

The Residual Volume Approach II: Simple Prediction of Ionic Conductivity of Ionic Liquids

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Dedicated to Professor Dr. Gerhard Maas on the occasion of his 60th birthday

The Residual Volume Approach (RVA), a recently developed method for the prediction of fundamental physical properties of ionic liquids (ILs) is extended and now allows the estimation of ionic conductivity of unknown ILs, using a simple linear correlation between the ionic conductivity and previously defined substituent parameters – β^X . The proposed method is applied to the conductivity correlations of 61 *n*-alkyl substituted imidazolium, tetraalkylammonium, pyrrolidinium, piperidinium, sulfonium and phosphonium homologous ILs, containing $[\text{BF}_4]^-$, $[\text{Tf}_2\text{N}]^-$, $[\text{C}_2\text{F}_5\text{PF}]^-$, $[\text{CF}_3\text{BF}_3]^-$, $[\text{C}_2\text{H}_5\text{BF}_3]^-$, $[\text{F}(\text{HF})_{2.3}]^-$, $[\text{Br}]^-$, $[\text{I}]^-$, and $[\text{formate}]^-$ as anions. The influence of the ion type – both anion and cation – on the property changes is discussed. Moreover, it is shown that relatively rigid cations with C_2 symmetry decrease the expected conductivity in the same manner as they increase the viscosity of the ILs.

Key words: Ionic Liquids, Predictive Methods, Ionic Conductivity, Viscosity, Structure-Property Relationships