Supporting information

Density, viscosity, and conductivity of [VAIM][TFSI] in mixtures for lithium ion battery electrolytes

Yingjun Cai[†,‡], Nicolas von Solms[†], Suojiang Zhang[‡], Kaj Thomsen[†]*

[†]Center for Energy Resources Engineering (CERE), Department of Chemical and Biochemical Engineering, Technical University of Denmark, Søltofts Plads, 2800, Kgs. Lyngby, Denmark

kth@kt.dtu.dk*

[‡]Beijing Key Laboratory of Ionic Liquids Clean Process, Key Laboratory of Green Process and Engineering, State Key Laboratory of Multiphase Complex Systems, Institute of Process Engineering, Chinese Academy of Sciences, Beijing 100190, P. R. China

The lines in figures S4 to S6 are tendency lines created by OriginLab software.[1]

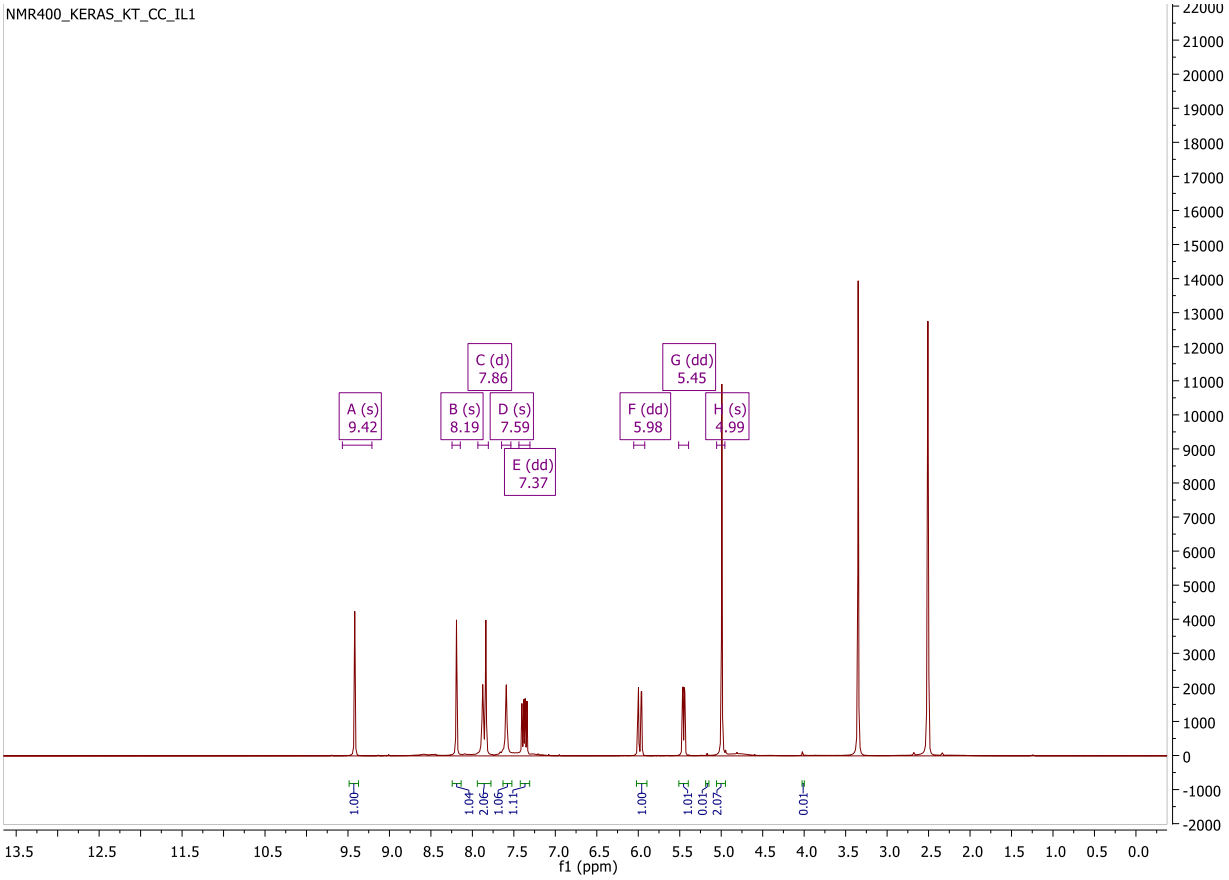
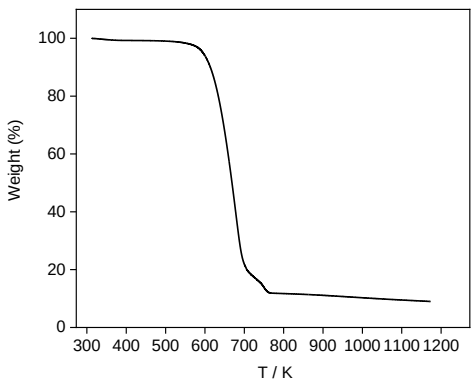


Figure S1. [1]H spectrum for the synthesized ionic liquid [VAIM][TFSI]. Peak integrals are indicated for hydrogen peaks.

The chemical shifts appear as follows: ^{1}H NMR (400 MHz, DMSO) δ 9.42 (s, 1H), 8.19 (s, 1H), 7.86 (d, *J* = 15.1 Hz, 2H), 7.59 (s, 1H), 7.37 (dd, *J* = 15.6, 8.8 Hz, 1H), 5.98 (dd, *J* = 15.6, 2.3 Hz, 1H), 5.45 (dd, *J* = 8.7, 2.3 Hz, 1H), 4.99 (s, 2H).



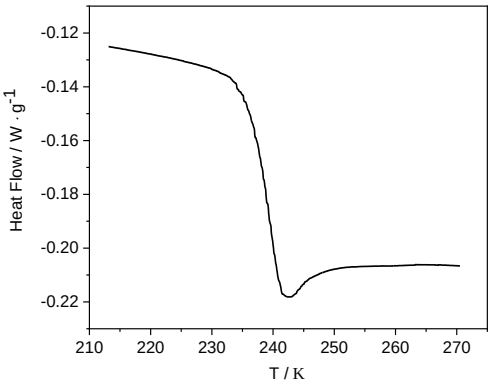


Figure S2. TGA curve for pure ionic liquid [VAIM][TFSI] **Figure S3.** DSC curve for pure ionic liquid [VAIM][TFSI]

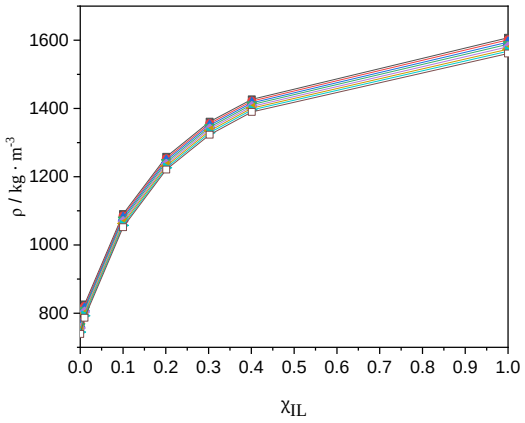


Figure S4. Densities of the binary mixtures [VAIM][TFSI] and acetonitrile as a function of mole fraction of IL at different temperatures: ■, 298.15 K; ●, 303.15 K; ▲, 308.15 K; ▼, 313.15 K; ♦, 318.15 K; ◄, 323.15 K; ►, 328.15 K; □, 333.15 K.

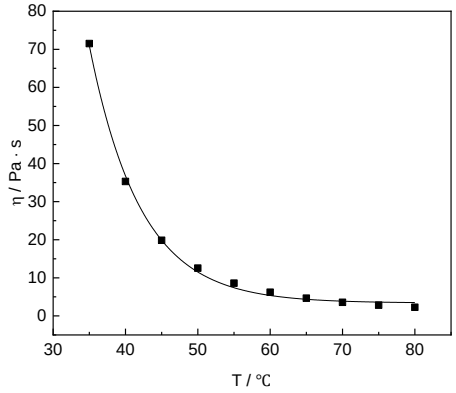


Figure S5. Viscosity of pure ionic liquid [VAIM][TFSI] at different temperatures.

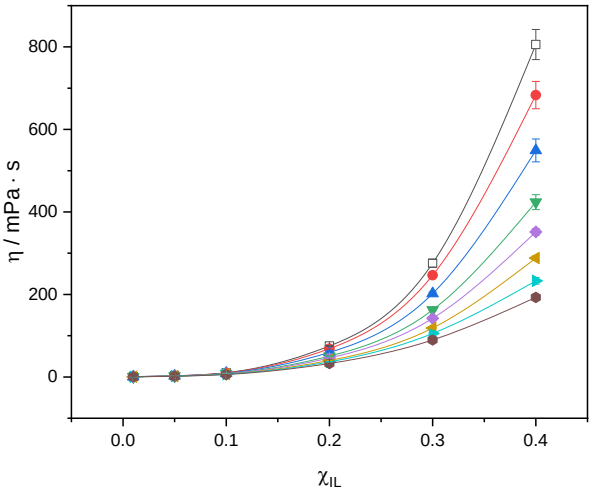


Figure S6. Viscosities of the binary mixtures of ionic liquid [VAIM][TFSI] and acetonitrile at different temperatures: ■, 298.15 K; ●, 303.15 K; ▲, 308.15 K; ▼, 313.15 K; ♦, 318.15 K; ◄, 323.15 K; ►, 328.15 K; □, 333.15 K.

Table S1. Densities (ρ, kg·m^{-3}) of pure acetonitrile at different temperatures (T) from 298.15 K to 333.15 K.

T / K	kg·m^{-3}, our work	kg·m^{-3}, Korosi and Kovars[2]
298.15	777.7	777.3
303.15	772.3	771.8
308.15	766.8	766.3
313.15	761.3	760.9
318.15	755.7	755.9
323.15	750.2	749.2
328.15	744.5	743.6
333.15	738.9	737.3

[a]Standard uncertainties are $u(T)$ = 0.01 K, u(p) = 0.01 MPa. Expanded uncertainty for density is $u(\rho)$ = 0.5 kg·m^{-3} (0.95 level of confidence). T is the Kelvin temperature.

Table S2. Viscosity (η, mPa·s) of pure acetonitrile at different temperatures (T) from 298.15 K to 333.15 K.

T / K	mPa·s, our work	mPa·s, Moumouzias et al[3]
298.15	0.3441	0.3440
303.15	0.3236	0.3280
308.15	0.3078	0.3080
313.15	0.2926	0.2965
318.15	0.2770	0.2890
323.15	0.2624	0.2715
328.15	0.2462	0.2690
333.15	0.2195	0.2590

[a]Standard uncertainties are u(x_{IL}) = 0.0003, $u(T)$ = 0.01 K, u(p) = 0.01 MPa. Relative standard uncertainty for viscosity u_r (η) is 0.15. T is the Kelvin temperature.

Table S3. Conductivities (σ, S·m^{-1}) of the binary mixtures [VAIM][TFSI] and acetonitrile at different temperatures from 298.15 K to 333.15 K, at 0.1 MPa.

x_{IL}	T =298.15 K	T =303.15 K	T =308.15 K	T =313.15 K	T =318.15 K	T =323.15 K	T =328.15 K	T =333.15 K
0.010	1.29	1.34	1.40	1.47	1.53	1.58	1.65	1.69
0.020	2.52	2.64	2.78	2.90	3.01	3.13	3.25	3.35
0.047	3.16	3.32	3.52	3.70	3.87	4.03	4.19	4.34
0.070	3.32	3.51	3.74	3.96	4.16	4.36	4.58	4.79
0.080	3.26	3.47	3.72	3.95	4.17	4.39	4.61	4.77
0.100	3.06	3.28	3.53	3.80	4.02	4.25	4.49	4.72
0.200	1.60	1.77	1.98	2.19	2.38	2.58	2.80	3.00
0.393	0.39	0.48	0.60	0.73	0.86	1.00	1.16	1.33
1.000	0.01	0.02	0.03	0.05	0.07	0.10	0.14	0.20

[a]Standard uncertainties are u(x_{IL}) = 0.0003, $u(T)$ = 0.01 K, u(p) = 0.01 MPa. Relative uncertainty (u) for conductivity is u_r (σ) = 0.004. x_{IL} = mole fraction of ionic liquid. T is the Kelvin temperature.

Table S4. Conductivities (σ, S·m^{-1}) of the electrolytes, different mass fraction of lithium salt in acetonitrile, without [VAIM][TFSI] at different temperatures from 298.15 K to 333.15 K, at 0.1 MPa.

w (salt)	T =298.15 K	T =303.15 K	T =308.15 K	T =313.15 K	T =318.15 K	T =323.15 K	T =328.15 K	T =333.15 K
0.1286	2.67	2.79	2.91	3.03	3.14	3.24	3.34	3.47
0.1813	3.11	3.23	3.34	3.47	3.58	3.7	3.81	3.92
0.228	3.53	3.68	3.85	4.01	4.16	4.29	4.43	4.57
0.2696	3.93	4.1	4.25	4.47	4.64	4.81	4.99	5.16
0.307	4.07	4.25	4.45	4.63	4.8	4.97	5.14	5.28
0.3407	3.93	4.12	4.33	4.53	4.7	4.87	5.05	5.24
0.3713	3.82	4.01	4.14	4.35	4.52	4.74	4.95	5.17
0.3992	3.65	3.84	4.05	4.26	4.45	4.63	4.82	4.99

[a]Standard uncertainties are u(w(salt)) = 0.0001, $u(T)$ = 0.01 K, u(p) = 0.01 MPa. Relative standard uncertainty (u) for conductivity is u_r (σ) = 0.004. w (salt) = mass fraction of lithium salt. T is the Kelvin temperature.

Table S5. Conductivities (σ, S·m^{-1}) of the electrolytes with 3 wt % [VAIM][TFSI]. The remaining 97 wt % consists of variable mass fractions of lithium salt in acetonitrile, at different temperatures from 298.15 K to 333.15 K, at 0.1 MPa.

w (salt)	T =298.15 K	T =303.15 K	T =308.15 K	T =313.15 K	T =318.15 K	T =323.15 K	T =328.15 K	T =333.15 K
0.1248	2.73	2.83	2.96	3.07	3.17	3.3	3.4	3.53
0.1759	3.51	3.66	3.82	3.97	4.11	4.25	4.39	4.51
0.2211	3.85	4.02	4.2	4.38	4.53	4.69	4.83	4.97
0.2615	4.03	4.21	4.41	4.6	4.77	4.94	5.1	5.25
0.2978	4.11	4.28	4.51	4.71	4.9	5.08	5.26	5.43
0.3305	3.97	4.15	4.38	4.58	4.77	4.97	5.16	5.34
0.3602	3.8	4	4.22	4.44	4.64	4.83	5.03	5.21
0.3872	3.67	3.86	4.09	4.3	4.51	4.71	4.92	5.13

[a]Standard uncertainties are u(w(salt)) = 0.0001, $u(T)$ = 0.01 K, u(p) = 0.01 MPa. Relative standard uncertainty (u) for conductivity is u_r (σ) = 0.004. w (salt) = mass fraction of lithium salt. T is the Kelvin temperature.

Table S6. Conductivities (σ, S·m^{-1}) of the electrolytes, with 5 wt % [VAIM][TFSI. The remaining 95 wt % consists of variable mass fractions of lithium salt in acetonitrile, at different temperatures from 298.15 K to 333.15 K, at 0.1 MPa.

w (salt)	T =298.15 K	T =303.15 K	T =308.15 K	T =313.15 K	T =318.15 K	T =323.15 K	T =328.15 K	T =333.15 K
0.1222	3.1	3.22	3.36	3.49	3.61	3.73	3.84	3.95
0.1722	3.56	3.7	3.87	4.02	4.18	4.31	4.48	4.6
0.2166	3.82	3.97	4.16	4.33	4.48	4.63	4.77	4.9
0.2561	3.96	4.13	4.33	4.52	4.68	4.85	5.01	5.15
0.2916	4.05	4.22	4.44	4.62	4.8	4.96	5.13	5.28
0.3237	3.98	4.16	4.37	4.56	4.74	4.95	5.13	5.28
0.3527	3.94	4.14	4.37	4.54	4.73	4.92	5.08	5.24
0.3792	3.56	3.72	3.93	4.13	4.31	4.5	4.68	4.85

[a]Standard uncertainties are u(w(salt)) = 0.0001, $u(T)$ = 0.01 K, u(p) = 0.01 MPa. Relative standard uncertainty (u) for conductivity is u_r (σ) = 0.004. w (salt) = mass fraction of lithium salt. T is the Kelvin temperature.

Table S7. Conductivities (σ, S·m^{-1}) of the electrolytes, with 44 wt % [VAIM][TFSI. The remaining 56 wt % consists of variable mass fractions of lithium salt in acetonitrile, at different temperatures from 298.15K to 333.15K, at 0.1 MPa.

w (salt)	T =298.15 K	T =303.15 K	T =308.15 K	T =313.15 K	T =318.15 K	T =323.15 K	T =328.15 K	T =333.15 K
0.0720	3.43	3.66	3.92	4.17	4.42	4.67	4.92	5.19
0.1015	3.24	3.48	3.75	4.02	4.28	4.56	4.85	5.15
0.1277	3.05	3.29	3.56	3.81	4.07	4.32	4.61	4.91
0.1510	2.87	3.1	3.36	3.61	3.87	4.13	4.37	4.68
0.1719	2.65	2.87	3.11	3.35	3.58	3.82	4.06	4.3
0.1908	2.47	2.68	2.93	3.16	3.38	3.61	3.85	4.14
0.2079	2.4	2.62	2.86	3.09	3.29	3.52	3.77	4.03

[a]Standard uncertainties are u(w(salt)) = 0.0001, $u(T)$ = 0.01 K, u(p) = 0.01 MPa. Relative standard uncertainty (u) for conductivity is u_r (σ) = 0.004. w (salt) = mass fraction of lithium salt. T is the Kelvin temperature.

References

(1) OriginLab 2018b(9.55) version. Copyright: 1991-2018 OriginLab.

(2) Korosi, G.; Kovars, E. Density and surface tension of 83 organic liquids. *J. Chem. Eng. Data* **1981**, *26*, 323–332.

(3) Moumouzias, G.; Panopoulos, D.; Ritzoulis, G. Excess Properties of the Binary Liquid System Propylene Carbonate + Acetonitrile. *J. Chem. Eng. Data* **1991**, *36*, 20–23.