Artificial Neural Networks and the Melting Temperature of Imidazolium- and Ammonium-type Ionic Liquids

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The use of artificial neural networks (ANN) for the correlation and prediction of the melting temperature of ionic liquids (Tm) is analyzed in this paper. In the study 297 selected data of imidazolium-type ionic liquids and 236 ammonium-type ionic liquids were considered. Several network architectures were analyzed for each set of data and results compared with others from the literature. The independent variables considered for training the ANN (those that could have influence on the melting temperature) were: groups forming the molecules, mass of the cation, mass of the anion and mass connectivity index. These properties are easily available or calculated from information available in the open literature. As a measure of the accuracy of the method the average deviation and the average absolute deviation are evaluated. Results of this work and others from the literature indicate that appropriate selection of data, a good combination of architecture and variables can lead to acceptable correlation of data but accurate predictions with ANN are not yet possible. To make progress in this area of estimating Tm of ionic liquids using ANN it is necessary to standardize the experimental determination of this property so good experiments guarantee reproducibility and elimination of wrong data could be done. Also, it is necessary to know better the structure of the ILs, the characteristics of the anion and cation and which are the variables that may affect Tm to define the most appropriate variables for ANN training. With the present data one cannot obtain good results, especially in predicting the melting temperature of ILs using ANN, at least in the way done until now. Literature information and our own studies indicate better experimental data are needed and that chemical descriptors seem to be the way for making progress in correlating and predicting the Tm of ionic liquids.