

**Probing Lithium-ion Induced Micro-environment Changes in Pyrrolidinium-Based  
Mono-cationic and Di-cationic Ionic Liquid**

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## Supplementary Materials

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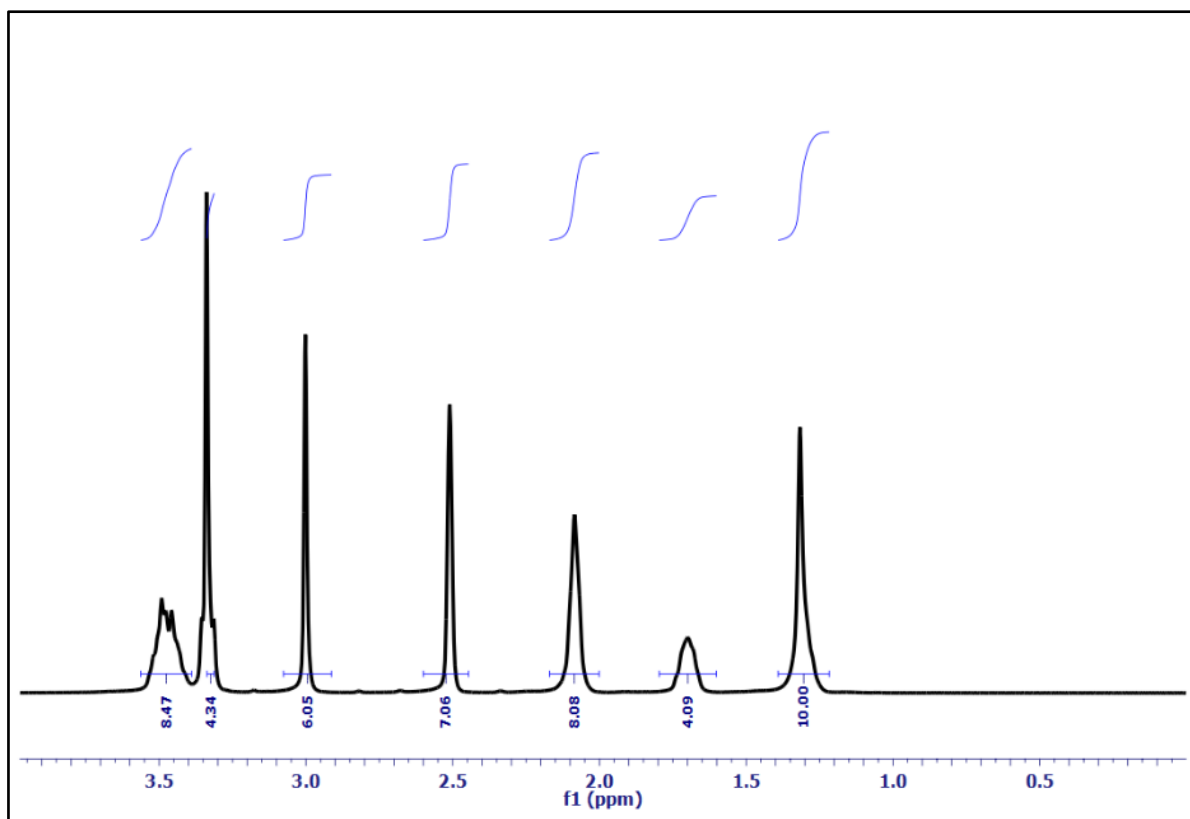
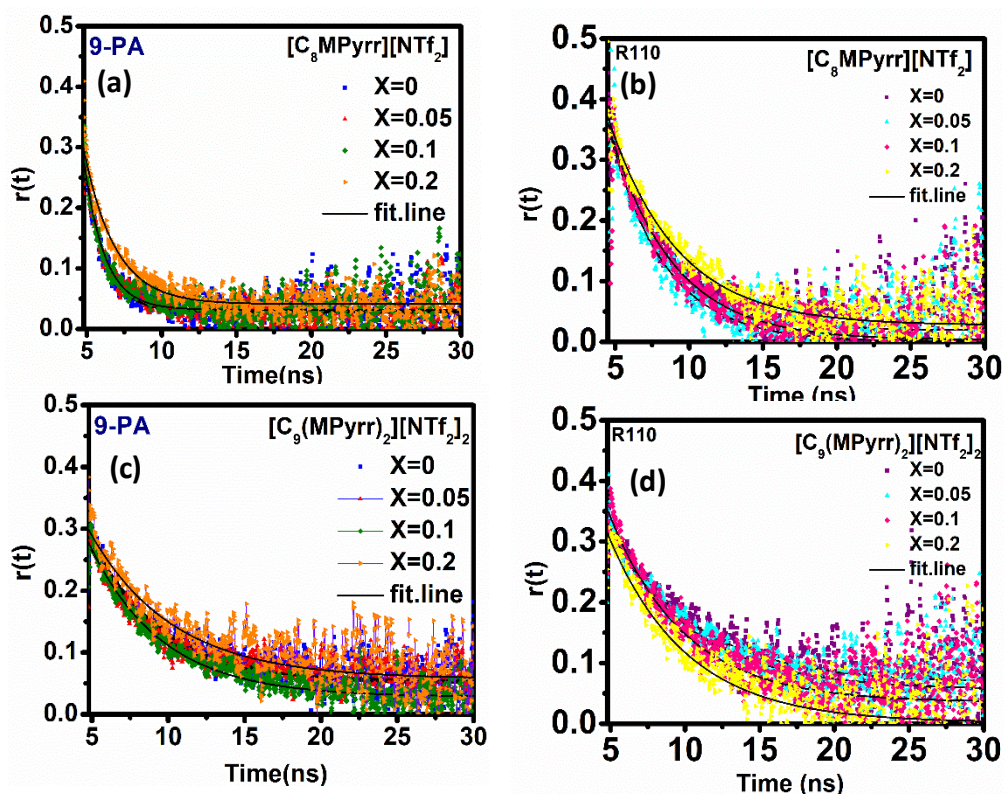


Fig S1.  $^1\text{H}$  NMR spectra of synthesized DIL  $[\text{C}_9(\text{MPyrr})_2][\text{NTf}_2]_2$



**Fig S2:** Anisotropy decay profile of 9-PA and R110 in MIL and DIL in absence and presence of various mole-fraction of Lithium-salt.

**Table S1.** Simulation details of the studied system.

| System                   | Cations (MIL/DIL) | Li <sup>+</sup> Ions | Anions (TFSI) | Li <sup>+</sup> /TFSI Ratio |
|--------------------------|-------------------|----------------------|---------------|-----------------------------|
| MIL                      | 250               | 0                    | 250           | N.A.                        |
| MIL + LiNTf <sub>2</sub> | 250               | 250                  | 500           | 1:2                         |
| DIL                      | 125 (+2 Charge)   | 0                    | 250           | N.A.                        |
| DIL + LiNTf <sub>2</sub> | 125 (+2 charge)   | 250                  | 500           | 1:2                         |