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

Structures of glyme-Li^+ complexes and their interactions with anions in equimolar mixtures of glymes and Li[TFSA]: Analysis by molecular dynamics simulations

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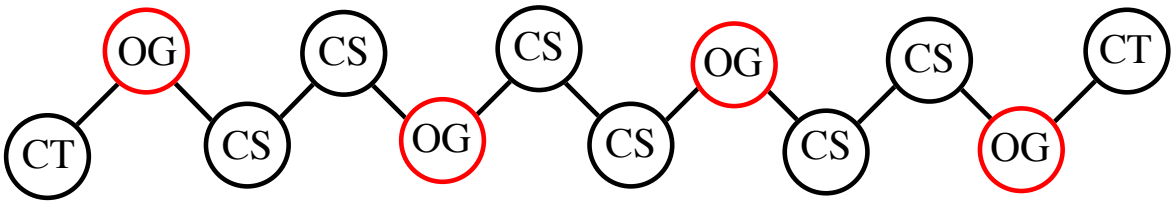

Figure 1S. Atom types used for tryglyme. Red and black circles correspond to oxygen and carbon atoms, respectively. The atom type HG was used for all hydrogen atoms of glymes. The same atom types were used for tetraglyme.

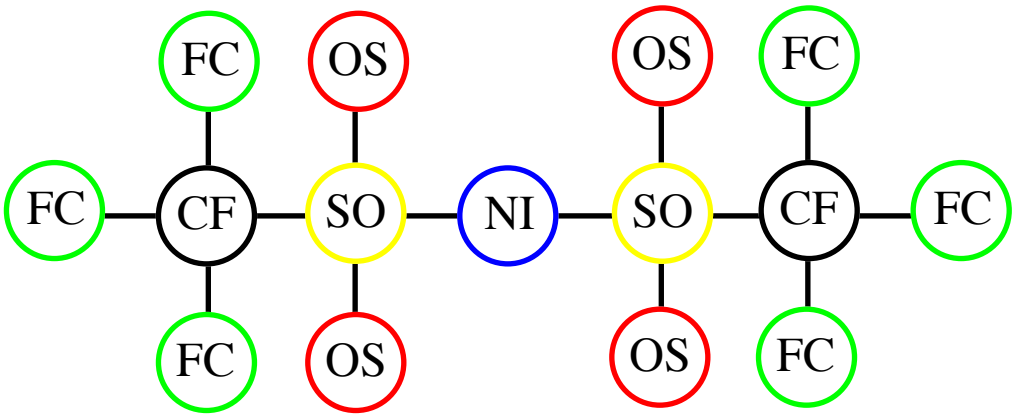

Figure 2S. Atom types used for $[TFSA]^-$ anion. Red, black, blue, yellow and light green circles correspond to oxygen, carbon, nitrogen, sulfur and fluorine atoms, respectively.

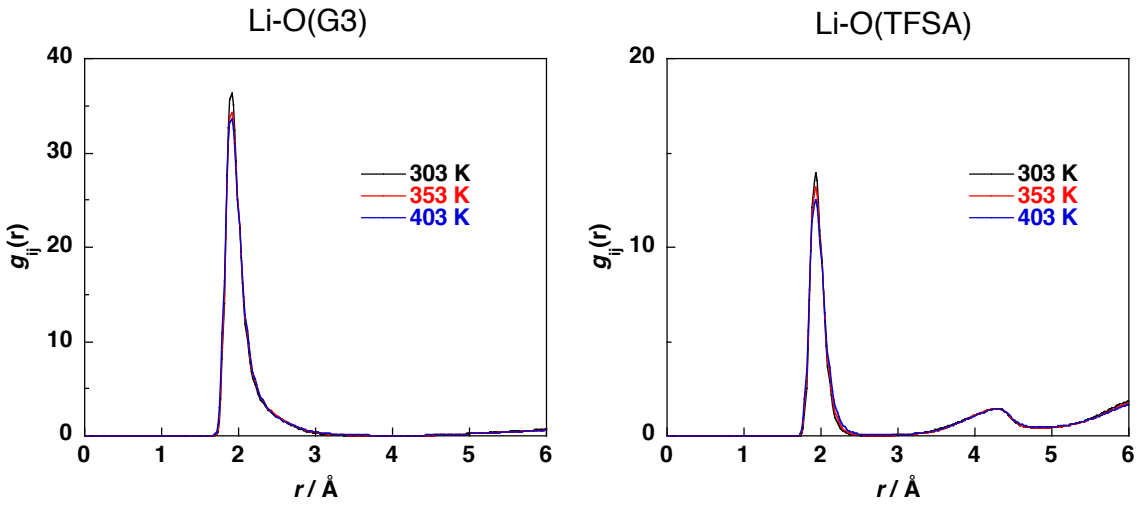

Figure 3S. Temperature dependence of site-site intermolecular radial distribution function between the Li^+ and oxygen atoms of the triglyme and that between Li^+ and oxygen atoms of the $[TFSA]^-$ in the [Li(G3)][TFSA].

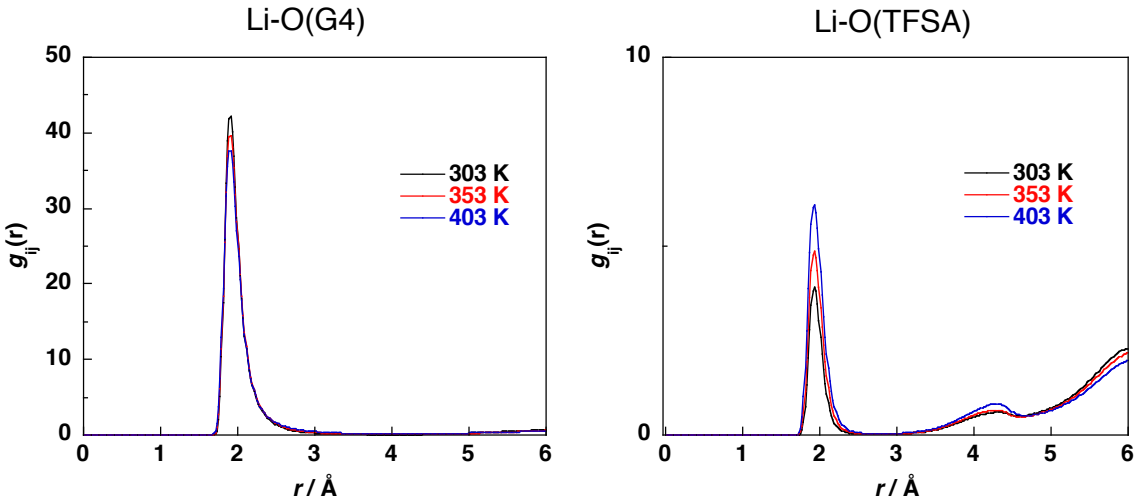

Figure 4S. Temperature dependence of site-site intermolecular radial distribution function between the Li^+ and oxygen atoms of the tetraglyme and that between Li^+ and oxygen atoms of the $[TFSA]^-$ in the [Li(G4)][TFSA].

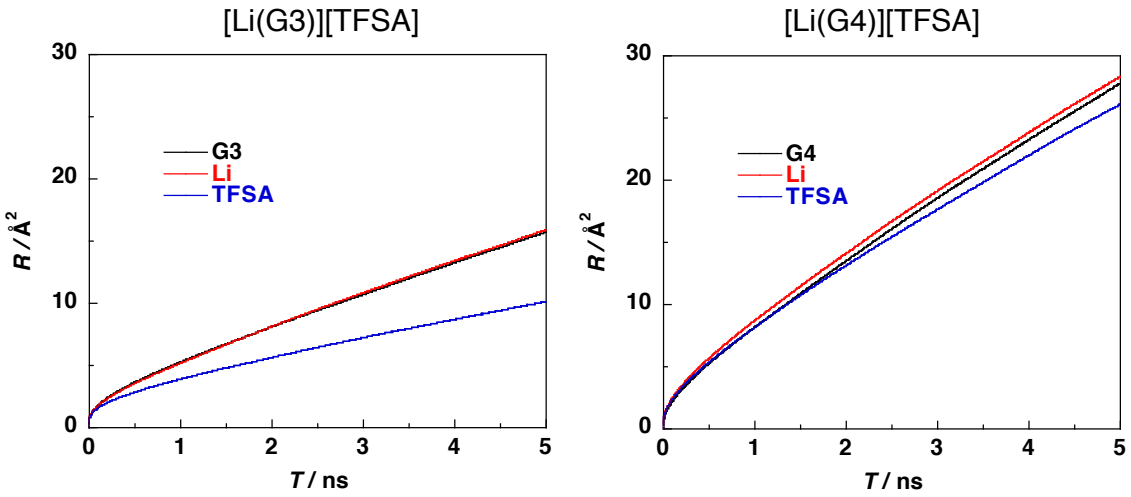

Figure 5S. Mean-square displacements of the ions in the [Li(G3)][TFSA] and [Li(G4)][TFSA] at 403 K.

Table 1S. Force field parameters used for glymes and Li^+ (Atom types were explained in Figures 1S and 2S).

Nonbonding parameters

atom	q (e)	σ (Å)	ε (kJ mol^{-1})
CT	0.32	3.5	0.066
CS	0.32	3.5	0.066
OG	−0.64	3.2	0.21
HG	0.0	2.6	0.03
Li	1.0	1.46	0.191
CF	0.52	3.5	0.066
OS	−0.54	3.26	0.21
NI	−0.72	3.45	0.17
FC	−0.18	2.95	0.053
SO	0.96	3.55	0.25

$E_{nonbond} = 4\varepsilon [(\sigma / r)^{12} - (\sigma / r)^{6}]$

Bond stretching parameters

bond	k_s (kJ mol^{-1} $Å^{-2}$)	r_0 (Å)
CS–CS	268.0	1.529
CT–HG	331.0	1.09
CS–HG	331.0	1.09
CT–OG	570.0	1.408
CS–OG	570.0	1.408
CF–FC	884.0	1.340
SO–CF	471.0	1.835
SO–OS	1274.0	1.450
NI–SO	744.0	1.600

$E_{str} = k_s (r - r_0)^2$

Angle bending parameters

angle	k_θ (kJ mol^{-1} rad^{-2})	θ_0 (deg)
CS-CS-HG	37.43	110.7
CT-OG-CS	55.0	106.8
CS-OG-CS	55.0	106.8
CS-CS-OG	80.0	109.0
OG-CT-HG	35.0	109.0
OG-CS-HG	35.0	109.0
HG-CS-HG	33.0	107.8
HG-CT-HG	33.0	107.8
CF-SO-OS	208.0	102.6
CF-SO-NI	195.0	100.2
FC-CF-FC	187.0	108.6
SO-CF-FC	166.0	110.4
OS-SO-OS	232.0	120.2
OS-SO-NI	189.0	111.4
SO-NI-SO	80.0	121.0

$$E_{bend} = k_\theta (\theta - \theta_0)^2$$

Tonsional parameters

dihedral	V_1 (kJ mol^{-1})	V_2 (kJ mol^{-1})	V_3 (kJ mol^{-1})
CT-OG-CS-CS	−2.4	−0.97	0.25
CS-OG-CS-CS	−0.98	−0.97	0.25
OG-CS-CS-OG	4.0	4.0	0.202
HG-CS-CS-HG	0.0	0.0	0.318
CS-OG-CS-HG	0.0	0.0	0.67
CS-OG-CT-HG	0.0	0.0	0.67
CT-OG-CS-HG	0.0	0.0	0.67
OG-CS-CS-HG	0.0	0.0	0.366
FC-CF-SO-OS	0.0	0.0	0.171

FC-CF-SO-NI	0.0	0.0	0.0
SO-NI-SO-CF	7.833	2.490	-0.764
SO-NI-SO-OS	0.0	0.0	-0.004

$E_{torsion} = \Sigma\ V_n/2\ (1 + \cos(n\phi))$