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Silvia RANG, A. TALVARI, O. EISEN

50 eV MASS SPECTRA OF SOME 1- AND 3-MONOSUBSTITUTED CYCLOPENTENES

In our previous paper [1] mass spectra of 1- and 3-*n*-alkylsubstituted cyclopent-1-enes and *n*-alkyl-cyclopentanes C₆—C₁₂ were reported. In this work mass spectra of some 1- and 3-isoalkylcyclopent-1-enes with isopropyl, isobutyl and isopentyl groups in a side chain, 1- and 3-allyl- and 3-phenylcyclopent-1-enes, not described so far, are discussed to elucidate the influence of a side chain structure on the fragmentation upon electron impact.

The experimental technique was analogical to that described in [1]. The relative intensities of ions in the text are given in per cent of total ion intensities, if not indicated otherwise.

Results and discussion

Mass spectra of investigated cyclopentenes are given in Tables 1, 2. Peaks with intensities less than 1 per cent (in B) are omitted.

1- and 3-iso-alkylsubstituted cyclopent-1-enes

The regularities found for *n*-alkylcyclopentenes [1] are also observed in the fragmentation of isoalkylcyclopentenes. The principal fragmentation path is elimination of the side chain isoalkyl group from the molecular ion to form an ion (C₅H₇)⁺. In case of 3-isomers it corresponds to the cleavage of the C—C-bond located in β-position to the ring double bond.

Mass spectra of the investigated 3-*n*-alkyl- [1] and 3-isoalkylcyclopentenes C₈—C₉, as well as those of 1-*n*- and 1-isopentylcyclopentenes are nearly identical, and these isomers cannot be differentiated by their mass spectra. 1-isopropyl- and 1-isobutylcyclopentenes differ correspondingly by high abundances of ions (C₇H₁₁)⁺ with *m/e* 95 (64 % from the base peak) and ions (C₆H₉)⁺ with *m/e* 81 (48 % from the base peak) which enable their identification. Ions (C₇H₁₁)⁺ result after the elimination of a methyl group from the molecular ion of 1-isopropylcyclopentene, and ions (C₆H₉)⁺ after the elimination of the isopropyl group from the molecular ion of 1-isobutylcyclopentene. In both cases the carbon-carbon bond beta to the ring double bond at the tertiary carbon atom of the side chain is interrupted favourably.

In the cyclopentane series the isoalkyl group, instead of the corresponding normal alkyl C₃—C₄ in a side chain, diminishes notably (~3—5

Table 1

Mass spectra 1- and 3-isoalkyl substituted cyclopentenes

m/e	Side chain											
	1-Isopropyl		1-Isobutyl		1-Isopentyl		3-Isopropyl		3-Isobutyl		3-Isopentyl	
	B	Σ	B	Σ	B	Σ	B	Σ	B	Σ	B	Σ
27	10.5	2.58	12.9	2.96	11.8	3.11	6.4	2.75	8.2	3.13	4.5	1.83
28	7.2	1.77	1.2	0.28	3.4	0.89	2.2	0.97			1.3	0.52
29	3.5	0.85	5.1	1.18	10.9	2.88	1.6	0.70	5.2	1.96	4.7	1.88
39	18.6	4.57	14.1	3.24	13.2	3.47	10.5	4.51	10.2	3.88	7.6	3.08
40	3.5	0.85	2.8	0.65	2.5	0.67	2.2	0.97	2.3	0.87	1.7	0.70
41	25.9	6.36	28.3	6.49	33.0	8.71	17.8	7.61	20.7	7.91	18.0	7.27
42	1.8	0.44	2.1	0.48	2.2	0.59	1.5	0.63	1.6	0.61	1.7	0.70
43	5.2	1.28	19.7	4.53	6.4	1.70	4.3	1.86	7.0	2.69	6.6	2.67
50	1.0	0.25										
51	3.8	0.92	3.1	0.70	2.2	0.59	1.5	0.65	1.6	0.63		
52	2.0	0.48	2.4	0.56	1.7	0.44			1.1	0.42		
53	8.1	1.99	11.7	2.68	9.2	2.44	2.8	1.21	4.3	1.65	2.9	1.19
54	2.4	0.59	3.9	0.90	5.0	1.33			1.7	0.65	1.5	0.59
55	11.3	2.78	8.1	1.85	10.1	2.66	2.5	1.09	3.4	1.30	5.1	2.05
56	1.6	0.38	2.8	0.65	8.4	2.22			1.9	0.73	2.3	0.92
57			8.1	1.85	16.8	4.44			8.2	3.13	5.2	2.11
63	1.3	0.33										
65	6.1	1.49	4.4	1.01	3.9	1.04	6.1	2.60	3.2	1.22	4.3	1.73
66	13.0	3.18	10.1	2.31	4.8	1.26	21.0	9.02	14.5	5.52	13.2	5.34
67	100.0	24.51	100.0	22.97	100.0	26.39	100.0	42.89	100.0	38.13	100.0	40.42
68	13.0	3.18	14.5	3.33	6.7	1.77	10.0	4.30	10.2	3.88	8.6	3.49
69	13.8	3.38	2.6	0.59	2.8	0.74	4.5	1.93	1.3	0.48	1.6	0.65
70					1.7	0.44					2.4	0.97
71											1.9	0.76
77	6.9	1.70	6.5	1.49	4.2	1.11	2.5	1.07	2.2	0.83	2.4	0.97
78	1.7	0.42	1.7	0.39								
79	6.7	1.63	18.9	4.35	10.1	2.66	1.8	0.77	4.2	1.61	4.1	1.68
80	2.0	0.50	8.5	1.94	3.4	0.89			2.3	0.86	2.1	0.86
81	10.5	2.58	47.8	10.99	14.3	3.77	1.6	0.70	13.3	5.07	5.2	2.11
82	6.1	1.49	27.2	6.24	31.9	8.43	1.3	0.56	9.0	3.43	16.8	6.78
83	1.0	0.25	2.9	0.67	6.4	1.70			1.3	0.50	3.9	1.57
91	4.3	1.06	2.1	0.48	1.5	0.39	1.7	0.72				
93	5.8	1.42	1.2	0.28	2.0	0.52	1.8	0.79				
94	1.0	0.25			1.7	0.44						
95	63.6	15.60	5.6	1.29	20.2	5.34	4.3	1.86	1.5	0.57	2.7	1.08
96	4.3	1.06	1.1	0.26	2.0	0.52						
109	2.4	0.59	14.9	3.42					4.1	1.57	1.6	0.65
110	25.2	6.17	1.4	0.33			10.2	4.38				
111	2.4	0.59										
124			25.0	5.43					9.4	3.58		
125			2.4	0.56								
138					14.8	3.92					4.0	1.62
139					1.4	0.37						

times) the molecular ion stability [2]. In the cyclopentene series, with close W_m values for *n*- and isoalkylcyclopentenes, this substituent branching effect is negligible. Similarly to *n*-alkylcyclopentenes, 1-isoalkylcyclopentenes reveal higher molecular ion stabilities (~ 1.5 – 2 times) than the corresponding 3-isoalkylcyclopentenes. The W_m values [3] in isoalkylcyclopentene series decrease with a lengthening of the side chain $C_3 \dots C_5$ from 6.7 to 4.3 (1-isoalkyl-) and from 4.8 to 1.8 per cent for 3-isoalkylcyclopentenes (Fig. 1).

The abundances of the ions $(C_5H_7)^+$ in the mass spectra of isoalkylcyclopentenes C_8 – C_{10} (Fig. 2) are lower than those of *n*-alkylcyclopent-

Mass spectra of 1- and 3-allyl- and 3-phenylcyclopent-1-enes

m/e	Side chain					
	1-Allyl		3-Allyl		3-Phenyl	
	B	Σ	B	Σ	B	Σ
1	2	3	4	5	6	7
27	5.6	1.06	4.4	2.32	4.7	0.72
28			2.2	1.16	1.1	0.16
38	2.2	0.41			1.3	0.20
39	37.7	7.18	13.4	7.06	19.6	2.98
40	5.7	1.09	2.2	1.16	3.9	0.59
41	20.9	3.97	17.9	9.41	8.5	1.29
43	1.1	0.21				
50	3.6	0.68			6.4	0.97
51	10.4	1.99	2.4	1.24	20.2	3.06
52	6.7	1.27	1.1	0.58	4.7	0.72
53	10.4	1.99	1.9	0.99	2.2	0.33
54	4.8	0.92	2.0	1.06		
55	2.9	0.56				
58					1.6	0.24
62					2.3	0.35
63	3.1	0.59	1.0	0.53	10.1	1.53
64					3.3	0.50
65	17.9	3.40	8.9	4.71	15.9	2.41
66	11.4	2.17	9.5	5.00	25.3	3.83
67	100.0	19.03	100.0	52.64	9.6	1.45
68	5.7	1.09	5.0	2.63		
70					2.0	0.31
71					7.4	1.13
74					1.9	0.28
75					2.6	0.39
76					3.2	0.48
77	30.2	5.75	2.6	1.39	13.8	2.09
78	8.4	1.61			6.4	0.97
79	52.8	10.06	2.3	1.21	1.3	0.20
80	17.4	3.31				
81	3.1	0.59				
87					1.1	0.17
89					6.4	0.97
90					1.1	0.16
91	25.8	4.91	1.5	0.77	15.4	2.33
92	2.9	0.56			1.3	0.20
93	66.0	12.57				
94	4.8	0.92				
102					6.4	0.97
103					8.5	1.29
104					2.2	0.33
105	2.2	0.41				
107	4.0	0.77				
108	37.7	7.18	1.0	0.53		
109	3.1	0.59				
114					1.3	0.20
115					35.7	5.41
116					8.5	1.29
117					4.0	0.61
127					11.7	1.77
128					50.5	7.66
129					91.7	13.90
130					9.6	1.45
139					2.1	0.32
141					11.1	1.69

	1	2	3	4	5	6	7
142						5.8	0.89
143						75.0	11.37
144						100.0	15.16
145						11.1	1.69
146						2.7	0.40

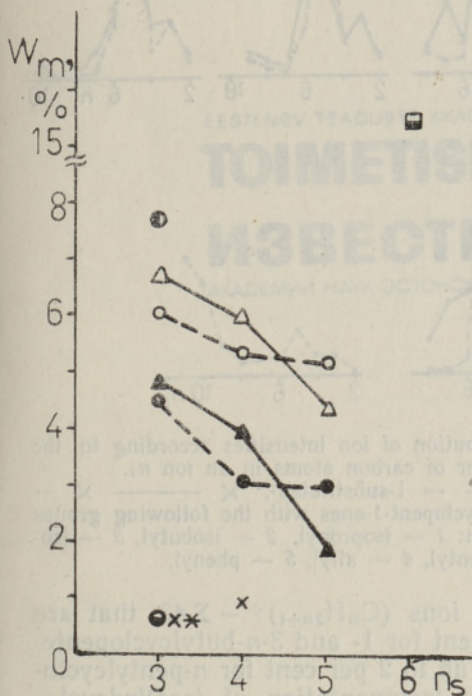
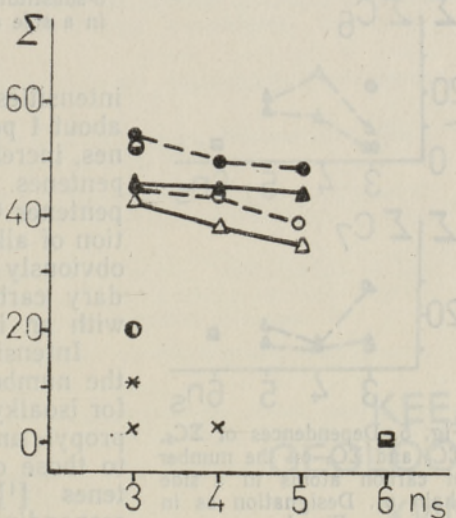
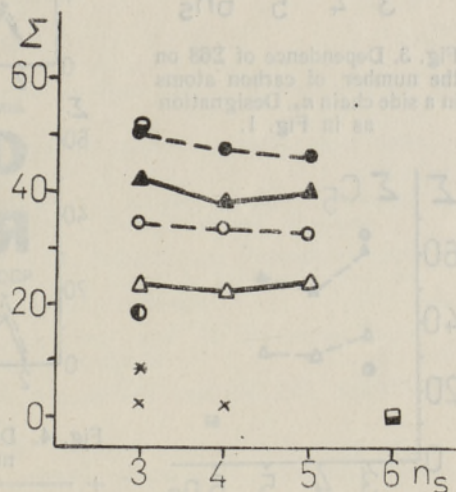


Fig. 1. Stability of molecular ions for monosubstituted cyclopentenes

○ — 1-*n*-alkylcyclopent-1-enes; ● — 3-*n*-alkylcyclopent-1-enes; △ — 1-isoalkylcyclopent-1-enes; ▲ — 3-isoalkylcyclopent-1-enes; ○ — 1-allylcyclopent-1-ene; ○ — 3-allylcyclopent-1-ene; ◻ — 3-phenylcyclopent-1-ene; × — literature data for isoalkylcyclopentanes and × — for allylcyclopentane.

Fig. 2. Dependences of relative intensities of principal ions $(C_5H_7)^+$ (above) and characteristic sums $\Sigma 67$ on the number of carbon atoms in a side chain n_s . Designation as in Fig. 1.



tenes — 38—43 (3-isoalkyl-), 46—51 (3-*n*-alkyl-), 23—26 (1-isoalkyl-) and 28—36 (1-*n*-alkylcyclopentenes) per cent. Total intensities of ions $(C_nH_{2n-3})^+ - \Sigma 67$ are lower for isoalkylcyclopentenes than for corresponding *n*-alkylcyclopentenes, too (Fig. 2). $\Sigma 68$ is slightly higher for 1-isoalkylcyclopentenes than for 3-isoalkylcyclopentenes (Fig. 3).

Both lengthening and branching of the side chain alkyl group increase the abundances of alkyl ions in the mass spectra of cyclopentenes. Total

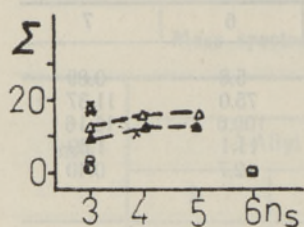


Fig. 3. Dependence of Σ_{68} on the number of carbon atoms in a side chain n_s . Designation as in Fig. 1.

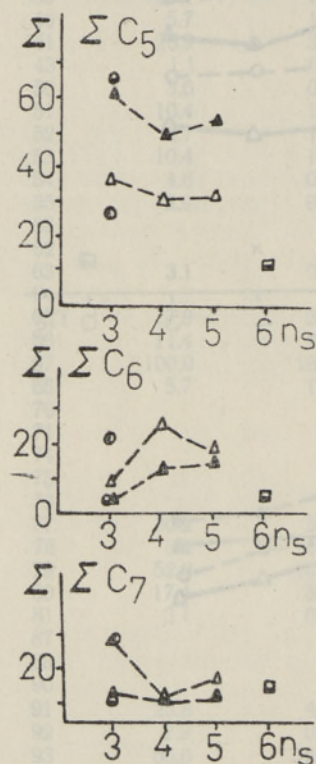


Fig. 5. Dependences of Σ_{C_5} , Σ_{C_6} and Σ_{C_7} on the number of carbon atoms in a side chain n_s . Designation as in Fig. 1.

intensities of ions $(C_nH_{2n+1})^+ - \Sigma_{43}$, that are about 1 per cent for 1- and 3-*n*-butylcyclopentenes, increase up to 2 per cent for *n*-pentylcyclopentenes. The fragmentation of isoalkylcyclopentenes C_9-C_{10} is accompanied by the formation of alkyl ions in quantities of 5–6 per cent, obviously due to the increased stability of secondary carbon ions formed from a substituent with an isostructure.

Intensity distribution curves according to the number of the carbon atoms in an ion n_i for isoalkylcyclopentenes (Fig. 4), except 1-isopropyl- and 1-isobutylcyclopentenes, are similar to those of the corresponding *n*-alkylcyclopentenes [1]. There are three maxima corresponding to Σ_{C_3} , Σ_{C_5} and to the molecular ion group. The plots of 3-isoalkylcyclopentenes differ by their sharp maxima at Σ_{C_5} (50–61%) that exceed the maxima at Σ_{C_3} (15–16%) about 3–4 times. The Σ_{C_5} maximum for 1-isoalkylcyclopentenes is lower (30–37%), being more wide for 1-isobutyl- and 1-isopentylcyclopentenes because of the higher intensities of ions with six and seven carbon atoms ($\Sigma_{C_6} - 26$ and 19, $\Sigma_{C_7} - 3$ and 7%). 1-Isopropylcyclopentene has a high Σ_{C_7} value — 20 per cent, corresponding to the third maximum on its intensity distribution plot. 1-Isobutylcyclopentene differs from 1-*n*-butylcyclopentene by a higher Σ_{C_6} value. The dependences of Σ_{C_5} , Σ_{C_6} and Σ_{C_7} on n_s for investigated compounds are given in Fig. 5.

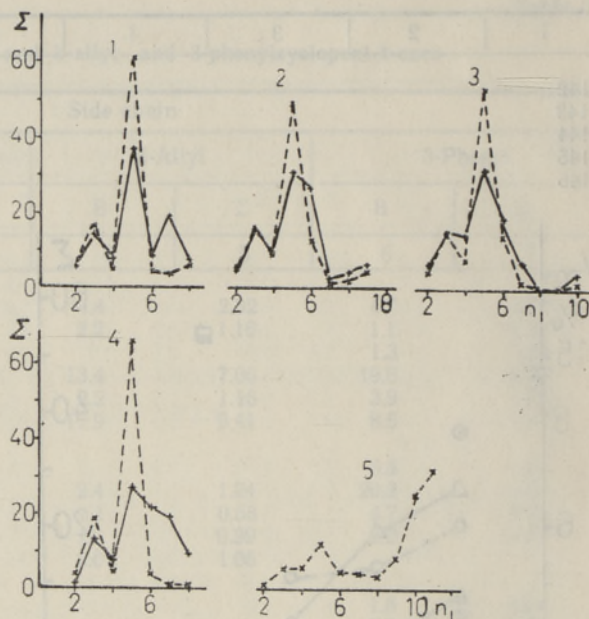


Fig. 4. Distribution of ion intensities according to the number of carbon atoms in an ion n_i . + — 1-substituted, × — 3-substituted-cyclopent-1-enes with the following groups in a side chain: 1 — isopropyl, 2 — isobutyl, 3 — isopentyl, 4 — allyl, 5 — phenyl.

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1- and 3-allylcyclopent-1-enes

The effect of an allyl group on the fragmentation of cyclopentenes upon the electron impact depends on its position. If located at the ring double bond, its effect is more appreciable. Analogically to alkylcyclopentenes, the principal degradation path of 1- and 3-allylcyclopentenes is elimination of the side chain (allyl group), yielding ions $(C_5H_7)^+$. Mass spectrum of 3-allylcyclopentene does not differ markedly from that of 3-*n*-propylcyclopentene, if the molecular ion mass 108 and its low intensity (0.5%) are excluded. The three most intensive peaks in the mass spectrum of 3-allylcyclopentene correspond to the ions $(C_5H_7)^+$ — 53, $(C_3H_5)^+$ — 9 and $(C_3H_3)^+$ — 7 per cent. Abundances of all other peaks are lower than 5 per cent. Ions $(C_5H_7)^+$ and $(C_3H_5)^+$ are obviously formed by an interruption of the C—C-bond located in β -position to the ring double bond at the one side, and at the other side — to the double bond of an allyl side group, the positive charge locating mainly on the larger fragment with m/e 67 and, to a lesser amount, on the fragment with m/e 41. Ions $(C_3H_3)^+$ may arise from ions $(C_3H_5)^+$ by elimination of H_2 .

The mass spectrum of 1-allylcyclopentene with the base peak of m/e 67 is more complicated. It markedly differs from those of 3-allyl- and other *n*- and isoalkylcyclopentenes in much higher abundances of larger, hydrogen-deficient fragment ions $(C_5H_5)^+$, $(C_6H_5)^+$, $(C_6H_6)^+$, $(C_6H_7)^+$, $(C_6H_8)^+$, $(C_7H_7)^+$ and $(C_7H_9)^+$ with m/e 65, 77, 78, 79, 80, 91 and 93. Their total intensities make 42 per cent in the mass spectrum of 1-allylcyclopentene, for 3-allyl- and 1-*n*-propylcyclopentenes — 9, and for 3-*n*-propylcyclopentene — 6 per cent. The fragmentation of 1-allylcyclopentene obviously proceeds by multistep degradation accompanied by hydrogen elimination and rearrangement.

The three most abundant ions in the fragmentation pattern of 1-allylcyclopentene are $(C_5H_7)^+$ with m/e 67 (19%), $(C_7H_9)^+$ with m/e 93 (13%) and $(C_6H_7)^+$ with m/e 79 (10%). They arise by an elimination of allyl, methyl and ethyl groups from the molecular ion, respectively. Metastable ion with apparent mass 80.1, corresponding to the transition m/e 108 $\xrightarrow{-15}$ m/e 93, was observed in its spectrum. Obviously the ions with m/e 93 result from cleavage of the ring, followed by migration of a hydrogen atom and subsequent elimination of a methyl group. In the mass spectra of 1- and 3-*n*-propylcyclopentenes the intensity of the peak with m/e 79 is 3.9 and 1.7 per cent (Σ), correspondingly, and the intensity of the peak with m/e 93 is lower than 1 per cent of the base peak intensity. The total intensity of the peaks with m/e 79 and 93 in the mass spectrum of 3-allylcyclopentene is about 1 per cent.

Total intensities of ions $(C_nH_{2n-5})^+$ with m/e 65, 79, 93 etc. are for 1-allylcyclopentene 27 per cent, but for 1- and 3-*n*-propyl- and 3-allylcyclopentenes — 6, 4 and 6 per cent. In turn, the ions $(C_6H_9)^+$ with m/e 81 are formed in considerably smaller quantities (below 1%) from 1-allyl- and 3-allylcyclopentenes than from 1-*n*-propylcyclopentene (7%).

The molecular ion stability of 1-allylcyclopentene is 7.7 per cent, i.e. higher as compared to 1-*n*-propylcyclopentene (6.1%), but more than ten times higher than that of 3-allylcyclopentene (0.6%, Fig. 1).

For 3-allylcyclopentene $\Sigma 67$ is 53 per cent, i.e. about 2.5 times higher than for 1-allylcyclopentene (20%), and close to 3-*n*-propylcyclopentene (55%, Fig. 2). $\Sigma 68$ does not exceed 3 per cent for both allylcyclopentenes (Fig. 3).

The intensity distribution curve, according to the number of carbon atoms in the ion for 3-allylcyclopentene, has two maxima corresponding to ΣC_3 and ΣC_5 (Fig. 4). These plots with sharp high maxima at ΣC_5 (66, 62 and 61%) and smaller ones at ΣC_3 (19 and 16%) are similar for 3-allyl-, 3-*n*- and 3-isopropylcyclopentenes. 3-*n*-Propylcyclopentene shows higher ΣC_8 values (5%) than 3-allylcyclopentene (1%). Analogically to 1-alkylcyclopentenes, the distribution curve for 1-allylcyclopentene is more scattered, the maxima at ΣC_5 and ΣC_3 being lower (27 and 13%) and ΣC_6 , ΣC_7 and ΣC_8 values being higher (22, 19 and 9%) as compared to those of 3-allylcyclopentene — 66, 19, 4, 1 and 1%, accordingly.

For allylcyclopentenes, the general regularity of higher *m/e* 67, $\Sigma 67$ and ΣC_5 values and of decreased intensity of molecular ion for 3-isomer, as compared to those of 1-isomer, is more strikingly revealed than for alkylcyclopentenes, due to the specific effect of the position of an allyl group on fragmentation. Thus, the isomeric 1- and 3-allylcyclopentenes may be distinguished on the ground of their mass spectra.

3-Phenylcyclopent-1-ene

A phenyl group as a substituent completely alters the degradation paths of the cyclopentenes upon electron impact. Two rings — cyclopentene and aromatic ones — form quite a stable system. The molecular ion stability of 3-phenylcyclopentene is 15.5 per cent, being the highest peak in the spectrum. Other more abundant ions are $(C_{11}H_{11})^+$ — 11, $(C_{10}H_9)^+$ — 14, $(C_{10}H_8)^+$ — 8 per cent, $(C_9H_7)^+$ — 5 per cent, with *m/e* 143, 129, 128 and 115. The sum of the relative intensities of these five peaks with general formulas $(C_nH_{2n-11})^+$, $(C_nH_{2n-12})^+$ is 54 per cent, i.e. a half of all ions formed. More abundant in the mass spectrum of 3-phenylcyclopentene are still ions with *m/e* 39, 51, 65, 66, 77 and 91. Some of them, e.g. the ions with *m/e* 51, 77 and 91 are represented in small quantities in the mass spectra of alkylsubstituted cyclopentenes. Peaks with *m/e* 81, 82 and 95, which are quite intensive in the *n*-alkylcyclopentene mass spectra, are of a low intensity in the 3-phenylcyclopentene spectrum.

In general, ions $(C_nH_{2n-2})^+$, $(C_nH_{2n-1})^+$ and $(C_nH_{2n})^+$ are formed in small quantities from 3-phenylcyclopentene.

The relative intensity of the peak *m/e* 67 is 1.5 per cent in 3-phenylcyclopentene mass spectrum, but for 3-*n*-hexylcyclopentene it is 44 per cent. Obviously, here the influence of the higher mass aromatic ring predominates, and principal fragmentation paths of cyclopentene series are excluded. Fragmentation of 3-phenylcyclopentene results in prevailing amounts (80%) of larger, hydrogen-deficient fragment ions with *m/e* above 67. Ions with *m/e* 67 and lower are formed in the amounts of ~20 per cent from 3-phenylcyclopentene, and ~70 per cent from 3-*n*-hexylcyclopentene.

These peculiarities of fragmentation of 3-phenylcyclopentene are seen in Fig. 4. The intensity distribution curve according to the number of carbon atoms has two maxima that correspond to ions with five (11,9%) and ten to eleven carbon atoms (ΣC_{10} and ΣC_{11} are 25 and 32%, accordingly). For 3-*n*-hexylcyclopentene the ΣC_5 , ΣC_{10} and ΣC_{11} values are 55, 0.1 and 3 per cent. These differences in the relative intensity distribution allow an identification of 3-phenylcyclopentene in the mixture of alkyl- and allylcyclopentenes. From these and our previous results [1], as well

as from literature data [2] it follows that fragment ion distribution and molecular ion intensity in the spectra of monosubstituted cyclopentenes depend on the structure, length and position of the side chain. 1-Isomers have higher molecular ion stability as compared to that of the corresponding 3-isomers. If the side chain structure allows specific fragmentation paths characteristic of the side chain position, the mass spectra of 1- and 3-isomers will be quite different (mainly quantitatively). In such cases, the 1- and 3-isomers are distinguishable on the ground of their mass spectra, e.g. 1- and 3-isopropyl- and 1- and 3-allylcyclopentenes.

The great similarity of the fragmentation patterns of isomeric monosubstituted *n*-alkylcyclopentenes suggests the extensive double bond isomerization in a molecular ion. But the observed quantitative differences in ion intensity distribution for isomeric molecules which obviously arise from differences in molecular ion stability show that no equilibrium between the isomeric structures is reached before fragmentation.

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Academy of Sciences of the Estonian SSR,
Institute of Chemistry

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Silvia RANG, A. TALVARI, O. EISEN

1- JA 3-MONOASENDATUD TSÜKLOPENTEENIDE MASSISPEKTRID 50 eV JUURES

Uurimuses võrreldakse 1- ja 3-isopropüül-, -isobutüül-, -isopentüül-, -allüül- ning 3-fenüül-1-tsüklopenteenide massispektreid ning selgitatakse kõrvalahela struktuuri ja asendi mõju nende dissotsiativsele ionisatsioonile elektroni löögi toimet. Leiti, et 1- ja 3-isopropüül- ning 1- ja 3-allüül-1-tsüklopenteenide massispektrid on erinevad. Uhesuguse kõrvalahela puhul on molekulaarse iooni stabiilsus 1-isomeeridel suurem kui 3-isomeeridel. Kõigi uuritud ühendite puhul, välja arvatud 3-fenüül-1-tsüklopenteen, on peamiseks lõhus-tumissaaduseks tsüklopentenüülioon ($C_5H_7^+$) massiarvuga 67. Uurimuses esitatud massispektrid on kasutatavad nimetatud ühendite identifitseerimiseks, eeskätt aga keeruliste segude analüüsimiseks kromato-massispektromeetrilisel meetodil.

Сильвия РАНГ, А. ТАЛВАРИ, О. ЭЙЗЕН

МАСС-СПЕКТРЫ 1- И 3-МОНОЗАМЕЩЕННЫХ ЦИКЛОПЕНТЕНОВ ПРИ 50 эВ

Установлены корреляции между структурами и масс-спектрами 1- и 3-изопропил-, -изобутил-, -изопентил-, -аллил- и 3-фенил-1-циклопентенов. Рассмотрено влияние структуры и положения боковой цепи на процесс диссоциативной ионизации под действием электронного удара. Показано, что масс-спектры 1- и 3-изопропил- и -аллилциклопентенов различны. При одинаковой боковой цепи стабильность молекулярного иона для 1-изомеров выше, чем для 3-изомеров. Для всех исследованных соединений, кроме 3-фенилциклопентена, распад молекулярного иона приводит к преимущественному образованию цикlopентенилиона ($C_5H_7^+$) с m/e 67. Приведенные масс-спектры могут быть использованы для идентификации указанных соединений в первую очередь при анализе смесей методом хромато-масс-спектрометрии.