

Supporting information for

Determination of Hansen Solubility Parameters of Ionic Liquids by Using Walden Plots

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Table S1 HSPs for organic solvents used in this work.

IL	δ_d	δ_p	δ_h	Source ^a	Purity
	/(MPa) ^{1/2}	/(MPa) ^{1/2}	/(MPa) ^{1/2}		(GC) [%]
Acetone	15.5	10.4	7	Wako	> 99.0
Acetonitrile	15.3	18	6.1	Junsei	> 98.0
Acetophenone	18.8	9	4	TCI	> 98.5
Benzyl alcohol	18.4	6.3	13.7	TCI	> 99.0
2-Butoxyethanol	16	5.1	12.3	TCI	> 99.0
γ -Butyrolactone	18	16.6	7.4	TCI	> 99.0
1-Chlorobutane	16.2	5.5	2	TCI	> 99.0
Chloroform	17.8	3.1	5.7	Junsei	> 99.0
Cyclohexanone	17.8	8.4	5.1	TCI	> 99.0
Diethylene glycol	16.6	12	19	TCI	> 99.5
<i>N,N</i> -dimethylacetamide	16.8	11.5	9.4	Wako	> 98.0
<i>N,N</i> -dimethylformamide	17.4	13.7	11.3	Junsei	> 99.0
Dimethyl sulfoxide	18.4	16.4	10.2	Junsei	> 99.0
1,4-Dioxane	17.5	1.8	9	Junsei	> 98.0
Ethanol	15.8	8.8	19.4	Junsei	> 99.5
Ethyl acetate	15.8	5.3	7.2	Junsei	> 99.0
Heptane	15.3	0	0	Wako	> 99.0
Isopropanol	15.8	6.1	16.4	Junsei	> 99.5
Methyl ethyl ketone	16	9	5.1	Junsei	> 98.0
Methyl isobutyl ketone	15.3	6.1	4.1	Wako	> 99.5
<i>N</i> -Methyl-2-pyrrolidone	18	12.3	7.2	Junsei	> 99.0
2-Methoxyethanol	16	8.2	15	TCI	> 99.0
Propylene carbonate	20	18	4.1	TCI	> 98.0

Table S1 continued.

IL	δ_d	δ_p	δ_h	Source ^a	Purity
	/MPa ^{1/2}	/MPa ^{1/2}	/MPa ^{1/2}		
Pyridine	19	8.8	5.9	Junsei	> 99.0
Tetrahydrofuran	16.8	5.7	8	Junsei	> 99.0
Toluene	18	1.4	2	Junsei	> 99.0

^a Wako: FUJIFILM Wako Pure Chemical, Junsei: Junsei Chemical, TCI: Tokyo Chemical Industry.

Table S2 Molecular weights (MW), densities (ρ), conductivities (σ), and viscosities (η) of ILs at 25 °C.

IL	MW / g mol ⁻¹	ρ / g cm ⁻³	σ / mS cm ⁻¹	η / mPa s	A^d
[TBLP][TFSI]	651.8	1.13 ^a	0.16 ^b	338 ^c	0.505
[TOMA][TFSI]	648.9	1.11 ^a	0.06 ^b	635 ^c	0.653
[OMI][TFSI]	475.5	1.32 ⁽¹⁾	1.32 ⁽¹⁾	105 ⁽¹⁾	0.302
[OPy][TFSI]	472.5	1.33 ⁽²⁾	1.18 ⁽³⁾	114 ⁽³⁾	0.318

^a Measured with a density meter.

^b Measured with a handheld conductivity meter.

^c Measured with a viscometer.

^d The parameter A was calculated from these properties by using equation (7).

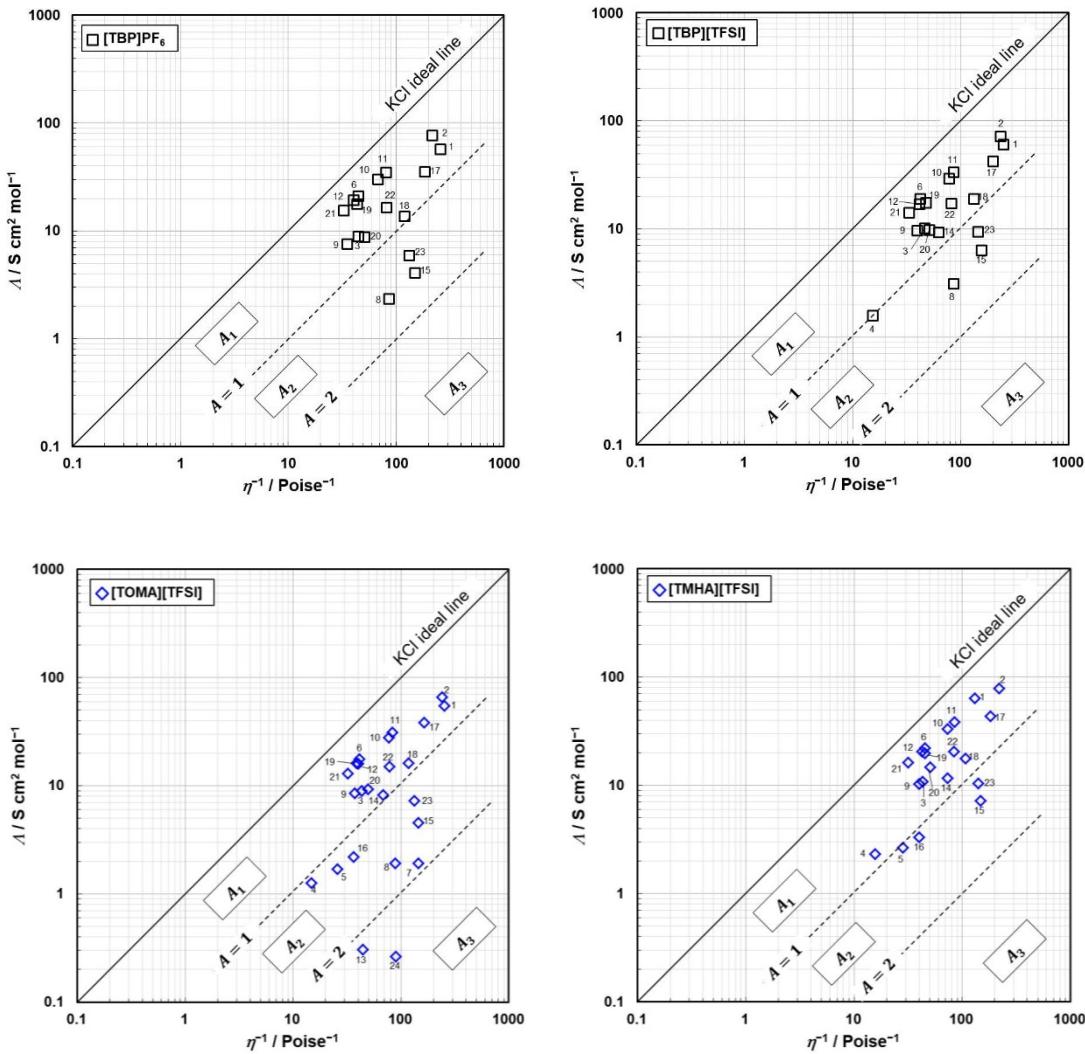


Figure S1 Walden plots of IL solutions at concentration 0.1 g mL⁻¹ at 25 °C. 1: Acetone, 2: acetonitrile, 3: acetophenone, 4: benzyl alcohol, 5: 2-butoxyethanol, 6: γ -butyrolactone, 7: 1-chlorobutane 8: chloroform, 9: cyclohexanone, 10: *N,N*-dimethylacetamide, 11: *N,N*-dimethylformamide, 12: dimethyl sulfoxide, 13: 1,4-dioxane, 14: ethanol, 15: ethyl acetate, 16: isopropanol, 17: methyl ethyl ketone, 18: methyl isobutyl ketone, 19: *N*-methyl-2-pyrrolidone, 20: 2-methoxyethanol, 21: propylene carbonate, 22: pyridine, 23: tetrahydrofuran, and 24: toluene.

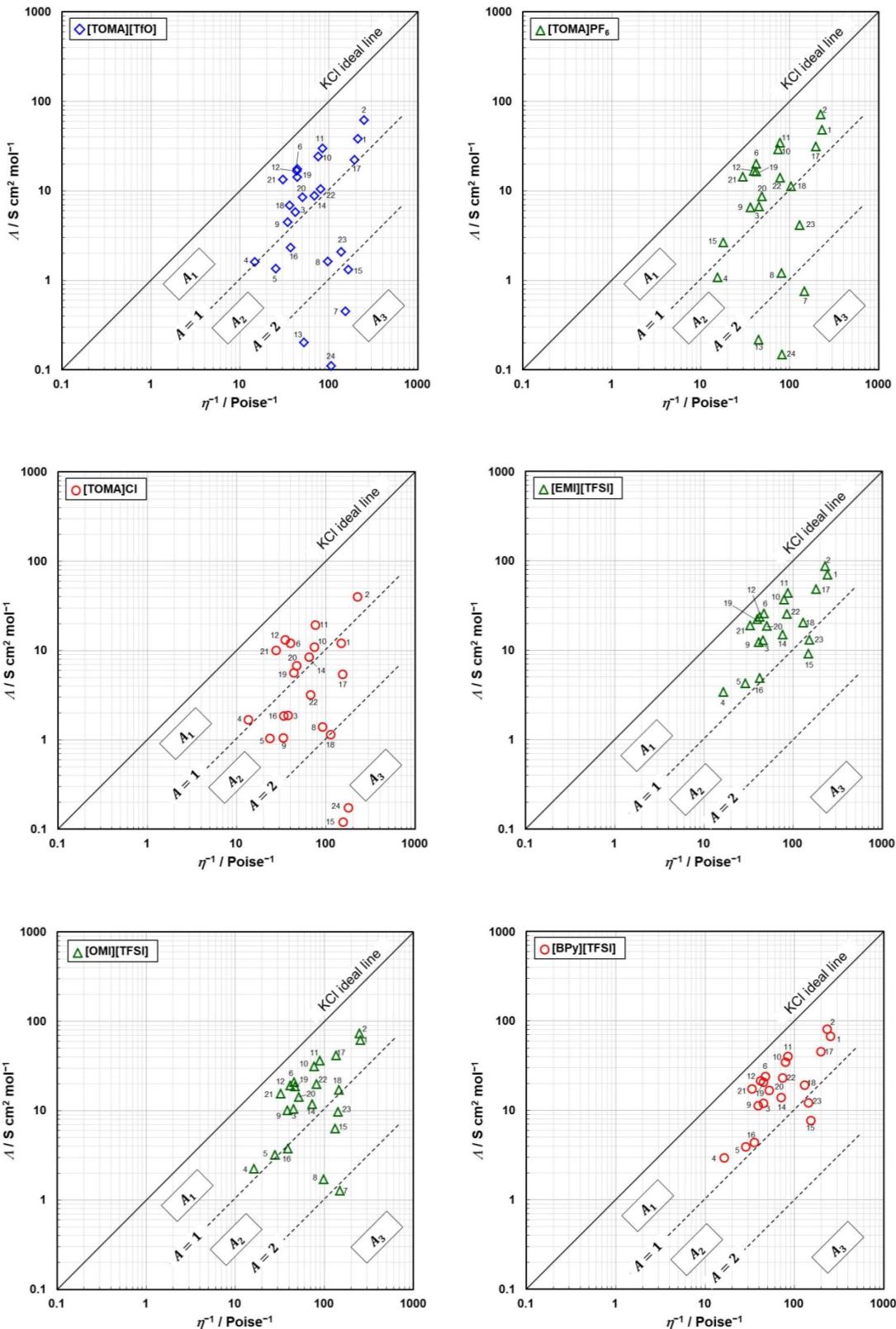


Figure S1 continued.

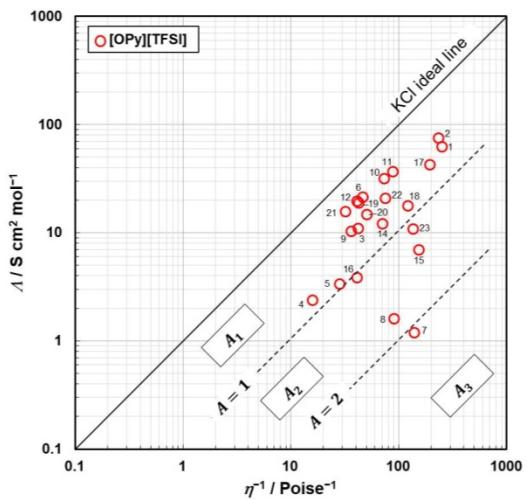


Figure S1 continued.

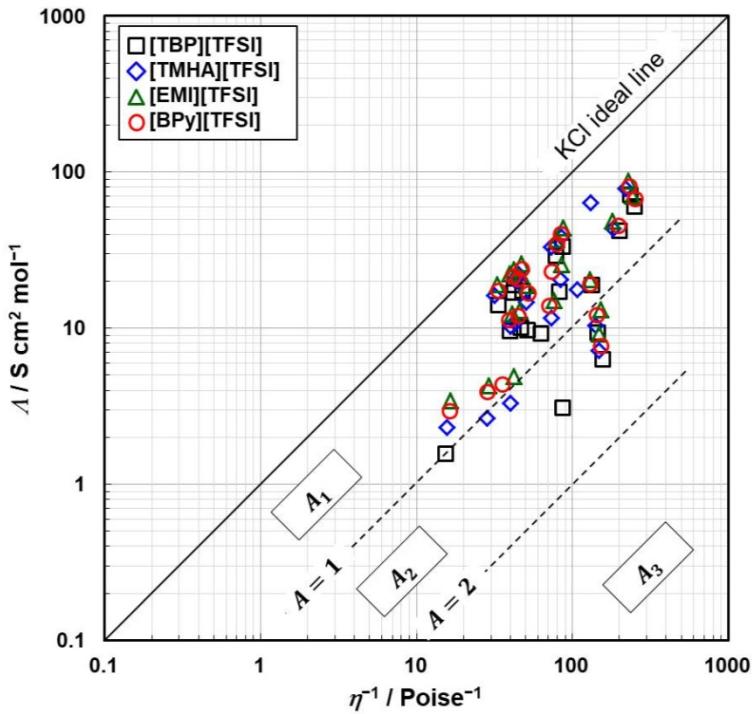


Figure S2 Walden plots of $[\text{TBP}][\text{TFSI}]$, $[\text{TMHA}][\text{TFSI}]$, $[\text{EMI}][\text{TFSI}]$, and $[\text{BPy}][\text{TFSI}]$ solutions at concentration 0.1 g mL^{-1} at 25°C .

Table S3 HSP results for ILs calculated from Hansen solubility spheres.

IL	δ_d /(MPa) ^{1/2}	δ_p /(MPa) ^{1/2}	δ_h /(MPa) ^{1/2}	δ_t /(MPa) ^{1/2}	R_0	Fitting	R_a ^{a)}
[TBP][TFSI]	17.8	15.6	7.4	24.8	12.1	0.920	2.4
[TBP]PF ₆	17.5	11.7	7.5	22.3	8.5	1.000	5.4
[TBLP][TFSI]	14.9	17.4	2.6	23.1	17.2	0.888	7.1
[TMHA][TFSI]	16.8	13	9.7	23.3	9.8	1.000	1.7
[TOMA][TFSI]	17.7	9.4	8.6	21.8	10.5	1.000	8.6
[TOMA][TfO]	17.7	9.4	8.6	21.8	10.5	1.000	5.4
[TOMA]PF ₆	17.9	9.7	6.2	21.3	9.4	1.000	5.8
[TOMA]Cl	17.7	9.4	8.8	21.9	10.7	1.000	—
[EMI][TFSI]	16.8	13	9.7	23.3	9.8	1.000	3.2
[OMI][TFSI]	16.4	12.5	9.1	22.6	10.1	1.000	3.1
[BPy][TFSI]	16.8	13.0	9.7	23.3	9.8	1.000	2.9
[OPy][TFSI]	17.3	12.2	9.9	23.3	9.7	1.000	5.8

a) R_a is the distance between the HSP calculated by the Hansen ionicity sphere and that of the Hansen solubility sphere.

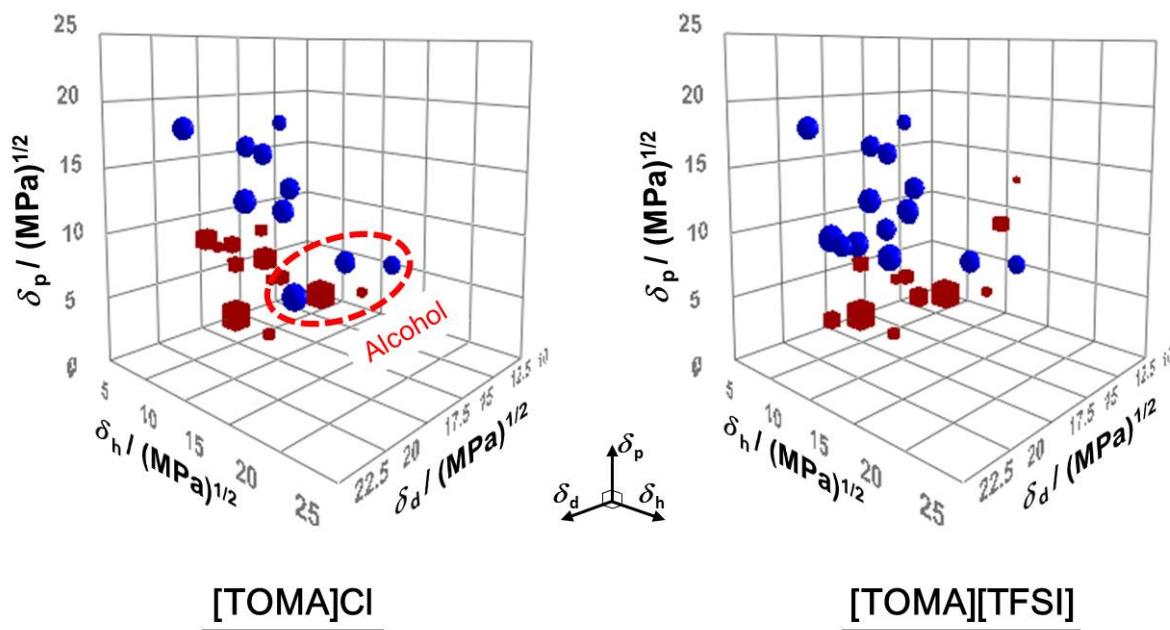


Figure S3 Hansen solubility results for [TOMA]Cl and [TOMA][TFSI]. Blue and red plots indicate solvents in solutions that showed A_1 and the other properties, respectively. Hansen sphere is calculated with blue plots inside the sphere, and red plots outside the sphere.

REFERENCES

- (1) Tokuda, H.; Hayamizu, K.; Ishii, K.; Susan, M. A. B. H.; Watanabe, M. Physicochemical Properties and Structures of Room Temperature Ionic Liquids. 2. Variation of Alkyl Chain Length in Imidazolium Cation. *J. Phys. Chem. B* **2005**, *109*(13), 6103–6110.
- (2) Yunus, N. M.; Mutalib, M. I. A.; Man, Z.; Bustam, M. A.; Murugesan, T. Thermophysical Properties of 1-Alkylpyridinium Bis(trifluoromethylsulfonyl)imide Ionic Liquids *J. Chem. Thermodyn.* **2010**, *42*(4), 491–495.
- (3) Tu, T.; Bao, X.; Assenmacher, W.; Peterlik, H.; Daniels, J.; Dotz, K. H. Efficient Air-stable Organometallic Low-molecular-mass Gelators for Ionic Liquids: Synthesis, Aggregation and Application of Pyridine-bridged Bis(benzimidazolylidene)-palladium Complexes. *Chemistry* **2009**, *15*(8), 1853–1861.