Supplementary material

Transport coefficients, Raman spectroscopy, and computer simulation of lithium salt solutions in an ionic liquid

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	ηo / cP	B/K	To/K	B/To
BMMITFSI	0.20±0.05	763±50	178±20	4.3
+ 1 M LiTFSI	0.21±0.04	733±34	197±10	3.7
+ 2 M LiTFSI	0.28±0.02	718±17	208±10	3.5

Table 1s - VTF equation parameters of viscosity data. Errors reported here are the standard errors of the non-linear least-squares fit to experimental data.

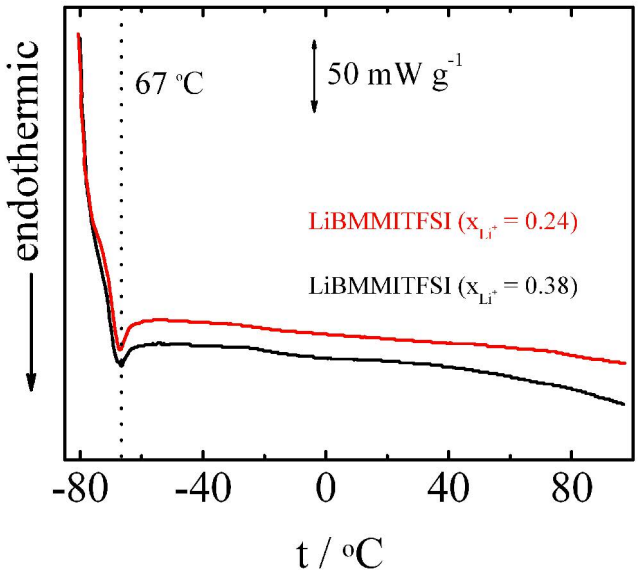

Figure 1s - DSC curves of BMMITFSI with two different LiTFSI concentrations.

	σo /S cm^{-1}	**B/K**	**To/K**	**B/To**
BMMITFSI	1.0±0.3	722±70	165±10	4.4
+ 1 M LiTFSI	1.0±0.5	888±120	164±9	5.4
+ 2 M LiTFSI	1.0±0.4	1000±100	169±10	5.9

Table 2s - VTF equation parameters of conductivity data. Errors reported here are the standard errors of the non-linear least-squares fit to experimental data.

Molecular dynamic parameters used in the simulation

	k_b (10^{-20} J Å^{-2})	r_{eq} (Å)
N3 – C7	153.01	1.477
N3 – C2	278.19	1.34
N3 – C4	278.19	1.39
C4 – C5	285.15	1.37
C2 – C11	154.75	1.53
N1 – C5	278.19	1.39
N1 – C2	279.19	1.34
N1 – C6	153.01	1.477
C7 – C8	139.10	1.53
C8 – C9	154.75	1.534
C9 – C10	154.75	1.534
C-S	327.240	1.818
S-N	517.110	1.570
C-F	614.120	1.323
S-O	885.540	1.442

Table 3s

	k_θ (kJ mol^{-1} rad^{-2})	θ_{eq}
C2-N3-C7	90.42	125.8
C4-N3-C7	90.42	125.8
C2-N3-C4	90.42	108.3
N3-C4-C5	90.42	107.2
N3-C2-N1	90.42	109.1
N1-C2-C11	90.42	125.9
N3-C2-C11	90.42	125.9
C4-C5-N1	90.42	107.2
C2-N1-C5	90.42	108.3
C2-N1-C6	90.42	125.9
C5-N1-C6	90.42	125.9
N3-C7-C8	97.38	112.6
C7-C8-C9	40.62	111.6
C8-C9-C10	40.62	111.6
F-C-F	129.730	107.1
F-C-S	115.220	111.8
C-S-N	135.540	100.2
S-N-S	111.460	125.6
C-S-O	144.510	102.6
O-S-O	160.960	118.5
O-S-N	131.060	113.6

Table 4s

	$k_{\psi,n}$ (10^{-20} J Å^{-2})	N	δ (ângulo)
C6–N1–C5–C4	9.73	1	0
C7–N3–C4–C5	9.73	1	0
C7–N3–C2–N1	9.73	1	0
C6–N1–C2–N3	9.73	1	0
C4–N3–C2–N1	9.73	2	180
N3–C2–N1–C5	9.73	2	180
N3–C4–C5–N1	9.73	2	180
C5–C4–N3–C2	9.73	2	180
C2–N1–C5–C4	9.73	2	180
C2–N3–C7–C8	0.06977	1	180
C4–N3–C7–C8	0.13953	1	0
C7–C8–C9–C10	0.10465	1	0
C5–N1–C2–C11	9.73	0	0
C4–N3–C2–C11	9.73	0	0
C–S–N–S	2.7200	1	0
C–S–N–S	-0.8650	2	180
C–S–N–S	-0.2650	3	0
S–N–S–O	-0.0012	3	180
F–C–S–N	0.1100	3	0
F–C–S–O	0.1200	3	0

Table 5s

Atom	Epsilon (10^{-20} J)	Sigma (Å)	Charge (e)
N1	0.10615	3.58	-0.154
C2	0.066229	4.27	0.522
N3	0.10615	3.58	-0.317
C4	0.066229	4.27	0.217
C5	0.066229	4.27	0.168
C6	0.129319	4.153	0.435
C7	0.073705	4.296	0.555
C8	0.073705	4.296	-0.192
C9	0.073705	4.296	0.114
C10	0.1094262	4.296	-0.173
C11	0.129319	4.153	-0.176
C_{tfsi}	0.034	3.566	0.299
S_{tfsi}	0.134	3.420	0.485
N_{tfsi}	0.106	3.066	-0.426
O_{tfsi}	0.063	3.082	-0.359
F_{tfsi}	0.037	2.910	-0.118
Li^+	0.00001	3.100	1.000

Table 6s