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PREDICTION OF THE SOLUBILITY OF 1-1 ELECTROLYTES IN NONAQUEOUS SOLVENTS WITH THE USE OF THE RADIAL BASIS FUNCTION ARTIFICIAL NEURAL NETWORK

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Determination of the solubility of electrolytes in a wide range of temperatures and pressures is a one of the experimental problems of modern electrochemistry. Currently has considerable theoretical and experimental data on the solubility of substances in water. Much less material is devoted to solubility in nonaqueous solvents.

The main tasks of our work are literature search of the experimental data on the solubility 1-1 electrolytes in nonaqueous solvents and using this information for prediction of the solubility of 1-1 electrolytes in nonaqueous solvents with the use of the radial basis function artificial neural network (RBFANN) at the new composition of the mixed solvent. 1-1 electrolytes and solvents used in this work are shown in Table.

№	Electrolyte	Solvent	Mole fraction of solvent	Temperature, K
1	$CsClO_4$	Mixture of propylene glycol and ethanol	0.000, 0.105, 0.196, 0.292, 0.393, 0.491, 0.577, 0.651, 0.801, 0.898, 1.000 (propylene glycol)	288.15, 298.15, 308.15, 318.15, 328.15
2	NaCl	Mixture of acetonitrile and methanol	0.000, 0.074, 0.128, 0.249, 0.359, 0.465, 0.568, 0.665, 0.753, 0.839, 0.922, 0.964 (methanol)	288.15, 298.15, 308.15, 318.15
3	NaBr	Mixture of nitromethane and methanol	0.000, 0.250, 0.350, 0.450, 0.650, 0.800, 0.900, 0.950, 1.000 (nitromethane)	293.15, 303.15, 313.15, 323.15

Equations of the following forms have also been used for prediction of solubility of electrolytes:

$$S = (a_0 + a_1 \cdot T) + (b_0 + b_1 \cdot T) \cdot x + (c_0 + c_1 \cdot T) \cdot x^2, \quad (1)$$

$$S = a_0 + b_0 \cdot x + c_0 \cdot x_1, \quad (2)$$

where S *– solubility,*

a_0, a_1, b_0, b_1, c_0, c_1 *– coefficients,*

x *– mole fraction of solvent,*

x_1 *– temperature.*

The best description of the experimental data has been obtained with the use of RBFANN (see Figure), maximum value of relative standard deviation from the experimental values is 1.7 %. Also we obtained satisfactory results for solubility of electrolytes at new compositions of mixed solvents. Using equations (1), (2) do not lead to satisfactory results and sometimes produce negative solubility. The results of the work make it possible to predict the solubility of 1-1 electrolytes in mixed solvent without making experimental research.

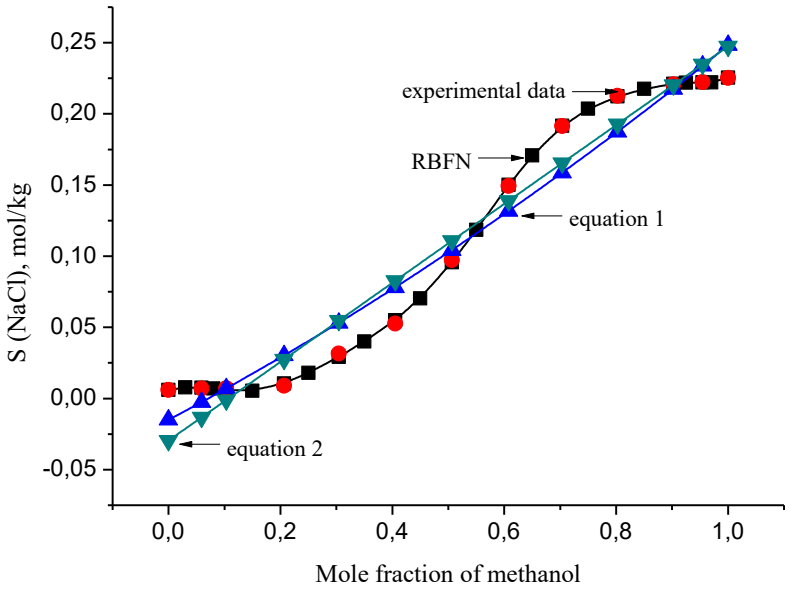

Fig. **Dependence of solubility of NaCl on the mole fraction of methanol at temperature 288.15 K**