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Organic Chemistry

Peculiarities of Fragmentation in Mass-Spectra of Dipyrrolonaphthalene Amide Derivatives

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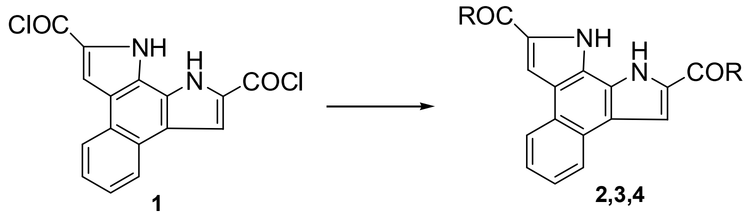
ABSTRACT. In the present work fragmentation of molecular ions in mass-spectra of benzo[e]pyrrolo[3,2-g]indole dichloranhydride and diamides (hydrazine) obtained on its basis are compared to fragmentation of benzopyrroloindole, dihydrazides of indolo[4,5-e]indole and indolo[5,4-e]indole, and hydrazidohydrazones obtained on their basis. At starting stages elimination of side radicals (R) of molecular ions occurs and [OC-HeT-CO]$^+$ fragments containing dicarbonyl group are produced, having high-intensity peaks in the mass spectra. For these ions quinoid structure is offered which, presumably, conditions their stability. *© 2011 Bull. Georg. Natl. Acad. Sci.*

Key words: *dipyrrolonaphthaline, indoloindole, benzopyrroloindole, condensation, dihydrazide, hydrazidohydrazone, fragmentation.*

The work presents mass-spectra analysis of benzopyrroloindole dichloranhydride 1, synthesized previously by us, and that of diamides (hydrazine) 2,3,4 obtained on its basis [1] (Fig.1).

Data on the mass-spectra of compounds 1-4 are compared with isomeric dihydrazides 5,6,7 synthesized by us [2] and with hydrazidohydrazone 8-12 obtained as a result of interaction between dihydrazides and carbonylic compounds [3]. Mass-spectrum 5 of dyhydrazide of indolo[4,5-e]indole [2] is also considered (Fig.2).

Molecular ion peak within mass-spectrum of dichloranhydride 1 was relatively low in intensity. At the first and second stages consecutive elimination of two molecules of hydrogen chloride occurs. The peak of the derived ion [M-HCI-HCI]$^+$ was of maximal intensity. The subsequent fragmentation of this ion 258(100) proceeds in two ways. The first way is consecutive loss of fragments N=C=C=O (decay of pyrrole nuclei) that considerably differs from known schemes of indole fragmentation. The spectrum showed also the second way for decay of



2 R = -NH-Ph; **3** R = -NH-C$_6$H$_4$-Cl(p); **4**R = -N(CH$_3$)$_2$;

Fig. 1. Scheme of synthesis of diamides 2-4

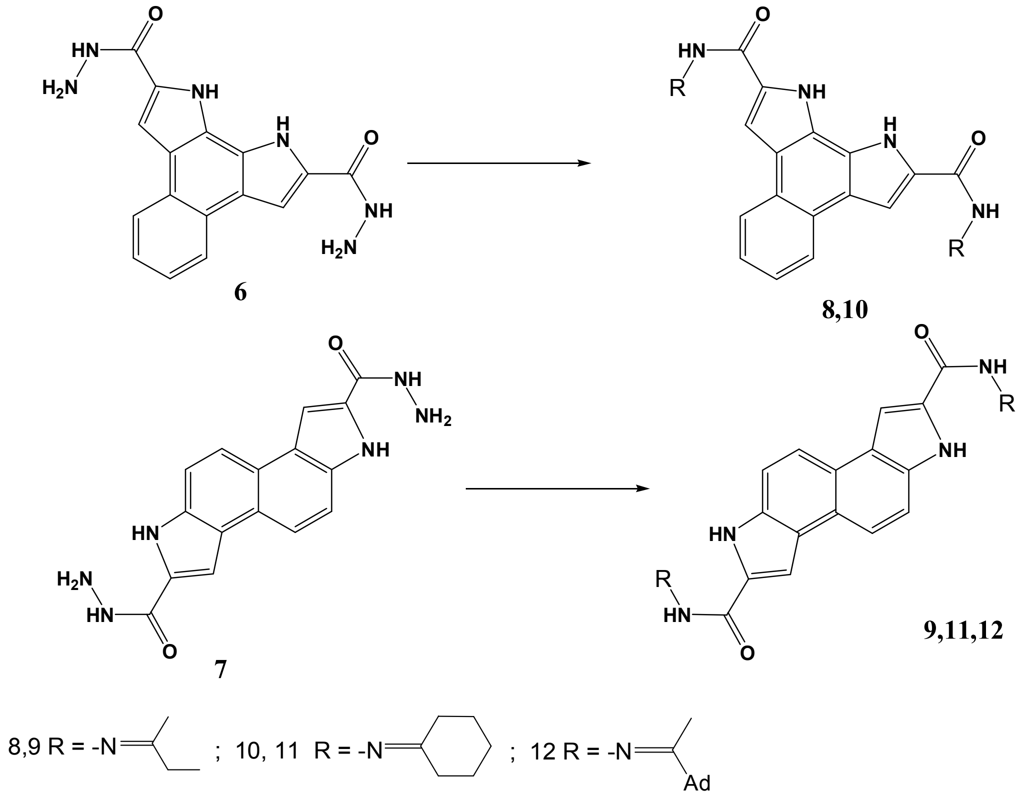


Fig. 2. Scheme of obtaining hydrazidohydrazones 8-12

$[M\text{-}HCI]^+$ ion 294(38) to form ion 259(68). Formation of this ion is also significant in the fragmentation process of diamides 2, 3, 4.

The most convincing scheme of the decay of compound 1 considering all peaks is the following:

In the course of fragmentation of molecular ions of compounds 2,3,4, after bond breakage with both carbonyl groups due to elimination of corresponding particles or molecules a fragment was formed with mass 259 and with a peak of maximal or high intensity in the spectrum.

Compound 1:

$$\begin{tikzcd}
M^+\ 330(23) \arrow[r, "-HCI"] & 294(38) \arrow[r, "-HCI"] \arrow[d, "-CI"] & 258(100) \arrow[r, "-N=C=C=O"] \arrow[d, "-2CO"] & 204(25) \arrow[r, "-N=C=C=O"] & 150(11) \\
& 259(68) \arrow[d, "-CO"] & 202(62) \arrow[r, "-CN"] & 176(32) & \\
203(19) & 231(25) \arrow[l, "-CO"'] \arrow[r, "-N=C=C=O"] & 177(13) & &
\end{tikzcd}$$

Compound 2:

$$\begin{tikzcd}
M^+\ 444(86) \arrow[r, "-H_2N\text{-}C_6H_5"] \arrow[dr, "-C_6H_5NCO"'] & 351(69) \arrow[r, "-HN\text{-}C_6H_5"] & 259(100) \arrow[r, "-HCN"] & 232(62) \arrow[r, "-CO"] & 204(55) \arrow[d, "-CN"] \\
& 325(31) \arrow[r, "-C_6H_5NCO"] & 206(28) & & 178(27)
\end{tikzcd}$$

Compound 3:

$$\begin{tikzcd}
M^+\ 512(8) \arrow[r, "-H_2NC_6H_4CI"] \arrow[dr, "-CIC_6H_4NCO"'] & 385(5) \arrow[r, "-HNC_6H_4CI"] & 259(26) \arrow[r, "-HCN"] & 232(100) \arrow[r, "-CO"] & 204(68) \arrow[d, "-CN"] \\
& 359(21) \arrow[r, "-CIC_6H_4NCO"] & 206(60) & & 178(53) \arrow[d, "-CO"] \\
{[CIC_6H_4N=C=O]^+\ 153(20)} & & & & 150(16)
\end{tikzcd}$$

Compound 4:

$$\begin{tikzcd}
M^{+}\ 348(64) \arrow[r, "-NH(CH_3)_2"] & 303(100) \arrow[r, "-N(CH_3)_2"] & 259(58) \arrow[r, "-HCN"] & 232(23) \arrow[r, "-CO"] & 204(29) \arrow[d, "-HCN"] \\
 & & & & 177(23)
\end{tikzcd}$$

Dihydrazide 5:

$$\begin{tikzcd}
\mathbf{(M\text{-}1)^{+}\ 321(64)} \arrow[r, "-NH-NH_2"] & \mathbf{290(16)} \arrow[r, "-N_2H_4"] & \mathbf{258(84)} \arrow[r, "-CO"] & \mathbf{230(90.4)} \arrow[r, "-CN"] & \mathbf{204(92)} \arrow[r, "-CO"] & \mathbf{176(73.6)} \arrow[r, "-CN"] & \mathbf{150(51.2)}
\end{tikzcd}$$

Dihydrazide 6:

$$\begin{tikzcd}
M^{+}\ 322(8) \arrow[r, "-NHNH_2"] & 291(5) \arrow[r, "-N_2H_4"] & 259(13) \arrow[r, "-HCN,-CN"] \arrow[d, "-CO"] & 206(100) \arrow[r, "-CO"] & 178(17) \arrow[r, "-CO"] & 150(5) \\
 & & 231(25) \arrow[r, "-CN"] & 205(43) \arrow[r, "-HCN"] & 178(17) \arrow[r, "-CO"] & 150(5)
\end{tikzcd}$$

Dihydrazide 7:

$$\begin{tikzcd}
M^{+}\ 322(33) \arrow[r, "-NHNH_2"] & 291(38) \arrow[r, "-N_2H_4"] & 259(100) \arrow[r, "-HCN,-CN"] \arrow[d, "-CO"] & 206(178) \arrow[r, "-HCN"] & 177(62) \arrow[r, "-CO"] & 149(10) \\
 & & 231(35) \arrow[r, "-HCN"] & 204(58) \arrow[r, "-CO"] & 176(70) \arrow[r, "-CN"] & 150(18)
\end{tikzcd}$$

Thereupon HCN and CO groups were consecutively lost. Similar fragmentation took place also in the mass spectra of dihydrazides 5-7. In the spectra of diamides 2 and 3 elimination of arylisocyanates from molecular ions was also observed. Splitting of arylisocyanate ions with masses 119 (compound 2) and 153 (compound 3) was recorded in the spectrum as single peaks.

In spectra of hydrazidohydrazones 8-12 an analogous fragmentation of molecular ions was observed. After breaking bonds with both carbonyl groups and consecutive splitting corresponding particles or molecules, fragment ion with mass 259 was recorded too here. Similarly to the case of diamides, when this ion decayed, fragment N=C=C=O was lost (decay of pyrrole nucleus).

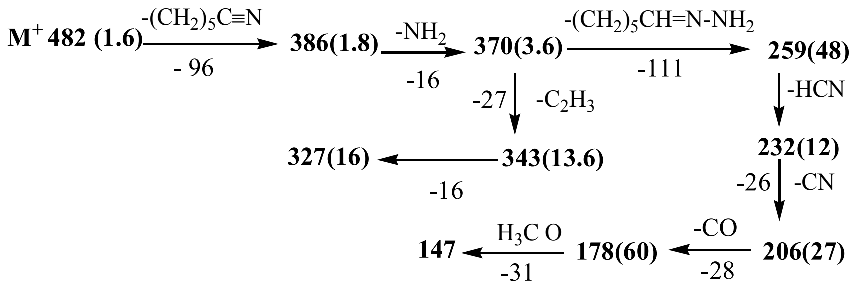
Compound 8:

$$\begin{tikzcd}
\mathbf{430(14.4)} \arrow[r, "C_3H_4", "-40"'] & \mathbf{390(92)} \arrow[r, "-CH_2-NH-NH_2", "-45"'] & \mathbf{345(18.4)} \arrow[r, "-C_3H_4", "-40"'] & \mathbf{305(100)} \arrow[r, "CH_3-NH-NH_2", "-46"'] & \mathbf{259(51.2)} \arrow[r, "-CO", "-28"'] & \mathbf{231(20.8)} \arrow[r, "-HCN", "-27"'] \arrow[d, "-N=C=C=O", "-54"'] & \mathbf{204(33.6)} \arrow[r, "-N=C=C=O", "-54"'] & \mathbf{150} \\
 & & & & & \mathbf{177(21.6)} & &
\end{tikzcd}$$

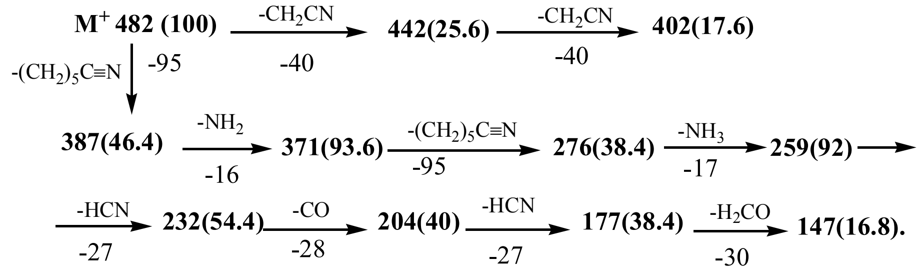
Compound 9:

$$\begin{tikzcd}
\mathbf{430(76)} \arrow[r, "CH\equiv C-CH_3", "-40"'] \arrow[rrr, bend left, "-2C_4H_8", "-112"'] & \mathbf{390(11.2)} \arrow[r, "-CH_2-NH-NH_2", "-45"'] & \mathbf{345(25.6)} \arrow[r, "-CH=CH_2", "-27"'] & \mathbf{318(58.4)} \arrow[r, "CH_3-\dot{C}H-NH-NH_2", "-59"'] & \mathbf{259(100)} \arrow[r, "-CN", "-26"'] \arrow[dr, "-NH=CH=C=O"'] & \mathbf{233(49.6)} \arrow[r, "-N=C=C=O", "-54"'] & \mathbf{179(27.2)} \\
 & & & & & \mathbf{204(28)} \arrow[r, "-N-C=C=O"] & \mathbf{150(9.6)}
\end{tikzcd}$$

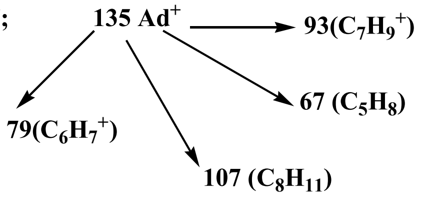
Compound 10:



Compound 11:



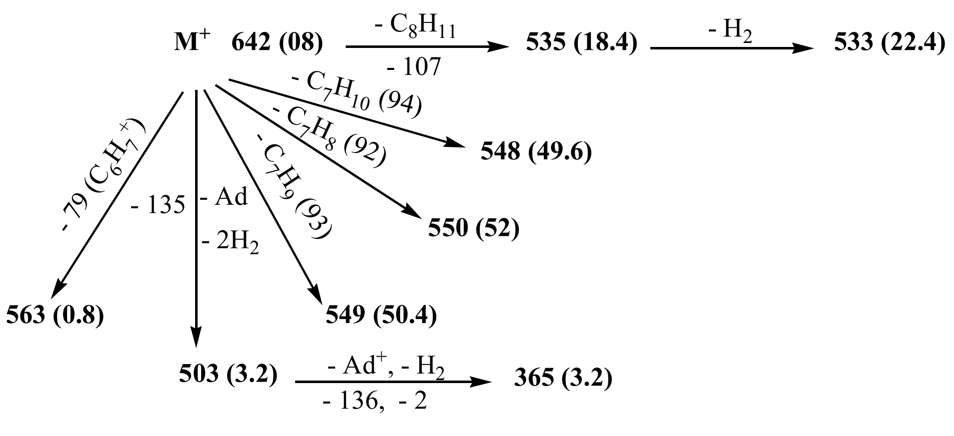
Ions eliminated from side chains of molecular ions were also recorded in mass spectra as single peaks of corresponding mass. For example, in the case of compound 9 intensive peak with mass 111 could be radical C_8H_{15} obtained as a result of binding two radicals of eliminated butylene; in the mass spectra of compound 12 high intensity peaks of adamantyl radical and those of characteristic ions formed at its following fragmentation [4] are recorded. It is known [4] that at fragmentation of molecular ions in the adamantane mass spectra fragment ions are formed having the following values of *m*/*z*:



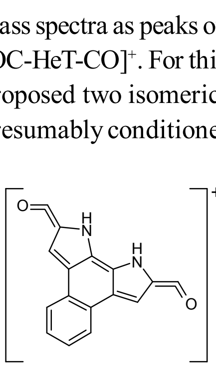
Proceeding from the above and taking into consideration the peaks in mass spectra of compound 12 we can say that elimination of ions produced as a result of decay of adamantane radical occurred at the starting stage. Eliminated fragment ions were registered in the spectra: radical $(Ad\text{-}1)^+$ (100) in the form of maximal intensive peak and ions with masses 107(9.6), 93(16.8), 79(128) in the form of relative low intensive peaks.

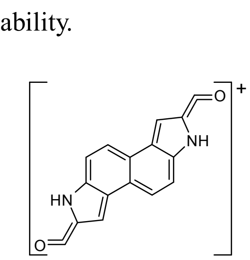
At the next stage splitting of corresponding particles from the side chain continued; as a result of bond cleavage with both carbonyl groups an ion with mass 259 was produced. Successive fragmentation of this ion occurred analogously to that of compounds 8-11 by consecutive cleaving HCN and CO groups.

General scheme of molecular ions of amide derivatives of dipyrolonaphthalenes elimination of side radicals was established by comparison of mass spectra of com-



pounds 1-12. At starting stages radicals (R) were consecutively eliminated and a fragment containing dicarbonyl group was produced with corresponding masses m/z=259 or m/z=258, which were recorded in the mass spectra as peaks of maximal (100%) or high intensity [OC-HeT-CO]$^+$. For this general fragment ion m/z=259 we proposed two isomeric quinoid structures 13, 14, which presumably conditioned their stability.


13


14

The following fragmentation of these ions happens mainly by consecutive splitting off groups HCN and CO. In some cases an interesting alternative way of their decay differing considerably from the known scheme of decay of indoles: elimination of fragment -N=C=C=O, is recorded in the spectra (decay of pyrrole nucleus).

Experimental part. The reaction course, monitoring the purity of products, and determination of the R_f values were carried out on Silufol UV-254 plates. Silica gel with particle size 100-250 μm was used as the adsorbent in column chromatography. The mass spectra of compounds 5-12 were obtained on a Finnigan MAT 95 mass spectrometer (USA) (at the Organic Chemistry Laboratory, Saarbrücken University) and those of compounds 1-4 – on a quadrupole chromatography mass spectrometer Nermag R10-10B with data processing system Spider (ionizing-electron energy 70 eV).

The IR spectra were obtained on a Termo Nikolet Avatar-370 spectrometer equipped with FTIR in vaseline mull. The UV spectra were obtained on a Varian Carry 100 UV-Vis spectrometer. The ^{1}H NMR spectra were obtained on a Bruker AM-400 spectrometer at 400 MHz with TMS as the internal standard. The error of the chemical shift measurement was δ±0.01 ppm and the error for the coupling constant was ±0.1 Hz (DMSO- d_6).

Synthesis of compounds 1-4 is given in [1].

2,9-Di(carbohydrazide)-3H,8H-indolo[4,5-e]indole (5). 1g (3 mmol) suspension of diethoxycarbonyl indolo[4,5-e]indole [5] was heated in 59 ml isopropyl alcohol, hydrazinhydrate was added. It was boiled for 2 hr, filtered in the hot state, washed with isopropyl alcohol, ether and dried. Cream-coloured crystals were insoluble in water and hardly dissolved in organic solvents. The yield was 0.9 g(85 %), mp 330°C. IR spectrum, ν cm^{-1}: 3100-3300 (NH indole and hydrazine), 3430 (NH$_2$), 1610, 1640 (CO-amide band 1), 1530, 1570 (CO-amide band 2). ^{1}H-NMR spectrum, δ ppm: 11.78 (2H, w. s, 3-H, 8-H), 9.49 (2H, w. s, NH-hydrazide), 8.00 (2H, s, 1-H, 10-H), 7.69 (2H, d, 5-H, 6-H), 7.52 (2H, d, 4-H, 7-H), 4.45 (4H, w. s, NH$_2$), $J_{4,5}$=6.77 Hz; mass-spectrum (70 eV), m/z; found: [M$^+$] 322, $C_{16}H_{14}N_6$. Calculated M=322 [2].

2,9-Di(carbohydrazide)-1H,10H-benzo[e]pyrrolo[3,2-g]indole (6). 0.2g (0.57mmol) 2,9-diethoxycarbonyl-1H,10H-benzo[e]pyrrolo[3,2-g]indole [6] was dissolved in 20 ml isopropyl alcohol and boiled, then 10ml hydrazine hydrate was added to it. Reaction mixture was heated to 80 °C for 3 h mixing permanently. Isolated sediment was filtered, washed with isopropyl alcohol and dried with ether. Brown sediment was got. The yield was 0.17g (85%). m.p. 403°C. R_f 0.35 (isopropyl alcohol-hexane, 10:1), IR spectrum, ν cm^{-1}: 3430 (NH$_2$), 3330 (NH-indole), 3250-3280 (NH-hydrazide), 1610-1670(CO-amide band 1), 1510-1580 (CO amide band 2). UV spectrum, max λ(lg ε): 227(3.16), 238 (3.25), 255 (3.21), 270 (3.32), 282 (3.31), 345 (3.25), 255 nm(3.24). ^{1}H-NMR spectrum, δ ppm: 11.66 (2H, w. s, 1-H,10-H), 9.55 (2H, w. s, NH-hydrazide), 8.10 (2H, s, 4-H, 7-H), 7.68(2H, d, 3- H, 8 -H), 7.45 (2 H,d, 5-H, 6-H), 4.41 (4H w. s, NH$_2$), $J_{4,5}$=6,21 Hz. $J_{4,6}$=3,29 Hz. Mass-spectrum (70 eV), m/z; found: [M$^+$] 322, $C_{16}H_{14}N_6$. Calculated: M=322 [2].

2,7-Di(carbohydrazide)-3H,8H-indolo[5,4-e]indole (7). 0.1g (0.29 mmol) solution of 2,7-diethoxycarbonyl-3H,8H-indolo[4,5-e]indole [5] dissolved in 10 ml isopropyl alcohol was boiled and 7 ml hydrazine hydrate added. Reaction mixture was heated to 80 °C for 3 h mixing permanently. Isolated sediment was filtered, washed with isopropyl alcohol and dried with ether. Yellow sediment was got. R_f 0.49 (isopropyl alcohol-hexane, 10:1). The yield was 0.09 g (80%), T_{decomp}>300 °C. IR spectrum, ν, cm^{-1}: 3470 (NH$_2$), 3320 (NH-indole), 3200-3290 (NH-hydrazide), 1640 (CO-amide band 1), 1550(CO-amide band 2). ^{1}H-NMR spectrum, δ (ppm), J,Hz : 11.85 (2H, s, NH indole), 9.73 (2H, s, NH hydrazide), 4.49 (4H, br. s, NH$_2$), 7.70 (2H, br.. s, 1-H, 6-H), 7.90 (2H, d, 4-H, 9-H), 7.63 (2H, d, 5-H, 10-H), $J_{4,5}$=9.0. Mass-spectrum (70 eV), m/z; found: [M$^+$] 322, $C_{16}H_{14}N_{6.}$ Calculated: M=322.

Methylethylketone benzo[e]pyrrolo[3,2-g]indole-2,9-yl-di(carbohydrazidohyrdazone) (8). 0.3 ml methylethylketone was heated to 50 °C, 0.05g (0.17 mmol) dicarbohydrazide 6 and 1-2 drops of acetic acid were added and heated to 78-80 °C for 2 h. Isolated sediment was filtered, washed with isopropyl alcohol and dried with diethyl ether. R_f 0.62 (isopropyl alcohol-ether, 6:1). The yield was 0.057g(78 %), m.p. 303-305°C. IR spectrum, ν cm^{-1}: 3340 (NH-indole, 3200, 3240 (NH-amide), 1640 (CO-amide), 1600 (C=N). ^{1}H-NMR spectrum (DMSO-d_6), δ (ppm), J,Hz: 11.88 (2H, br s, NH-indole), 10.34 (2H, s, NH-hydrazide), 7.99 (2H, d, 3-H, 8-H), 8.15 (2H, dd, 4-H, 7-H), 7.47 (2H, dd, 5-H, 6-H), 2.02 (6H, s, =C-CH_3), 2.36-2.42 (4H, m. CH_2-Et), 1.06-1.24 (6H, m, CH_3-Et), $J_{1,3}$=3.2; $J_{4,5}$=5.2, $J_{4,6}$=3.2,$J_{5,6}$=6.0, $J_{5,7}$=2.8. Mass-spectrum (70 eV), *m/z*; found: [M^+] 430. $C_{24}H_{26}N_6O_2$. Calculated: M=430.

Methylethylketone indolo[5,4-e]indole-2,9-yl-di(carbohydrazidohydrazone) (9). 0.3 ml methylethylketone was heated to 50 °C. 0.05 g (0.16 mmol) dihydrazide 7 and 1-2 drops of acetic acid were added mixing permanently. Reaction medium was heated to 80-82 °C. In 2 hours 8 ml methylethylketone was added. Brown-coloured sediment was filtered, washed with isopropyl alcohol and dried with diethyl ether. The yield was 0,04g (58%). $T_{decomp.}$>240 °C. R_f 0.30 (isopropyl alcohol-ether, 6:1). IR spectrum, v cm^{-1}: 3350 (NH-indole), 3170-3280 (NH-amide), 1640, 1660 (CO amide), 1580 (C=N). ^{1}H-NMR spectrum (DMSO-d_6), δ(ppm), J, Hz: 11.97 (2H, s, NH indole), 10.32 (2H, s, NH amide), 7.88 (2H, br s, 1-H, 6-H), 8.03 (2H, d, 4-H,9-H), 7.68 (2H, d, 5-H, 10-H), 2.03(6H, s, =C-CH_3), 2.39(4H, br s, -CH_2), 1.16 (br s, -CH_2-CH_3), $J_{4,5}$=8.6. Mass-spectrum (70 eV), *m/z*; found: [M^+] 430. $C_{24}H_{26}N_6O_2$. Calculated: M= 430.

Cyclohexanone benzo[e]pyrrolo[3,2-g]indole-2,9-yl-di(carbohydrazidohydrazone) (10). 2 ml cyclohexanone was heated to 50-60 °C, 0.04g (0.12 mmol) dihydrazide benzo[e]pyrrolo[3,2-g]indole 6 and 2-3 drops of acetic acid were added. White-colored sediment gradually became light brown. Reaction medium was heated to 100 °C for 2 h. Isolated sediment was filtered and washed with isopropyl alcohol. The yield was 0.03 g (53%), T_{decomp}>300^{0}C. R_f 0.50 (isopropyl alcohol -ether, 6:1). IR spectrum, v, cm^{-1}: 3370 (NH-indole), 3250-3260 (NH-hydrazone), 1670 (CO-amide), 1610 (C=N). 1H-NMR spectrum (DMSO-d_6), δ(ppm), J, Hz: 11.85 (2H, s, NH indole), 10.59 (2H, s, NH amide), 7.94 (2H, d, 3-H, 8-H), 8.18 (2H, m, 4-H, 7-H), 7.46 (2H, dd, 5-H, 6-H), 1.61-1.77 (12H, m, H_b-H_c), 2.35-2.46 (8H, m, H_a), $J_{4,5}$=6.0, $J_{4,6}$=3.2. Mass-spectrum(70 EV), *m/z*; found: [M^+] 482. $C_{28}H_{32}N_6O_2$. Calculated: M= 482.

Cyclohexanone indolo[5,4-e]indole-2,9-yl-di(carbohydrazidohydrazone) (11). 2 ml cyclohexanone was heated to 50-60 °C, 0.04g (0.12 mmol) di(carbohydrazide)-3H,8H- indolo[5,4-e]indole (7) and 2-3 drops of acetic acid were added. Reaction mixture was heated to about 100 °C for 2 h, held for 24 s and settled with diethyl ether. Brown-coloured sediment was formed. R_f 0.50 (diethyl ether-hexane, 9:1). The yield was 0.03 g (50%), T m.p. 230-232° C. IR spectrum, v, cm^{-1}: 3247(NH-amide), 3350(NH-indole), 1697 (Co-amide), 1643 (C=N). ^{1}H-NMR spectrum(DMSO-d_6) δ(ppm), J, Hz: 11.98 (2H, br s, NH indole), 10.58 (2H, s, NH amide), 7.86 (2H, br s, 1-H, 6-H), 8.04 (2H, d, 4-H,9-H), 7.66 (2H, d, 5-H, 10-H), 1.64-1.77 (12H, m, =H_b-H_c), 2.25-2.40 (8H, m., H_a), J_{45} =7.2. Mass-spectrum(70 eV), *m/z*; found: [M^+] 482, $C_{28}H_{32}N_6O_2$. Calculated: M= 482.

Acetyladamantane indolo[5,4-e]indole-2,9-yl-di(carbohydrazidohydrazone) (12). 0.06g Acetyladamantane was dissolved in small amount of isopropyl alcohol, 0.05g (0.16mmol) indoloindole dihydrazide 7 dissolved in dimethylformamide was added. Reaction medium was heated up to about 80 °C for 3 h, sediment was filtered and dried with diethyl ether. The yield was 0.06 g (56%). $T_{decomp.}$>300 ^{0}C. R_f 0.55 (isopropyl alcohol-ether, 6:1). IR spectrum, v cm^{-1}: 3301(NH-indole), 3193 (NH-amide), 2676, 2723 (Ad), 1627 (CO-amide), 1535 (C=N). ^{1}H-NMR spectrum(DMSO-d_6) δ(ppm), J, Hz: 11.99 (2H, br s, NH indole), 10.60 (2H, br s, NH amide), 7.89 (2H, br s, 1-H, 6-H), 8.06 (2H, d, 4-H, 9-H), 7.71 (2H, d, 5-H, 10-H), 1.48-1.81 (30H, Ad), 1.70-1.81(C-CH_3), J_{45}=7.6. Mass-spectrum (70 eV), *m/z*; found: [M^+] 642, $C_{40}H_{46}N_6O_2$. Calculated: M= 642.

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წარმოდგენილია ბენზო[e]პიროლო[3,2-g]ინდოლის დიქლორანჰიდრიდისა და მის საფუძველზე მიღებული დიამიდების მას-სპექტრებში მოლეკულური იონების ფრაგმენტაციის თავისებურებანი. იგი შედარებულია ბენზოპიროლოინდოლის, იზომერული ინდოლო[4,5-e]ინდოლისა და ინდოლო[5,4-e]ინდოლის დიჰიდრაზიდებისა და მათ საფუძველზე მიღებულ ჰიდრაზიდოჰიდრაზონების ფრაგმენტაციასთან. გაკეთებულია დასკვნა სინთეზირებული ამიდური ნაწარმების მას-სპექტრებში ფრაგმენტაციის ზოგადი კანონზომიერების შესახებ: საწყის სტადიებზე ხდება მოლეკულური იონების გვერდითი რადიკალების (R) ელიმინირება და დიკარბონილის ჯგუფის შემცველი ფრაგმენტების [OC-HeT-CO]$^+$ წარმოქმნა, რომელიც მას-სპექტრებში დაფიქსირებულია ან მაქსიმალური(100%), ან მაღალი ინტენსიურობის პიკების სახით. ამ იონებისათვის მოწოდებულია ქინოიდური სტრუქტურა, რომელიც სავარაუდოდ მათ მდგრადობას განაპირობებს. შემდგომი ფრაგმენტაცია მიმდინარეობს ძირითადად CO და HCN ჯგუფების თანდათანობით მოხლეჩით. ზოგიერთ შემთხვევაში კი დაფიქსირებულია მათი დაშლის საინტერესო ალტერნატიული გზაც, სპექტრებში ფიქსირდება -N=C=C=O ფრაგმენტის ელიმინირება (პიროლის ბირთვის დაშლა), რომელიც განსხვავდება ინდოლების დაშლის ცნობილი სქემისაგან.

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