Cohesive Energy and Volatility of Protic Ionic Liquids

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Cohesive energies are intimately related with the volatilities of ionic liquids, which may be decisive for their use as replacements of conventional volatile industrial solvents. The determination of cohesive energies of protic ionic liquids (PILs) is, however, a practically unexplored topic. This problem was addressed here by using a combination of calorimetric and high-accuracy explicitly correlated quantum chemistry methods, namely the W1-F12 and CCSD(T)-F12 methodologies. The work involved a series of [HB]A PILs (HB = 1-methylimidazolium, 1-ethylimidazolium, 1-butylimidazolium, 1-octylimidazolium, and 1,1,3,3-tetramethylguanidinium; A = nitrate, chloride, perchlorate, and ethanoate), which are expected to cover a significant range of ionicity, given the differences in acidity/basicity strengths between their acid (HA) or base (B) precursors. The relationship between the obtained cohesive energies, the extent of HA to B proton transfer, and the vaporization channels that are likely to determine the volatility PILs will be discussed.

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