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Prediction of Activity Coefficients at Infinite Dilution for Organic Solutes in Ionic Liquids [BMPYR][TCM] by Artificial Neural Network

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Introduction

Infinite dilution activity coefficient (γ_{13}^{∞}) is an important physicochemical property of solution, useful in separation. The values of (γ_{13}^{∞}) depends on the type of ionic liquid, so measuring the (γ_{13}^{∞}) is important. The ionic liquid used in this study is 1-butyl-1-methylpyrrolidinium tricyanomethanide [BMPYR] [TCM] which has quite a high selectivity for the separation of aromatic and aliphatic hydrocarbons. There are some analytical methods for determining the (γ_{13}^{∞}) [1]. Experimental methods are expensive and time consuming, but theoretical and computational methodologies such as quantitative structure property relationship QSPR can be helpful in the estimation of the (γ_{13}^{∞}) in ionic liquid of [BMPYR] [TCM] instead. This paper provides effective methods for predicting (γ_{13}^{∞})of organic compounds in [BMPYR] [TCM]. It also reveals that artificial neural network (ANN) can be used as a powerful tool of chemo metrics for QSPR studies

Methods

In this investigation, the average experimental activity coefficients at infinite dilution,(γ_{13}^{∞}), for 354 data points (59 solutes in 6 temperatures) of organic solutes were taken from the ref [2]. It is clear that, when we used from one data set in several different conditions (such as temperature), we should be repeated this data with respect the number of different conditions by using the related values for a response parameter such as (γ_{13}^{∞}) in their conditions (see the ref [3]). The chemical structures of the studied organic solutes were drawn with HYPERCHEM software (ver.7.0) and optimization was done with the AM1 semi empirical method. For each molecule, 1481 molecular descriptors were taken from DRAGON software, 21 molecular descriptors from HYPERCHEM and The experimental descriptor of temperature were also packed in the SPSS software. The dataset was randomly divided into

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three sets including training, test and validation sets consisting of 249, 52 and 53 members respectively. The stepwise regression (SR) and genetic algorithm (GA) based on partial least square (GA-PLS) methods were used to select the best descriptors to construct the model. The selected variables were used as the input of artificial neural network (ANN) to predict (γ_{13}^{∞}) for these compounds.

Result and Discussion

12 and 10 most significant descriptors were selected by stepwise regression (SR) and genetic algorithm (GA) methods respectively. These descriptors were used as the inputs for the neural network. The important parameters of network including the number of nodes in the hidden layer, weights and biases learning rates and momentum values were optimized. The optimized parameters of stepwise regression-artificial neural network (SR-ANN) and genetic algorithm-artificial neural network (GA-ANN) models are shown in Table 1.

Table1 Optimized parameters of SR-ANN and GA-ANN models

Optimized parameters	SR-ANN	GA-ANN
Input neurons	12	10
Hidden neurons	10	10
Output neurons	1	1
Momentum	0.0683	0.0679
Number of iteration	256	148

Figures 1and 2 show a plot of predicted values by the SR-ANN and GA-ANN against experimental values of the (γ_{13}^{∞}) of test sets. These figures show good correlation between predicted and observed (γ_{13}^{∞}).

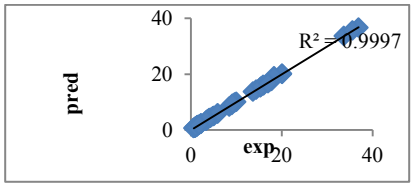

Fig 1.Plot of predicted (γ_{13}^{∞}) by SR-ANN Against the experimental values

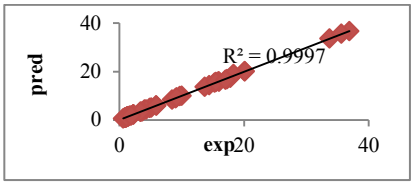

Fig 2: Plot of predicted (γ_{13}^{∞}) by GA-ANN Against the experimental values

Conclusions

The results show a satisfactory data agreement with $R^2 = 0.9997$ and MSE=0.0293 for testing data when using SR-ANN and $R^2 = 0.9997$ and MSE=0.0248 for testing data when using GA-ANN.

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