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A novel method for predicting melting point of ionic liquids

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Abstract

For industrial applications, it is important to know phase transition properties such as melting points of ionic liquids (ILs). A novel correlation is introduced to predict melting points of important classes of ILs including imidazolium-, pyridinium-, pyrrolidinium-, ammonium-, phosphonium-, and piperidinium-based ILs and different type of anions with specific cation/anion moieties. It is based only on the number of some of atoms in cationic and anionic structures as well as two correcting functions for the presence of some specific cation/anion moieties. The numbers of carbon, hydrogen and nitrogen atoms are used for cation. Meanwhile, the numbers of hydrogen, nitrogen, bromine, chlorine and aluminum atoms are applied for anion. The measured data of 195 different types of ILs were used to derive the new correlations. The calculated Download English Version:

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