Chemoinformatics methods in the thermodynamics of equilibrium. Potassium monocoronates (18C6K+).

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Abstract

Multiple linear regression and neural network modeling were applied to the analysis and prediction of the Gibbs energy (constants) stability of the complexes of 18-crown-6 with potassium cations in water - organic solvents. The comparison of results of the solvation-thermodynamic analysis and the regression analysis was carried out. The significant factors which influence the stability of potassium corontes were identified. The neural network model (three-layer perceptron) was constructed and a perspective of application of neural networks for prediction of stability constants of potassium monocoronates in water-organic solvents was showed.