Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Towards large-scale, fully *ab initio* calculations of ionic liquids

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SUPPLEMENTARY INFORMATION

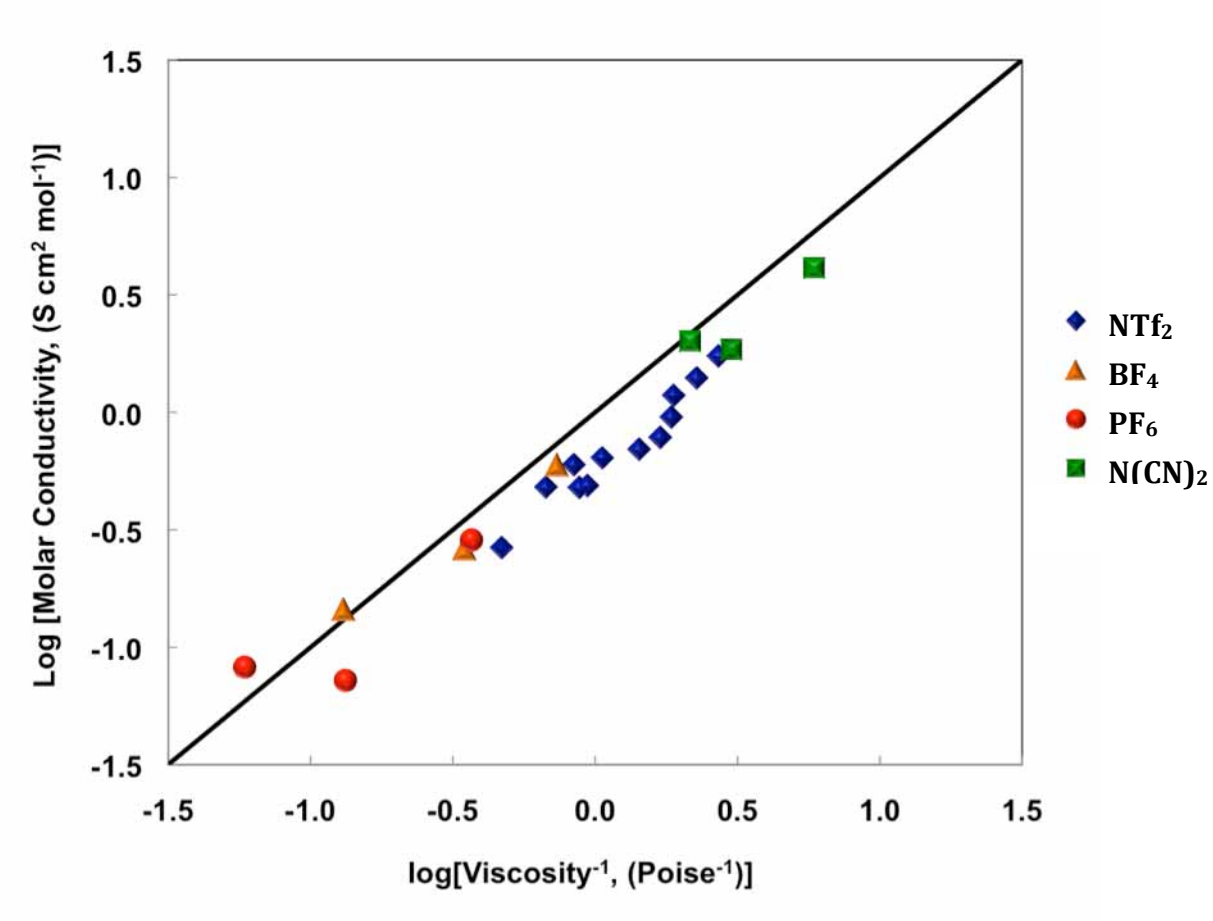

Figure S1. Walden plot for ionic liquids studied in ref. 11. Ionic liquids were grouped with respect to anions.

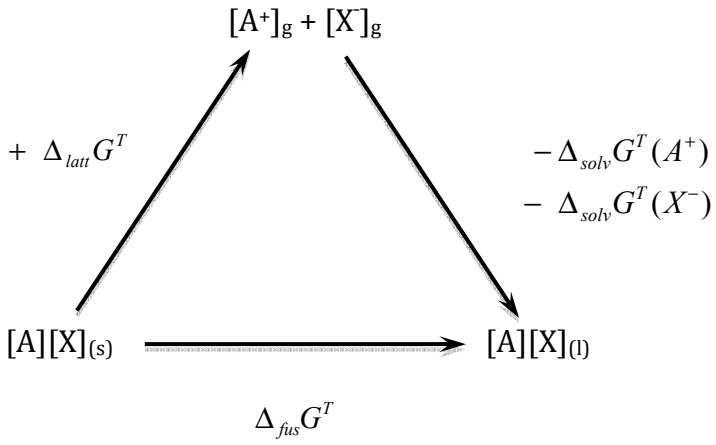

Figure S2. Born-Fajans-Haber cycle for calculating $\Delta_{fus}G^{T}$.

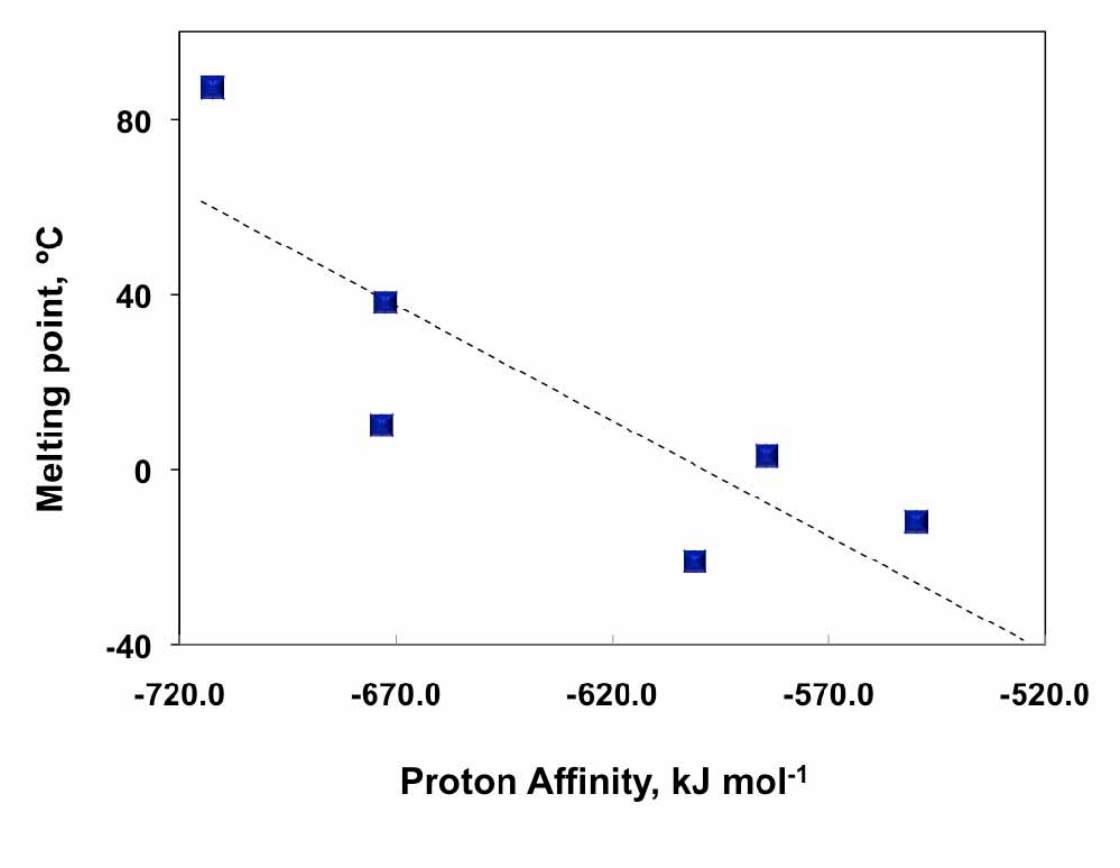

Figure S3. Correlation between the proton affinity and melting point for C_2mim-based ionic liquids incorporating anions: NTf_2, $N(CN)_2$, Cl, NO_3, CF_3SO_3 and $(SO_2CH_3)N(SO_2CF_3)$.