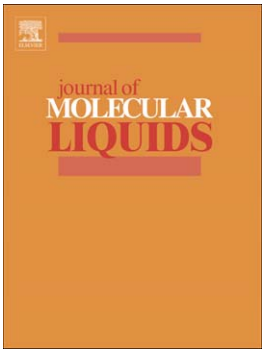

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Predicting Ionic Liquid Melting Points using Machine Learning

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Abstract

The melting point (T_m) of an ionic liquid (IL) is of crucial importance in many applications. The T_m can vary considerably depending on the choice of the anion and cation. This study explores the use of various machine learning (ML) methods to predict the melting points (-96°C - 359°C range) of structurally diverse 2212 ILs based on a combination of 1369 cations and 141 anions. Among the ML models applied to independent training and test sets, tree-based ensemble methods (Cubist, random forest and gradient boosted regression) were found to demonstrate slightly better performance over support vector machines and k-nearest neighbour approaches. In comparison, quantum chemistry based COSMOtherm predictions were generally found to have significant deviations with respect to the experimental values. However, classification models were more efficient in discriminating between ILs with $T_m > 100$°C and those below 100°C.

Keywords: QSPR, ionic liquids, melting point, machine learning, experimental, quantum chemistry

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