INVESTIGATIONS IN THE SERIES OF HETEROCYCLES.

53.* MASS SPECTRA OF 5-ARYLIDENEBARBITURIC ACIDS AND THEIR 2-THIO- AND 2-SELENO-ANALOGS

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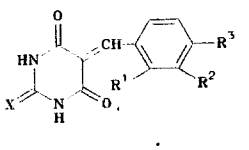
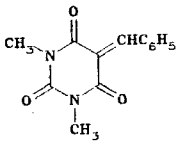
The mass spectra of 5-arylidenebarbituric acids, their 2-thio- and 2-seleno-analogs, barbituric, 2-thio- and 2-selenobarbituric acid, as well as selenourea, were obtained. The molecular ions of these compounds, as a rule, the main ones in intensity, may break down along several pathways, the ratio of which depends substantially on the nature of the atom bound to the carbon atom in the 2-position of the pyrimidine ring. The influence of substituents in the benzene ring on the direction of decomposition of the molecular ions is negligible.

The mass spectra of barbituric acid, its alkyl and aryl-derivatives, as well as a series of their 2-thio-analogs, were studied earlier in rather great detail [2-6]. The presence of an α,β-unsaturated fragment conjugated with the benzene ring and carbonyl in the molecules of organic compounds, examples of which are the 5-arylidenebarbituric acids, leads to the appearance of substantial peculiarities in the behavior of these substances under the action of electron impact [7]. At the same time, it might be expected that replacement of the carbonyl oxygen atom in the 2-position of the pyrimidine ring by sulfur or selenium atoms and variation of the substituent in the benzene ring will substantially affect the behavior of the molecular ions of 5-arylidenebarbituric acids. In connection with this, we made a mass spectrometric investigation of three series of compounds: 5-arylidenebarbituric acids (I), their 2-thio- (II) and 2-seleno-analogs (III), as well as 1,3-dimethyl-5-benzylidenebarbituric acid (IV).



I–III



IV

I X=O; II X=S; III X=Se; I—III a $R^1=NO_2$, $R^2=R^3=H$; b $R^1=R^2=H$; $R^3=NO_2$; c $R^4=R^3=H$, $R^2=NO_2$; d $R^1=R^3=H$, $R^2=Br$; e $R^1=R^3=H$, $R^2=Cl$; f $R^1=R^3=H$, $R^2=COOH$; g $R^1=R^2=H$, $R^3=Br$; h $R^1=R^2=H$, $R^3=Cl$; i $R^1=R^2=H$, $R^3=I$; j $R^1=R^3=H$, $R^2=OH$; k $R^1=R^3=H$, $R^2=OCH_3$; *l* $R^1=R^2=H$, $R^3=F$; m $R^1=R^2=R^3=H$; n $R^1=H$, $R^2=R^3=OCH_3$; o $R^1=R^2=H$, $R^3=CH_3$; p $R^1=R^2=H$, $R^3=OCH_3$; q $R^1=R^3=OCH_3$, $R^2=H$, r $R^1=R^2=H$, $R^3=N(CH_3)_2$; s $R^1=R^2=H$, $R^3=N(C_2H_5)_2$

Just as in the case of 5-arylidenebarbituric acids (I) [7], in the mass spectra of thio- (II) and seleno-derivatives (III), with rare exceptions (Tables 1-3), the peaks of molecular ions are observed with maximum intensity. The pathways of decomposition of the molecular ions $M^{+\cdot}$ of compounds I-IV are presented in scheme 1. It should be noted that in addition to the pathways of decomposition of the molecular ions (C and D) presented in [7], there are supplementary pathways (A, B, E, F, G). We should also indicate the fact that in contrast to unsubstituted barbituric acids (V) and its seleno-analog (VII) (scheme 2, Table 4), as well as other hydroxy- and thiopyrimidines, in the mass spectra of compounds I-IV no elmination of the fragment $HN_{(3)}C_{(2)}X$ is observed at the first stages of decomposition of the molecular ions. General pathways of fragmentation of $M^{+\cdot}$ for all three series of compounds are: A) with the

*For Communication 52, see [1].

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TABLE 1. Mass Spectra of 5-Arylidenebarbituric Acids (I)[a]

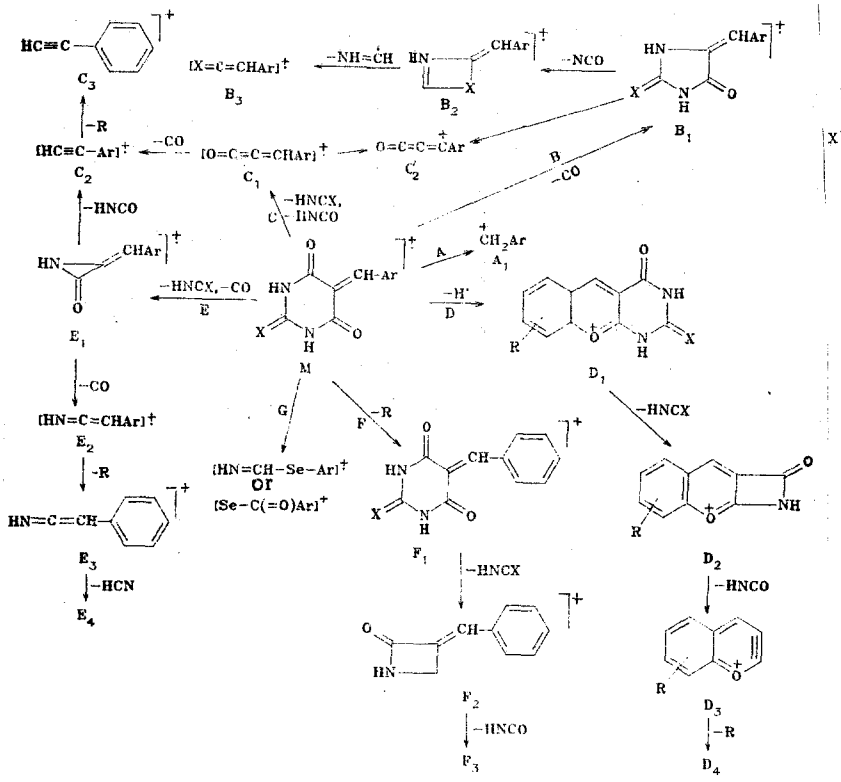
Compound	R^3	R^4	$M^{+\cdot}$	Pathway A, A_1	Pathway B, B_2	Pathway C		
						C_1	C_2	C_2'
Ic	NO_2	H	261	—	163 (12)	175 (5)	—	174 (14)
Ie	Cl	H	250/252	125/127 (20/9)	152/154 (17/5)	164/166 (14/4)	136/138 (30/11)	163/165 (23/10)
If	COOH	H	260	135 (4)	—	—	—	173 (8)
Ig	H	Br	294/296	169/171 (25/23)	196/198 (12/10)	208/210 (10/8)	180/182 (26/24)	207/209 (24/22)
Ii	H	I	342	217 (4)	—	256 (3)	228 (3)	255 (16)
Ij	OH	H	232	107 (33)	134 (10)	146 (10)	118 (22)	145 (25)
Ik	OCH_3	H	246	121 (24)	—	160 (12)	132 (8)	159 (18)
Im	H	H	216 (90)	91 (16)	118 (12)	130 (4)	102 (40)	129 (28)
Im[b]	H	H	218 (50)	92 (4)	118 (20)	130 (6)	102 (34)	129 (20)
Io	H	CH_3	230	105 (26)	132 (8)	144 (8)	116 (19)	143 (20)
Io[b]	H	CH_3	232 (30)	106 (12)	132 (16)	144 (8)	116 (28)	143 (35)
Ip	H	OCH_3	246	121 (29)	—	160 (9)	132 (13)	159 (12)
Ir	H	$N(CH_3)_2$	259	134 (30)	—	—	—	172 (10)
Is	H	$N(C_2H_5)_2$	287	162 (16)	—	201 (7)	—	—
IV	H	H	244 (80)	91 (23)	—	130 (33)	116 (16)	129 (12)

[a]The values of m/z (relative intensity, %) are cited. The if it is 100%. [b]The spectra of 1,3-dideuteroderivatives.

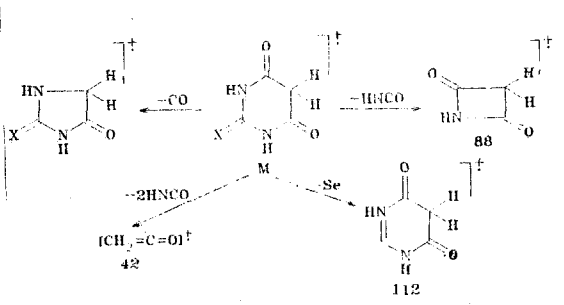
Pathway D			Pathway E		Pathway F		Other ions
D_1	D_2	D_3	E_1	E_2	F_1	F_2	
260 (38)	217 (26)	174 (14)	190 (13)	162 (12)	215 (20)	172 (36)	263 (7), 262 (20), 246 (3), 245 (20), 244 (93), 228 (14), 218 (6), 214 (82), 201 (6), 173 (16), 171 (30), 161 (8), 158 (14), 145 (10), 144 (26), 143 (8), 132 (4), 130 (4), 128 (22), 127 (6), 126 (4), 117 (14), 116 (42), 115 (18), 114 (6), 105 (13), 104 (13), 101 (32), 90 (10), 89 (38), 77 (12), 75 (25)
249/251 (90/32)	206/208 (42/20)	163/165 (23/10)	179/181 (17/5)	151/153 (12/4)	215 (50)	172 (38)	253 (10), 216 (12), 173 (6), 162 (22), 150 (6), 129 (4), 128 (4), 116 (12), 101 (20), 89 (16)
259 (64)	216 (32)	179 (8)	189 (3)	—	215 (44)	172 (23)	261 (27), 244 (20), 189 (3), 166 (20), 134 (4), 128 (11), 105 (4)
293/295 (83/81)	250/252 (43/41)	207/209 (24/22)	223/225 (12/10)	195/197 (11/10)	215 (72)	172 (54)	297 (16), 214/216 (24/20), 173 (12), 144 (6), 129 (6), 128 (22), 116 (6), 101 (25), 89 (18)
341 (55)	298 (40)	255 (16)	271 (3)	243 (4)	215 (44)	172 (50)	344 (6), 343 (30), 232 (14), 231 (6), 216 (14), 144 (4), 129 (12), 128 (33), 116 (12), 101 (33), 91 (8), 89 (16)
231 (70)	188 (55)	145 (25)	161 (15)	133 (44)	215 (44)	172 (23)	234 (12), 233 (20), 162 (10), 132 (6), 128 (16), 89 (10)
245 (58)	202 (41)	159 (18)	175 (5)	147 (4)	215 (37)	172 (25)	248 (16), 247 (20), 231 (10), 188 (10), 128 (6), 102 (14), 89 (12)
215 (100)	172 (66)	129 (28)	145 (8)	117 (11)	—	—	214 (24), 173 (14), 144 (2), 128 (20), 116 (6)
217 (84)	173 (50)	129 (20)	146 (4)	118 (20)	—	—	219 (12), 216 (100), 215 (68), 172 (52), 145 (6), 144 (2), 128 (20), 117 (6), 91 (9), 90 (6)
229 (63)	186 (53)	143 (20)	159 (7)	131 (12)	215 (90)	172 (40)	216 (14), 202 (4), 187 (12), 184 (10), 173 (6), 142 (12), 130 (13), 115 (32), 91 (6)
231 (56)	187 (32)	143 (35)	160 (5)	132 (16)	217 (26)	173 (24)	234 (3), 233 (6), 230 (100), 229 (64), 216 (56), 215 (88), 188 (4), 186 (60), 172 (42), 159 (8), 142 (20), 131 (22), 130 (22), 129 (6), 128 (3), 118 (6), 115 (50), 105 (21), 104 (10), 103 (10), 91 (10), 89 (6)
245 (58)	202 (42)	159 (12)	175 (4)	147 (4)	215 (24)	172 (11)	248 (8), 247 (20), 244 (12), 231 (8), 188 (6), 145 (8), 117 (6), 89 (8), 88 (6)
258 (55)	215 (28)	172 (10)	—	—	215 (28)	172 (10)	261 (10), 260 (22), 144 (10), 121 (8), 120 (8), 88 (70), 58 (40)
286 (20)	243 (12)	—	—	—	215 (3)	172 (3)	288 (14), 273 (24), 272 (100), 244 (26), 183 (4), 134 (8)
243 (100)	186 (41)	129 (12)	159 (9)	131 (25)	—	—	245 (24), 158 (11), 156 (8), 144 (6), 102 (34), 91 (22)

intensity of the peaks of the molecular ions is not indicated

Scheme 1



Scheme 2



formation of the corresponding benzyl cation; B) with the formation of a rearranged ion B_3; C) with simultaneous ejection of HNCX and HNCO, leading to the ions C_1 and C_2. The main pathway of decompositions of compounds I and IV is pathway D, for thio-derivatives II pathways B, D, and F, and for seleno-analogs III pathways B and C.

The formation of the benzyl cation A_1 (pathway A), characteristic of all the compounds I-IV, can occur by migration of a hydrogen atom from the nitrogen atom of the heterocycle or from a methyl group bonded to this nitrogen atom, as in compound IV, to the α-carbon atom of the exocylic C=C bond, according to scheme 3, which is confirmed by decomposition of the molecular ions of 1,3-dideutero-derivatives of compounds Im and Io, in which peaks corresponding to the ions $ArCHD^+$ appear.

For most of the compounds I-IV pathway B, leading to the formation of a rearranged ion B_3, is realized (migration of the atom X from $C_{(2)}$ to $C_{(5)}$). Moreover, the intensity of the peaks corresponding to these ions increases as we go from compounds I to compounds II and III. The low intensity of the peaks corresponding to the ions B_1 and B_2 in the mass spectra of seleno-derivatives III (the ions B_1 and B_2 can be considered as intermediate in the formation of the rearranged ion B_3) and the absence of these ions in the spectra of 5-arylidenebarbituric acids I and their 2-thio-analogs II are evidently explained by their very low stability. It should be noted that the first step in this pathway, accompanied by the ejection of CO, is also characteristic of unsubstituted 2-thio-, and 2-selenobarbituric acids (V-VII).

Noteworthy is the fact that pathway D with ejection of a hydrogen atom from the molecular ion, which is the main pathway in the case of compounds I and was studied in detail in [7], becomes commensurate in its significance with pathway B for 2-thio-analogs II and is virtually absent in 5-arylidene-2-selenobarbituric acid (III). The relative ease of formation of D_1 ions for derivatives of barbituric acid in comparison with S- and Se-analogs is in full agreement with the scheme of stripping of hydrogen (scheme 4), proposed by the authors of [7].

Actually, on the one hand, the electrophilicity of the oxygen atom of the $C_{(6)}=O$ group of the molecular ion should drop sharply with decreasing electronegativity of the X atom of the $C_{(2)}=X$ group, but on the other hand, with increasing energy of the electrons of this atom, the

TABLE 2. Mass Spectra of 5-Arylidene-2-thiobarbituric Acids (II)[a]

Compound	R^1	R^2	R^3	$M^{+\cdot}$	Pathway A, A_1	Pathway B, B_3	Pathway C			Pathway D			Pathway F		Other ions
							C_1	C_2	C_2'	D_1	D_2	D_3	F_1	F_2	
IIa	NO_2	H	H	277 (70)	—	—	—	—	174 (2)	276 (10)	—	174 (2)	231 (100)	172 (76)	233 (16), 232 (30), 230 (84), 218 (4), 213 (6), 202 (7), 188 (8), 187 (20), 186 (6), 173 (18), 171 (6), 163 (8), 159 (14), 146 (2), 145 (4), 144 (14), 143 (36), 131 (2), 130 (8), 128 (3), 119 (23), 116 (4), 115 (6), 104 (12), 103 (4), 93 (12), 92 (18), 91 (3)
IIb	H	H	NO_2	277	—	179 (34)	175 (10)	—	174 (2)	276 (22)	217 (4)	174 (2)	231 (4)	172 (4)	260 (10), 247 (10), 230 (26), 186 (16), 181 (2), 180 (4), 171 (6), 151 (10), 150 (10), 144 (16), 129 (6), 121 (4), 120 (2), 101 (14), 89 (4)
IIc	H	NO_2	H	277	—	179 (32)	175 (5)	—	174 (2)	276 (16)	217 (3)	174 (2)	231 (3)	172 (5)	260 (6), 247 (4), 232 (2), 230 (14), 186 (6), 181 (2), 180 (2), 171 (3), 151 (11), 150 (4), 144 (14), 133 (4), 129 (16), 116 (4), 101 (16)
IIf	H	COOH	H	276	135 (24)	178 (44)	174 (10)	146 (12)	173 (8)	275 (30)	216 (7)	173 (8)	231 (32)	172 (18)	274 (6), 260 (14), 258 (2), 232 (10), 215 (5), 188 (2), 187 (5), 186 (44), 180 (3), 179 (6), 175 (8), 171 (13), 157 (12), 155 (8), 150 (10), 148 (12), 144 (28), 129 (24), 128 (8), 116 (12), 105 (8), 101 (6)
IIi	H	H	I	358	217 (4)	260 (28)	256 (12)	—	255 (4)	357 (22)	298 (6)	255 (4)	231 (20)	172 (28)	257 (4), 232 (14), 186 (4), 173 (2), 144 (4), 129 (18), 129 (17), 127 (5), 116 (4), 101 (21), 89 (5)
IIl	H	H	F	250	109 (18)	152 (40)	148 (26)	120 (33)	147 (6)	249 (34)	190 (6)	147 (6)	231 (3)	—	248 (10), 186 (17), 171 (3), 154 (2), 153 (4), 144 (5), 135 (5), 124 (10), 123 (26), 122 (8), 121 (8), 109 (18)
IIm	H	H	H	232	—	134 (34)	130 (8)	102 (30)	129 (6)	231 (52)	172 (16)	129 (6)	—	—	158 (9), 146 (6), 145 (10), 144 (82), 136 (4), 135 (3), 131 (4), 116 (33), 105 (8)
IIn	H	OCH_3	OCH_3	292	151 (20)	194 (12)	—	—	—	291 (6)	232 (6)	—	261 (60)	202 (32)	263 (5), 262 (20), 260 (5), 217 (8), 203 (2), 191 (4), 161 (6), 144 (4), 138 (8), 121 (5)
IIo	H	H	CH_3	246	105 (7)	148 (30)	144 (8)	116 (4)	143 (7)	245 (33)	186 (18)	143 (7)	231 (40)	172 (18)	233 (2), 232 (10), 187 (2), 171 (2), 150 (3), 149 (5), 145 (2), 120 (4), 119 (16), 115 (16), 91 (3)
IIp	H	H	OCH_3	262	121 (10)	164 (28)	160 (12)	—	159 (2)	261 (36)	202 (12)	159 (2)	231 (20)	172 (6)	260 (6), 247 (5), 187 (3), 186 (25), 166 (2), 165 (3), 161 (12), 146 (3), 145 (4), 135 (5), 117 (5)
IIq	OCH_3	H	OCH_3	292	151 (18)	194 (22)	—	—	—	291 (6)	232 (7)	—	261 (66)	202 (34)	263 (8), 262 (14), 260 (8), 217 (15), 216 (6), 203 (6), 191 (5), 179 (5), 166 (14), 165 (8), 148 (6), 138 (6), 121 (8), 91 (4)
IIr	H	H	$N(CH_3)_2$	275	134 (26)	177 (31)	173 (12)	145 (6)	172 (22)	274 (30)	215 (10)	172 (22)	231 (3)	172 (22)	273 (10), 242 (7), 179 (2), 178 (4), 174 (23), 171 (6), 159 (8), 148 (8), 147 (3), 146 (4), 144 (24), 135 (6), 121 (26), 120 (26)

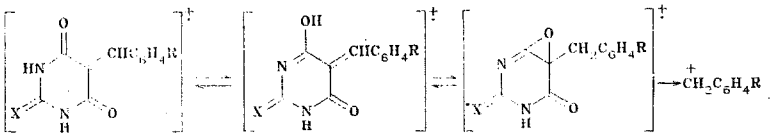
[a]The intensity of the molecular ions is 100% for all compounds except for IIa.

TABLE 3. Mass Spectra of 5-Arylidene-2-selenobarbituric Acids (III)[a]

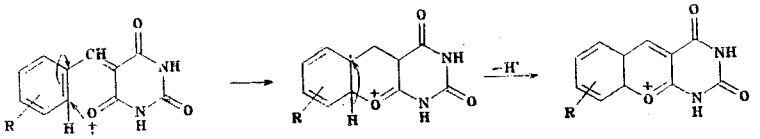
Compound	R^3	R^4	$M^{+\cdot}$[b]	Pathway A: A_2 A_1	Pathway B			Pathway C			Other ions
					B_1	B_2	B_3	C_1	C_2	C_2'	
IIIb	H	NO_2	325	—	297 (2)	—	227 (26)	175 (25)	147 (2)	—	277 (4), 230 (24), 215 (6), 192 (5), 176 (14), 160 (6), 151 (16), 129 (13), 117 (10), 107 (4), 101 (14), 89 (4)
IIIc	NO_2	H	325	—	297 (2)	—	227 (33)	175 (28)	—	—	230 (26), 215 (16), 192 (6), 176 (15), 172 (14), 160 (30), 151 (20), 136 (10), 129 (30), 117 (4), 116 (14), 107 (14), 101 (38), 89 (18)
IIId	Br	H	358/360 (100/96)	169/171 (2/1,6)	330/332 (1/0,8)	288/290 (12/10)	260 (22)	208/210 (16/14)	180/182 (18/16)	—	279 (8), 263/265 (16/14), 248/250 (10/8), 209/211 (10/8), 181/183 (6/4), 129 (4), 116 (3), 101 (16)
IIIh	H	Cl	314/316 (100/51)	125/127 (31/11)	—	244/246 (28/20)	216/218 (32/20)	164/166 (48/26)	136/138 (26/14)	—	234/236 (21/11), 219/221 (30/14), 217 (19), 215 (10), 214 (20), 204/206 (4/3), 192 (20), 190 (10), 172 (8), 165 (28), 162 (3), 160 (4), 158 (3), 140 (20), 139 (18), 137 (10)
IIIm	H	H	280	91 (10)	252 (3)	210 (16)	182 (36)	130 (40)	102 (52)	129 (10)	234 (6), 192 (10), 185 (26), 172 (10), 170 (10), 157 (6), 156 (4), 131 (20), 117 (8), 103 (16)
IIIn	OCH_3	OCH_3	340	151 (20)	—	—	242 (40)	190 (20)	162 (6)	189 (11)	325 (8), 309 (16), 276 (6), 259 (4), 234 (10), 232 (10), 227 (10), 218 (5), 217 (16), 202 (12), 192 (10), 191 (24), 176 (6), 175 (13), 166 (16), 165 (12), 147 (10), 112 (10), 19 (11)
IIIp	H	OCH_3	310	121 (15)	282 (2)	240 (10)	212 (32)	160 (25)	132 (10)	—	295 (3), 279 (2), 161 (20), 145 (14), 135 (12), 117 (12)
IIIr	H	$N(CH_3)_2$	323	134 (100)	295 (2)	—	255 (40)	173 (24)	145 (24)	172 (24)	275 (6), 268 (6), 242 (26), 190 (30), 188 (28), 175 (24), 174 (25), 171 (22), 160 (24), 159 (24), 158 (24), 148 (28), 146 (14), 144 (24), 135 (76), 126 (25), 121 (78), 120 (84), 107 (26), 106 (24), 105 (18), 91 (22)

[a]The peaks of the ions containing the isotope ^{80}Se are cited. [b]The intensity of the peaks of the molecular ions is 100%.

Scheme 3



Scheme 4



Scheme 5

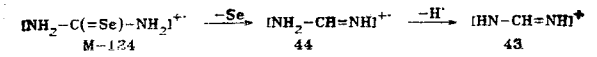


TABLE 4. Mass Spectra of Barbituric, 2-Thio-, and 2-Selenobarbituric Acids (V-VII) and Selenourea (VIII)

Compound	m/z (relative intensity, %)
V	128 (100), 100 (14), 85 (34), 42 (78)
VI	144 (100), 116 (38), 85 (3), 43 (24), 42 (3)
VII[a]	192 (100), 164 (70), 112 (10), 107 (30), 84 (11), 69 (28), 56 (12), 43 (14), 42 (22)
VIII[a]	124 (100), 44 (12), 43 (38)

[a]The peaks of the ions containing the isotope ^{80}Se are cited.

localization of the positive charge on it, and not on the oxygen atom of the carbonyl $C_{(6)}=O$, will also increase.

Fragmentation of M^+ along pathway C, which plays only a negligible role in the general decomposition, becomes predominant in the case of compounds I and II, together with pathway B, for 5-arylidene-2-selenobarbituric acids. In the mass spectra of compounds I-III there is almost always a peak corresponding to the C_2^1 ion. It is suggested [7] that it is formed by stripping of a fragment $H_2NC(=X)NHCO$ directly from the molecular ion. This pathway seems possible if the $(M-1)^+$ is formed on account of stripping of a hydrogen atom from the α-carbon atom of the exocyclic C=C bond. However, the intensity of the peaks of the ions $(M-1)^+$ decreases as we go from compounds I to compounds II, and they are virtually absent in the mass spectra of 5-arylidene-2-selenobarbituric acids (III). At the same time, the formation of the C_2^1 ion may occur as a result of fragmentation of other ions, for example, B_1 or C_1. Moreover, the ions C_2^1 and D_3 are characterized by the same values of m/z. Therefore the peaks corresponding to them are the most intense in the case of compounds I, for which pathway D predominates. Since pathway D is not characteristic of seleno-derivatives III, it can be assumed that exclusively the C_2^1 ions observed in the case of electron donor substituents in the benzene ring are responsible for the appearance of these ions in the mass spectra of compounds III, which also agrees with the concepts of stability of carbocations.

In contrast to unsubstituted 2-selenobarbituric acid, as well as selenourea (VIII) (Scheme 5, Table 4), no ejection of Se is observed in the mass spectra of compounds III. Another peculiarity of them is the presence of ions to whose values of m/z two structures may correspond: $[HN{=}CH{-}Se{-}Ar]^{+\cdot}$ or $[Se{-}C(=O){-}Ar]^+$ (pathway G); however, the available data are insufficient for an explanation of their formation.

We must also consider still another pathway of decomposition of $M^{+\cdot}$ ions, associated with the participation of a substituent in the benzene ring (pathway F). This pathway includes both elimination of the substituent whole and its fragmentation without stripping from the benzene ring. Elimination of the substituent from the benzene ring plays the greatest role in the case of compounds I and II, but for the selenoanalogs III this pathway is negligible. Just as for other compounds [8] containing the NO_2, OCH_3, $N(C_2H_5)_2$, and COOH groups, for the substances studied in this work ejections of the particles NO, CH_3, CO_2, etc., are observed.

Substituents in the benzene ring have no significant effect on the intensities of the peaks corresponding to one pathway of decomposition or another, with the exception of pathway A (formation of a benzyl cation) in the case of 5-arylidene-2-selenobarbituric acids. The significance of this pathway increases with increasing electron donor properties of the substituents in the benzene ring, and this pathway of decomposition of $M^{+\cdot}$ ions is the main one for 5-p-dimethylaminobenzylidene-2-selenobarbituric acid.

Thus, the greatest influence on the nature of the fragmentation of molecular ions of compounds I-III is exerted by the nature of the atom bonded to the carbon atom in the 2-position of the pyrimidine ring, whereas the role of substituents in the benzene ring is inconsequential.

EXPERIMENTAL

The synthesis of compounds I-III was performed according to the procedures described in [9-11].

The mass spectra were obtained on an MX-1303 instrument at an ionizing voltage of 30 eV, emission current 150 μA, and temperature of the ion source 150°C. The temperature of admission of substances to the ion source was 140-225°C.

5-p-Nitrobenzylidene-2-selenobarbituric acid (IIIb) was produced according to the method of [11]. Yield 78%, mp 290°C (with dec.). IR spectrum (liquid petrolatum): 2880 (NH), 1655, 1642 (C=O), 1515, 1345 cm^{-1} (NO_2). PMR spectrum (dioxane): 11.88 (1H, s, NH); 11.78 (1H, s, NH); 8.54 (1H, s, CH=C); 8.34 (2H, d, J = 8 Hz, aromatic o-protons) 8.14 ppm (2H, d, J = 8 Hz, aromatic m-protons). Found: C 39.2; H 2.2; N 12.3%. $C_{11}H_7N_3O_4Se$. Calculated: C 40.7; H 2.2; N 13.0%.

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