Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Molecular Simulation of Glycerol-Derived Triether Podands for Lithium Ion Solvation

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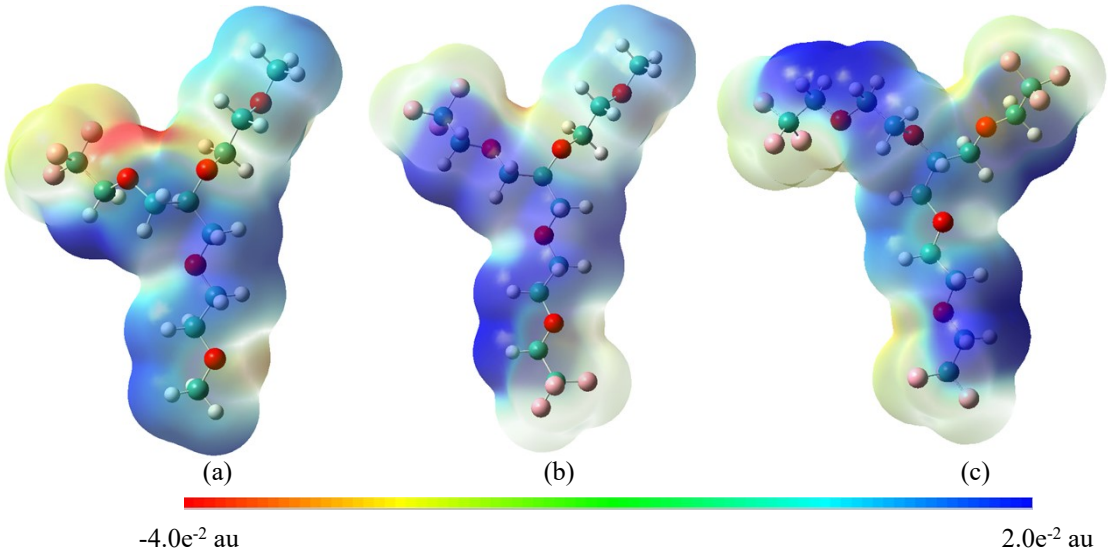

Figure S1. Electrostatic surface potential map of (a) TRF1, (b) TRF2, and (c) TRF3. The electrostatic potential is mapped onto the electron density surface with an isovalue of 0.0004 e^-/au^3.

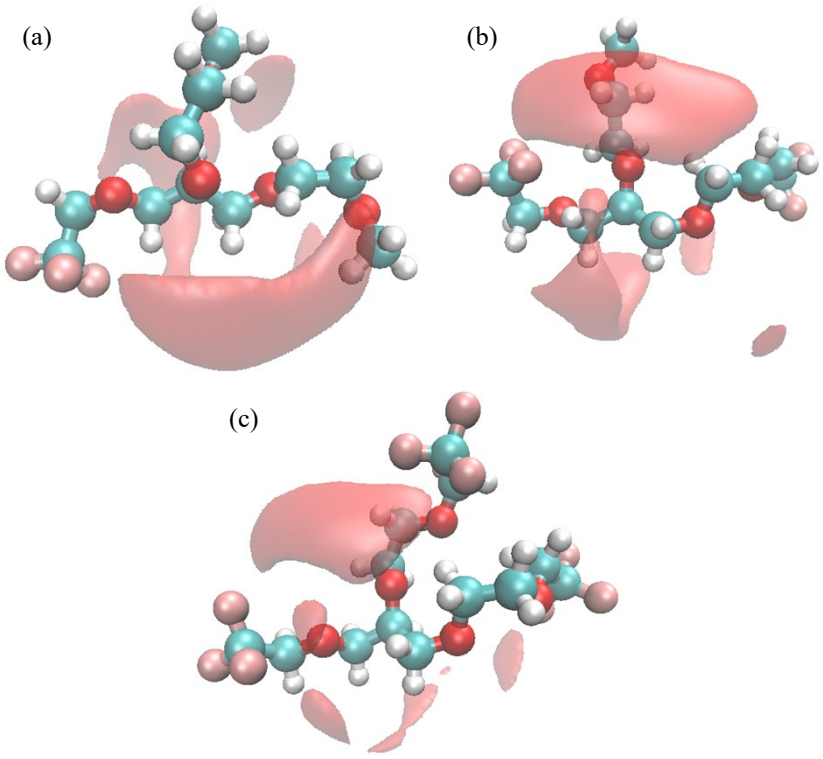

Figure S2. Spatial distribution function of oxygen (red isosurface) around (a) TRF1, (b) TRF2, and (c) TRF3 at 298 K. Color code: cyan = carbon; white = hydrogen; pink = fluorine.

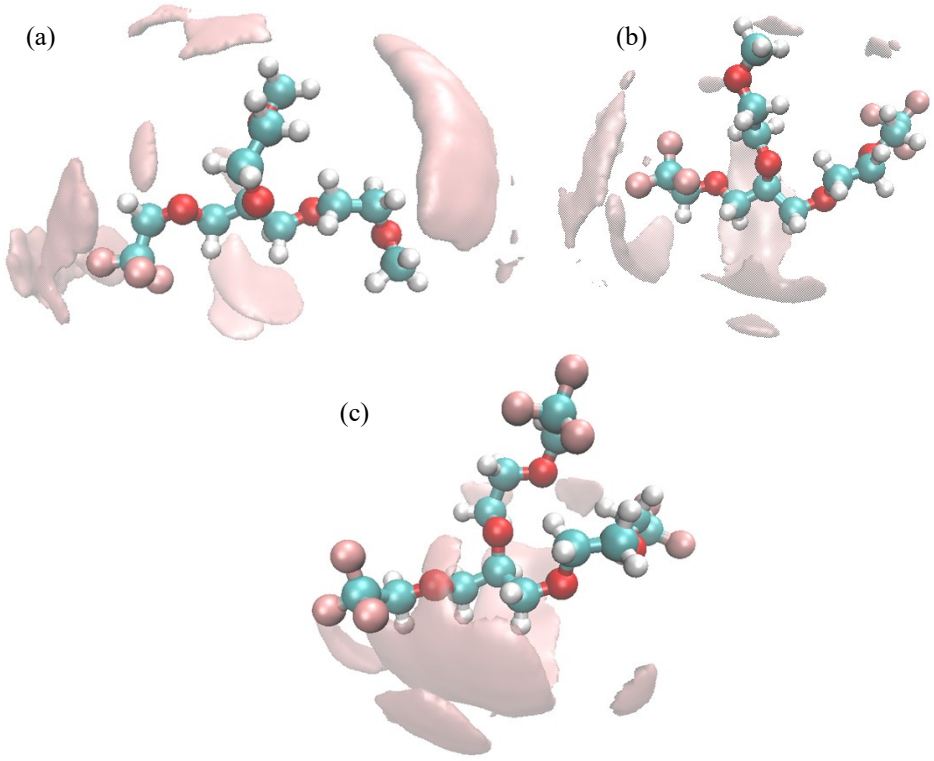

Figure S3. Spatial distribution function of fluorine (pink isosurface) around (a) TRF1, (b) TRF2, and (c) TRF3 at 298 K. Color code: cyan = carbon; white = hydrogen; pink = fluorine.

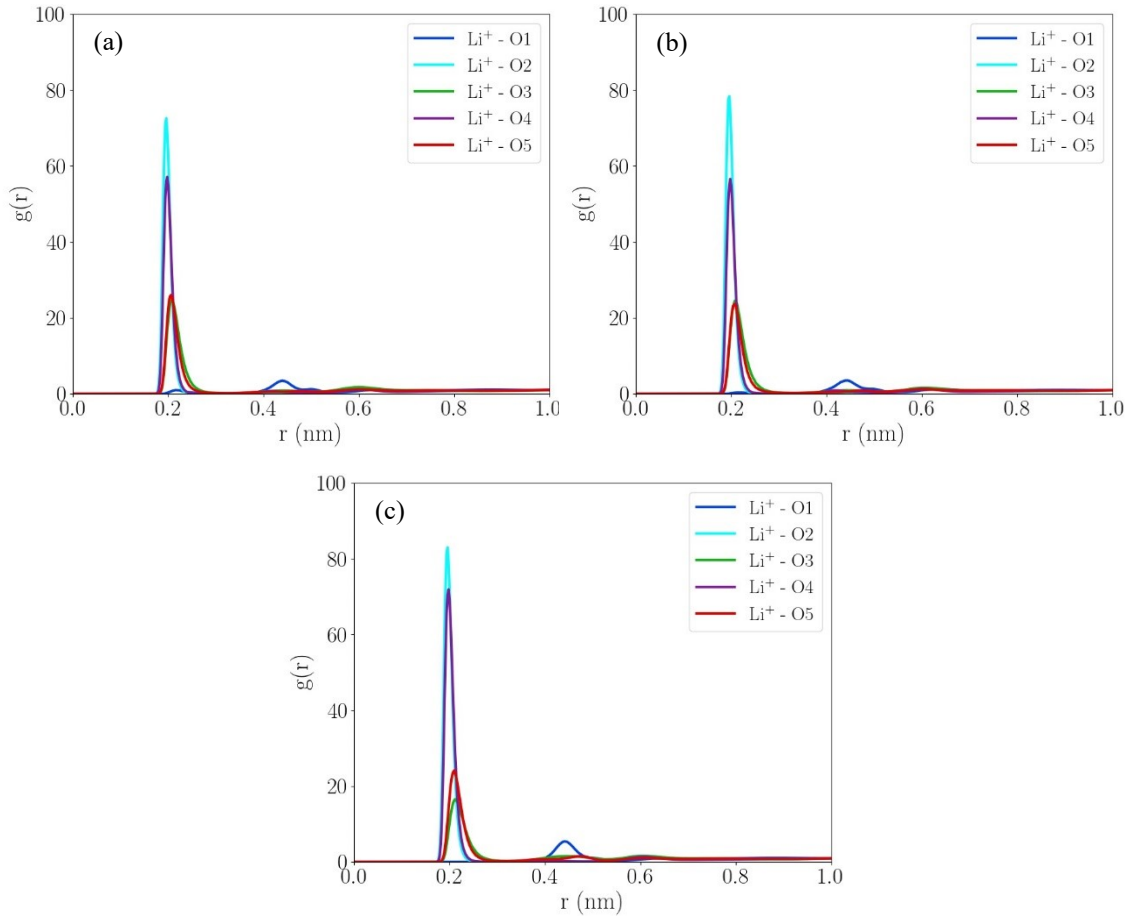

Figure S4. RDFs between Li^+ and different oxygen sites of TRF1 for the mixture of 100 $LiTf_2N$ + solvent at (a) 298 K, (b) 323 K, and (c) 348 K.

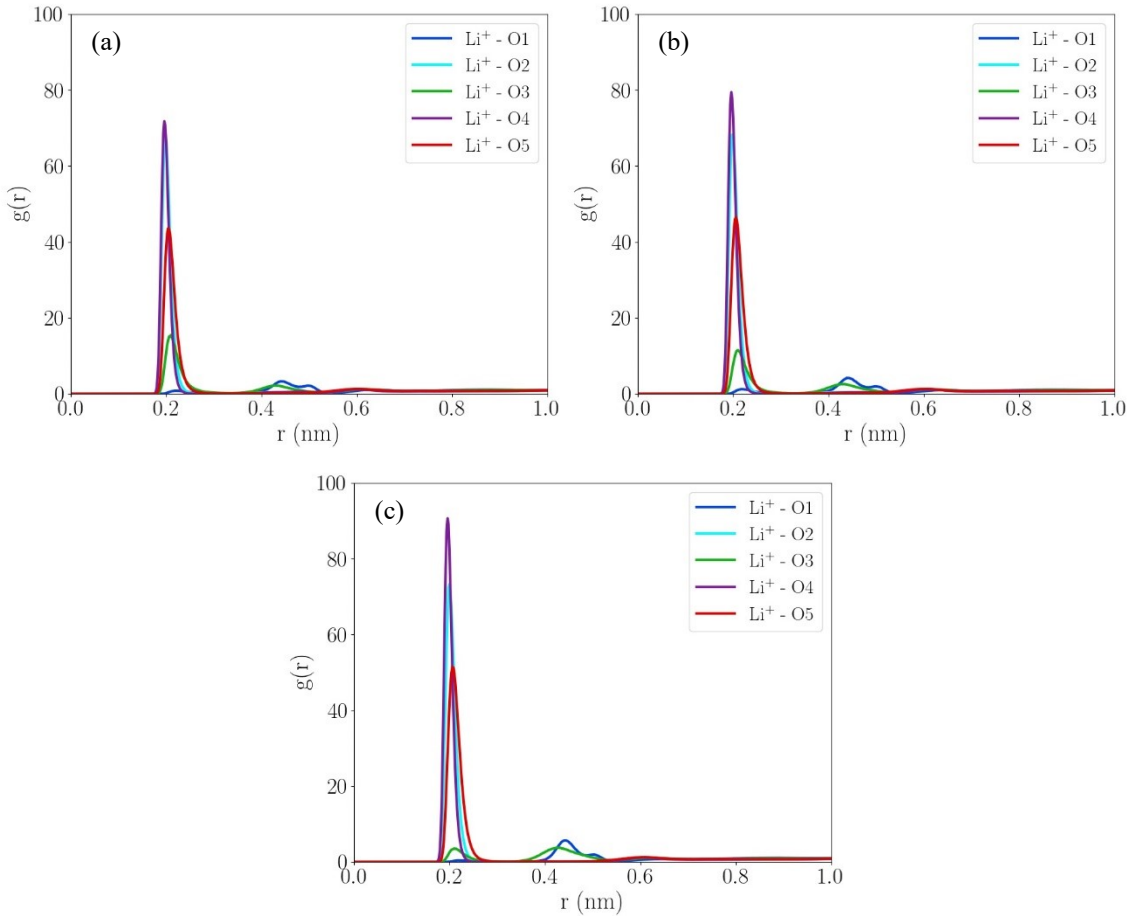

Figure S5. RDFs between Li^+ and different oxygen sites of TRF2 for the mixture of 100 $LiTf_2N$ + solvent at (a) 298 K, (b) 323 K, and (c) 348 K.

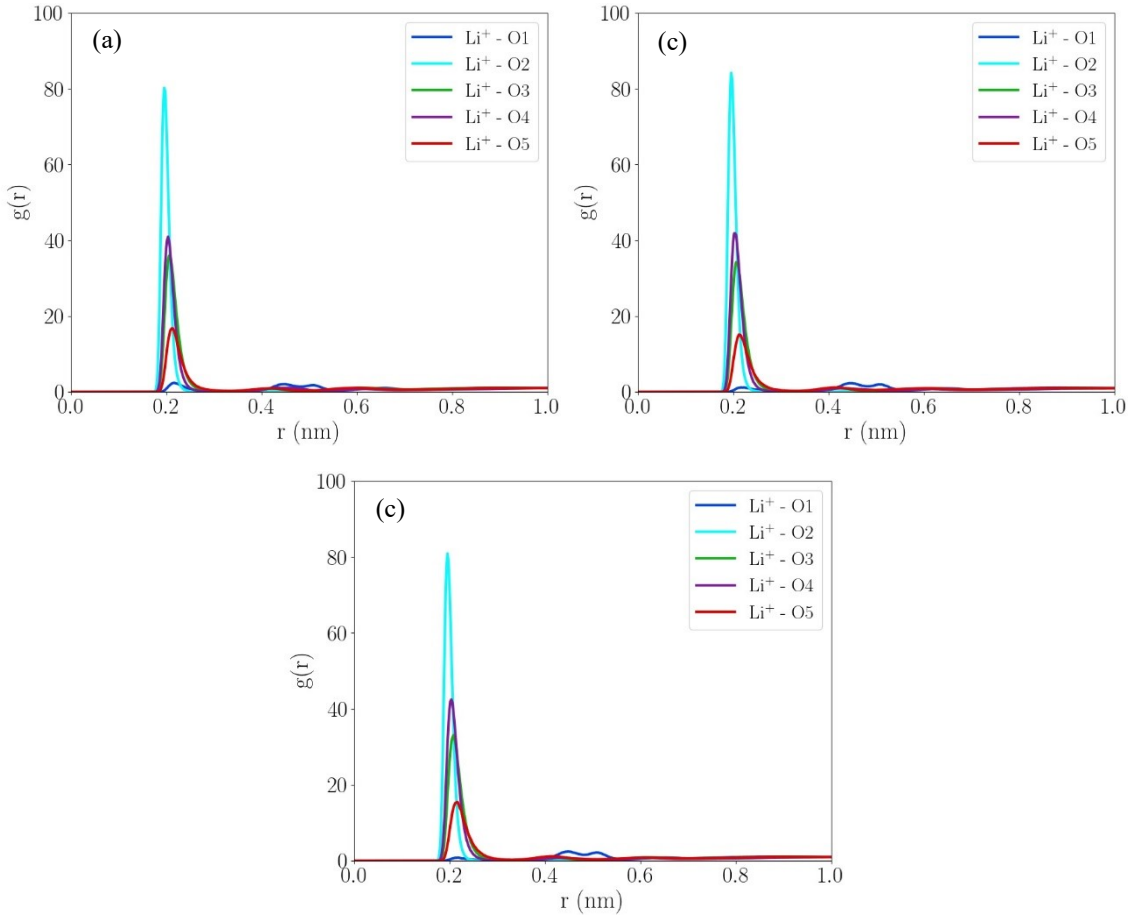

Figure S6. RDFs between Li^+ and different oxygen sites of TRF3 for the mixture of 100 $LiTf_2N$ + solvent at (a) 298 K, (b) 323 K, and (c) 348 K.

Table S1. Quantitative evaluation of the RDFs between Li^+ and different oxygen sites for the mixture of 100 LiTf2N + solvent: r_0 = most intense peak position; $g(r_0)$ = RDF value at r_0; $w(r_0)$ = the potential of mean force at r_0, calculated using $w(r_0) = -RT \cdot \ln(g(r_0))$; and N_c = coordination number up to 0.4 nm.

Solvent	Oxygen Site	Temp. (K)	r_0 (nm)	$g(r_0)$	$w(r_0)$ (kJ/mol)	N_c
TRF1	O1	298	0.44	3.46	-3.078	0.165
		348	0.44	5.40	-4.878	0.065
	O2	298	0.20	72.59	-10.616	1.730
		348	0.20	83.00	-12.786	1.996
	O3	298	0.21	24.74	-7.950	1.293
		348	0.21	16.53	-8.116	1.111
	O4	298	0.20	57.13	-10.023	1.393
		348	0.20	71.92	-12.371	1.924
	O5	298	0.21	26.01	-8.073	1.114
		348	0.21	24.13	-9.211	1.248
TRF2	O1	298	0.44	3.26	-2.930	0.160
		348	0.44	5.67	-5.020	0.055
	O2	298	0.20	67.46	-10.435	1.550
		348	0.20	73.31	-12.427	1.901
	O3	298	0.21	15.51	-6.792	0.918
		348	0.43	3.78	-3.845	0.411
	O4	298	0.20	71.81	-10.590	1.422
		348	0.20	90.67	-13.041	1.903
	O5	298	0.20	43.57	-9.352	1.405
		348	0.21	51.43	-11.401	1.861
TRF3	O1	298	0.22	2.37	-2.136	0.233
		348	0.45	2.44	-2.583	0.076
	O2	298	0.20	80.27	-10.866	1.540
		348	0.20	80.95	-12.713	1.554
	O3	298	0.21	35.95	-8.875	1.250
		348	0.21	33.06	-10.122	1.296
	O4	298	0.20	40.98	-9.200	1.181
		348	0.20	42.50	-10.849	1.306
	O5	298	0.21	16.78	-6.988	0.879
		348	0.22	15.48	-7.927	0.916

Table S2. Atomic charges (units of e) of the oxygen sites; these charges are obtained by the ChelpG method, as described in the simulation methodology section.

Solvent	Oxygen Site	Partial charge (e)
TRF1	O1	-0.431
	O2	-0.632
	O3	-0.518
	O4	-0.651
	O5	-0.512
TRF2	O1	-0.386
	O2	-0.595
	O3	-0.514
	O4	-0.654
	O5	-0.499
TRF3	O1	-0.358
	O2	-0.584
	O3	0.512
	O4	-0.498
	O5	-0.404

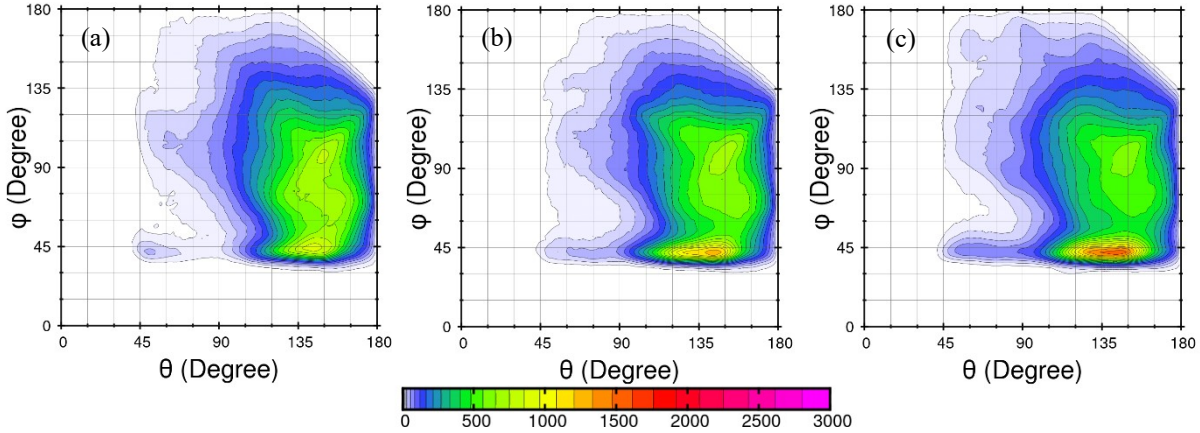

Figure S7. Combined distribution functions of the θ and φ angles of TRF1 at 298 K and 1 bar for the mixture of (a) 100, (b) 200, and (c) 300 $LiTf_2N$ + solvent. The color scale indicates the number of occurrences that fall within each angle bin.

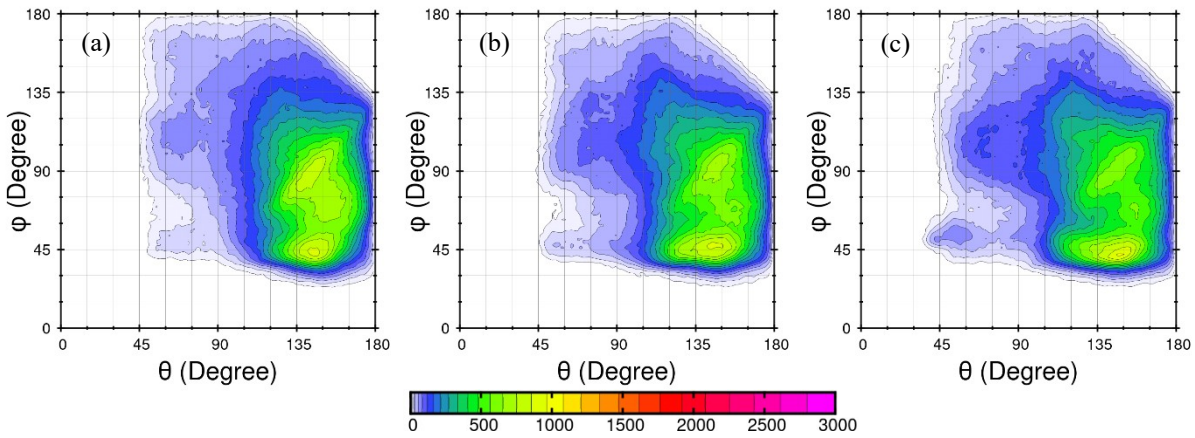

Figure S8. Combined distribution function of the θ and φ angles of TRF2 at 298 K and 1 bar for the mixture of (a) 100, (b) 200, and (c) 300 $LiTf_2N$ + solvent. The color scale indicates the number of occurrences that fall within each angle bin.

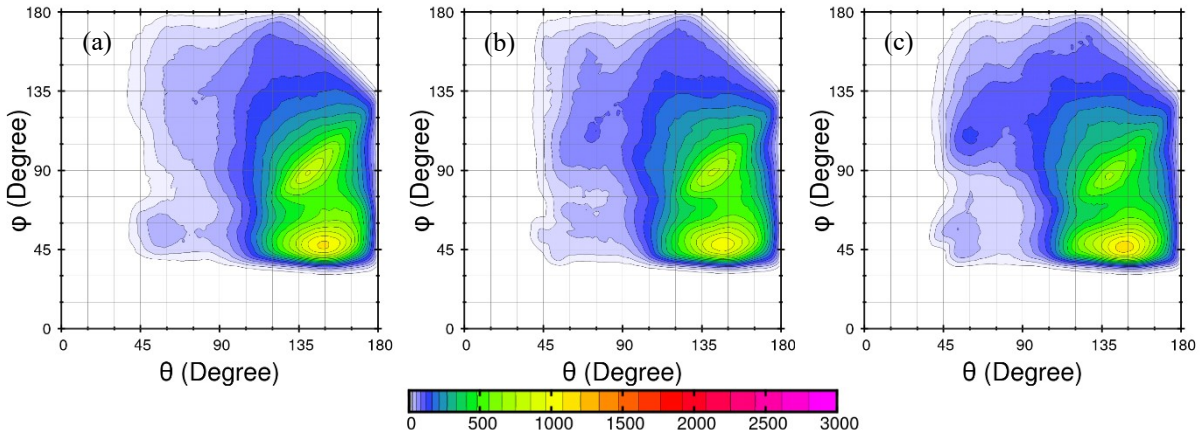

Figure S9. Combined distribution function of the θ and φ angles of TRF3 at 298 K and 1 bar for the mixture of (a) 100, (b) 200, and (c) 300 $LiTf_2N$ + solvent. The color scale indicates the number of occurrences that fall within each angle bin.

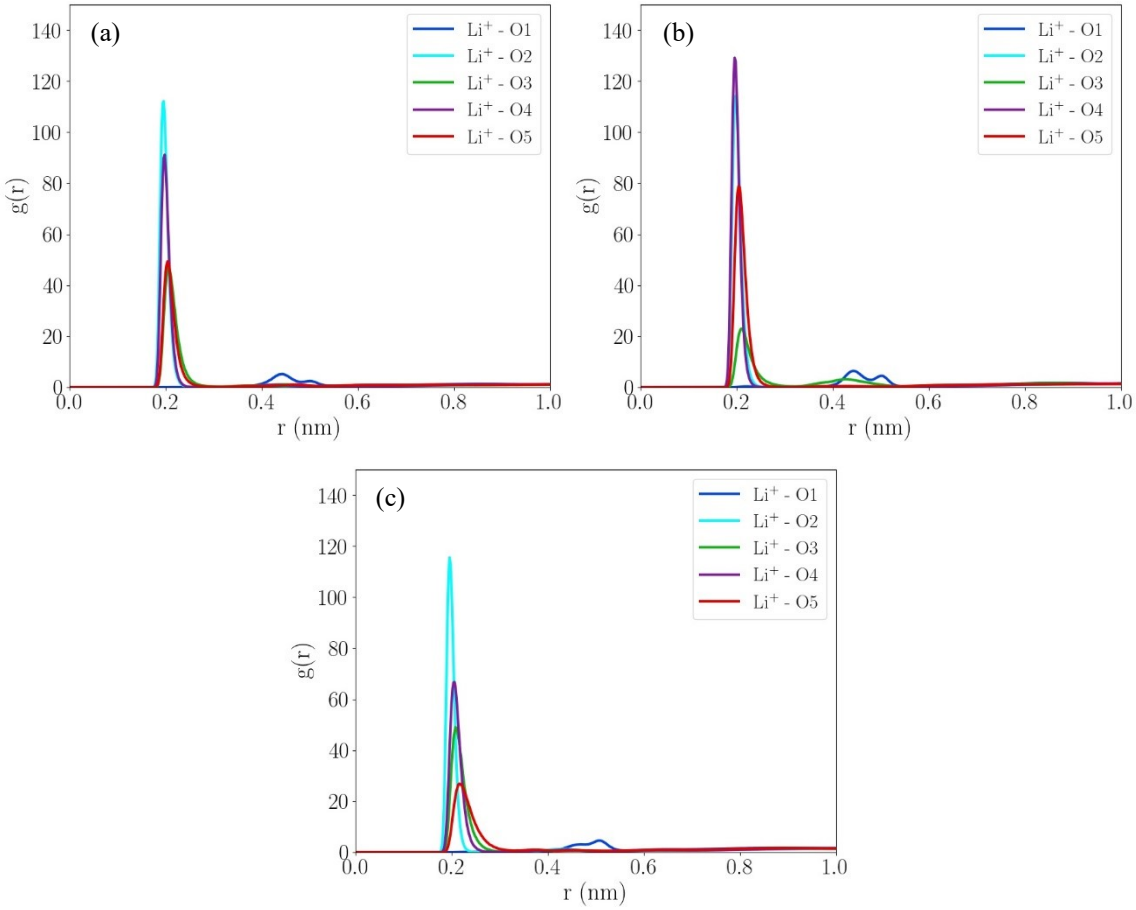

Figure S10. RDFs between Li^+ and different oxygen sites of (a) TRF1, (b) TRF2, and (c) TRF3 for the mixture of 1M $LiTf_2N$ brine + solvent at 298 K and 1 bar.

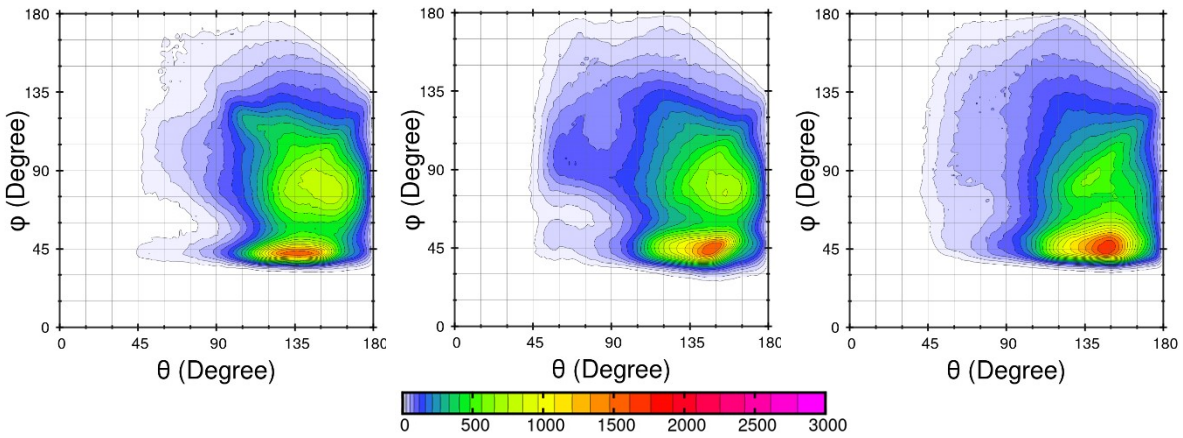

Figure S11. Combined distribution function of the θ and φ angles of (a) TRF1, (b) TRF2 and (c) TRF3 at 298 K and 1 bar for the mixture of $LiTf_2N$ 1M brine + solvent. The color scale indicates the number of occurrences that fall within each angle bin.