Unravelling Ion Dynamics and Interactions in an Ionic Liquid Electrolyte with a Protonated Anion for Lithium Batteries

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1. Density of the ILs

Table S1. The specific density (ρ) from 3 repetitions and the corresponding average den	sity (
$\overline{\rho}$), standard deviation (ρ_{SD}) and functional uncertainty (f_{FN}) for the ILs.	

	$ ho_1$ / kg L ⁻¹	$ ho_2$ / kg L ⁻¹	$ ho_3$ / kg L ⁻¹	$\overline{ ho}$ / kg L ⁻¹	$ ho_{ m SD}$ / kg L ⁻¹	<i>f</i> _{FN} / %
C ₃ mpyr LiDFTFSI	1.47	1.46	1.44	1.46	0.014	0.6
C ₂₀₁ mpyr LiDFTFSI	1.43	1.61	1.57	1.54	0.097	3.6

The experimental repetition uncertainties were systematically studied for density of the ILs, The standard deviation (ρ_{SD}) and fractional uncertainty (f_{FN}) of density were calculated using Eq. S [1], Eq. S [2],¹ respectively:

$$\rho_{\rm SD} = \sqrt{\Sigma(\rho_{\rm i} - \overline{\rho})^2 / (N - 1)} \qquad S[1]$$

$$f_{\rm FN} = \rho_{\rm SD} / (\sqrt{N \times \overline{\rho}}) \times 100\%$$
 S [2]

In Eq. S [1] and Eq. S [2], ρ_i is the density of sample i, $\overline{\rho}$ is the mean value of all the measured samples, and *N* is the number of measurements. The calculated values are shown in Table S1.

2. NMR spectra of LIDFTFSI



Figure S1: NMR spectra of the LiDFTFSI salt. The deuterated solvent for the NMR measurement is acetone- d_6 .

3. Temperature dependent correlation times of different nuclei in C₃mpyr LiDFTFSI

Table S2: Correlation times from ¹⁹F, ¹H and ⁷Li nuclei T₁ relaxation measurements extracted from BPP fitting at varying temperatures in C₃mpyr LiDFTFSI.

	¹⁹ F		¹ H			⁷ Li
Temperature (K)	CF ₃	CF ₂ H	Anion	C2	C6	
253	6.41E-10	9.78E-10	9.52E-10	7.91E-10	4.34E-10	1.50E-08
263	4.99E-10	7.55E-10	6.89E-10	5.86E-10	3.53E-10	1.06E-08
273	3.96E-10	5.95E-10	5.11E-10	4.44E-10	2.92E-10	7.71E-09
283	3.19E-10	4.76E-10	3.86E-10	3.43E-10	2.44E-10	5.72E-09
293	2.61E-10	3.87E-10	2.98E-10	2.70E-10	2.07E-10	4.33E-09
303	2.17E-10	3.19E-10	2.34E-10	2.16E-10	1.78E-10	3.34E-09
313	1.82E-10	2.66E-10	1.86E-10	1.75E-10	1.54E-10	2.62E-09
323	1.54E-10	2.24E-10	1.51E-10	1.44E-10	1.34E-10	2.08E-09
333	1.32E-10	1.91E-10	1.23E-10	1.19E-10	1.18E-10	1.68E-09
343	1.14E-10	1.64E-10	1.02E-10	1.00E-10	1.05E-10	1.37E-09
353	9.97E-11	1.43E-10	8.55E-11	8.50E-11	9.35E-11	1.14E-09

4. Temperature dependent correlation times of different nuclei in C₂₀₁mpyr LiDFTFSI

	¹⁹ F		¹ H			⁷ Li
Temperature (K)	CF ₃	CF ₂ H	Anion	C2	C6	
253	5.97E-10	1.04E-09	1.03E-09	1.07E-09	5.69E-10	1.15E-08
263	4.64E-10	7.88E-10	7.28E-10	7.61E-10	4.43E-10	8.12E-09
273	3.67E-10	6.09E-10	5.27E-10	5.57E-10	3.51E-10	5.88E-09
283	2.96E-10	4.79E-10	3.90E-10	4.17E-10	2.82E-10	4.36E-09
293	2.41E-10	3.83E-10	2.95E-10	3.18E-10	2.31E-10	3.30E-09
303	2.00E-10	3.11E-10	2.27E-10	2.47E-10	1.91E-10	2.54E-09
313	1.67E-10	2.55E-10	1.78E-10	1.95E-10	1.60E-10	1.99E-09
323	1.42E-10	2.13E-10	1.41E-10	1.57E-10	1.36E-10	1.58E-09
333	1.21E-10	1.79E-10	1.14E-10	1.27E-10	1.16E-10	1.27E-09
343	1.05E-10	1.52E-10	9.28E-11	1.05E-10	1.00E-10	1.04E-09
353	9.12E-11	1.30E-10	7.66E-11	8.69E-11	8.75E-11	8.59E-10

Table S3: Correlation times from ¹⁹F, ¹H and ⁷Li nuclei T₁ relaxation measurements extracted from BPP fitting at varying temperatures in C₃mpyr LiDFTFSI.

Reference

(1) Cohen, E. R. An Introduction to Error Analysis: The Study of Uncertainties in Physical Measurements. *Measurement Science and Technology* **1998**, *9* (6), 191–192.