Supplementary Information for: Effect of Organic Solvents on Li⁺ Ion Solvation and Transport in Ionic Liquid Electrolytes: A Molecular Dynamics Simulation Study.

Zhe Li, † Oleg Borodin, ‡ Grant D. Smith, § Dmitry Bedrov, †,*

[†] Department of Materials Science & Engineering, University of Utah, 122 S. Central Campus Dr., Rm 304, Salt Lake City, Utah, 84112, USA

[‡]Electrochemistry Branch, Army Research Laboratory, 2800 Powder Mill Rd., Adelphi,
Maryland 20783, United States

[§]Wasatch Molecular Inc., 825 North, 300 West, Salt Lake City, Utah, 84103, USA

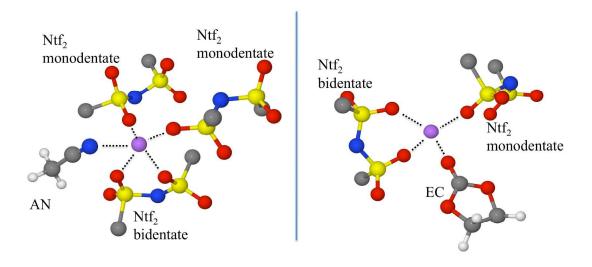


Figure SI.1. Representative snapshots of Li-ion first coordination shell in ILEs with 20% organic cosolvent. (Fluorine atoms are not shown).

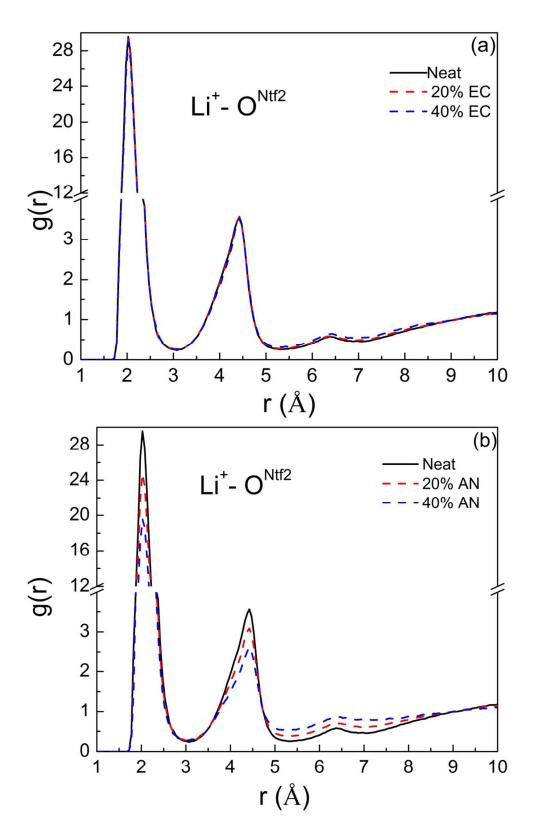


Figure SI.2. Radial distribution functions for Li^+ - O^{Ntf2} in ILEs with (a) EC and (b) AN at 363K.

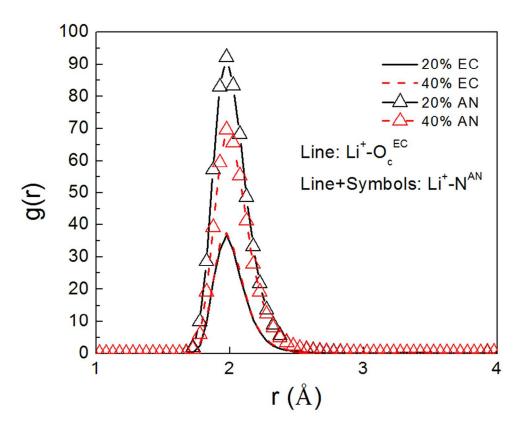
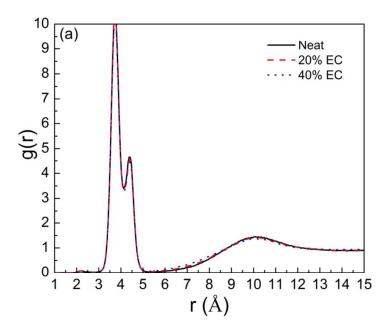


Figure SI.3. Radial distribution functions for $\text{Li}^+\text{-}O_c^{\ EC}$ and $\text{Li}^+\text{-}N^{AN}$ obtained from simulations of ILEs at 363K



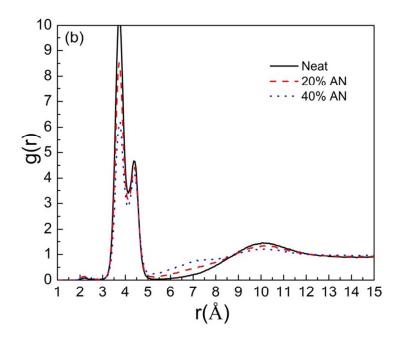


Figure SI.4. Radial distribution functions for Li⁺-N^{Ntf2} obtained from simulations of ILE at 363K.

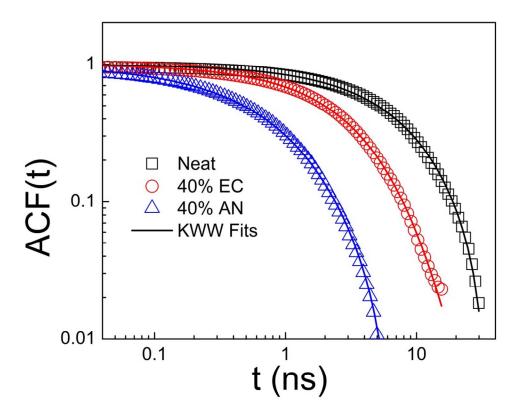


Figure SI.5. Evolution of Li⁺-N^{Ntf2} residence time auto correlation functions (ACF) and their KWW fits as obtained from MD simulations at 363K.