Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information

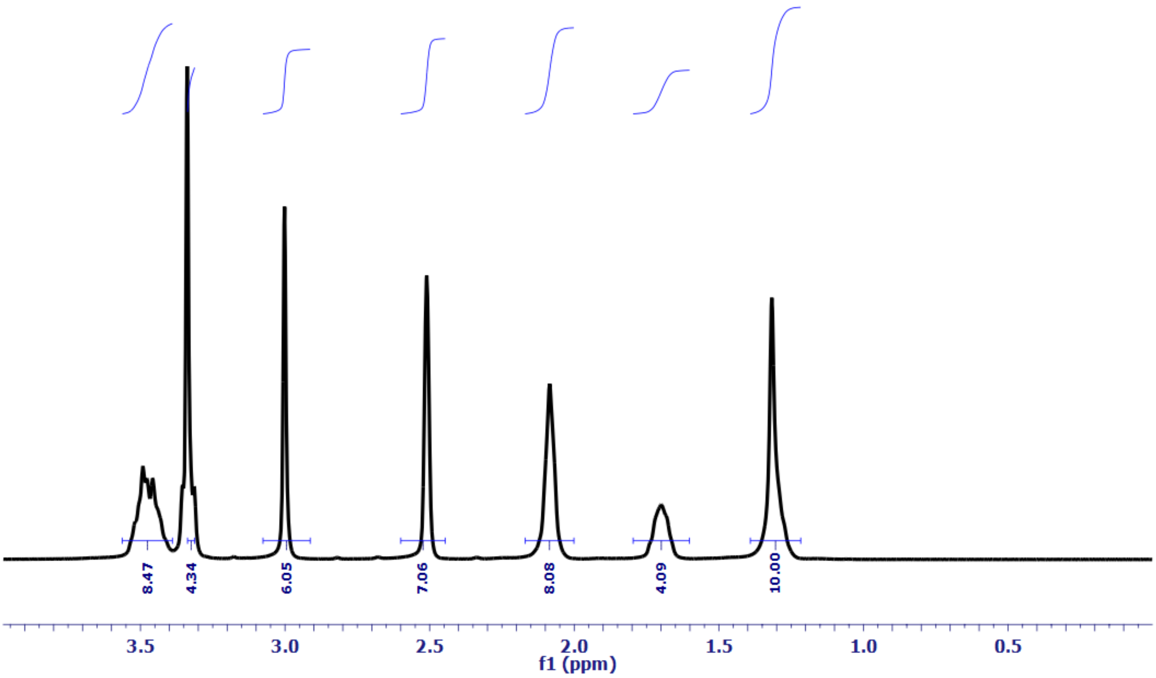
Comparison between Pyrrolidinium-based and Imidazolium-based Dicationic Ionic Liquids: Intermolecular Interaction, Structural Organization and Solute Dynamics

Amita Mahapatra,[a] Manjari Chakraborty,[a] Sahadev Barik[a] and Moloy Sarkar[a*]

[a]*School of Chemical Sciences, National Institute of Science Education and Research, HBNI, P.O. Jatni, Khurda, 752050, Bhubaneswar, Odisha, India*

*Corresponding author, Tel: +91-674-2494190 Fax: +91-674-2494004. Email: msarkar@niser.ac.in

(a)



(b)

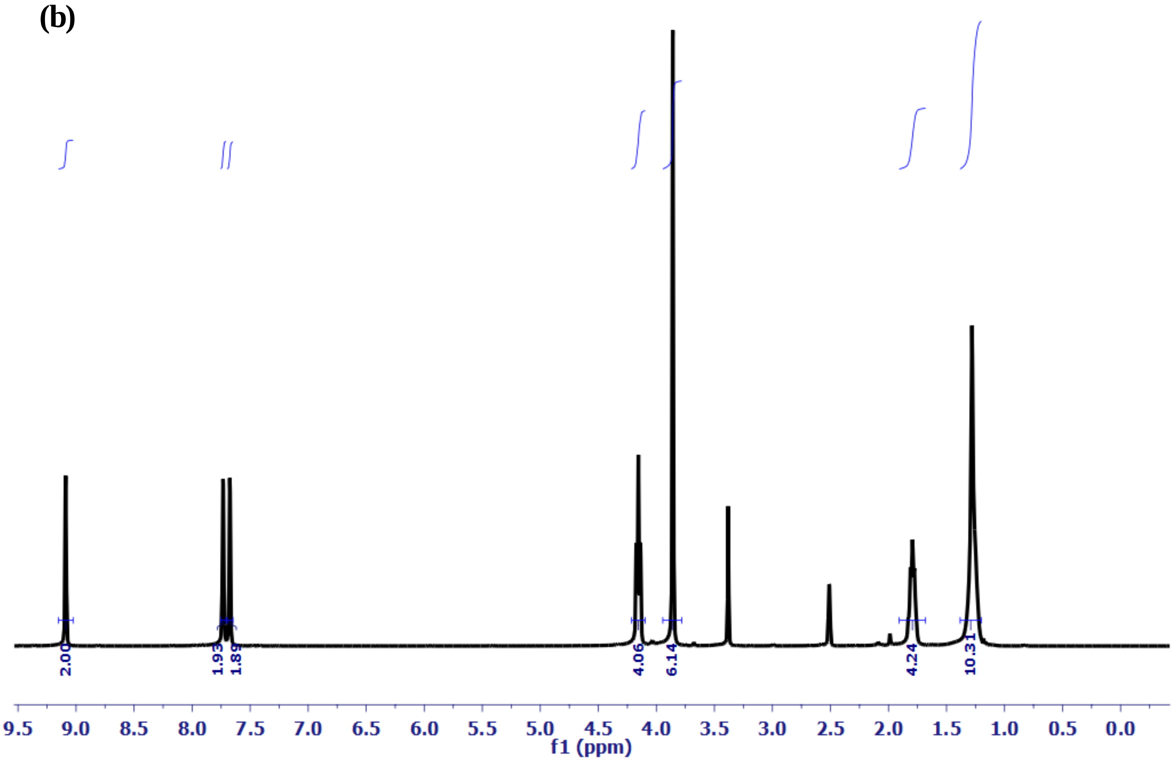


Fig. S1 ^{1}H NMR spectra of (a) $[C_9(MPyrr)_2][NTf_2]_2$ and (b) $[C_9(Mim)_2][NTf_2]_2$ in DMSO-d^6.

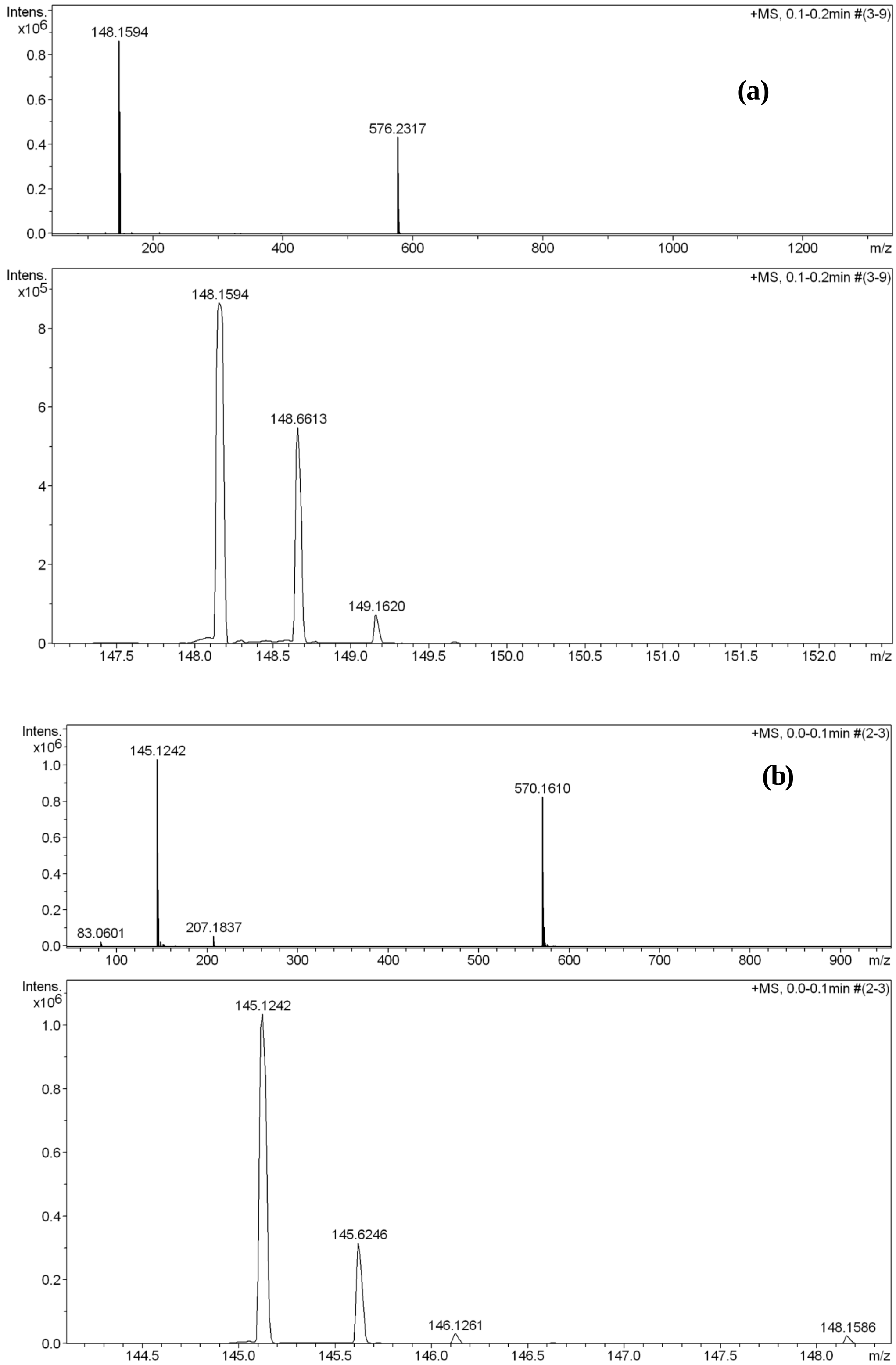


Fig. S2 ESI-Mass spectra of (a) $[C_9(MPyrr)_2][NTf_2]_2$ and (b) $[C_9(Mim)_2][NTf_2]_2$.

Table S1 Normalized emission maximum of C153 in MILs and DILs.

Systems	**λ_{max} (nm)**
$[C_4Mim][NTf_2]$	525
$[C_4MPyrr][NTf_2]$	519
$[C_9(Mim)_2][NTf_2]_2$	521
$[C_9(MPyrr)_2][NTf_2]_2$	520

Table S2 Viscosity of the MILs and DILs with standard error

T(K)	Viscosity (cP)					
	$[C_4Mim]$	$[C_4MPyrr]$	$[C_8Mim]$	$[C_8MPyrr]$	$[C_9(Mim)_2]$	$[C_9(MPyrr)_2]$
293	63.2±3.16	90.3±4.51	115±5.75	128.0±6.41	960.0±48.00	1024±51.2
298	49.6±2.48	73.2±3.66	90.3±4.51	99.4±4.97	655.9± 32.71	710.2± 35.51
303	40.4±2.02	58.9±2.94	72.1±3.60	81.1±4.05	486.6± 24.33	535.2± 26.76
308	33.4±1.67	48.4±2.42	57.0±2.85	62.8±3.14	361.5± 18.07	404.6± 20.23
313	27.5±1.375	39.2±1.96	45.6±2.26	51.0±2.55	272.8± 13.64	312.5± 15.62

Equation S1 Vogel-Tamman-Fulcher (VFT) equation:

$$\eta = \eta_0 \; exp\left[\frac{B}{(T-T_0)}\right] \qquad (1)$$

Where η_0 (cP), B (K), and T_0(K) are fitting parameters.

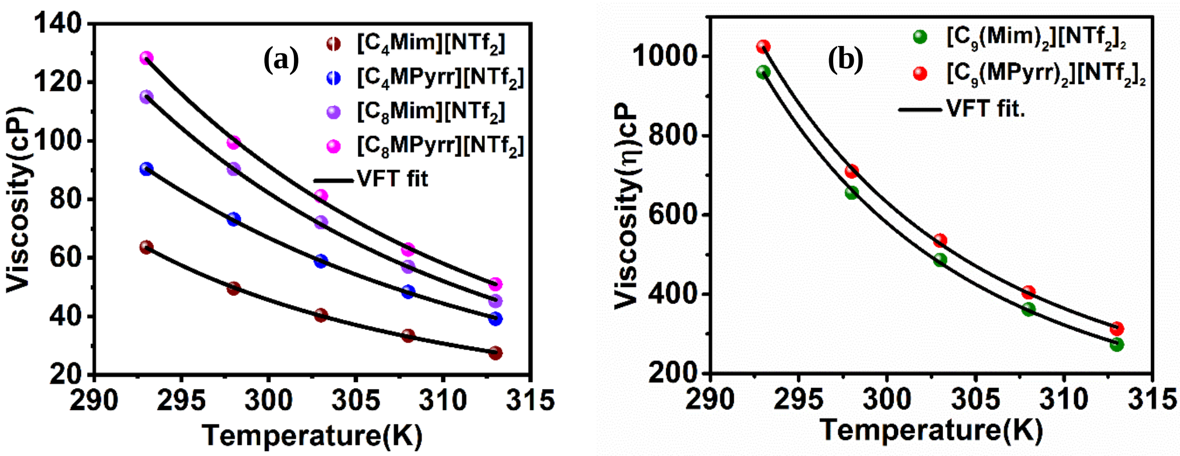
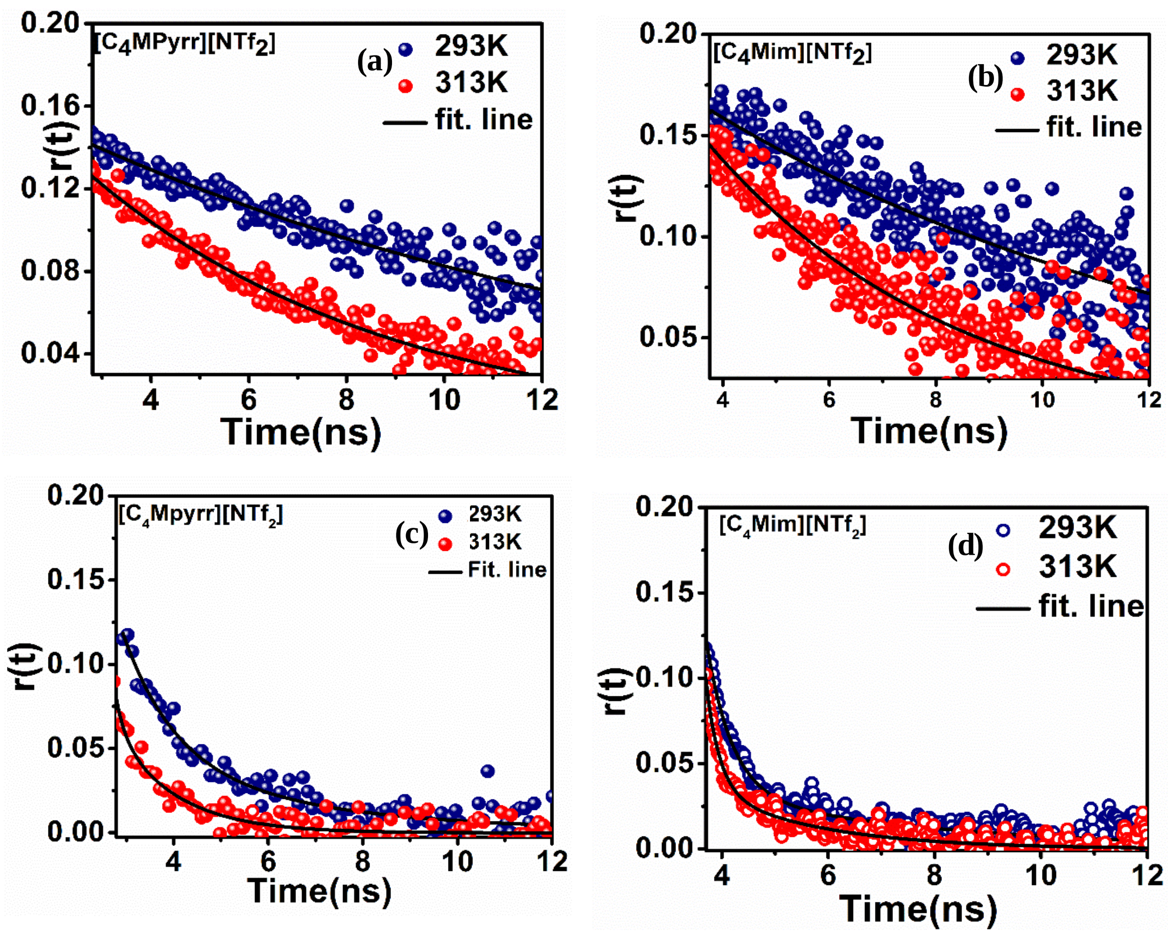


Fig. S3 Vogel-Tamman-Fulcher (VTF) fitting of Viscosity (η) (cP) of (a) MILs and (b) DILs with Temperature (K).



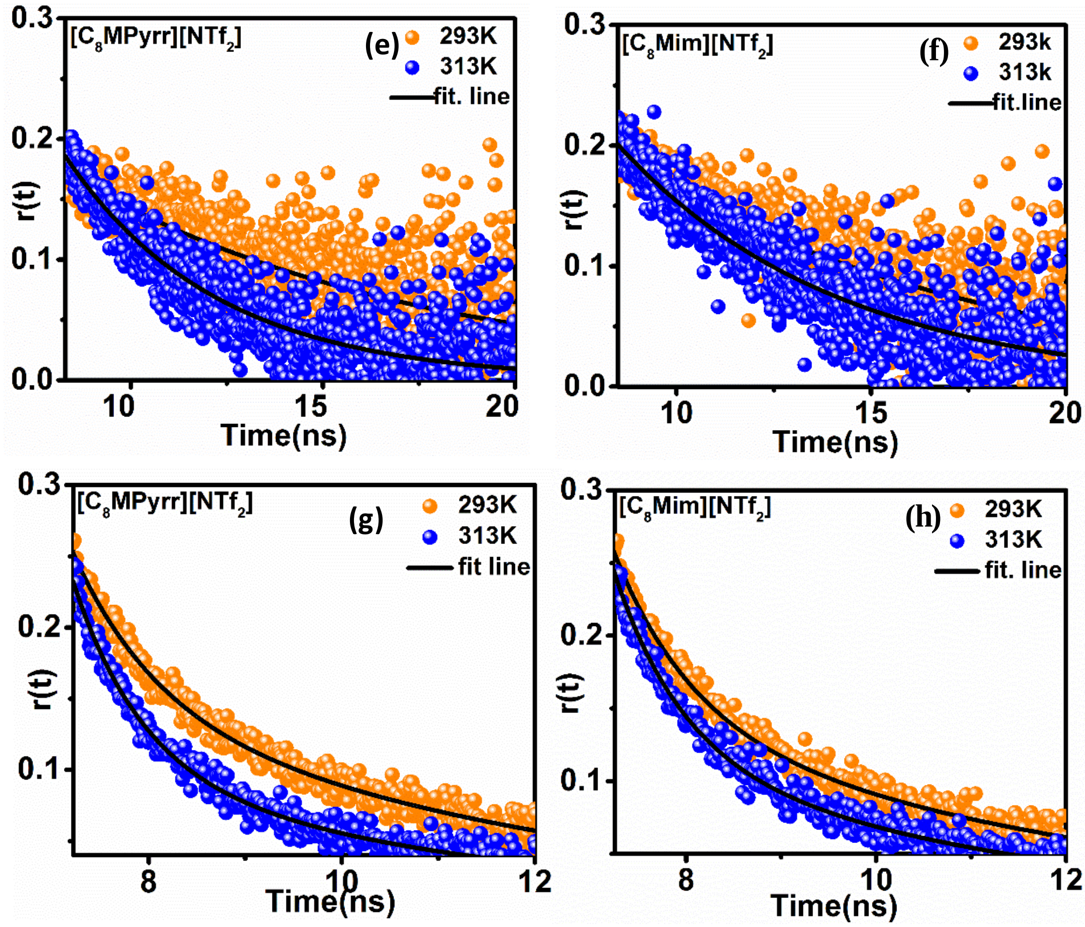


Fig. S4 Time-resolved fluorescence anisotropy decay for MPTS (a,b) and MPTS (c,d) in butyl chain containing MILs and for MPTS (e,f) and MPTS (g,h) in octyl chain containing MILs. The solid line in the figure represents the bi-exponential fit for perylene and single exponential fit for MPTS.

Table S3 Van der Waals Volumes (V), Shape Factor (*f*), and Slip Boundary (C_{slip}) Condition Parameters of Model probes

Solute	van der Waals volume (V) /Å ^{3}	shape factor (*f*)	C_{slip}
Perylene	225	1.76	0.085
MPTS	343	1.33	0.11

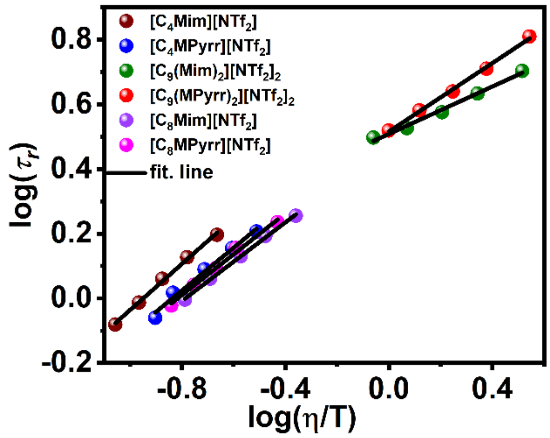


Fig. S5 Power law plot.