1698-1707 cm⁻¹, NH₂ 3183–3201, 3426–3520 cm⁻¹, vibrations of aromatic rings 1600–1620 cm⁻¹. In the ¹H NMR spectra of compounds **2a-c** we note the signals of a vinyl proton within 5,68–5,71 ppm, the signals of the protons at tertiary carbon atoms within 5,72–5,74 and 6,82–6,92 ppm, the signal of a NH2 group's protons at 9,97–9,99 ppm, the multiplet of aromatic rings within 7,17–7,69 ppm, the signal of the methyl group protons of an aromatic substituent (for compound **2b**) around 2,35 ppm, and that of a methoxylic group (for compound **2c**) at 3,82 ppm.

We also tried to implement reaction of 5-R¹-3-R²-3H-pyrrol-2-ones with 2-mercaptobenzymidazole under microwave radiation. Only the source compounds were detected in the reaction mixture, which means this reaction not proceeding under microwave radiation.

Experimental

IR spectra were recorded on an FSM-1201 Fourier spectrometer in KBr tablets, the spectral range being 400–4000 cm⁻¹. ¹H NMR spectra were obtained on a Varian-400 spectrometer within 20–25 °C in CDCl₃, TMS being the internal reference. The working frequency was 400 MHz.

3-(2-amino-2-R1-vinyl)-2-R2-2H-benzo[4,5] imidazo[2,1-b][1,3]thiazine-4(3H)-ones (2a-c). A mixture of 5-R-3-arylmethylidene-3H-furan-2-one (Ia, b, c) (0,01 mol) and 2-mercaptobenzymidazole (0,015 mol) was boiled in icy acetic acid with a catalytic amount of sulfuric acid during 30 hours, poured into cold water, and neutralized by a sodium carbonate solution. The crystals precipitated were filtered on a Schott filter and recrystallized from ethanol.

For **2a**: yield 73%; mp 263–265°C; ¹H NMR, δ : 5,70–5,71 (1H, d), 5,72–5,73 (1H,d), 6,86–6,90 (1H, t), 9,97 (2H, NH₂), 7,19–7,66 (13H, m, Ar). Found (%) C, 66,74; H, 3,94; N, 6,69; S, 7,65. Calc. for C₂₄H₁₈N₃SOC1 (%) C, 66,74; H, 4,17; N, 7,73; S, 7,42.

For **2b**: yield 71%; mp 249–251°C; ¹H NMR, δ : 5,70–5,71 (1H, d), 5,73–5,74 (1H,d), 6,89–6,92 (1H, t), 9,97 (2H, NH₂), 7,17–7,63 (13H, m, Ar), 2,23 (3H, s). Found (%) C, 67,92; H, 4,60; N, 4,05; S, 7,50 Calc. for C₂₅H₂₀N₃SOC1 (%) C, 67,33; H, 4,52; N, 9,42; S, 7,19

For **2c**: yield 68%; mp 141–142 °C; ¹H NMR, δ : 5,68–5,69 (1H, d), 5,72–5,73 (1H,d), 6,82–6,86 (1H, t), 9,99 (2H, NH₂), 7,20–7,69 (13H, m, Ar), 3,82 (3H, s). Found (%) C, 68,75; H, 4,33; N, 8,10; S, 7,44. Calc. for C₂₅H₂₁O₂N₃S (%) C, 69,40; H, 4,95; N, 9,83; S, 7,50.

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FUNDAMENTALS OF CHEMOMETRICS IN DIFFERENT BRANCHES OF CHEMICAL SCIENCE

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The article shows the possibility of applying the method of multilevel modeling in evaluating the physical and chemical variables.

In Nature, as well as in the natural sciences, everything is interconnected. This regular occurrence is usually not seen, if we bear in mind two functional parameters. But multiparameter functional relationship is observed when we apply not less than three characteristics to the sought-for parameter [1, 2, 3].

In the study of the method of multilevel modeling (MMLM), which permits to carry out mathematical modeling of certain chemical processes in different environments, and also to estimate absent (scarce) characteristics in physical-chemical methods of analysis, let's limit with the assumption that regression is linear and is determined by the following dependence:

$$Y = a + b_1 X_1 + b_2 X_2 + \dots + b_n X_n.$$
(1)

If we accept that a number of arguments is equal to two, then in terms of geometry, this equation defines the plane in the space of variables X_1 , X_2 , and Y_2 .

Y

To determine parameters $a, b_1, ..., b_n$ in equation (1) let's apply the method of least squares. After differentiation according to the variable parameters this method leads to the system:

$$\Sigma y = na + b_1 \Sigma X_1 + ... + b_n \Sigma X_n;$$
 (2-a)

$$\Sigma y X_1 = a \Sigma X_1 + b_1 \Sigma X_1^2 + \dots + b_n \Sigma X_1 X_2 \dots X_n;$$
 (2-b)

$$\Sigma y X_n = a \Sigma X_n + b_1 \Sigma X_1 X_2 + \dots + b_n \Sigma X_n^2. (2-c)$$

To solve this system we divide equation (2-a) to n, then we obtain:

$$a = y_{av} - b_1 X_{1(av)} - b_2 X_{2(av)} - \dots - b_n X_{n(av)}.$$

Substituting this value for a in formula (1) and equation (2-b) and (2-c), we find out that the formula MMLM with n variables has the following form:

$$Y-y_{av} = b_1(X_1 - X_{1(av)}) + b_2(X_2 - X_{2(av)}) + \dots + b_n(X_n - X_{n(av)}),$$
(3)

the coefficients $b_1, b_2, ..., b_n$ are found from the following system of linear equations:

$$b_{1}\Sigma x_{1}^{2} + b_{2}\Sigma x_{1}x_{2} + \dots + b_{n}\Sigma x_{1}x_{n} = \Sigma x_{1}y_{1};$$

$$b_{1}\Sigma x_{1}x_{2} + b_{2}\Sigma x_{2}^{2} + \dots + b_{n}\Sigma x_{2}x_{n} = \Sigma x_{2}y_{2};$$

$$\dots$$

$$b_{1}\Sigma x_{1}x_{n} + b_{2}\Sigma x_{2}x_{n} + \dots + b_{n}\Sigma x_{n}^{2} = \Sigma x_{n}y_{n},$$

where the following conventional signs are adopted:

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$$\begin{split} \Sigma x_1^{\ 2} &= \Sigma (X_1 - X_{1(av)});\\ \Sigma x_1 x_2 &= \Sigma (X_1 - X_{1(av)}) (X_2 - X_{2(av)});\\ \Sigma x_1 x_n &= \Sigma (X_1 - X_{1(av)}) (X_n - X_{n(av)});\\ \Sigma x_1 y_1 &= \Sigma (X_1 - X_{1(av)}) (Y_1 - Y_{1(av)}); \text{ м т.д.} \end{split}$$

Let's point out the important physical meaning of MMLM coefficients. For example, the coefficient b_1 in equation (3) respond to the question, how many units varies Y_1 , if X_1 changes by one unit on the assumption that X_2 retains a constant value.

Thus, the MMLM formula can eliminate the influence of factor X_2 , bound with the factor of X_1 on Y in its pure form.

The problem of various characteristics optimizing of all sorts of systems becomes relevant in connection with the intensive development of the theory and practice of electrolyte solutions, physical and chemical methods of research, the development of modern methods of processing the experimental results. For example, parameters for the method of pair correlations in comparative calculations of physicalchemical properties of substances (e.g., concentration is in the functional dependence of analytical signal) in most cases are poorly known and considerably scatter or non-existent. That problem hinders their choice for a variety of assessment operations.

A common reliable regular occurrence, linking changes in various properties of complex compounds in a solvent, hasn't been found so far, as well as the quantitative relationships between the major, basic, physical-chemical properties and various derivative properties of complex compounds in various media.

Derivation of multiple linkages and interdependence of properties and their changes for solvents, including water and electrolyte solutions is possible with deliberate and clear choice of benchmarks and with properly determined values of physical and chemical key properties of the studied systems [4].

Depending on whether a system (herein solvent) exchanges with the environment in matter and energy, it is thermodynamically isolated, closed or open and respectively is characterized by the microcanonical, canonical or macrocanonical Gibbs's distributions. This basis must be sufficiently complete and contain at least four parameters: thermochemical, electrical, kinetic and structural parameters. Their usefulness follows from the correspondence of solvent molecules to statistical Gibbs's ensembles with the main role of internal and external parameters:

$$\xi = \phi (a_1, a_2, ..., T),$$

where ξ is an internal parameter, $a_1, a_2, ..., T$ is an external parameter.

1. It is known that if the system (herein solvent) is in equilibrium conditions without exchange with the macroscopic environment, or environment in matter and energy, it is thermodynamically isolated. In these conditions, its characteristics are determined by the parameters of the internal structure, i.e. by the length and coupling constant, atom's masses, the number of electrons, etc.

2. If the system communicates with the environment only by energy, it is thermodynamically closed. The process can be described by thermochemical parameters of constant number of particles.

3. In case the system exchanges with the macroscopic environment both with energy and matter, the system is thermodynamically open, the number of particles in the system is variable. In such a situation the number of particles may change, to a first approximation, by the forces of electromagnetic origin, which determine the appropriate response of the electromagnetic characteristics of the investigated system.

4. Any movement of bodies at a certain speed in the condensed phase generates dissipative processes, mainly characterized by kinetic parameters: viscosity, diffusion, thermal conductivity or other parameters.

Theoretically modulating the processes of measurement, i.e. interaction between a system and a device, it is necessary to take into account all the situations observed above. This idea is the basis for the evaluation of dissociation constants of electrolytes in the studied solvents pK, the radii of solvent molecules R_s , the energies of intermolecular interactions in pure solvents ΔH and other physical and chemical characteristics of solvents and non-aqueous electrolyte solutions.

Table presents the data obtained from the thermodynamic constants of dissociation of hydrochloric acid, the titrant, in analytical chemistry $pK_{\rm HCl}$. Its systematic values, such basic properties of the solvent as a boiling point *T*, density ρ , viscosity η , a dipole moment of solvent molecule *p*, a molar mass of solvent *M*, an amount of bond lengths $\Sigma L \cdot 10^8$ cm, the radius of the solvent molecule $r_s \cdot 10^8$ cm and autoprotolysis constants (ionic product) of solvent pK_s are absent.

The program «MMLM» leads to the equation

$$pK_{\rm HCl} = -0.03220 \cdot T - 5.08662 \cdot \rho + 0.52392 \cdot \eta + 2.71678 \cdot p - 0.05334 \cdot M + 0.40049 \cdot \Sigma L + 3.40571 \cdot R_s - 0.07179 \cdot pK_s + 6.70942.$$
(4)

multilevel factor (multidimentional) of modeling is $K_{MMLM} = 0.9741$.

As it will be shown further, all the members of the right part of the equation have dimension mol/ dm³. Dimension in other cases of MMLM (like identifying the dimension $pK_{\rm HCl}$) are defined similarly.

The dimensional coefficients in MMLM, for example, in the same equation (4), can be obtained by solving the system of normal equations:

for *a*, *b*₁, *b*₂,..., *b*₈, where *i* is a number of variables (herein the number of solvents); $X_{i1} = T_{boiling}$; X_{i2} is a solvent density ρ , g/cm³; X_{i3} is viscosity of the solvent η , cП3; X_{i4} is a dipole moment of solvent molecule p_i , *D*; X_{i5} is a molar mass of solvent *M*, g/ mol, X_{i6} is an amount of bond lengths $\Sigma L \cdot 10^8$ cm, X_{i7} is a radius of the solvent molecules $R_s \cdot 10^8$ cm, X_{i8} is an indicator of autoprotolysis constants (ionic product) solvent pK_s , $y_{av}X_{1(av)}$, $X_{2(av)}$, $X_{3(av)}$, ..., $X_{8(av)}$ is an arithmetic functions (mathematical expectation) of the relevant parameters with the number of variables *i*. We obtain the following factors and their dimensions:

 $b_1 = -0,03220 \text{ mol/dm}^3 \cdot K; b_2 = -5,08662 \text{ mol/kg};$ $b_3 = 0,52392 \text{ mol/dm}^3 \cdot c\Pi;$

 $b_4 = 2,71678 \text{ mol/dm}^3 \cdot D; b_5 = -0,05334 \text{ mol}^2/\text{kg},$

 $b_6 = 0,40049 \text{ mol/dm}^2$, $b_7 = 3,40571 \text{ mol/dm}^2$,

 $b_{s} = -0.07179 \text{ mol}^{2}/\text{dm}^{6}$ and $a = 6.70942 \text{ mol}/\text{dm}^{3}$.

The basic parameters for assessing the physical and chemical properties of solvents and the results of evaluations of MMLM derivative characteristics

№ п/п	$T_{boiling}$	r	h	р	М	ΣL	R _s	pK _s	pK_{HCl} (ref. lit.)	$pK_{\rm HCl}$ according to eq.(4)
01.	373,2	0,9971	0,894	1,84	18,0	1,26	1,45	14,00	-0,98	-1,43
02.	338,2	0,7914	0,547	1,70	32,0	3,48	1,89	17,30	1,20	1,58
03.	351,5	0,7895	1,080	1,69	46,0	5,02	2,19	18,95	1,95	2,18
04.	370,4	0,7995	2,256	1,68	60,1	6,56	2,50	19,46	2,51	2,99
05.	390,4	0,8058	2,950	1,66	74,1	8,11	2,65	21,56	3,04	2,88
06.	411,2	0,8098	3,820	1,65	88,1	9,65	2,81	20,65	3,62	3,09
07.	329,4	0,7920	0,316	2,88	58,0	5,27	2,30	32,50	4,00	4,58
08.	352,8	0,8054	0,428	2,79	72,1	6,81	2,40	31,00	4,45	3,89
09.	375,7	0,8089	0,500	2,48	86,1	8,35	2,56	25,62	-	3,13
10.	400,7	0,8304	0,542	2,16	100,1	9,89	2,68	25,30	-	1,67
11.	425,7	0,9445	0,796	3,82	73,1	5,12	2,53	31,60	3,40	3,49
12.	438,7	0,9366	0,919	3,79	87,1	6,66	2,72	31,20	3,30	3,64
13.	508,2	1,0253	3,340	5,37	179,2	6,09	3,10	20,56	3,56	3,43
14.	462,2	1,1014	1,960	4,30	78,0	5,82	2,37	32,30	3,06	2,86
15.	558,2	1,2618	10,13	4,69	120,0	5,94	2,61	25,45	3,25	3,40
16.	475,2	1,0327	1,830	4,09	99,1	6,66	2,70	24,15	2,80	3,06
17.	353,3	0,7856	0,345	3,84	41,0	3,79	2,54	32,20	8,10	7,62
18.	514,9	1,0257	2,510	4,94	102,0	6,70	3,12	29,20	-	5,42

N o t e s: 1 – water, 2 – methanol, 3 – ethanol, 4 – propanol, 5 – butanol, 6 – pentanol, 7 – acetone, 8 – methylethylketone, 9 – metilpropilketon, 10 – metilbutilketon, 11 – dimethylformamide, 12 – dimethylacetamide, 13 – hexamethylphosphotriamide, 14 – dimethylsulfoxide, 15 – tetrametilensulfon, 16 – metilpirrolidon, 17 – acetonitrile, 18 – propylene carbonate.

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Thus, when applying heterogeneous units of initial parameters X_{i1} , X_{i2} , X_{i3} , ..., X_{i8} and equations of the method of multilevel modeling

$$y_{i} = y_{av} + b_{1}(X_{i1} - X_{1(av)}) + b_{2}(X_{i2} - X_{2(av)}) + b_{3}(X_{i3} - X_{i3(av)}) + \dots + b_{8}(X_{i8} - X_{8(av)})$$

units of measure and dimensional ratios y_i in mol/dm³ for the thermodynamic constants of dissociation of hydrochloric acid $pK_{\rm HCl}$ are obtained. The coefficient method of multilevel modeling $K_{\rm MMLM}$ is introduced to assess the ties between variables. It is defined by the formula:

$$K_{MMIM}^{2} = \Sigma (Y_{i} - Y_{av})^{2} / \Sigma (y_{i} - y_{av})^{2},$$

where y_i is the variable *Y*, taken from the correlation table 1 (reference value), and Y_i is the variable *Y*, calculated from the equation MMLM (4).

MMLM gains an evident advantage over the method of pair correlations. It is obviously seen when comparing the coefficients of multiple regression K_{MMLM} and pair correlations K_{pc} . The ratio K_{MMLM} of such basic parameters as $T_{boiling}$, ρ , η , p, M, $\Sigma L \cdot 10^8$, $R_s \cdot 10^8$ and pK_s by equation (4) for water, alcohols, ketons and other solvents is equal to 0.9741, while coefficients of pair correlations $pK_{HCI} - T$, $pK_{HCI} - \rho$, $pK_{HCI} - \eta$, $pK_{HCI} - p$, $pK_{HCI} - R_s$, $pK_{HCI} - pK_s$ are respectively: 0,0012; 0,0009; 0,0083; 0,1668;

0,00003; 0,15020 and 0,3713 which is considerably less than 0,9741.

Thus, using as a benchmark the thermochemical (boiling point, molar heat of vaporization, etc.) and kinetic (viscosity, etc.), electrical (dipole moment, etc.) properties and molecular characteristics (the sum of the lengths of chemical bonds in the molecule of solvent etc.) which are easily identified reference values, gives a satisfactory equivalence between the estimated values MMLM with real experimental values, regardless to the nature and class of substances. The method of multilevel (multidimensional) modeling permits to solve numerous problems in the absence of important characteristics in different branches of chemical science and technology.

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