841(4)	2238(4)	9860(11)	2373(3)	3060(3)
$C_{(11)}$	2632(5)	4177(3)	3590(11)	4865(14)	5337(4)	1526(5)	8062(13)	2557(3)	3624(4)
$C_{(12)}$	1593(5)	4774(3)	4856(9)	6423(13)	5319(4)	719(4)	7443(16)	3365(4)	4131(4)
$H_{(1)}$	577(3)	106(2)	456(6)	−53(11)	749(3)	353(4)	463(10)	−83(3)	260(4)
$H_{(71)}$	383(3)	178(2)	620(8)	−173(10)	633(3)	256(3)	608(9)	2(3)	380(3)
$H_{(72)}$	322(4)	123(3)	385(8)	68(10)	705(3)	219(3)	381(11)	38(3)	327(4)
$H_{(9)}$	496(3)	334(2)	−2(8)	206(10)	498(3)	337(3)	1067(10)	116(3)	246(3)
$H_{(10)}$	371(3)	485(2)	67(7)	610(10)	434(3)	236(3)	1131(10)	281(3)	289(3)

---

*The coordinates of the hydrogen atoms of the methyl groups are not presented; they can be obtained from the authors.

TABLE 4. Bond Lengths in the Independent A, B, and B_1 Molecules (Å)

Bond	A	B	B_1	Bond	A	B	B_1
$O_{(1)}—C_{(2)}$	1,333(3)	1,311(6)	1,342(6)	$C_{(3)}—C_{(4)}$	1,484(9)	1,492(10)	1,492(8)
$O_{(1)}—C_{(3)}$	1,457(6)	1,441(7)	1,432(5)	$C_{(3)}—C_{(5)}$	1,516(9)	1,529(10)	1,505(7)
$O_{(2)}—C_{(3)}$	1,429(7)	1,458(8)	1,454(6)	$C_{(7)}—C_{(8)}$	1,481(6)	1,503(9)	1,494(7)
$O_{(2)}—C_{(6)}$	1,348(4)	1,346(8)	1,352(6)	$C_{(7)}—H_{(71)}$	1,00(4)	1,06(5)	0,94(5)
$O_{(3)}—C_{(6)}$	1,188(4)	1,193(8)	1,195(7)	$C_{(7)}—H_{(72)}$	0,95(3)	0,95(5)	0,96(6)
$O_{(4)}—C_{(2)}$	1,210(4)	1,194(7)	1,190(6)	$C_{(8)}—C_{(9)}$	1,343(5)	1,345(8)	1,329(7)
$O_{(5)}—C_{(8)}$	1,375(5)	1,365(8)	1,382(6)	$C_{(9)}—C_{(10)}$	1,436(5)	1,419(9)	1,444(6)
$O_{(5)}—C_{(11)}$	1,384(6)	1,372(8)	1,379(6)	$C_{(9)}—H_{(9)}$	0,98(4)	1,02(5)	1,00(5)
$C_{(1)}—C_{(2)}$	1,501(4)	1,503(7)	1,506(7)	$C_{(10)}—C_{(11)}$	1,332(7)	1,327(9)	1,320(8)
$C_{(1)}—C_{(6)}$	1,514(3)	1,500(8)	1,508(7)	$C_{(10)}—H_{(10)}$	0,83(3)	1,09(5)	1,00(5)
$C_{(1)}—C_{(7)}$	1,531(6)	1,528(8)	1,538(7)	$C_{(11)}—C_{(12)}$	1,481(7)	1,486(9)	1,501(8)
$C_{(1)}—H_{(1)}$	0,90(3)	0,97(5)	1,00(5)				

TABLE 5. Bond Angles (deg) in the A, B, and B_1 Molecules

Angle	A	B	B_1	Angle	A	B	B_1
$C_{(2)}O_{(1)}C_{(3)}$	120,8(3)	123,5(4)	122,0(3)	$C_{(4)}C_{(3)}C_{(5)}$	115,1(5)	114,2(5)	115,5(5)
$C_{(3)}O_{(2)}C_{(6)}$	121,5(3)	119,4(5)	121,4(4)	$C_{(1)}C_{(7)}C_{(8)}$	114,4(3)	113,4(5)	113,6(4)
$C_{(2)}C_{(1)}C_{(6)}$	112,9(2)	112,1(4)	113,8(4)	$O_{(5)}C_{(8)}C_{(9)}$	109,5(3)	108,8(5)	109,9(4)
$C_{(2)}C_{(1)}C_{(7)}$	114,5(3)	112,9(4)	112,5(4)	$C_{(7)}C_{(8)}C_{(9)}$	136,8(4)	136,0(6)	136,3(5)
$C_{(6)}C_{(1)}C_{(7)}$	111,9(3)	113,6(4)	113,5(4)	$C_{(8)}O_{(5)}C_{(11)}$	107,0(4)	107,8(5)	106,5(4)
$C_{(7)}C_{(1)}H_{(1)}$	108(2)	105(3)	104(3)	$C_{(8)}C_{(9)}C_{(10)}$	106,7(3)	106,9(5)	106,5(4)
$O_{(4)}C_{(2)}C_{(1)}$	123,9(3)	125,6(5)	124,6(5)	$C_{(9)}C_{(10)}C_{(11)}$	107,3(3)	107,5(6)	107,2(5)
$O_{(3)}C_{(6)}C_{(1)}$	123,8(3)	123,9(6)	124,1(5)	$O_{(5)}C_{(11)}C_{(10)}$	109,5(4)	109,1(6)	110,0(5)
$O_{(1)}C_{(3)}O_{(2)}$	110,0(4)	107,6(5)	110,3(3)	$C_{(10)}C_{(11)}C_{(12)}$	135,2(4)	133,5(6)	135,2(6)

In conclusion, let us note the following. First, considering the results obtained by x-ray diffraction analysis in [1, 3, 4] and in the present research one may assume that the hybridization of the $C_{(5)}$ atom of the dioxanedione ring has a decisive effect on the geometry of the ring. In compounds with an sp^3-hybridized $C_{(5)}$ atom the dioxanedione ring has a boat conformation. Second, one should exclude the possibility of the formation of the "sandwich" structures proposed in [2], since a bulky substituent attached to the $C_{(5)}$ atom of the dioxanedione ring is always equatorially oriented.

EXPERIMENTAL

The IR spectra of solutions of the compounds in CCl_4 were recorded with a UR-20 spectrometer. The electronic spectra were obtained with a Specord UV-vis spectrophotometer. The PMR spectra of solutions in deuterochloroform were obtained with Tesla BS-467 (60 MHz) and Bruker WM-250 (250 MHz) spectrometers. The course of the reactions and the purity of the products were monitored by means of TLC on Silufol UV-254 plates in a toluene—ethanol system (20:3). The compositions of hydrogenation products IIa-f were confirmed by the results of elementary analysis for C and H; products IId,e were also analyzed for their halogen content.

2,2-Dimethyl-5-(5-methylfurfuryl)-1,3-dioxane-4,6-dione (IIb). A) A 0.7-g (30 mmole) sample of Ib was dissolved in 40 ml of ethanol, 2 g of inactivated Raney nickel was added, and hydrogenation was carried out in a "catalytic long-necked hydrogenation flask" for 70 min at room temperature. The catalyst was removed by filtration, the filtrate was diluted with water (100 ml), and the precipitated crystals were recrystallized.

Compound IIa was similarly obtained.

B) Sodium borohydride as added in ~0.05 portions [a total of 0.2 g (5 mmole)] with vigorous stirring at room temperature to a solution of 2.36 g (10 mmole) of Ib in 50 ml of ethanol until the solution became colorless, after which it was cooled and treated with 100 g of finely crushed ice. The aqueous mixture was acidified with dilute (1:10) hydrochloric acid to pH ≈ 6, and the resulting precipitate was washed with water and recrystallized.

Compounds IIa,c-f were similarly obtained.

Monoclinic crystals were obtained in the crystallization of IIb from toluene—hexane (2:1). These crystals had the following unit cell parameters: a = 8.527(2), b = 13.160(2), c = 5.370(2) Å. γ = 103.4°, V = 586.6(3) $Å^3$, space group $p2_1$, Z = 2. The parameters of the unit cell and the intensities of 874 independent reflections with I > 30 (I)were obtained with a PT Syntex automatic diffractometer (MOK_{α} emission, β filter, θ/2θ scanning to $2\theta_{max} = 55°$).

Monoclinic crystals with the following unit cell parameters were obtained by crystallization of IIb from ethyl acetate: a = 5.199(1), b = 15.066(3), c = 15.415(4) Å, γ = 94.08(2)°, V = 1204.4(6) $Å^3$, space group $P2_1$, Z = 4. The experimental data were similarly obtained. In all, 1529 independent reflections with $I > 3\sigma(I)$ were measured.

The structures were decoded by the direct method by means of a complex of SHELXTL programs [12] with a NOVA-3 computer and were refined within the anisotropic (isotropic for the hydrogen atoms) approximation up to divergence factors R = 0.03, R_{ω}= 0.032, and R = 0.042, R_{ω}= 0.042 for the first and second types of crystals, respectively.*

LITERATURE CITED

1. G. D. Krapivin, V. E. Zavodnik, V. K. Bel'skii, N. I. Val'ter, and V. G. Kul'nevich, Khim. Geterotsikl. Soedin., No. 11, 1453 (1988).
2. I. Schuster and P. Schuster, Terahedron, 25, 199 (1969).
3. A. Van Coppernolle, J. P. Declercq, J. M. Dereppe, G M. Germain, and M. Van Meersche, Bull. Soc. Chim. Belges, 88, 223 (1979).
4. G. E. Pfluger and P. D. Boyle, J. Chem. Soc., Perkin 2, No. 10, 1547 (1985).
5. G. D. Krapivin, V. G. Kul'nevich, and N. I. Val'ter, Khim. Geterotsikl. Soedin., No. 10, 1325 (1986).
6. G. Swoboda, J. Swoboda, and F. Wessely, Monatsh. Chem., 95, 1283 (1964).
7. A. Stephen and F. Wessely, Monatsh. Chem., 98, 184 (1967).
8. A. D. Wright, M. L. Haslego, and P. X. Smith, Tetrahedron Lett., 20, 2325 (1979).
9. D. M. Hrubowohak and F. X. Smith, Tetrahedron Lett., 24, 4951 (1983).

---

*The anisotropic temperature factors of the nonhydrogen atoms can be obtained from the authors.

10. A. E. Rozumaeva and P. M. Zorkii, Zh. Strukt. Khim., 21, 77 (1980).
11. P. M. Zorkii and A. E. Rozumaeva, Zh. Strukt. Khim., 20, 463 (1979).
12. G. M. Sheldrick, Computational Crystallography, Oxford University Press, New York–Oxford (1982), p. 506.

N-[3-NITRO(AMINO)COUMARIN-4-YL]ANTHRANILIC ACID AMIDES. SYNTHESIS OF 6,7,8,13-TETRAHYDRO[1]BENZOPYRANO[4,3-b][1,4] BENZODIAZEPINE-6,8-DIONE*

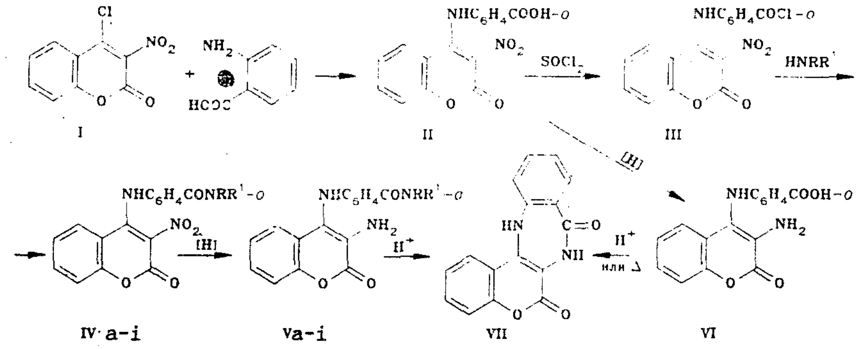
V. L. Savel'ev, O. S. Artamonova,
A. V. Makarov, V. S. Troitskaya,
A. V. Antonova, and V. G. Vinokurov

UDC 547.892'837.2'816:615.214

The reaction of 3-nitro-4-chlorocoumarin with anthranilic acid was used to synthesize N-(3-nitro-4-coumarinyl)-anthranilic acid, from which, through the acid chloride, we obtained a number of amides, which were reduced to N-(3-amino-4-coumarinyl)anthranilic acid amides The latter are cyclized under the influence of hydrochloric acid to 6,7,8,13-tetrahydro[1]benzopyrano-[4,3-b][1, 4]benzodiazepine-6,8-dione, which was also obtained from N-(3-amino-4-coumarinyl)anthranilic acid by its thermolysis or treatment with hydrochloric acid.

Substances with different forms of pharmacological activity have been found among derivatives of N-hetaryl-substituted anthranilic acids [2-6]. On the other hand, as we have previously shown [7, 8], 3-substituted 4-aminocoumarins have a depressive or stimulating effect on the central nervous system and also display a pronounced anticonvulsive effect [8].

In this connection by means of the reaction of 3-nitro-4-chlorocoumarin (I) with anthranilic acid we obtained N-(3-nitro-4-coumarinyl)anthranilic acid (II), which served as the starting compound for further syntheses via the following scheme:



IV, V a $R=R^1=H$; b $R=H$, $R^1=i\text{-}C_3H_7$; c $R=H$, $R^1=n\text{-}C_4H_9$; d $R=H$, $R^1=CH_2C_6H_5$; e $R=H$, $R^1=C_6H_5$; f $R+R^1=(CH_2)_4$; g $R+R^1=(CH_2)_5$; h $R+R^1=O(CH_2CH_2)_2$; i $R+R^1=CH_3N(CH_2CH_2)_2$

Characteristic absorption bands of an NH group are observed in the IR spectra of amides IVa-i at 3200-3300 cm^{-1}; absorption of the carbonyl group of the coumarin ring shows up in the form of intense bands at 1710-1740 cm^{-1}, while the frequency of the vibrations of the amido group ranges from 1610 to 1670 cm^{-1}, which is evidently explained by the possibility of the formation of intramolecular hydrogen bonds of two types (A and B), depending on the substituents in the amido group.

---

*See [1] for our preliminary communication.

Scientific-Research Institute of Pharmacology, Academy of Medical Sciences of the USSR, Moscow 125315. Translated from Khimiya Geterotsiklicheskikh Soedinenii, No. 9, pp. 1208-1212, September, 1989. Original article submitted January 4, 1988; revision submitted March 29, 1988.

0009-3122/89/2509-1011 $12.50