

Artificial Neural Network and Multiple Linear Regression for Prediction and Classification of Sustainability of Sodium and Potassium Coronates

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Abstract—Models of multiple linear regression and multilayer artificial neural network have been developed for modeling and predicting the stability constants of sodium and potassium coronates basing on the properties of aqueous-organic solvents (water–methanol, water–propan-2-ol, water–acetonitrile, and water–acetone). The values of the coronates stability constants in water–ethanol solvents have been predicted, and the predictions of the models of multiple linear regression and an artificial neural network models have been compared. The contributions of electrostatic, cohesive, and electron-donating interactions to the increase in the stability of the coronates have been quantitatively assessed basing on the models of multiple linear regression and the principle of free energies linearity. Neural network models based on unsupervised (multilayer perceptrons) and supervised (Kohonen networks) learning algorithms have been developed to classify the stability of sodium and potassium coronates. The neural network classifiers have fully confirmed the classification of the coronated stability via the *k*-means exploration method.

Keywords: multiple regression, multilayer perceptron, Kohonen network, prediction, neural network classifier

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Majority of conventional prediction methods are based on the assumption of linear dependence of the predicted (dependent) variable and the set of independent descriptors. The multiple linear regression models are built using the correlation and regression analysis methods.

Nonlinear relationships between the variables are conventionally modeled via fitting of nonlinear curves (quadratic, cubic, power, exponential, logarithmic, hyperbolic, or logistic ones) or their linearization. However, the artificial neural networks approach has been recognized as promising method to model nonlinear dependences in the prediction tasks over recent decades [1]. Major advantages of the artificial neural networks algorithms are their capability to learning, generalization, and prediction of the data, fault tolerance, parallel data processing, and fast computation procedures. This has been supported by the neural networks application in theoretical and computational chemistry, analytical chemistry, biochemistry, medicine, drugs chemistry, pharmaceuticals, and food products studies.

It should be noted that artificial neural networks have been applied to the chemometrics tasks since early 1990ies. Four applications of artificial neural networks

in chemical engineering have been comprehensively described [2]: fault detection, quality prediction, signal processing, and modeling and control of the processes. Various architectures of artificial neural networks and their applications in chemistry have been demonstrated [3], outlining the advantages and disadvantages in comparison with conventional chemometrics methods. A novel approach to prediction of biological activity of peptides and proteins, physics and chemistry-driven artificial neural network (Phys-Chem ANN), has been proposed [4]. The Phys-Chem ANN has been based on physical and chemical properties as well as structural features of proteins. The task on classification and prediction of the strength of weak organic acids in aqueous-organic solvents has been solved [5].

The neural networks method has been used to model individual wave kinetic curves [6], to demonstrate the importance of ^1H , ^{13}C , and ^{15}N chemical shifts of proteins for confirmation and refinement of their three-dimensional structure [7], to elaborate the algorithm of spectral studies of traces of gases [8], to predict the lipophilicity of chemicals [9, 10], to realize the method of prediction of the peptides ions drift time in mass spectrometry [11],

Table 1. Descriptive statistics on the initial data ($n = 33$)

Parameter	Mean	Minimum	Maximum	Dispersion	Standard deviation	Standard error of the mean
$\log K_{18C6Na^+}$	2.17	0.52	4.25	1.15	1.07	0.19
$\log K_{18C6K^+}$	3.50	2.04	5.85	1.02	1.01	0.18
$1/\varepsilon$	2.00	1.00	4.12	0.82	0.91	0.16
E_T	0.75	0.46	1.00	0.02	0.13	0.02
B_{KT}	0.51	0.19	0.89	0.04	0.19	0.03
δ^2	0.67	0.24	1.00	0.05	0.23	0.04

Table 2. Calculated values of the Kolmogorov–Smirnov criterion

Parameter	Criterion	Parameter	Criterion
$\log K_{18C6Na^+}$	0.0987	E_T	0.1230
$\log K_{18C6K^+}$	0.1383	B_{KT}	0.1250
$1/\varepsilon$	0.1773	δ^2	0.0782

to develop the model for prediction of calorific power of Slovenian coal [12], to simultaneously analyze two components of a powder drug (paracetamol and diphenhydramine hydrochloride) by means of IR spectroscopy [13], to quantitatively analyze potassium phenoxymethylpenicillin powder using the NIR spectroscopy data [14], to elucidate the effects of demographic, biochemical, and therapeutic parameters on the concentration of topiramate serum level [15], to build the models predicting the trypanocidal activity of quinonoid compounds [16], to investigate the antitumor (anticancer) activity of phenolic compounds [17], for drug development [18], to study the effect of cannabinoid compounds on mental activity [19], and to elucidate the influence of phenolic compounds on antioxidant activity of food products [20]. Novel technology of smart dynamic gas sensors [21] as well as algorithms of classification of quality of potato [22], wine [23–25], honey [26, 27], cheese [28], tea [29], olive oil [30], and vegetable oil [31] have been developed basing on the neural networks approach.

Artificial neural networks have been successfully applied to the spectra interpretation [32, 33], optimization of medical diagnostics of pathologies [34], modeling of the properties of fish antibiotics [35], and predicting rate constant of the reactions of hydroxyl-containing compounds [36], rate of dissolution of colemanite in water saturated with carbon dioxide [37], plasmons in silver nanorods [38], ionization potentials of the elements of groups I–III of the periodic table [39], survival of injured

patients [40], activity of cannabinoid ligands [41], and organic reactions [42].

This study consisted in modeling, predicting, and classification of stability of sodium and potassium coronates in aqueous-organic solvents by means of neural networks and multiple linear regression. The earlier determined stability constants of sodium and potassium coronates in aqueous-organic solvents (water–methanol, water–propan-2-ol, water–acetonitrile, and water–acetone) have been presented in [43], along with the reference data on the properties of the aqueous-organic solvents: dielectric constants, Dimroth–Reichardt parameter E_T , Kamlet–Taft parameter B_{KT} , and cohesion energy density δ^2 .

The neural network and multiple regression models were built and the results were analyzed using the STATISTICA 12 software package (Windows 10).

Multiple linear regression. The descriptive statistics on the initial data [$n \times m$] data matrix, $n = 33$ being the number of observations and $m = 6$ being the total number of dependent ($\log K_{18C6Na^+}$ and $\log K_{18C6K^+}$) and independent (four properties of the mixed solvents) variables] are collected in Table 1. Normality of the variables distribution was verified by calculating the Kolmogorov–Smirnov criterion (Table 2). The calculated values for all the variables were below the critical one ($D_{cr} = 0.2308$ for $n = 33$ and $\alpha = 0.05$). Hence, the empirical distributions of the variables did not differ from the normal one, and the multiple regression analysis of the studied processes

Table 3. Correlation analysis results

Parameter	Mean	Standard deviation	$1/\varepsilon$	E_T	B_{KT}	δ^2	$\log K_{18C6Na^+}$	$\log K_{18C6K^+}$
$1/\varepsilon$	2.00	0.91	1.000	-0.827	0.899	-0.641	0.352	0.511
E_T	0.75	0.13	-0.827	1.000	-0.763	0.732	-0.494	-0.648
B_{KT}	0.51	0.19	0.899	-0.763	1.000	-0.507	0.340	0.406
δ^2	0.67	0.23	-0.641	0.732	-0.507	1.000	-0.849	-0.970
$\log K_{18C6Na^+}$	3.50	1.01	0.352	-0.494	0.340	-0.849	1.000	0.928
$\log K_{18C6K^+}$	2.17	1.07	0.511	-0.648	0.406	-0.970	0.928	1.000

Table 4. Multiple regression results

Parameter	B_i	Standard error of B_i	$ t _{\text{calc}}(30)$	p -Level
Model: $\log K_{18C6Na^+} = B_1 + B_2\delta^2 + B_31/\varepsilon$ $R = 0.981, R^2 = 0.961, F_{\text{calc}}(2, 30) = 374.23, p = 0.00$				
B_1	6.08	0.24	25.53	0.00
δ^2	-5.18	0.22	23.35	0.00
$1/\varepsilon$	-0.22	0.06	4.03	0.00
Parameter	B_i	Standard error of B_i	$ t _{\text{calc}}(29)$	p -Level
Model: $\log K_{18C6K^+} = B_1 + B_2\delta^2 + B_31/\varepsilon + B_4B_{KT}$ $R = 0.914, R^2 = 0.835, F_{\text{calc}}(3, 29) = 48.75, p = 0.00$				
B_1	7.31	0.47	15.45	0.00
δ^2	-5.01	0.45	11.14	0.00
$1/\varepsilon$	-0.93	0.22	4.23	0.00
B_{KT}	2.76	0.93	2.97	0.01

of complex formation between sodium (potassium) ions and 18-crown-6 ether should be valid.

Table 3 shows the results of correlation analysis of the variables. The stability constants of the coronates ($\log K_{18C6Na^+}$ and $\log K_{18C6K^+}$) were strongly negatively correlated with the cohesion energy density, the correlation with the $\log K_{18C6Na^+}$ dependent variable with the $1/\varepsilon$ and E_T was average, and the weakest correlation was revealed for the $1/\varepsilon$ and B_{KT} descriptors with the $\log K_{18C6K^+}$ variable.

Variables selection for the regression model was performed using two methods implemented in STATISTICA 12 package: direct selection of the regressors and their reverse exclusion. Table 4 lists the results of the multiple regression analysis. As revealed by the determination coefficient values ($R^2 = 0.961$ for the $\log K_{18C6Na^+}$ model and

$R^2 = 0.835$ for the $\log K_{18C6K^+}$ model), the linear multiple regression explained 96.1 and 83.5% of the data variation relative to the mean level for the $\log K_{18C6Na^+}$ and $\log K_{18C6K^+}$ parameters, respectively. That fact evidenced strong dependence of the stability constants of sodium and potassium coronates on the selected independent parameters (regressors) of the aqueous-organic solvents.

The values of the Fisher criterion $F_{\text{calc}}(2, 30) = 374.23$ (at $\nu_1 = 2, \nu_2 = 30$ degrees of freedom) and $F_{\text{calc}}(3, 29) = 48.75$ (at $\nu_1 = 3, \nu_2 = 29$ degrees of freedom) confirmed the adequacy of the regression models. The corresponding critical values at the significance level $p = 0.05$ were $F_{\text{cr}}(2, 30) = 3.32$ and $F_{\text{cr}}(3, 29) = 2.93$; $F_{\text{calc}} > F_{\text{cr}}$.

The calculated values of the Student criterion of the multiple regression coefficients were: $|t|_{\text{calc}}(30)$

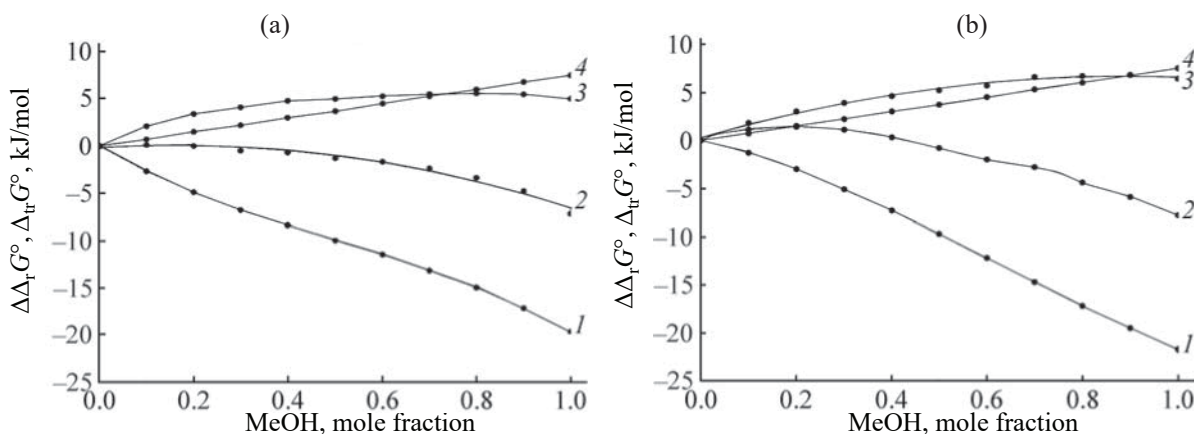


Fig. 1. Gibbs energy of the transfer of the complex formation reaction (1, $\Delta\Delta_1G^\circ$, $\Delta_{tr}G^\circ_{LM}$), its starting compounds (3, $\Delta_{tr}G^\circ_L$, 4, $\Delta_{tr}G^\circ_M$), and the products (2, $\Delta_{tr}G^\circ_{LM}$) from water to the water–methanol mixtures and methanol. (a) 18-crown-6Na⁺ and (b) 18-crown-6K⁺. $\Delta\Delta_1G^\circ_{LM} = \Delta_{tr}G^\circ_{LM} - \Delta_{tr}G^\circ_L - \Delta_{tr}G^\circ_M$ [43], where M = Na⁺ or K⁺.

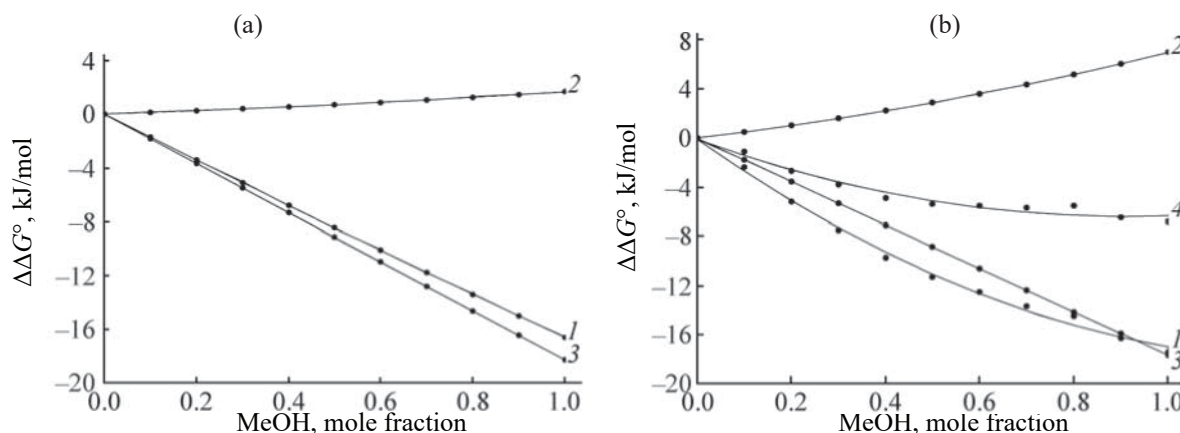


Fig. 2. Gibbs energy of the transfer of the complex formation reaction (1, $\Delta\Delta_1G^\circ_{LM}$) and its terms [2, $\Delta\Delta G^\circ_{LM}(1/\epsilon)$, 3, $\Delta\Delta G^\circ_{LM}(\delta^2)$, 4, $\Delta\Delta G^\circ_{LM}(B_{KT})$] as function of the composition of water–methanol mixture. (a) 18-crown-6Na⁺ and (b) 18-crown-6K⁺. $\Delta\Delta_1G^\circ_{LM} = \Delta\Delta G^\circ_{LM}(1/\epsilon) + \Delta\Delta G^\circ_{LM}(\delta^2) + \Delta\Delta G^\circ_{LM}(B_{KT})$, where M = Na⁺ or K⁺.

between 4.03 and 25.53 ($\nu = 30$ degrees of freedom) and $|t|_{\text{calc}}$ (29) between 2.97 and 15.45 ($\nu = 29$ degrees of freedom). Hence, the coefficients B_i of the analyzed regression models for $\log K_{18C6Na^+}$ and $\log K_{18C6K^+}$ were significant at the level of 95%, the corresponding critical values at $p = 0.05$ being $t_{cr}(30) = 2.04$ and $t_{cr}(29) = 2.05$; $t_{\text{calc}} > t_{cr}$.

The following regression models were obtained from the data in Table 4:

$$\log K_{18C6Na^+} = 6.08 \pm 0.49 - (5.18 \pm 0.45)\delta^2 - (0.22 \pm 0.12)1/\epsilon, \quad (1)$$

$$\log K_{18C6K^+} = 7.31 \pm 0.96 - (5.01 \pm 0.92)\delta^2 - (0.93 \pm 0.45)1/\epsilon + (2.76 \pm 1.91)B_{KT}. \quad (2)$$

To verify the validity of the obtained regression models, we analyzed the residuals using the Kolmogorov–Smirnov criterion. The calculated values

of the criterion ($D_{\text{calc}} = 0.156$ for the $\log K_{18C6Na^+}$ model and $D_{\text{calc}} = 0.154$ for the $\log K_{18C6K^+}$ model) were lower than the critical one ($D_{cr} = 0.231$ at $n = 33$ and $p = 0.05$). Hence, it could be suggested that the regression models residuals were normally distributed, and the models adequately described the dependence of the stability constants on the solvent properties.

Comparison of the results of our earlier solvation-thermodynamic analysis [43] (Fig. 1) and the multiple regression analysis (Fig. 2) revealed the nature of the interactions in the considered aqueous-organic solvent–salt (NaCl or KCl)–crown ether systems, the energy of which determined the increase in the stability constant of the coronates with the increase in the fraction of the organic component in the mixed solvent.

According to the solvation-thermodynamic model, the increase in the stability of sodium and potassium coro-

Table 5. Statistical parameters of the MP 4-7-2 perceptron^a

Subset	MP 4-7-2		Correlation coefficient	
	productivity	learning error	$\log K_{18C6Na^+}$	$\log K_{18C6K^+}$
Training	0.9978	0.0038	0.9971	0.9985
Validation	0.9997	0.0099	0.9995	0.9999
Test	0.9993	0.0077	0.9992	0.9995

^a Training, validation, and test productivity: ratio of the standard deviation of prediction to that of the input data for the corresponding subset. Training, validation, and test error: error of the network for the corresponding subset.

nates ($\Delta\Delta_r G_{LM}^\circ < 0$) upon the introduction of methanol into the solvent was due to the reduced stability of the solvates of the cations ($\Delta_r G_M^\circ > 0$) and the crown ether ($\Delta_r G_L^\circ > 0$) as well as the enhanced stabilization of the solvated coronates ($\Delta_r G_{LM}^\circ < 0$) (Fig. 1).

Analysis of the multiple regression models (Fig. 2) revealed that the increase in the stability of sodium coronate in the aqueous-methanolic solvents was due to the influence of the cohesion forces [$\Delta\Delta G_{LM}^\circ(\delta^2) < 0$], whereas a similar effect for potassium coronate was due to cohesion [$\Delta\Delta G_{LM}^\circ(\delta^2) < 0$] and electron-donating interactions [$\Delta\Delta G_{LM}^\circ(B_{KT}) < 0$]. The electrostatic effects reduces the stability of sodium and potassium coronates with the increase in the methanol fraction [$\Delta\Delta G_{LM}^\circ(1/\varepsilon) > 0$].

The revealed effects could be rationalized as follows. The decrease in the cohesion energy density in aqueous-methanolic solvents in comparison with water facilitated the formation of voids in the solvent, which stronger stabilized the solvates of sodium and potassium coronates. The decrease in the dielectric constant of the solvent enhanced the interionic electrostatic interaction (Na^+-Cl^- and K^+-Cl^-), thus hindering the complex formation of the M-L pair due to the competition for the cation. The introduction of methanol into the solvent increased the electron-donating properties of the medium, which was reflected in the additional stabilization of potassium coronate in the aqueous-methanolic solvents.

Approximators of neural network and multiple linear regression. Thousand of neural networks (radial basis or multilayer perceptron) were constructed in Statistica Neural Networks [44, 45], and the optimal structure was selected as judged by the statistical merits; that was the MP 4-7-2 perceptron. The network consisted of three layers: the input one with four neurons, the output one with two neurons, and the hidden one with seven neurons (Table 5).

The three-layer perceptron was trained [46] using the single-step quasi-Newton BFGS (Broyden-Fletcher-Goldfarb-Shanno) algorithm [47]. The learning was complete in 85 epochs with the training error 0.0038, validation error 0.0099, and test error 0.0077. Those errors were determined, respectively, for the training (70%), validation (15%), and test (15%) subsets of the input dataset of the coronates stability constants and the properties of the mixed solvents. The data in the training subset were used for the network learning. The validation subset was used to verify the training quality (to avoid overtraining and determine the finish point of the training). The test subset data were not used in the training to allow for independent determination of the network prediction quality. The training was stopped when the minimum validation error was achieved [44-46]. The error of the neural network training is the mean-square deviation of the network predictions from the corresponding empirical stability constants of the coronates. Neurons of the hidden and output layers were activated, respectively, with logistic and linear (identical) functions.

One of the ways to estimate the quality of approximations was to compare the observed values $\log K_{exp}$ and the ones $\log K_{calc}$ predicted by means of multiple linear regression and using the MP 4-7-2 perceptron. Analysis of those data for the water-acetonitrile solvents (Table 6) revealed that both methods gave highly accurate precision, yet the neural network was more efficient since it showed lower prediction error.

The conclusion was further confirmed by the predictions of the coronates stability constants in the water-acetone solvents (Table 7). It is important to notice that those data were not used in the construction of the multiple linear regression models and in the training of the neural network, and therefore they could be used in the independent testing of the multiple linear regression and approximators of multilayer perceptrons.

Table 6. Results of the approximation of stability constants of sodium and potassium coronates in the water–acetonitrile mixed solvents

CH ₃ CN mole fraction	log <i>K</i> (18-crown-6Na ⁺)			log <i>K</i> (18-crown-6K ⁺)		
	log <i>K</i> _{exp}	multiple linear regression	multilayer perceptron	log <i>K</i> _{exp}	multiple linear regression	multilayer perceptron
0.0	0.52	0.68	0.63	2.04	1.89	2.14
0.1	1.18	1.03	1.06	2.42	2.57	2.41
0.2	1.46	1.39	1.33	2.74	2.95	2.67
0.3	1.55	1.74	1.61	3.02	3.24	2.96
0.4	1.64	2.09	1.86	3.28	3.46	3.23
0.5	2.17	2.45	2.19	3.53	3.71	3.51
0.6	2.69	2.81	2.66	3.80	4.04	3.83
0.7	3.20	3.17	3.17	4.08	4.36	4.15
0.8	3.65	3.53	3.64	4.41	4.60	4.36
0.9	4.01	3.90	4.00	4.78	4.81	4.80
1.0	4.25	4.26	4.26	5.20	5.01	5.18
Mean error of approximation, %		10.2	5.5		5.6	1.4

Table 7. Prediction of stability constants of sodium and potassium coronates in the water–acetone mixed solvents

Acetone mole fraction	log <i>K</i> (18-crown-6Na ⁺)			log <i>K</i> (18-crown-6K ⁺)		
	log <i>K</i> _{exp}	multiple linear regression	multilayer perceptron	log <i>K</i> _{exp}	multiple linear regression	multilayer perceptron
0.00	0.52	0.68	0.64	2.04	1.90	2.14
0.10	1.29	1.05	1.01	2.53	2.66	2.44
0.20	1.77	1.41	1.28	2.99	3.08	2.81
0.30	2.04	1.77	1.51	3.41	3.27	3.18
0.40	2.24	2.13	1.76	3.80	3.38	3.44
0.50	2.50	2.48	2.17	4.13	3.52	3.54
0.55	2.68	2.65	2.49	4.29	3.65	3.54
Mean error of prediction, %		12.8	20.0		8.6	7.4

Table 8 lists the constants of 18-crown-6 ether complex formation with Na⁺ and K⁺ obtained using the derived multiple linear regression and neural networks approximators basing on the descriptors of water–ethanol mixed solvents (dielectric constant, cohesion energy density, Dimroth–Reichardt parameter, and Kamlet–Taft parameter). It should be noted that the corresponding data are missing in the reference literature to the best of our knowledge.

Neural network classifiers. We have earlier performed clusterization of the stability of sodium and potassium coronates via the *k*-means method [48]. The cluster analysis allowed interpretation of three clusters (classes).

Cluster 1 contained coronates which were moderately stable in the mixed solvents of intermediate composition (log *K*_{NaL} = 1.5–2.5, 10 stability constants; log *K*_{KL} = 3.1–3.9, 7 stability constants).

Table 8. Predicted values of stability constants of sodium and potassium coronates in aqueous-ethanolic solvents

EtOH mole fraction	log $K(18\text{-crown-6Na}^+)$		log $K(18\text{-crown-6K}^+)$	
	multiple linear regression	multilayer perceptron	multiple linear regression	multilayer perceptron
0.0	0.52	0.52	2.04	2.04
0.1	1.00	0.86	2.40	2.32
0.2	1.32	1.38	3.11	2.80
0.3	1.63	1.66	3.41	3.24
0.4	1.94	1.92	3.61	3.74
0.5	2.25	2.22	3.82	4.27
0.6	2.56	2.61	4.03	4.70
0.7	2.88	3.06	4.23	4.82
0.8	3.19	3.56	4.47	4.73
0.9	3.51	4.01	4.77	4.76
1.0	3.83	4.27	4.95	4.72

Table 9. Basic parameters of the MP 4-4-3 and MP 4-3-3 classifiers^a

Training algorithm	Error function	Neurons activation functions		Number of classes members		
		hidden layer	output layer	class 1	class 2	class 3
MP 4-4-3 18-crown-6Na ⁺						
BFGS 42	SOS	Logistic	Tanh	10	12	11
MP 4-4-3 18-crown-6K ⁺						
BFGS 11	Entropy	Logistic	Softmax	7	10	16

^a (SOS) mean-square error $E = 1/P[\sum_{k=1}^P(\log K_{\text{calc},k} - \log K_{\text{exp},k})^2]$, (P) number of examples in subset; (Entropy) cross-entropy [51] $H(p, q) = -\sum p(x)\log q(x)$, (p and q) non-related random variables; (Logistic) logistic function $\sigma(x) = 1/[1 + \exp(-tx)]$, $[0, 1]$; (Tanh) hyperbolic tangent $th(Ax) = (e^{Ax} - e^{-Ax})/(e^{Ax} + e^{-Ax})$, $[-1, 1]$; (Softmax) generalization of logistic function for multivariate case $\sigma(z_j) = e^{z_j}/\sum_{k=1}^K e^{z_k}$, $[0, 1]$.

Cluster 2 contained the complexes stable in the mixed solvents rich in the organic component and in pure non-aqueous solvents (log $K_{\text{NaL}} = 2.6\text{--}4.3$, 12 stability constants; log $K_{\text{KL}} = 4.0\text{--}5.2$, 10 stability constants).

Cluster 3 contained the coronates weakly stable in water and the mixed solvents with high water content (log $K_{\text{NaL}} = 0.5\text{--}1.4$, 11 stability constants; log $K_{\text{KL}} = 2.0\text{--}3.0$, 16 stability constants).

That classification was confirmed in [48] by the discriminant Fisher analysis with 96.97% confidence (for both coronates) and by construction of the decision making trees with 90.9% (18-crown-6Na⁺) and 97.0% (18-crown-6K⁺) confidence.

In this study, the k -means cluster analysis results were confirmed with 100% confidence using the artificial neural network classification algorithms: multilayer perceptron and self-organizing map (SOM) also known as Kohonen network [49, 50]. In contrast to the multilayer perceptron (supervised learning), the Kohonen network is the competing neural network for unsupervised learning.

Tables 9 and 10 give the basic parameters of the MP 4-4-3 and SOM 7-3 classifiers for sodium coronate and of MP 4-3-3 and SOM 5-3 ones for potassium coronate.

Overall, the study of stability of sodium and potassium coronates in aqueous-organic solvents by means of multiple linear regression and neural network methods

revealed that different data analysis approaches should be used to confirm the validity of the solutions of multivariate analysis tasks (nonlinear regression) and classification of the coronates stability. Conventional statistical method (multiple linear regression) and the neural networks approach (with supervised training) were equally applicable for approximation of the complexes stability using the descriptors of aqueous-organic solvents. The multiple linear regression method gave somewhat less accurate predictions in comparison with the multilayer perceptron, yet the results of the former approach allowed quantitative estimation of the energy contributions of electrostatic, cohesion, and donor-acceptor interactions to the increase in stability of sodium and potassium coronates using the free energies linearity principle [52].

Artificial neural networks could be successfully applied to modeling, prediction, and classification of the coronates stability in the mixed solvents, similarly to the multiple linear regression method. Stability constants of sodium and potassium coronates in water–mixtures were predicted using the elaborated artificial neural network and multiple linear regression models. The algorithms of supervised multilayer perceptron and the Kohonen network learning fully confirmed the classification of the coronates stability by the *k*-means method.

CONFLICT OF INTEREST

No conflict of interest was declared by the authors.

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