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Vishwesh Venkatraman, Sigvart Evjen, Hanna K. Knuutila, Anne Fiksdahl, Bjørn Kåre Alsberg

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# Predicting Ionic Liquid Melting Points using Machine Learning

Vishwesh Venkatraman<sup>a,\*</sup>, Sigvart Evjen<sup>a</sup>, Hanna K. Knuutila<sup>b</sup>, Anne Fiksdahl<sup>a</sup>, Bjørn Kåre Alsberg<sup>a</sup>

<sup>a</sup>*Department of Chemistry, Norwegian University of Science and Technology, 7491, Trondheim, Norway*

<sup>b</sup>*Department of Chemical Engineering, Norwegian University of Science and Technology (NTNU), 7491 Trondheim, Norway*

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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 ( $-96^\circ\text{C}$  -  $359^\circ\text{C}$  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  $T_m > 100^\circ\text{C}$  and those below  $100^\circ\text{C}$ .

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

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\*Corresponding author  
Email address: vishwesh.venkatraman@ntnu.no ()

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