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ТЕРМОДИНАМИЧЕСКИЕ СВОЙСТВА ОРГАНИЧЕСКИХ КИСЛОТ И ИХ НЕКОТОРЫХ ПРОИЗВОДНЫХ

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Теплоты парообразования, сгорания, образования, энтропии и теплоемкости в различных фазах различных карбоновых кислот и их производных: ацетатов, эфиров с жирными радикалами, двух-, трех- и четырехосновных кислот (52 соединения) были проанализированы в рамках однопараметровых математических уравнений. Экспериментальные данные всех выбранных одно-, двух-, трех- и четырехосновных кислот были проанализированы и определено, что все термодинамические функции этих типов соединений зависят от числа валентных электронов N, из которого вычитается сумма неподеленных пар электронов g, как это представлено в уравнениях $\Delta_{vap,c,f}H° = i \pm f(N\text{-}g)$ ***и*** $S°(C_p) = i \pm f(N\text{-}g)$***. Коэффициент f в уравнениях находится в рамках 104-113 кДж моль***$^{-1}$ ***электрон***$^{-1}$***, что соответствует таким же значениям f, которые упомянуты в ранее опубликованных нами работах по определению теплот сгорания органических кислот. Что касается коэффициента i в полученных уравнениях, то необходимо отметить, что ситуация не такая однозначная, как с коэффициентом f. Значения этого коэффициента различны в уравнениях для испарения, сгорания, образования, так же, как и в уравнениях энтропии и теплоемкости. На базе литературных экспериментальных данных рассчитано 29 новых уравнений, которые могут быть использованы для вычисления тех же термодинамических функций других, новых органических кислот, и особенно биоорганических веществ с полезными свойствами. Необходимо добавить, что полученные уравнения могут служить дополнительным материалом для расчета энергий связей жирных кислот и их производных в газовой фазе.***

Ключевые слова: кислота, жирные кислоты, ацетат, эфир, двойные кислоты, тройные и четверные кислоты

THERMODYNAMIC PROPERTIES OF ORGANIC ACIDS AND SOME THEIR DERIVATIVES

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The heats of vaporization, combustion, formation, entropy and the heat capacities in different phases of different carbonic acids and their derivatives: acetates, esters with fatty radicals, two-, three- and four-basic acids (52 compounds) were analysed in the framework of one-parametric mathematic equations. The experimental data of all chosen one-, two-, three- and four-basic acids were analyzed. It was determined, that all thermodynamic functions of these types of compounds depend on the number of valence electrons N, from which the sum of lone electron pairs g as represented in the equations $\Delta_{vap,c,f}H° = i \pm f(N\text{-}g)$ ***and*** $S°(C_p) = i \pm f(N\text{-}g)$ ***is excluded. The coefficients f in the first equations is in the range of 104-113 kJ mol***$^{-1}$ ***electron***$^{-1}$***, that corresponds***

to the same values f in the equations, which are mentioned in our earlier papers on the determination of the heats of combustion of organic acids. As concerned of coefficient i in the received equations, necessary to note that situation is not synonymous as with the coefficient f. The magnitudes of this coefficient are different in the equations of vaporization, combustion, formation also as in the equations of entropy and the heat of capacity. On the base of literary experimental data we calculated the 29 new equations, which can be used for the calculation of the same thermodynamic functions for other new organic acids and especially bioorganic substances with the useful properties. Necessary to add, that the received equations can serve as additional material for the calculation of the bond energies of fatty acids and their derivatives in gas phase.

Key words: acid, fatty acids, acetate, ester, two-, three- and four-basic acids

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INTRODUCTION

It is known during a long time that organic acids are a very important and used class of the carbon derivatives in industry, agriculture and pharmaceutical industries and medical products [1]. In this connection it is possible to recollect such names of medical preparations as acetylsalicylic, gluconic, galactonic, valproic and lactic acids and their metallic derivatives [2, 3]. This class of compounds is a subject of an intensive research of the scientists in the different fields: the study of synthesis, stereoelectronic effects, mechanisms of reaction, thermodynamics and others directions in our time also. Many books and reference books have been written on this topic [4, 5].

However, not only thermochemical properties of linear carbonic, fat acids of different structure are important for the medical, technical needs and theoretical studies. Different acetates, esters and polyfunctional acids represent a large significance also. On this reason the analysis and mathematical treatment of all thermodynamic functions of these classes of derivatives of carbon acids are summed and considered in this review.

It is known, that all mentioned above classes and types of compounds exist in condensed and gaseous phases. Taking this circumstance into account, we believed that consideration of their thermochemical properties, which are represented in Table, should begin first of all from the analysis of the heat of vaporization ($\Delta_{\text{vap}}H^{\text{o}}$), because this functioncan connect the both phases.

This parameter can be obtained at the use of Clausius-Clapeyron experimental approach and the half-empirical theoretical calculations with the use of Trouton and Wadsö equations for the liquids, which have the hydrogen bonds or include the boiling points [6-9]. There is a especial method, based on the calculation of topological solvation index of the first order (${}^{1}\chi^{s}$) of investigated molecules [10].

The analysis of other thermodynamic functions ofdifferent organic compounds can be made by any ways also. In our previous works [10-15] it has been shown that all thermodynamic functions $\Delta_{vap,\text{c,f}}\Psi^{\text{o}}$ (Ψ^{o} is the heat (ΔH^{o}) of vaporization, combustion, formation and entropy (S^{o}) and heat capacity (Cp)) of investigated organic molecules) are connected with a parameter (N-g) in the range of one-factor correlation analysis, where N is a general number of valence electrons, g is a number of lone electron pairs of heteroatomes in molecules in general equation 1.1:

$$\Delta_{vap,\text{c,ff}}\Psi^{\text{o}} = i \pm f\,(N\text{-}g) \qquad (1.1)$$

The parameter g is equal 2 for trivalence nitrogen and phosphorus atoms and similar elements of the group, g is 4 for oxygen, sulfur etc., g is zero for five valence nitrogen and phosphorus etc., g is 6 for halogens [10-12, 14, 15]. The parameters i and f are stoichiometric coefficients. This equation a little differs from the equation (1.2), suggested earlier and mentioned in some papers on the heats of combustion process of organic compounds [10-16].

$$\Delta_{\text{c}}H^{\text{o}} = -109.0\cdot(4a + b - c) + \Sigma(hc_{\text{i}})\cdot d_{\text{i}} \qquad (1.2)$$

In last equation the number -109.0 (kJ mol^{-1} electron^{-1}) has been deduced from the heat of combustion of n-octane. The parameters a and b are the numbers of all four valence carbon and mono valence hydrogen atoms correspondingly, c is a number of the moving electrons from carbon to electronegative heteroatoms. The sum of $\Sigma(hc_{\text{i}})*d_{\text{i}}$ represents the number of the heat corrections in the heat of combustion of the organic substance for identical structural groups in molecule [11, 12, 16].

In the next parts of review we consequently will represent thermodynamic data of different acids andacetates. In the aims of the convenience of the perception of thermodynamic material all compounds have a general numeration. Necessary to add, that practically all earlier obtained experimental data, including also the data received in the period from 2000 to 2017, for the review were taken from recognized handbooks on organic chemistry of Pedley, Neylor, Kirby [2], Karapetyanz M.X., Karapetyanz M.L. [4], Cox and Pilcher [6] and National International Standard and Technology Institute (NIST) of United States of America [7].

RESULTS AND DISCUSSION

1. Acids

1.1. Acids withlinear C_1-C_{12} radicals

The analysis of the heat of vaporization ($\Delta_{vap}H^o$) of acids (1-9, Table [2, 4, 6, 7]) with the number of carbon atoms from 1 to 12 in the frame of one-factor correlation treatment shows a good dependence (2.1), in which (here and in other correlation equations) r is a correlation coefficient, S_o is a standard deviation and n is the number of data used for calculation)

$$\Delta_{vap}H^o = (35.0 \pm 7.1) + (1.2 \pm 0.2)\,(N\text{-}g) \tag{2.1}$$

r 0.913, S_o 9.2, n 9 (compounds **1-9**).

The similar equations (2.2-2.7) were found for other thermodynamic functions: the heats of combustion and formation, entropy and the heat of capacity in condensed and gaseous phases of the same compounds.

$$\Delta_cH^o = (-11.6 \pm 7.3) - (108.7 \pm 0.2)\,(N\text{-}g) \tag{2.2}$$

r 0.999, S_o 8.6, n 9 (compounds **1-9**)

$$\Delta_fH^o_{cond} = (-444.0 \pm 6.1) - (4.5 \pm 0.2)\,(N\text{-}g) \tag{2.3}$$

r 0.995, S_o 8.0, n 9 (compounds **1-9**)

$$\Delta_fH^o_{gas} = (-399.0 \pm 6.6) - (3.7 \pm 0.1)\,(N\text{-}g) \tag{2.4}$$

r 0.992, S_o 8.0, n 9 (compounds **1-9**)

$$S^o_{cond} = (114.2 \pm 1.3) + (5.5 \pm 0.05)\,(N\text{-}g) \tag{2.5}$$

r 0.999, S_o 1.3, n 5 (compounds **1-4, 6**)

$$S^o_{gas} = (208.9 \pm 41.2) + (8.3 \pm 2.1)\,(N\text{-}g) \tag{2.6}$$

r 0.969, S_o 27.4, n 3 (compounds **1, 3, 4**)

$$Cp_{cond} = (44.4 \pm 41.2) + (6.5 \pm 0.7)\,(N\text{-}g) \tag{2.7}$$

r 0.958, S_o 34.3, n 9 (compounds**1-9**)

Necessary to note that the parameter f in equations (2.2) has practically the same value, which was received earlier in our works [10-16] $f = 109.0$ kJ·mol^{-1} electrons^{-1} for the combustion of different organic compounds.

As to i and f coefficients in other equations (2.3-2.7), their values are essentially differ each from other in every case.

1.2. Fatty acids

Fatty acids are an interesting and important type of acids because they make up a main chain of the structure of lipids. Such acids have usually an even number of carbon atoms and form an unbranched chain. Many fatty acids have one or several double bonds; they are titled as unsaturated fatty acids. Such type of acids plays an important role in biochemistry of the living organisms and in industry also.

The analysis of thermodynamic functions of dodecanoic (**10**), miristic (**11**), palmitic (**12**), margarinic (**13**), stearic (**14**) and arachidic acids (**15**) [2, 6, 7, 18-20] (Table) gave the similar equations (2.8-2.11).

$$\Delta_{vap}H^o = (27.1 \pm 17.9) + (1.4 \pm 0.2)\,(N\text{-}g) \tag{2.8}$$

r 0.974, S_o 7.3, n 6 (compounds **10-15**)

$$\Delta_cH^o = (5.7 \pm 80.5) - (108.7 \pm 0.8)\,(N\text{-}g) \tag{2.9}$$

r 0.999, S_o 32.0, n 6 (compounds **10-15**)

$$\Delta_fH^o_{cond} = (-433.5 \pm 50.1) - (4.9 \pm 0.5)\,(N\text{-}g) \tag{2.10}$$

r 0.977, S_o 20.4, n 6 (compounds **10-15**)

$$Cp_{cond} = (201.7 \pm 17.7) + (2.9 \pm 0.2)\,(N\text{-}g) \tag{2.11}$$

r 0.992, S_o 7.2, n 6 (compounds **10-15**)

As can be seen, the correlation parameters i and f of similar equations for acids with C_1-C_{12} carbons and fatty acids, having from 12 to 20 carbon atoms in their own structures are practically equal, but have a different errors for i and f coefficients.

1.3. Acids with branched carbon radicals

There are a large number of saturated acids, the organic radicals of which have a different space form. However it will be difficult to compare thermodynamic functions of acids, which have a cyclic, iso- and tertiary radicals at carboxyl group. Taking into account this situation, we chose a little number of acids with not long and branched radical. It is the acids (**16-20**) in Table and on the base of their thermodynamic properties [2, 6, 7] the equations (2.12-2.15) were calculated.

$$\Delta_{vap}H^o = (27.9 \pm 1.4) + (1.1 \pm 0.04)\,(N\text{-}g) \tag{2.12}$$

r 0.999, S_o 0.8, n 3 (compounds **16, 17, 19**)

$$\Delta_cH^o = (-6.2 \pm 12.5) - (108.9 \pm 0.4)\,(N\text{-}g) \tag{2.13}$$

r 0.999, S_o 5.5, n 3 (compounds **17-19**)

$$\Delta_fH^o_{cond} = (-446.7 \pm 11.3) - (4.2 \pm 0.3)\,(N\text{-}g) \tag{2.14}$$

r 0.997, S_o 5.0, n 3 (compounds **17-19**)

$$\Delta_fH^o_{gas} = (-411.0 \pm 11.3) - (3.4 \pm 0.3)\,(N\text{-}g) \tag{2.15}$$

0.995, S_o 5.0, n 3 (compounds **17-19**)

No wonder, what the correlations coefficients in all three groups of mentioned acids have practically comparable values, because their room structures are not especially differ each to other.

1.4. Two-, three- and four-basic acids

These types of organic acids have a large importance for different domains of industry, pharmacology and others [8, 9]. Thermodynamic data of two-basic acids (**21-27**) together with such acids as citric, glycolic and others (**28-33**, Table) form the following equations (2.16-2.20), which similar to given higher.

$$\Delta_{vap}H^o = (104.9 \pm 3.1) + (1.1 \pm 0.1)\,(N\text{-}g) \tag{2.16}$$

r 0.963, S_o 4.0, n 7 (compounds **21-27**)

$\Delta_c H^o = (19.4 \pm 10.3) - (108.6 \pm 0.4)\ (N\text{-}g)$ (2.17)

r 0.999, S_o 10.3, n 6 (compounds **21-26**)

$\Delta_f H^o{}_{cond} = (-865.5 \pm 10.1) - (4.7 \pm 0.4)\ (N\text{-}g)$ (2.18)

r 0.985, S_o 10.1, n 6 (compounds **21-26**)

$\Delta_c H^o = (-411.6 \pm 129.2) - (92.9 \pm 4.7)\ (N\text{-}g)$ (2.19)

r 0.995, S_o 154.4, n 6 (compounds **28-33**)

$\Delta_f H^o{}_{cond} = (-1037.7 \pm 244.7) - (19.5 \pm 7.6)\ (N\text{-}g)$ (2.20)

r 0.876, S_o 181.7, n 4 (compounds **28, 30, 32, 33**)

Necessary to note, that the parameters of equations (2.16-2.18), which are related to two-basic acids, not bad correspond to parameters of equations for normal, fatty and branched acids. However the same parameters in equations (2.19) and (2.20) for the heats of combustion and formation of three- and four-basic acids very differ from others. Probably this effect is possible to explain by strong inner hydrogen connection between carboxylic groups of such type of acids.

2. Acetates and esters of fatty acids

The analysis thermodynamic properties of the large class of esters is useful for beginning with various functions of acetates, which have an important significance in theory of organic compounds and in different brunch of industry [1-5, 8, 9]. The approach to this aim is the same, which was used in previous parts: the creation of the definite number of equations, which reflect the interrelation of thermodynamic functions with the number of valence electrons of the examined molecules (Table).

The dependences of the heats of vaporization, combustion, formation and heat of capacity of acetates (34-41, Table) and their interrelations with parameter (N-g), as shown in the previous parts, are reflected in the equations (2.21-2.26).

$\Delta_{vap} H^o = (22.7 \pm 1.0) + (0.7 \pm 0.03)\ (N\text{-}g)$ (2.21)

r 0.995, S_o 1.1, n 8 (compounds **34-41**)

$\Delta_c H^o = (24.1 \pm 170.0) - (113.1 \pm 6.1)\ (N\text{-}g)$ (2.22)

r 0.997, S_o 116.5, n 4 (compounds **34,35,37,38**)

$\Delta_f H^o{}_{cond} = (-306.6 \pm 28.5) - (9.3 \pm 1.2)\ (N\text{-}g)$ (2.23)

r 0.991, S_o 15.9, n 3 (compounds **34,35,37**)

$\Delta_f H^o{}_{gas} = (-288.5 \pm 19.1) - (8.3 \pm 0.8)\ (N\text{-}g)$ (2.24)

r 0.995, S_o 10.6, n 3 (compounds **34,35,37**)

$Cp_{cond} = (72.5 \pm 3.1) + (4.8 \pm 0.1)\ (N\text{-}g)$ (2.25)

r 0.999, S_o 1.7, n 4 (compounds **34-37**)

$Cp_{gas} = (5.1 \pm 12.3) + (5.6 \pm 0.6)\ (N\text{-}g)$ (2.26)

r 0.994, S_o 5.7, n 3 (compounds **34-36**)

Thermodynamic data of esters of fatty acids presented in the literature [2, 6, 7] with more examples than acetates (**42-52**, Table), what gave a possibility to calculate the equations (2.27-2.29).

$\Delta_{vap} H^o = (4.8 \pm 10.6) + (0.9 \pm 0.1)\ (N\text{-}g)$ (2.27)

r 0.967, S_o 4.1, n 10 (compounds **42-46, 48-52**)

$\Delta_c H^o = (-54.7 \pm 171.7) - (109.1 \pm 1.6)\ (N\text{-}g)$ (2.28)

r 0.999, S_o 72.6, n 11 (compounds **42-52**)

$\Delta_f H^o{}_{cond} = (-201.3 \pm 205.5) - (6.5 \pm 2.0)\ (N\text{-}g)$ (2.29)

r 0.880, S_o 72.6, n 4 (compounds**42-44, 50**)

CONCLUSIONS

Thermodynamic parameters (heat of vaporization, combustion, formation in different phases, entropy and the heat of capacity) of 52 derivatives of carbonic acids and their derivatives were analyzed for the first time and it was determined that all functions depend on the number of valence electrons N from which is excluded the sum of lone electron pairs g as represented in 29equations $\Delta_{vap,c,f} H^o = i \pm f\,(N\text{-}g)$ and $S^o(Cp) = i \pm f\,(N\text{-}g)$. Necessary to note, that the stoichiometric coefficient f in the first equation is in the range 104-113 kJ mol^{-1} electron^{-1} in the received dependences, that corresponds to the same values f in the works, which are mentioned in introduction. Other coefficient i differs for each type of compounds and not necessity in the discussion.

Table

Thermodynamic properties (kJ mol^{-1} and J mol K^{-1}) of acids with C1-C12 carbons, fatty, branched, two-, three- and four-basic acids. The data are compiled from [2,4,6,7]

Таблица. **Термодинамические свойства (кДж моль$^{-1}$ и J моль K^{-1}) кислот с атомами углерода C1-C12, жирных, разветвленных, двух-, трех- и четырехосновных кислот; данные заимствованы из [2,4,6,7]**

No	Compound, formula, ($N-g$)	$\Delta_{vap}H^o$	$-\Delta_c H^o$	$-\Delta_f H^o$	$-\Delta_f H^o$	S^o	S^o	C_p	C_p
				cond	**gas**	**cond**	**gas**	**cond**	**gas**
1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**
	Acids with C_1-C_{12} carbons								
1	Acetic, $C_2H_4O_2$, 8	51.6 ± 1.5	874.2 ± 0.2	484.5 ± 0.2	433.0 ± 3.0 $^{a)}$	158.0	282.8	123.1	63.0 ± 0.1
2	n-Propanoic, $C_3H_6O_2$, 14	55.0 ± 2.0	1527.3 ± 0.1	510.8 ± 0.1	455.8 ± 2.0	191.0		152.8	
3	n-Butanoic, $C_4H_8O_2$, 20	58.0 ± 4.0	2183.5 ± 0.6	533.9 ± 0.6	475.9 ± 4.0	225.3	353.3	177.7	

1	2	3	4	5	6	7	8	9	10
4	*n*-Pentanoic acid, $C_5H_{10}O_2$, 26	57.9	2850.1 ± 5.9	560.2 ± 0.7	491.0 ± 20.0 a)	259.8	439.8 ± 0.6	197.0	
5	*n*-Hexanoic acid, $C_6H_{12}O_2$, 32	73.2 ± 2.0	3490.4 ± 0.5	585.7 ± 0.5	512.0 ± 4.0			225.1	
6	*n*-Heptanoic acid, $C_7H_{14}O_2$, 38	72.0 ± 1.5	4144.0 ± 0.6	611.5 ± 0.6	539.5 ± 1.6	323.3		267.3	
7	n-Octanoic Acid, $C_8H_{16}O_2$, 44	82.9 ± 1.0	4797.9 ± 0.5	636.9 ± 0.5	556.6 ± 1.1			297.9	
8	Nonanoic acid, $C_9H_{18}O_2$, 50	85.3 ± 2.0	5452.2 ± 1.0	661.9 ± 1.0	579.5 ± 1.0			362.4	
9	*n*-Decanoic, (capric) acid, $C_{10}H_{20}O_2$, 56	119.0 ± 2.0	6079.3 ± 0.9	714.1 ± 3.5	624.2 ± 5.0			475.6	
Fatty acids									
10	Dodecanoic acid, $C_{12}H_{24}O_2$, 68	127.9	7377.0 ± 0.9	775.1				404.3	
11	*n*-Tetradecanoic (miristic) acid, $C_{14}H_{28}O_2$, 80	139.7 ± 3.8	8676.7 ± 1.4	834.1 ± 4.2				432.0	
12	n-Hexadecanoic acid (palmitic) acid, $C_{16}H_{32}O_2$, 92	154.4 ± 4.2	10028.6 ± 1.9	848.4 ± 2.2		452.3		463.4	
13	Heptadecanoic acid (margarinic) acid, $C_{17}H_{34}O_2$, 98		10624.4 ± 1.7	924.4				475.7	
14	Octadecanoic acid, Stearic acid, $C_{18}H_{36}O_2$, 104	166.5 ± 4.2	11336.8 ± 2.1	947.2 ± 2.2		435.6		501.5	
15	Eicosanoic acid (arachidic) acid $C_{20}H_{40}O_2$, 116	199.6 ± 7.5	12574.2 ± 1.5	1012.6 ± 5.1				545.1	
Branched acids									
16	*i*-Butyric acid, $C_4H_8O_2$, 20	50.9						173.0	
17	3-Methylbutanoic acid, $C_5H_{10}O_2$, 26	55.8	2835.1 ± 5.9	561.6 ± 5.9	502.5 ± 6.6			197.1	
18	2-Methylbutanoic acid, $C_5H_{10}O_2$, 26		2842.2 ± 5.9	554.5 ± 5.9	495.4 ± 6.6				
19	2-Ethylhexanoic acid, $C_8H_{16}O_2$, 44	76.3 ± 0.9	4799.6 ± 1.7	635.1 ± 2.0	559.5 ± 2.1				
20	Heptanoic acid, 2-ethyl-, $C_9H_{18}O_2$, 50	63.4							
Two-, three- and four-basic acids									
21	Propanedioic acid, $C_3H_4O_4$, 8	111.4 [17] ± 0.7	861.1 ± 0.6	891.1 ± 0.4		149.0		127.6	
22	Butanedioic acid, $C_4H_6O_4$, 14	120.3 ± 4.4	1491.0 ± 3.0 a)	940.0 ± 2.0 a)		167.3		152.9	

1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**
23	Pentanedioic acid, $C_5H_8O_4$, 20	119.8 [17] ± 1.2	2150.3 ± 0.7	960.5 ± 1.1					
24	Hexanedioic acid, $C_6H_{10}O_4$, 26	133.6 [17] ± 1.3	2792.0 ± 0.4	998.2 ± 0.4					
25	Heptanedioic acid, $C_7H_{12}O_4$, 32	139.9 [17] ± 1.0	3460.2 ± 1.0	1009.4					
26	Octanedioic acid, $C_8H_{14}O_4$, 38	147.8 [17] ± 3.8	4110.9 ± 1.3	1038.0					
27	Tartronic acid, $C_3H_4O_5$, 6	116.4 ± 0.3	1159.3	1068.4 ± 1.4	952.0 ± 1.5			184.5	
28	Citric Acid, $C_6H_8O_7$, 18		1960.6 ± 4.6	1543.8 ± 4.6					
29	(Z)-1-propene-1,2,3-ricarboxylic acid, $C_6H_6O_6$, 18		2001.6						
30	(E)-1-propene-1,2,3-ricarboxylic acid, $C_6H_6O_6$, 18		1985.8 ± 2.5	1233.0 ± 3.0					
31	Mesotartaric acid, $C_4H_6O_6$, 6		1172.0						
32	Ethylenediamine tetraacetic acid, $C_{10}H_{16}N_2O_8$, 42		4458.1 ± 3.6	1761.7 ± 3.7					
33	Ethylenediamine-N,N'-disuccinic acid, $C_{10}H_{16}N_2O_8$, 42		4271.6 ± 3.9	1950.2 ± 3.9					
Acetates									
34	Methyl acetate, $C_3H_6O_2$, 14	33.4	1592.2 ± 0.7	445.8	410.0			140.6	86.0 ± 0.12
35	Ethyl Acetate, $C_4H_8O_2$, 20	36.7	2238.5 ± 0.5	480.6 ± 0.8	445.4 ± 0.8	259.4	362.7	169.6	113.6
36	Propyl acetate, $C_5H_{10}O_2$, 26	38.6 ± 0.1						196.1	153.6
37	Butyl acetate, $C_6H_{12}O_2$, 32	43.0 ± 0.1	3467.0	609.6	566.0			228.4	
38	Pentyl acetate, $C_7H_{14}O_2$, 38	48.6 ± 0.4	4372.1	383.2					
39	Hexyl acetate, $C_8H_{16}O_2$	51.9 [18] ± 0.3							
40	Heptyl acetate, $C_9H_{18}O_2$, 50	57.1 [18] ± 0.2							
41	Octyl acetate, $C_{10}H_{20}O_2$, 56	60.7 [18] ± 0.4							

1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**
Esters with fatty radicals									
42	Methyl dodecanoate, $C_{13}H_{26}O_2$, 74	70.7 [19] ± 0.2	8117.0 ± 0.4	714.6					
43	Methyl hexadecanoate, $C_{17}H_{34}O_2$, 98	96.8 [19] ± 0.6	10669.0 ± 0.4	879.5		495.1		474.5	
44	Methyl palmitoleate, $C_{17}H_{32}O_2$, 96	96.4 [20] ± 0.7	10547.9 ± 1.5	715.1					
45	Methyl octadecanoate, $C_{19}H_{38}O_2$, 110	105.9 [19] ± 1.4	11962.0 ± 0.4	945.6					
46	Methyl elaidate, $C_{19}H_{36}O_2$, 108	77.2	11885.0 ± 12.0	731.7					
47	Methyl linoleate, $C_{19}H_{34}O_2$, 106		11690.1 ± 1.5	645.7					
48	Methyl linolenate, $C_{19}H_{32}O_2$, 104	110.5 [20] ± 0.5	11506.0 ± 1.5	544.0					
49	Methyl oleate, $C_{19}H_{36}O_2$, 108	104.0 ± 6.0 a)	11832.4 ± 1.5	727.6					
50	Methyl eicosanoate, $C_{21}H_{42}O_2$, 122	116.4 ± 1.5	13263.0 ± 0.4	1003.0					
51	Methyl ester of *cis*-11-eicosenoic acid, $C_{21}H_{40}O_2$, 120	115.8 [20] ± 0.7	13190.0	791.0					
52	Butyl ester of oleic acid, $C_{22}H_{42}O_2$, 126	97.7 [20]	13843.0 ± 14 0	816.9					

Note: a) average from 6-8 values

Примечание: а) среднее из 6-8 значений

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