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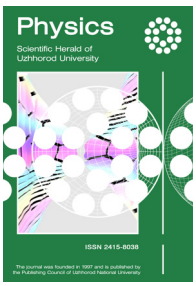

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Mass Spectrometric Studies of Valine Molecules by Electron Shock in the Gas Phase

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Abstract

Relevance. Valine is one of the eight amino acids not synthesised by the human body, necessary for the synthesis and growth of body tissues, muscle coordination; regulation of nervous processes, nitrogen metabolism, and stabilisation of the hormonal background. Since α-amino acids contain an asymmetric carbon atom, they can exist as optical isomers (mirror antipodes) that play an essential role in protein biosynthesis. The structure of matter and the physical processes that occur in it are studied using the method of mass spectrometry and spectral analysis. This indicates the relevance of the problem that was studied in this paper.

Purpose. Mass spectrometric studies of the formation of ionic products of single and dissociative ionisation of the valine molecule ($C_5H_{11}NO_{2)}$ with electrons according to the method of beams intersecting within the energy range of bombarding electrons 6-70 eV. To consider the mechanisms of formation of the most intense ion fragments during dissociative ionisation by electron shock.

Methods. The experiment was conducted on an installation with a monopole mass spectrometer of the MX-7304A type, which belongs to the class of dynamic mass analysers with electron shock ionisation in the range of mass numbers 0-120 Da. The mass spectra of molecules were investigated at different temperatures of the source of molecules in the range of 300-600 K.

Results. The obtained results are compared with the mass spectra of the D-, L-, and DL-enantiomeric forms of the valine molecule with data from the NIST and SDBS databases. The features of the processes of formation of ion fragments of valine molecules by electronic shock are analysed in detail, and the dynamics of the yield of ion fragments in the range of evaporation temperatures of the initial substance of 300-440 K is also studied. The total relative ionisation cross-section of the molecule under study was measured according to mass spectrometric method with an ionising electron energy of 5-60 eV. Based on the results of experimental studies, a threshold section of the dependence of the total relative cross-section of valine ionisation is determined and given in this paper.

Conclusions. A detailed analysis of the processes of formation of fragment ions in the mass spectra allows demonstrating the influence of the structural forms of valine enantiomers on the redistribution of relative intensities of product ions

Keywords: electron, mass spectrometry, ionisation, amino acid

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Introduction

Among all the molecules present in a living cell, the first place is occupied by proteins that account for at least half of the dry weight of the cell. Proteins perform various functions and serve as molecular tools by which genetic information finds its real embodiment. To build all proteins, whether they are proteins from the oldest bacteria or from higher organisms, the same set of 20 amino acids is used, covalently bound to each other in a certain sequence inherent only in this protein. Each amino acid, due to the specific features of its side chain, has a chemical individuality [1].

Valine is one of the eight amino acids not synthesised by the human body. At the same time, this aliphatic α-amino acid is necessary for the synthesis and growth of body tissues, muscle coordination; regulation of nervous processes, nitrogen metabolism, and stabilisation of the hormonal background [2]. Valine belongs to a group of simple aliphatic nonpolar α-amino acids that exist as various conformers. Two types of amino acid isomerism are known: structural isomerism, which is associated with the structural features of the carbon skeleton and the relative location of functional groups, and optical isomerism (spatial). Since α-amino acids contain an asymmetric carbon atom, they can exist as optical isomers (mirror antipodes) that play an essential role in protein biosynthesis.

The structure of matter, mechanisms, and features of physical processes occurring in it are investigated using methods of interaction with slow electrons, which include electron mass spectroscopy, i.e., the study of mass spectra, temperature dependences of the occurrence of positive ion fragments, dissociative ionisation of amino acid molecules under the action of low-energy (430 eV) electrons and determination of the appearance energies of ionised fragments [3; 4]. This indicates the relevance of the problem that was studied in this paper.

Ionising radiation, interacting with a living organism, can cause various changes in the genotype due to its effect on the genetic DNA and RNA macromolecules. This radiation, penetrating the body, generates streams of low-energy secondary electrons, the energy of which can range from 0.1 to tens of electron volts [5]. Secondary electrons initiate the processes of excitation [6; 7] and ionisation [8], which lead to destructive changes in DNA and RNA. According to the existing ideas [9], it is with slow electrons that the main part of destructive changes at the molecular level of biostructures is associated, and the main target is genetic macromolecules [10]. Assessment of the effects of physical excitation and ionisation processes caused by electron shock in biostructures requires obtaining information about the most probable channels of fragmentation of biomolecules. This was one of the tasks of this study.

The purpose of this paper was to investigate the process of electron ionisation of valine molecules in the gas phase according to mass spectrometric method at different evaporation temperatures of the first substance. It was also important to compare the relative intensities of practically all the peaks of the mass spectra obtained in this study with data from other authors and from the well-known NIST and SDBS databases. A detailed analysis of the processes of formation of fragment ions in the mass spectra allows demonstrating the influence of the structural forms of valine enantiomers on the redistribution of relative intensities of product ions.

Materials and Methods

The experiment was performed on a monopole mass spectrometer MX 7304A, which was described in detail earlier [8; 11]. This mass spectrometer is a single-pole version of the quadrupole analytical instrument and comprises an ion source, an analysis system, and a useful signal detection system. This device was placed in a vacuum installation with oil-free pumping. The system provided a residual gas vapour pressure of at least 210^{-6} Torr in working conditions. The ion source of the mass spectrometer allowed obtaining electron beams of regulated energy from 6 to 70 eV, a current in the range of 0.05-0.5 Ma, with a minimum energy spread of DE½ = 200 meV, where this value is the full width at half the maximum electron energy distribution. The range of recorded masses was 1-120 DA, with a resolution not worse than ΔM=1 Da. The concentration of the valine molecules under study in the region of interaction with electrons was $10^{10} \div 10^{11}$ cm^{-3}. The temperature of the source of molecules was maintained in the range of 300-600 K [2].

The mass scale was calibrated for isotopes of Ar and Xe atoms, and control mass spectra were measured for freon, sulphur hexafluoride, and krypton. The energy scale was calibrated from the initial section of the ionisation section of the Kr atom, which allowed determining the electron energy with an accuracy of ± 0.08 eV.

Valine of the Sigma Aldrich company was used for research (purity 0.999, No. CAS72-18-4, the presence of water molecules was excluded). The structural formula of valine is represented by in Figure 1A. The experiment was carried out in two stages: at the first stage, mass spectra in the range of 1-120 Da were carefully measured at ionisation energies (E_i) 20, 30, 40, 50 and 70 eV, and in the second case, the energy dependences of the relative dissociative ionisation cross-sections of the valine molecule were measured in the energy range of ionising electrons from 5 to 60 eV. The measurement method was reduced to simultaneous measurement of fragment ions; for this, the energy range was first set, then the test masses were set (no more than 20), and the total measurement time was calculated using the Formula (1):

$$T_{full} = t_1 \times n \times C \quad (1)$$

where t_1 is the measurement time of a single fragment; n is the number of fragments; C is the number of cycles determined depending on the value of the useful signal.

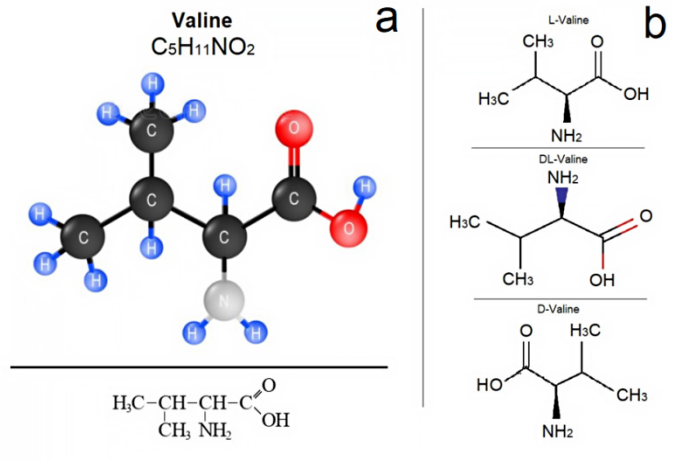

Figure 1. (a) structural formulas of valine and its enantiomers L-, DL-, and (b) D-forms

Results and Discussion

Before proceeding to the discussion of the results, it is advisable to consider the structural diagrams of the valine $C_5H_{11}NO_2$ molecule shown in Figure 1 and its enantiomers of L-, DL-, and D-forms. A distinctive feature of the valine molecule is the presence of hydrogen atoms bound to 4 substitutes, namely the 1st is a hydrogen atom, the 2nd is a carboxyl COOH group, the 3rd is an NH_2 amino group, the 4th, the most significant is an alkyl group, i.e., a side chain of Cα atoms, the composition of which determines the main properties of this amino acid. Valine enantiomers should have similar energy characteristics: ionisation potentials, heat of formation, activation energies, and mass spectra of fragments formed by dissociation of molecular ions. Enantiomers differ only in vector characteristics, which determine the properties of a molecule depending on its structure. Notably, α-amino acids contain an asymmetric carbon atom (C_α-atom) and can exist as optical isomers. The carboxyl group can rotate, and the hydrogen atom can be oriented both towards nitrogen and in the opposite direction. Conformational variability of molecules contributes to the reorientation of flexible carboxyl (-COOH) and amino (-NH_2) groups (Fig. 1b), forming various intramolecular hydrogen bonds. For example, the bond of a lone pair of a nitrogen atom with a hydrogen of a hydroxyl group (N...HO) or a bond between a hydrogen atom of an amino group and a carbonyl oxygen atom (NH...O= B) and hydroxyl (NH...OH) in groups.

Figure 2 demonstrates the mass spectrum of valine with ionising electron energies Ue=70 eV and a molecular source temperature of 393 K, as can be seen, the highest intensity corresponds to ions with m/z = 28, 42, 56 and 72 Da. Next, in the mass spectrum, the peak corresponding to the mother ion (m/z=117) is practically absent, which is inherent in aliphatic amino acids with low stability of the molecular ion formed during ionisation [12]. Inherent in most α-amino acids is that the main dissociation channel upon electron impact is conditioned upon the breaking of the C-Cα bond, and therefore, in the case of valine, an ion with a mass of m/z=72 is formed as a result of the cleavage of the COOH carboxyl group.

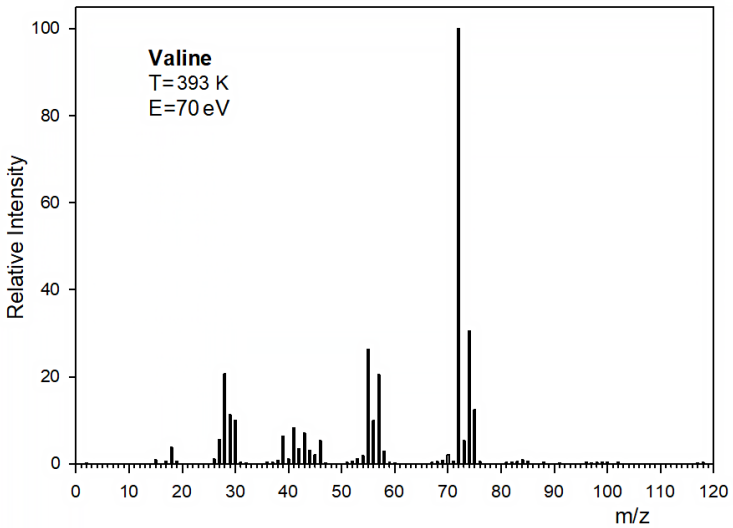

Figure 2. Mass spectrum of the valine molecule

Source: [2]

To analyse the mass spectra obtained by the authors, it was interesting to compare the relative intensities of the mass peaks of the valine molecule from various sources. This comparison is demonstrated in Table 1 from the NIST [13], SDBS [14] databases and studies [15; 16; 29].

Table 1. Comparison of relative intensities of valine peak masses

m/z	NIST [13]		SDBS [14]				V.Vukstich et al. [29]	P. Papp et al. [15]	W. Jochims, et al. [16]	OUR DATA
	DL-	D-	DL-	L-	DL-Nor	D-				
2			0.1	0.15						0.12
14	0.2		0.2	0.14	0.1	0.1				0.14
15	0.7		0.7	0.9	1.1	1.2				0.92
16				0.1				0.11		0.12
17	0.6		0.6	0.61	0.2	0.5				0.61
18	2.6		2.6	3.76	3.7	3.2		1.64		3.74
19	0.5		0.5	0.5	0.3	0.6		0.26		0.5
26	0.7	1.31	0.7	1.09	0.8	0.7		0.27		1.09
27	6.7	11.3	6.7	5.5	6.1	7.4	18.7	6.79	6	5.5
28	19.6	18.2	19.6	20.61	14.9	24.7	63.0	12.54	36	20.61
29	10.8	10.1	10.8	11.31	5.3	14.2	30.0	10.01	36	11.31
30	8.1	12.6	8.1	9.9	10.5	10.5	24.5	6.43	19	9.92
31	0.2	0.5	0.2	0.3	0.7	0.2		0.63		0.33
32	0.1		0.1	0.2	0.2	0.3		0.21		0.23
33	0.1		0.1	0.1	0.1					0.11
34				0.1		0.1				
36				0.4		0.4				0.43
37	0.2	0.5	0.2	0.25	0.2					0.25
38	0.8	1.2	0.8	0.71	0.6	0.5	17.7	0.71		0.71
39	6.7	8	6.7	6.35	3.5	7.2		4.69	3	6.35
40	0.7	3.3	0.7	1.05	0.6	0.9		0.74		1.05
41	8.4	12.6	8.4	8.21	3.7	8.7	13.5	6.43	9	8.21
42	2.8	5.9	2.8	3.49	4.9	3.1	6.8	2.54		3.49
43	7.2	10.5	7.2	7.04	4.7	6.7	8.3	4.98	13	7.03
44	1.2	7.7	1.2	2.97	7.8	1.6	5.2	2.43		2.97
45	1.5	5.1	1.5	2.1	1.6	2.1	9.4	1.38	6	2.1
46	5.4	5.1	5.4	5.3	3.1	6.4	13.5	3.6	13	5.3
47		0.2		0.2				0.22		0.2
49	0.1		0.1	0.1						0.1
50	0.1		0.1	0.14	0.2	0.2				0.14
51	0.4	0.5	0.4	0.36	0.2	0.4				0.36
52	0.6	0.7	0.6	0.52	0.2	0.6				0.52
53	1.1	1.5	1.1	1.1	0.6	1.2				1.1
54	2.1	2.5	2.1	1.84	0.8	1.9				1.84
55	28.7	24.9	28.7	26.33	6.1	31.4	33.9	28.91	64	26.33
56	9.8	12.2	9.8	9.86	3	12	21.9	5.46		9.86
57	19.1	26.7	19.1	20.48	3	24.5	30.7	26.08	60	20.48
58	3.2	3.9	3.2	2.9	0.1	3.3	6.2	1.96		2.9

Table 1, Continued

m/z	NIST [13]		SDBS [14]				V.Vukstich et al. [29]	P. Papp et al. [15]	W. Jochims, et al. [16]	OUR DATA
	DL-	D-	DL-	L-	DL-Nor	D-				
60	0.2	0.5	0.2	0.22		0.1				0.22
67	0.4	0.6	0.4	0.31		0.2				0.31
68	0.5	1	0.5	0.44	0.2	0.3				0.44
69	1	2.1	1	0.77	0.1	0.4				0.77
70	2.5	2.9	2.5	2.16	1.1	2.1		1.78		2.16
71	0.6	1	0.6	0.57	0.2	0.6				0.57
72	100	100	100	100	100	100	100	100	100	100
73	5.7	5.3	5.7	5.28	4.9	5		5.66		5.28
74	34.5	13.2	34.5	30.46	24	34	24	35.82	45	33.46
75	14	8.6	14	12.35	2.1	15.3	10.4	13.67	12	12.35
76	0.6	0.5	0.6	0.43	0.1			0.42		0.43
77				0.13		0.1				0.13
78	0.1		0.1	0.12		0.1				0.12
79	0.1		0.1	0.14						0.14
81	0.4		0.4	0.28		0.1				0.28
82	0.5	0.8	0.5	0.41	0.1	0.3		0.37		0.41
83	0.5	1	0.5	0.44		0.2				0.44
84	1	1	1	0.96		0.8				0.96
85	0.4	1.5	0.4	0.54		0.3		1.11		0.54
88		0.5		0.43	0.3					0.43
91	0.2		0.2	0.23						0.23
92	0.1		0.1	0.11						0.11
93	0.1		0.1	0.13						0.13
95	0.1		0.1	0.12						0.12
96	0.3		0.3	0.34						0.34
97	0.3		0.3	0.22		0.1				0.22
98	0.2	0.6	0.2	0.27		0.3				0.27
99	0.2	1	0.2	0.28						0.28
100	0.2	1.8	0.2	0.42		0.1				0.42
102	0.2	0.3	0.2	0.28		0.3				0.28
117		0.2		0.25					1	0.12
118		0.3		0.33						0.22

The results of studying the mass spectra of enantiomers of the L-, DL-, and D- forms of the valine molecule, obtained in various laboratories, presented in the table, give the most complete picture of the processes of formation of ion fragments. Comparison of the relative intensities demonstrated in the table shows a satisfactory agreement, but for some there are differences: not all ions with masses m/z=2, 16, 34, 36 are detected; the relative intensities of ion formation of fragments of enantiomers of L-, DL-, and D-forms with masses m/z=28, 29, 57, 58 differ (see Table 1).

Enantiomers must have the same mass spectra of ion fragments formed during dissociation of molecular ions [17]. However, analysis of the available data on the mass spectra of fragments formed upon ionisation of amino acids by electron shock reveals substantial differences for a number of D- and L-amino acids [16-18]. These differences can obviously only be related to the different probability of formation of any fragments according to the structural formula of enantiomers.

Thus, the results presented in the table allow considering the mechanisms of formation of the most intense

ion fragments upon dissociative ionisation by electron shock. As mentioned above, ionisation and electron removal lead to a weakening of the bonds in the molecular ion compared to the neutral molecule. In all optimal structures of the parent amino acid cations, the positive charge is mainly localised on the carbon atom of the carboxyl group, and the dissociation process occurs due to charge transfer to the carbon chain. This is confirmed by the relatively low intensity (see Table 1) in the mass spectrum of the COOH ion peak$^+$ (m/z=45). Analysing the data of the most intense ion fragments presented in the table, the processes leading to their formation can be suggested as follows:

m/z=72. The main most intense ion fragment occurs as a result of effective dissociation of the parent ion of the valine molecule upon CC bond break [2] with the formation of a neutral fragment of the COOH carboxyl group according to reaction (2):

$$C_5H_{11}NO_2 + e^- \rightarrow NH_2(CH_3)_2(CH)_2 + (COOH) + 2e^- \quad (2)$$

m/z=74. The ion with this mass has a peak with an intensity of 33% of the main one and is associated with the dissociation of the side chain and the formation of the C_3H_7 propyl (3):

$$C_5H_{11}NO_2 + e^- \rightarrow NH_2CHOCOOH + (CH_3)_2CH + 2e^- \quad (3)$$

m/z=57. The appearance of a rather intense (20% of the main) peak of such a mass is associated with dissociation of the amino group and the formation of neutral water and propylene C_3H_6 molecules (4):

$$C_5H_{11}NO_2 + e^- \rightarrow NHCHC(OH)^+ + H_20 + CH_3CHCH_2 + 2e^- \quad (4)$$

m/z= 39, 41, 43. These peaks belong to hydrocarbon ions and amino and carboxyl groups (5-7) are not involved in the formation of these fragments:

$$C_5H_{11}NO_2 + e^- \rightarrow CHCHCH^+ + C_2H_6N0 + H_2O + 2e^- \quad (5)$$

$$C_5H_{11}NO_2 + e^- \rightarrow CH_2CCH_3{}^+ + C_2H_5NO_2 + H + 2e^- \quad (6)$$

$$C_5H_{11}NO_2 + e^- \rightarrow (CH_3)_2CH^+ + NH_2CH_2{+}CO_2 + 2e^- \quad (7)$$

m/z= 27, 28, 29, 30. Unambiguous interpretation of peaks in this group is complicated by the alternativeness of the occurrence of certain neutral fragments, which is manifested in different intensities of peak masses obtained by interaction with electrons and photons (Table 1). For example, the appearance of the peak m/z=28 may correspond to isobar CO^+ and CH_2N^+ ions according to the following reactions (8):

$$C_5H_{11}NO_2 + e^- \rightarrow CO^+ + NH_2CH(OH)CH(CH_3)_2 + 2e^- \quad (8)$$

or (9)

$$C_5H_{11}NO_2 + e^- \rightarrow NHCH^+ + COOH + CH_3CH_2CH_3 + 2e^- \quad (9)$$

Preference should be given to reaction (9), since the formation of this HC-NH fragment dominates the processes of dissociation of amino acid molecules [19].

Analysis of the interaction processes of an electron with the valine molecule under study suggests that the carboxyl – COOH group – is initially separated due to a simple break in the bond between C_1-C_2 atoms.

The consequence is the formation of the main peak of the most intense in the mass spectrum with m/z=72. Energetically remarkably close to the process of separation of the entire carboxyl group is the separation of two neutral fragments H and CO_2, which is energetically more beneficial than the separation of two neutral OH and CO fragments [20].

Notably, in the mass range m/z=2-20, the interpretation of the appearance of peaks in the mass spectrum is quite difficult due to probable alternative channels of dissociative ionisation. This is especially true for the peak with m/z=2, which was also found in [14] for L- and DL-form enantiomers (Table 1).

The comparison of the relative intensities of mass peaks made in Table 1 with the data in NIST [13], SDBS [14], as well as in [15; 16] generally indicates a satisfactory agreement between them, and the evaporation temperature of valine molecules is given only in [14], which may make adjustments to the values of mass peaks. However, a more thorough analysis of the available mass spectra of fragments formed during electron shock ionisation of amino acids reveals substantial differences for a number of D- and L-amino acids [14; 16; 17]. Therewith, there are noticeable differences in the mass spectra of ions-fragments of compounds used by the authors [29] to identify 2,3-diaminopropanic acid. A more complete analysis of processes using theoretical calculations of the energies, lengths, and bond orders of mother, daughter fragment ions, and neutral molecules should be the result of a separate study, similar to the one conducted in [16] for photoionisation processes.

Undoubtedly, the influence of the temperature of the molecules under study on the dissociative ionisation process is essential [21-23]. This is also evidenced by the study [24]. Fig. 3 demonstrates the temperature dependences for the most intense ions of NH fragments$_2$(CH3)$_2$(CH)$^+$ (m/z=72), $NH_2CHCOOH^+$ (m/z=74), $NHCHC(OH)^+$ (m/z=57), $(CH_3)_2CH^+$ (m/z=43), $CH_2CCH_3{}^+$ (m/z=41) and CH_3 (m/z=15). Three segments are observed in Figure 3: a segment with an almost linear increase in intensity, a segment with exponential growth, with saturation in the temperature range of 400-418 K and a sharp decline, the cause of which is the beginning of decomposition of the substances under study [2]. Features on the measured dependences – the change in the slope of the curves at some temperatures, apparently, should be attributed to the passage of the processes described above (2-9).

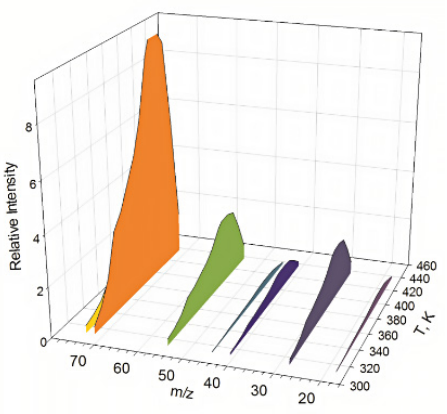

Figure 3. Dependence of the formation of positive ion fragments of the valine molecule on temperature. Electron energy 70 eV

Source: [2]

When the potentials on the deflecting electrodes of the mass spectrometer were turned off, the total (total) current of positive ions to the collector formed as a result of the interaction of the valine molecules under study with electrons was measured. By smoothly changing the energy of ionising electrons, it is possible to obtain the energy dependence of the total relative cross-section of the formation of positive ions in a given range of electron energies.

Figure 4 demonstrates the energy dependence of the total relative ionisation cross-section of the valine molecule in the energy range 5-60 eV, and also shows the threshold section of this dependence, which is approximated according to the least squares method [19; 22]. Evidently, the fitting results correlate well with the experimental curve, which allows determining the ionisation energies of the valine molecule, which turned out to be equal to: E_{IE}=8.66±0.22 eV.

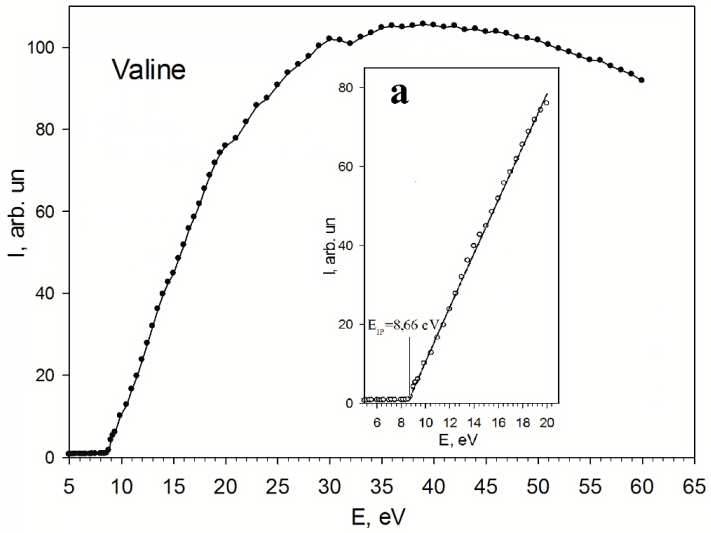

Figure 4. Energy dependence of the total ionisation cross-section of the valine molecule. On the tab: threshold section of the experiment point, solid approximation

The authors of this study compared it with the data of other authors [26-28] (see Table 2). In addition, the best agreement is observed with experimental data from the studies [15; 25] and with calculations according to the G3MP2 method [16].

Table 2. Value of the ionisation energy (eV) of the valine molecule

Experiment					Calculation		
Electronic shock				Photons	G3MP2	OVGF	OVGF
Our data	[25]	[26]	[15]	[16]	[16]	[27]	[28]
8.66± 0.20	8.71	9.86	8.91±0.05	8.9	8.89	9.54	9.50

Conclusions

Experimentally, the mass spectra of the valine molecule were investigated according to the mass spectrometry method in the range of mass numbers 0-120 Da within evaporation temperatures of the initial substance at 300-440 K. A detailed analysis of the processes of formation of ions-fragments of valine molecules by electron shock-was carried out. It was shown that the difference in the structural forms of valine enantiomers is reflected in the mass spectra as a redistribution of the relative intensity values of daughter ions. Information on the relative mass intensities of the L-, DL-, and D-form valine molecules obtained in various laboratories provides a more complete picture of the processes of ion fragment formation.

As a result of measurements of the total relative cross-section of the ionisation of the valine molecule by electrons in the energy range of 5-60 eV and the approximated threshold section of the energy dependence of the cross-section, the ionisation energy of the valine molecule was determined, which turned out to be equal to: $E_{IE}=8.66\pm0.22$ eV. This ionisation potential is compared with the available experimental and theoretical data, which showed a satisfactory agreement of the results obtained by the authors with the compared data. In conclusion, mass spectrometric studies of amino acids by electron shock in the gas phase provide rich information about their unique properties, allow determining the degree of fragmentation in the process of interaction with electrons, and evaluate the parameters of intermolecular bonds.

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Мас-спектрометричні дослідження молекул валіну електронним ударом в газовій фазі

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Анотація

Актуальність. Валін є однією з восьми амінокислот несинтезованих людським організмом, необхідною для синтезу і росту тканин тіла, м›язової координації; регулювання нервових процесів, азотного обміну, стабілізації гормонального фону. Оскільки α-амінокислоти містять асиметричний атом вуглецю, то вони можуть існувати у вигляді оптичних ізомерів (дзеркальних антиподів), які відіграють важливу роль в процесах біосинтезу білка. Структуру речовини та фізичні процеси, які відбуваються в ній досліджують за допомогою методу мас-спектрометрії і спектрального аналізу. Що свідчить про актуальність задачі, яка досліджувалася у цій роботі.

Мета. Мас-спектрометричні дослідження утворення іонних продуктів однократної та дисоціативної іонізації молекули валіну ($C_5H_{11}NO_{2)}$ електронами методом пучків, що перетинаються в діапазоні енергій бомбардуючих електронів 6–70 eV. Розглянути механізми утворення найінтенсивніших іонів-фрагментів при дисоціативній іонізації електронним ударом.

Методи. Експеримент проводився на установці з монопольним мас-спектрометром типу МХ-7304А, який відноситься до класу динамічних аналізаторів мас з іонізацією електронним ударом у діапазоні масових чисел 0–120 Da. Мас-спектри молекул досліджено за різних температур джерела молекул в діапазоні 300–600 К.

Результати. Проведено порівняння отриманих результатів з мас-спектрами D-, L- та DL-енантіомерних форм молекули валіну з даними баз NIST та SDBS. Детально проаналізовано особливості процесів утворення іонів-фрагментів молекул валіну електронним ударом, а також досліджено динаміку виходу іонів-фрагментів в інтервалі температур випаровування вихідної речовини 300–440 К. Було проведено вимірювання повного відносного перерізу іонізації досліджуваної молекули мас-спектрометричним методом з енергією іонізуючих електронів 5–60 eV. За результатами експериментальних досліджень визначено та наведено в даній роботі порогову ділянку залежності повного відносного перерізу іонізації валіну.

Висновки. Детальний аналіз процесів утворення іонів-фрагментів у мас-спектрах дозволяє показати вплив структурних форм енантіомерів валіну на перерозподіл відносних інтенсивностей іонів-продуктів.

Ключові слова: електрон, мас-спектрометрія, іонізація, амінокислота