

Supplementary Information

Organic salts utilising the hexamethylguanidinium cation: the influence of the anion on the structural, physical and thermal properties.

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NMR data

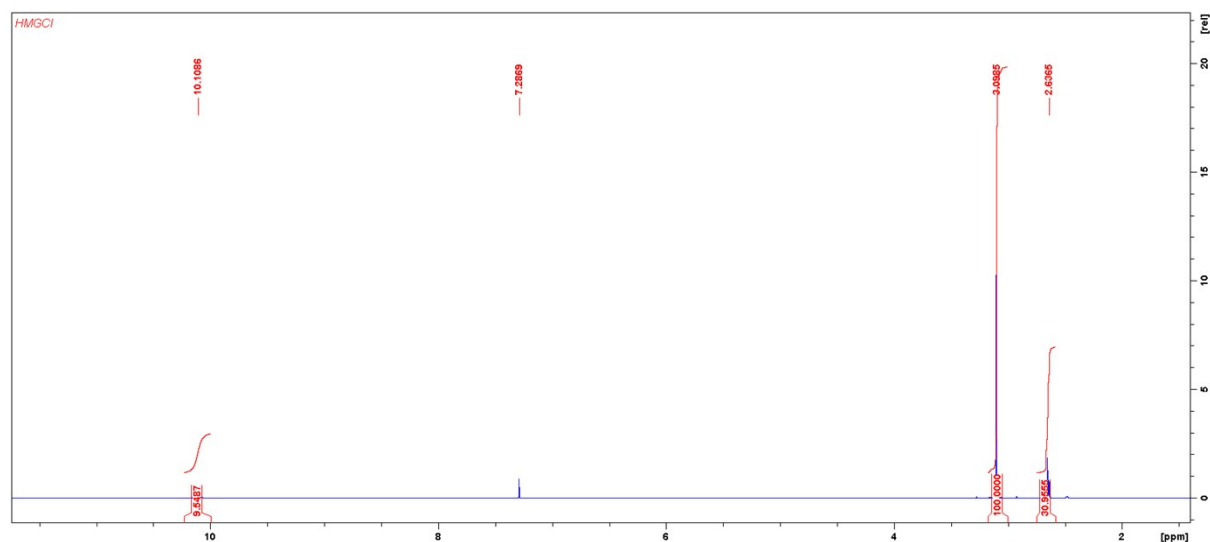


Figure S1; ¹H NMR for Hexamethylguanidinium chloride, $[(\text{CH}_3)_2\text{N}]_3\text{C}[\text{Cl}]$, [HMG][Cl]

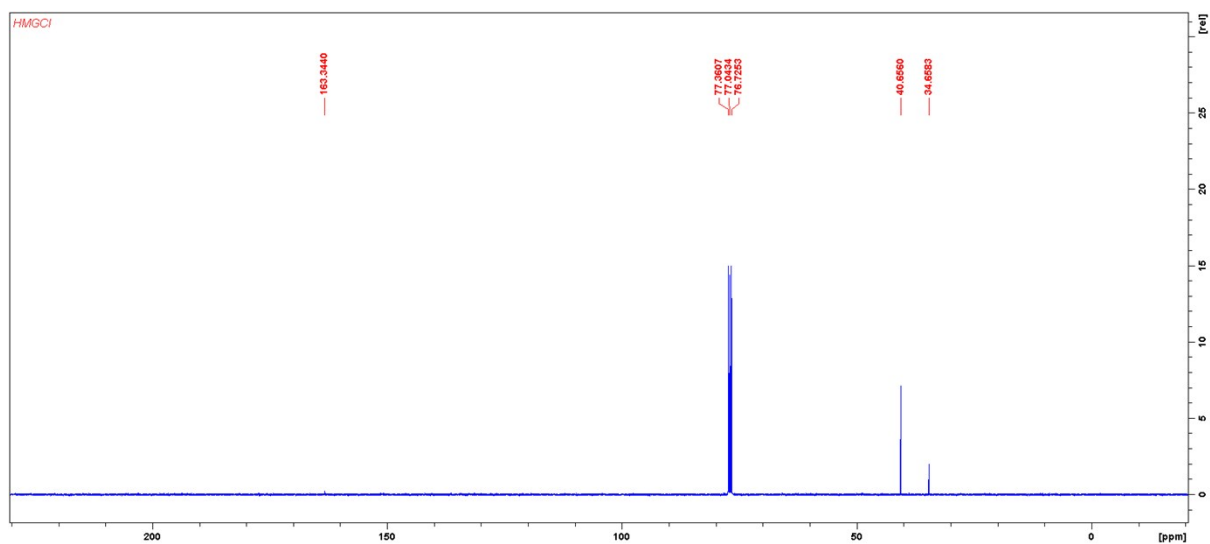


Figure S2; ¹³C NMR for Hexamethylguanidinium chloride, [((CH₃)₂N)₃C]Cl, [HMG][Cl]

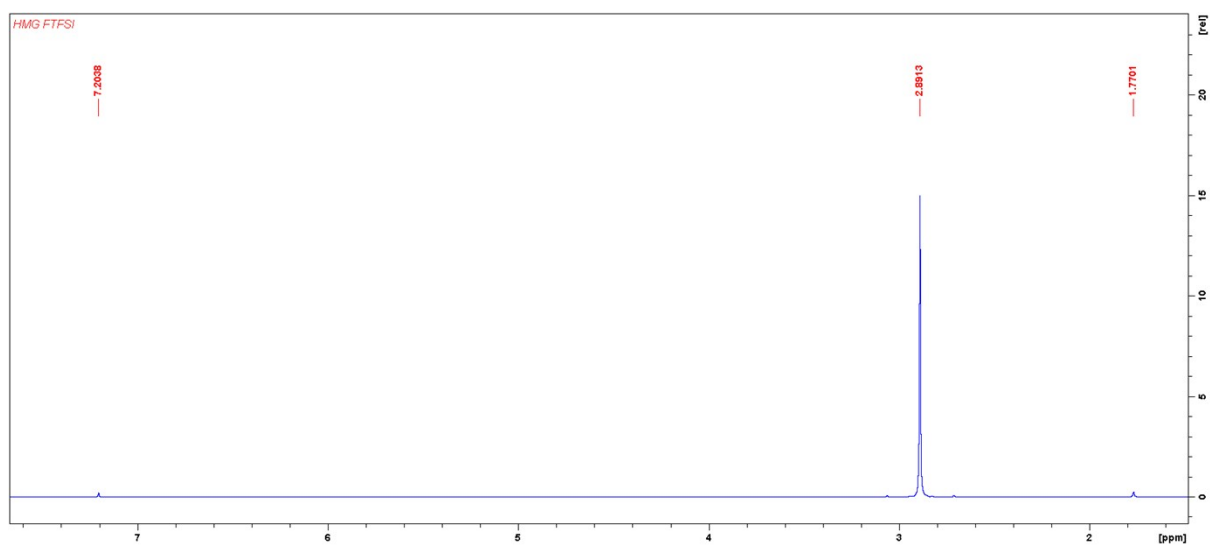


Figure S3; ¹H NMR for Hexamethylguanidinium trifluoromethanesulfonyl(fluorosulfonyl)imide, [((CH₃)₂N)₃C][FTFSI], [HMG][FTFSI]

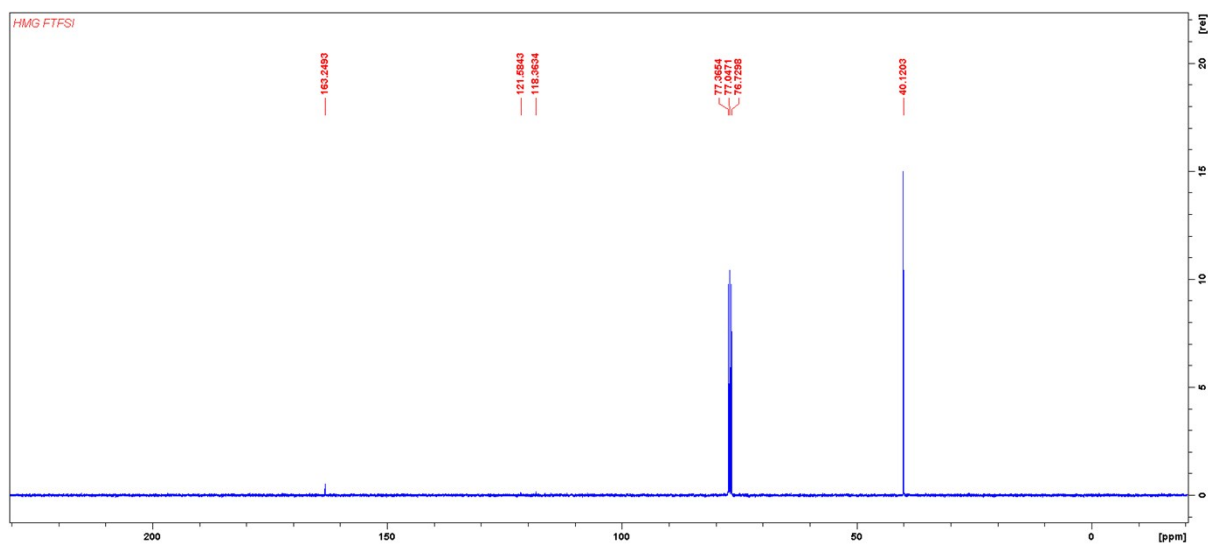


Figure S4; ¹³C NMR for Hexamethylguanidinium trifluoromethanesulfonyl(fluorosulfonyl)imide, $[(\text{CH}_3)_2\text{N}]_3\text{C}[\text{FTFSI}]$, $[\text{HMG}][\text{FTFSI}]$

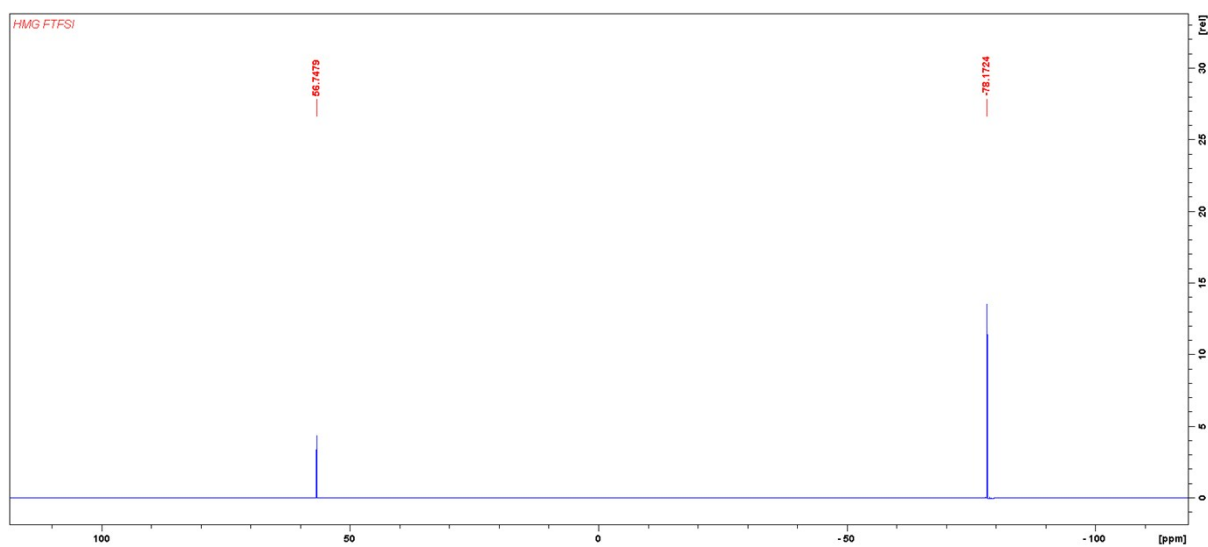


Figure S5; ¹⁹F NMR for Hexamethylguanidinium trifluoromethanesulfonyl(fluorosulfonyl)imide, $[(\text{CH}_3)_2\text{N}]_3\text{C}[\text{FTFSI}]$, $[\text{HMG}][\text{FTFSI}]$

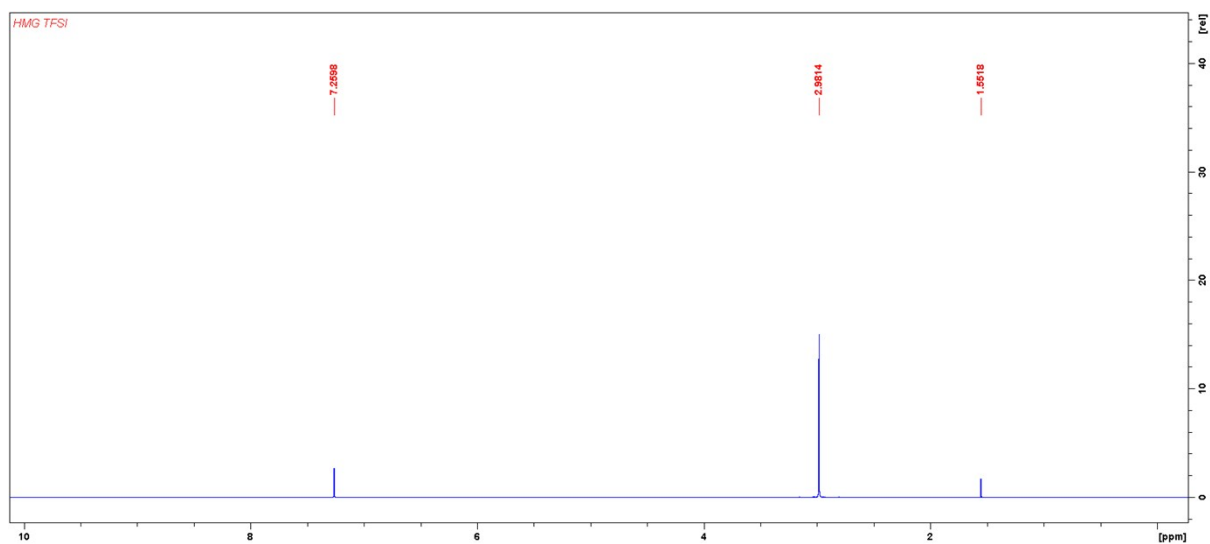


Figure S6; ^1H NMR for Hexamethylguanidinium bis(trifluoromethanesulfonyl)imide, $[\text{HMG}][\text{TFSI}]$

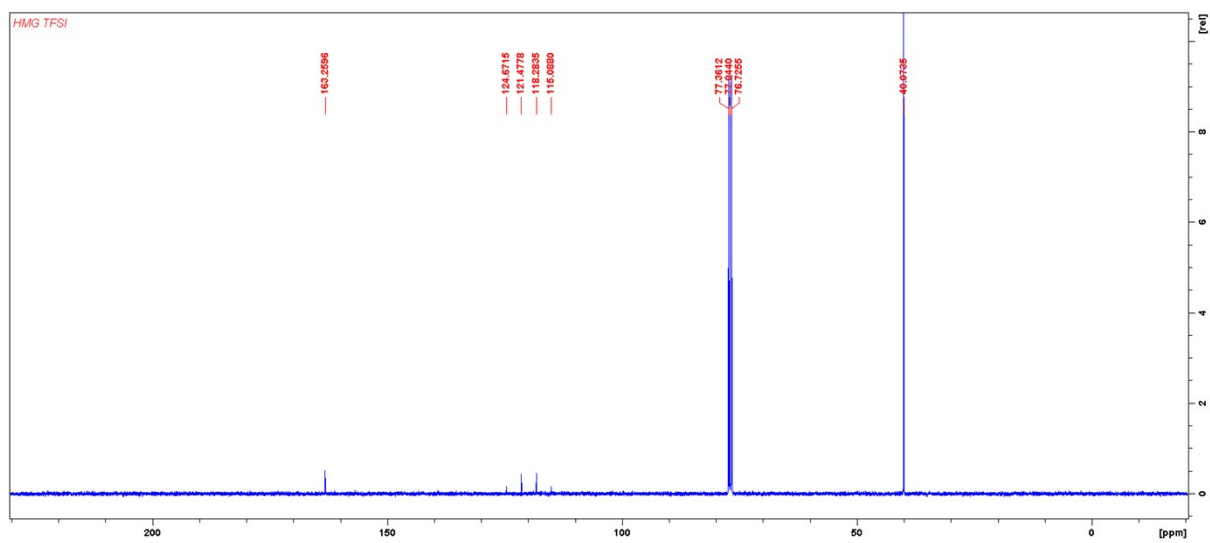


Figure S7; ^{13}C NMR for Hexamethylguanidinium bis(trifluoromethanesulfonyl)imide, $[\text{HMG}][\text{TFSI}]$

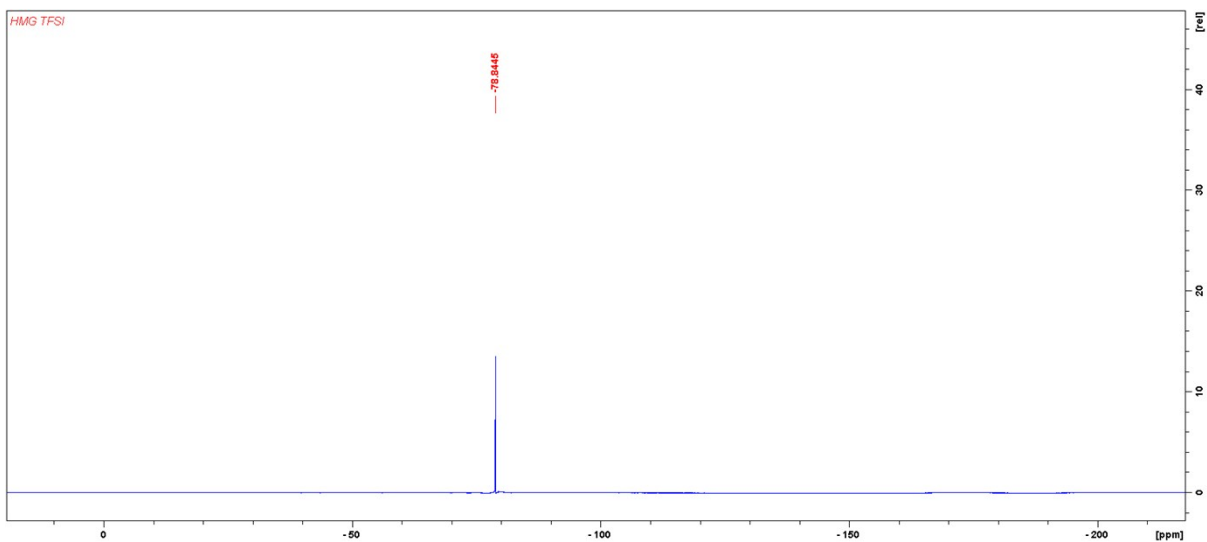


Figure S8; ^{19}F NMR for Hexamethylguanidinium bis(trifluoromethanesulfonyl)imide, $[((\text{CH}_3)_2\text{N})_3\text{C}][\text{TFSI}]$, $[\text{HMG}][\text{TFSI}]$

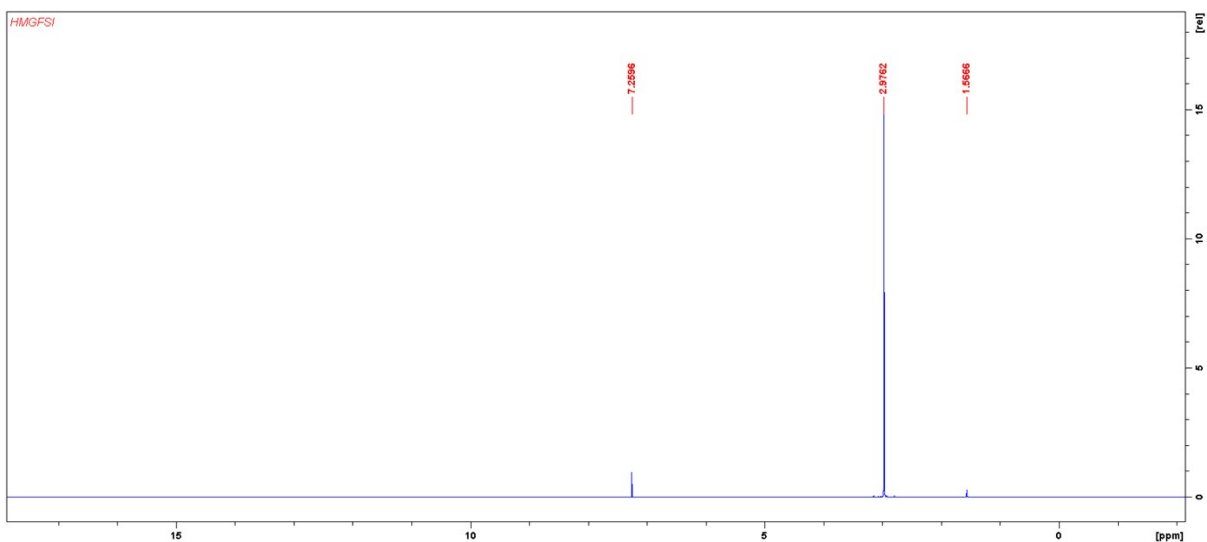


Figure S9; ^1H NMR for Hexamethylguanidinium bis(fluorosulfonyl)imide, $[((\text{CH}_3)_2\text{N})_3\text{C}][\text{FSI}]$, $[\text{HMG}][\text{FSI}]$

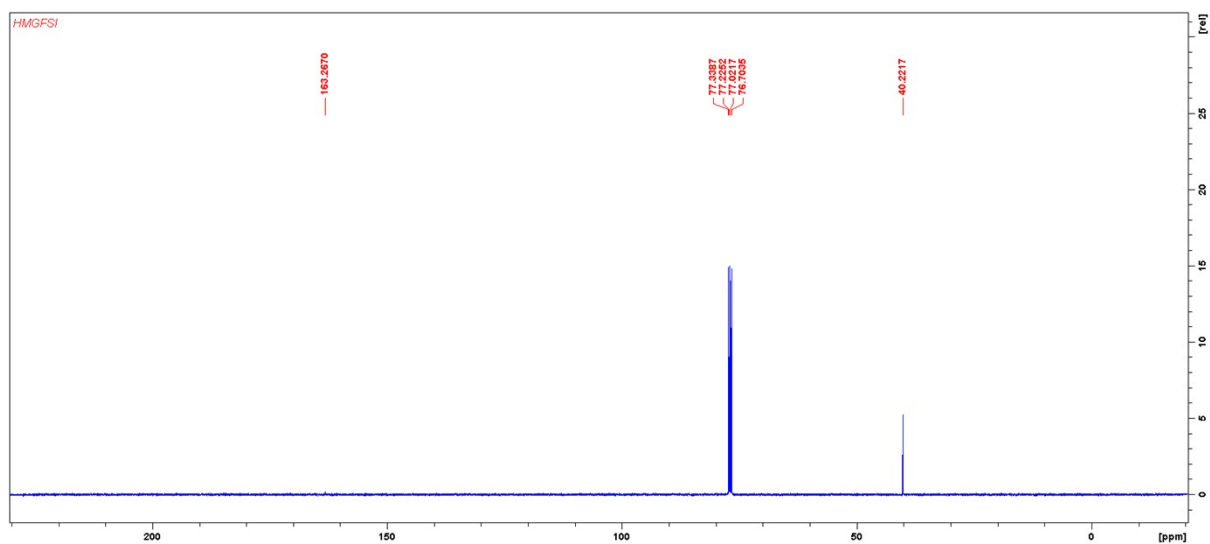


Figure S10; ^{13}C NMR for Hexamethylguanidinium bis(fluorosulfonyl)imide, $[(\text{CH}_3)_2\text{N}]_3\text{C}[\text{FSI}]$, $[\text{HMG}][\text{FSI}]$

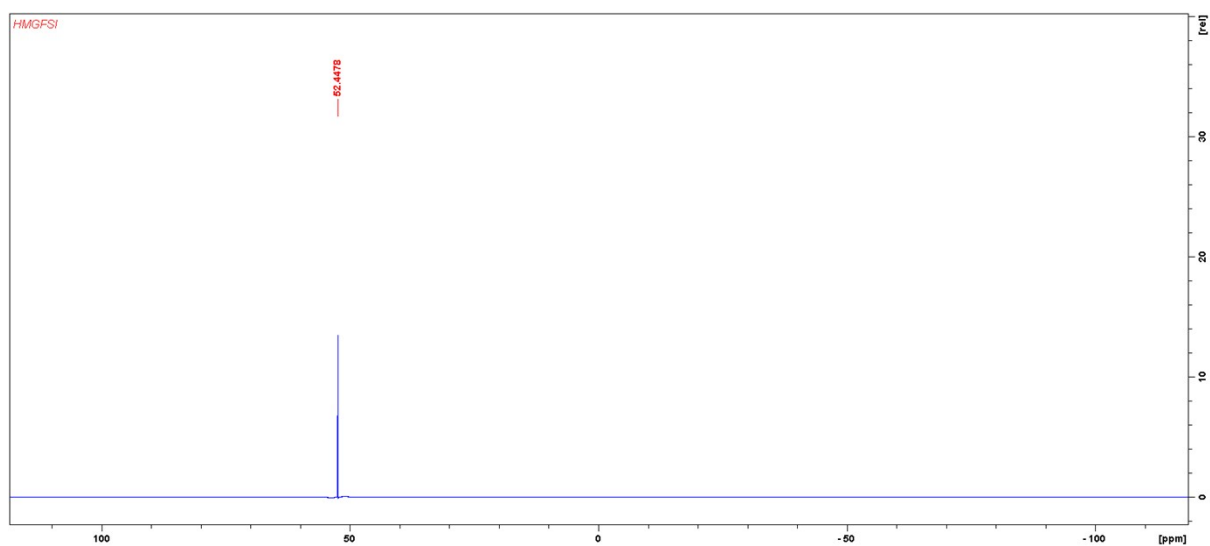


Figure S11; ^{19}F NMR for Hexamethylguanidinium bis(fluorosulfonyl)imide, $[(\text{CH}_3)_2\text{N}]_3\text{C}[\text{FSI}]$, $[\text{HMG}][\text{FSI}]$

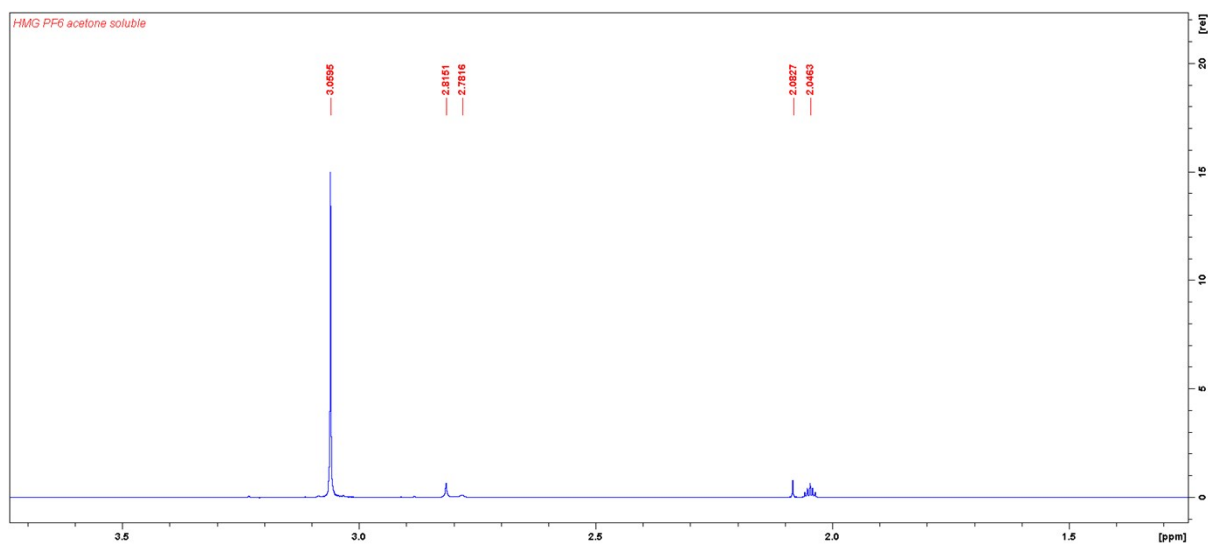


Figure S12; ¹H NMR for Hexamethylguanidinium hexafluorophosphate, $[(\text{CH}_3)_2\text{N}]_3\text{C}][\text{PF}_6]$, [HMG][PF₆]

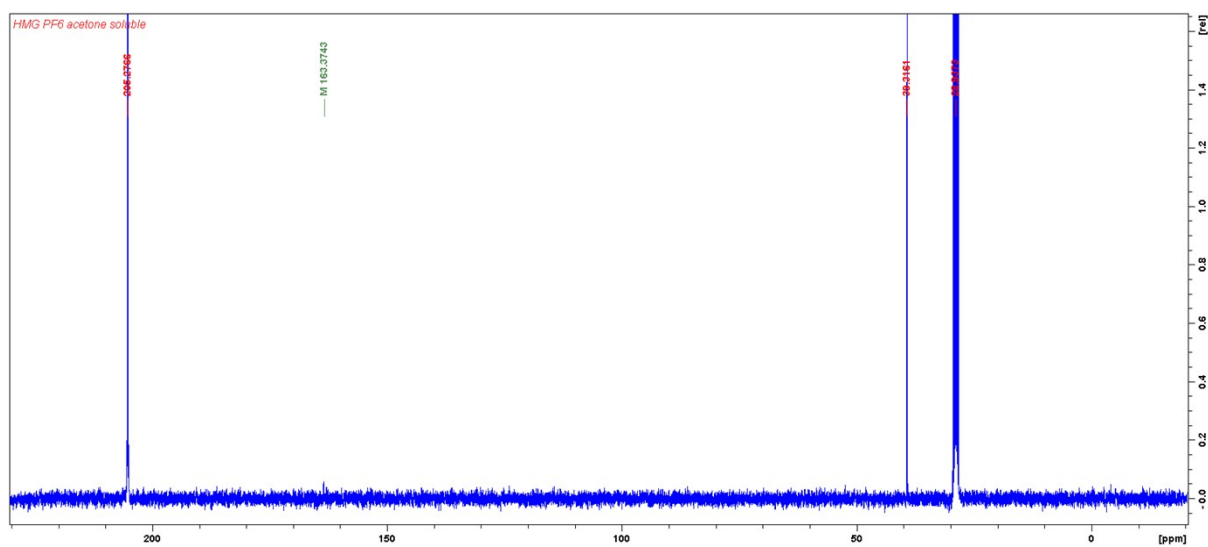


Figure S13; ¹³C NMR for Hexamethylguanidinium hexafluorophosphate, $[(\text{CH}_3)_2\text{N}]_3\text{C}][\text{PF}_6]$, [HMG][PF₆]

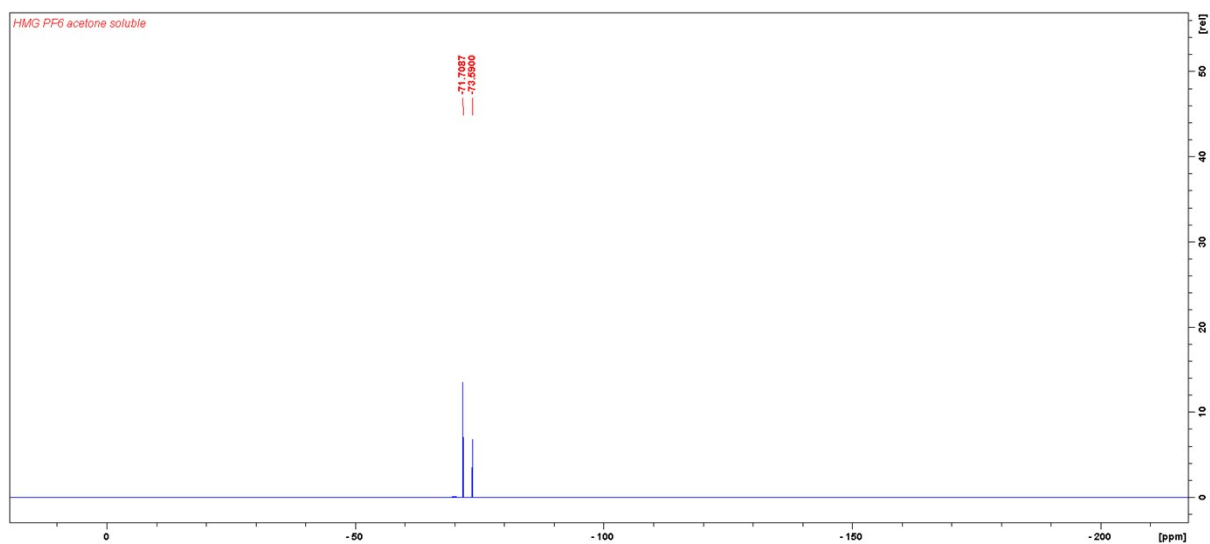


Figure S14; ^{19}F NMR for Hexamethylguanidinium hexafluorophosphate, $[((\text{CH}_3)_2\text{N})_3\text{C}][\text{PF}_6]$, $[\text{HMG}][\text{PF}_6]$

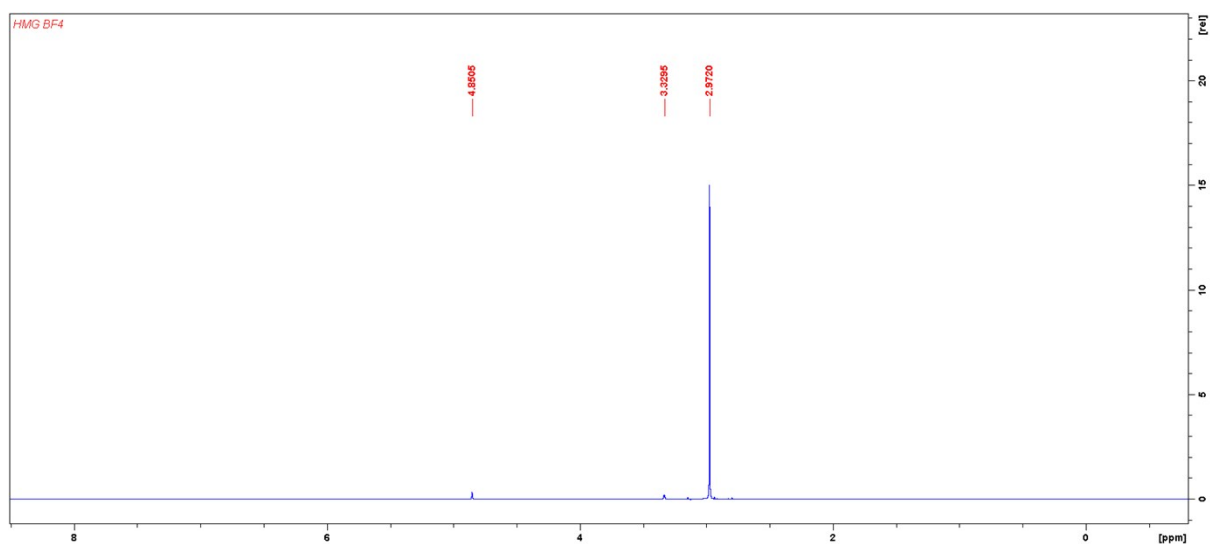


Figure S15; ^1H NMR for Hexamethylguanidinium tetrafluoroborate, $[((\text{CH}_3)_2\text{N})_3\text{C}][\text{BF}_4]$, $[\text{HMG}][\text{BF}_4]$

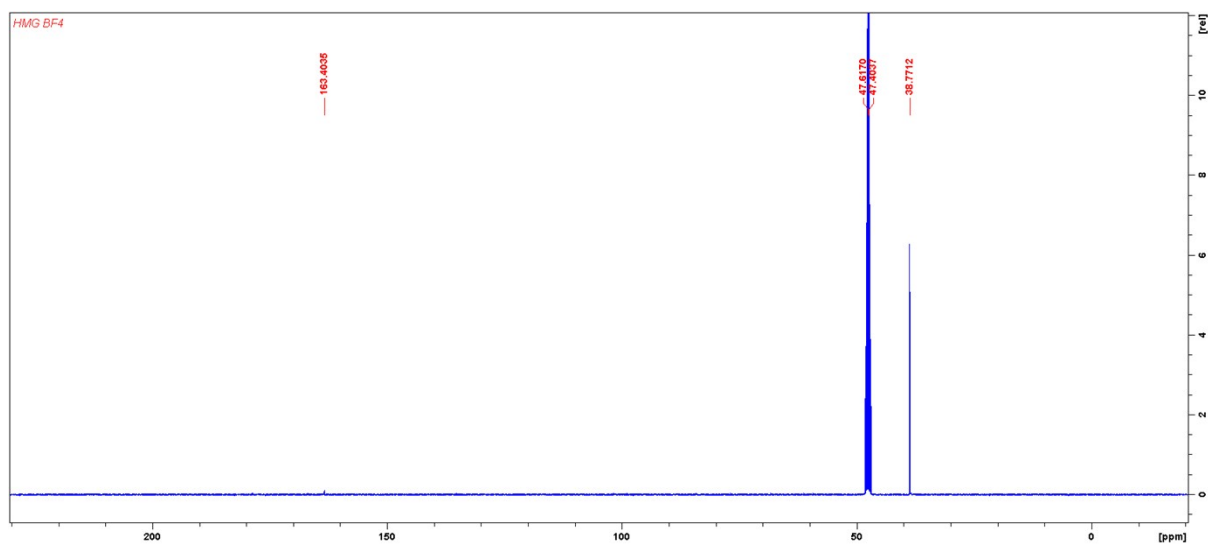


Figure S16; ^{13}C NMR for Hexamethylguanidinium tetrafluoroborate, $[\text{((CH}_3)_2\text{N)}_3\text{C}][\text{BF}_4]$, $[\text{HMG}][\text{BF}_4]$

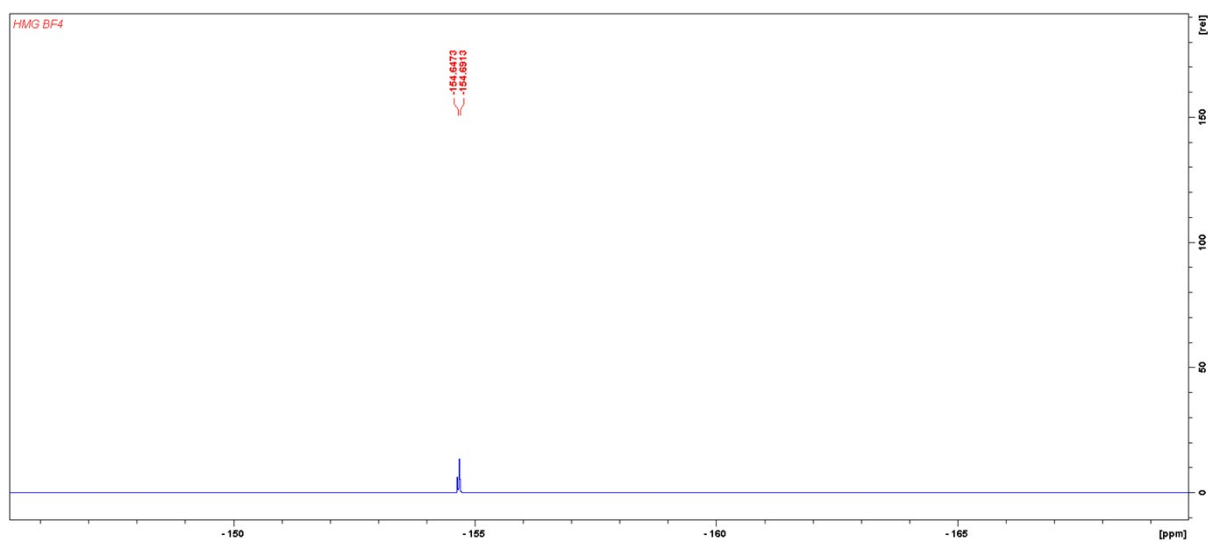


Figure S17; ^{19}F NMR for Hexamethylguanidinium tetrafluoroborate, $[\text{((CH}_3)_2\text{N)}_3\text{C}][\text{BF}_4]$, $[\text{HMG}][\text{BF}_4]$

Powder X-ray diffraction.

Room temperature PXRD of $[\text{HMG}][\text{PF}_6]$, $[\text{HMG}][\text{TFSI}]$ and $[\text{HMG}][\text{BF}_4]$.

HMG PF6 (Coupled TwoTheta/Theta)

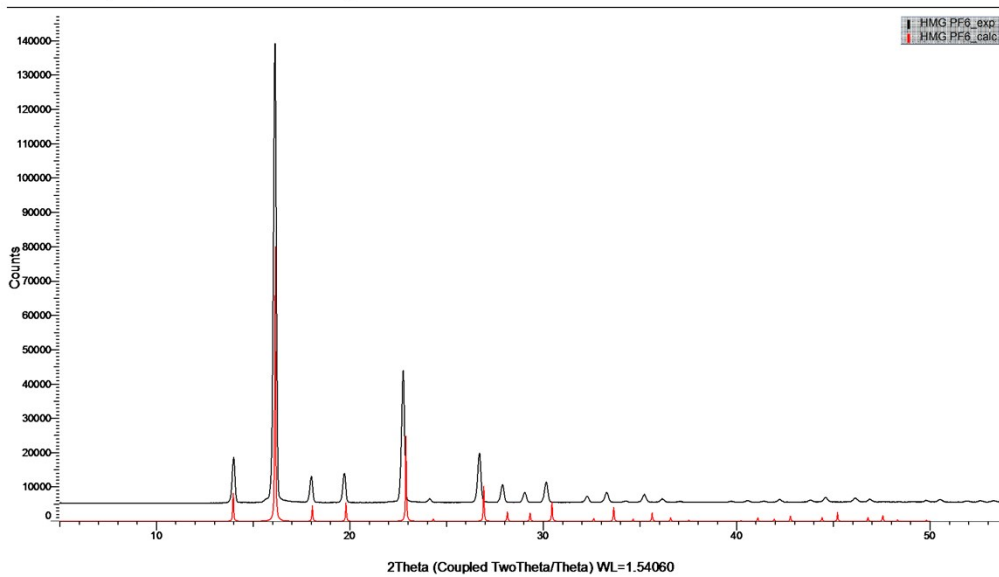


Figure S18; Experimental (black) and calculated (red) PXRD for [HMG][PF₆]

HMG TFSI (Coupled TwoTheta/Theta)

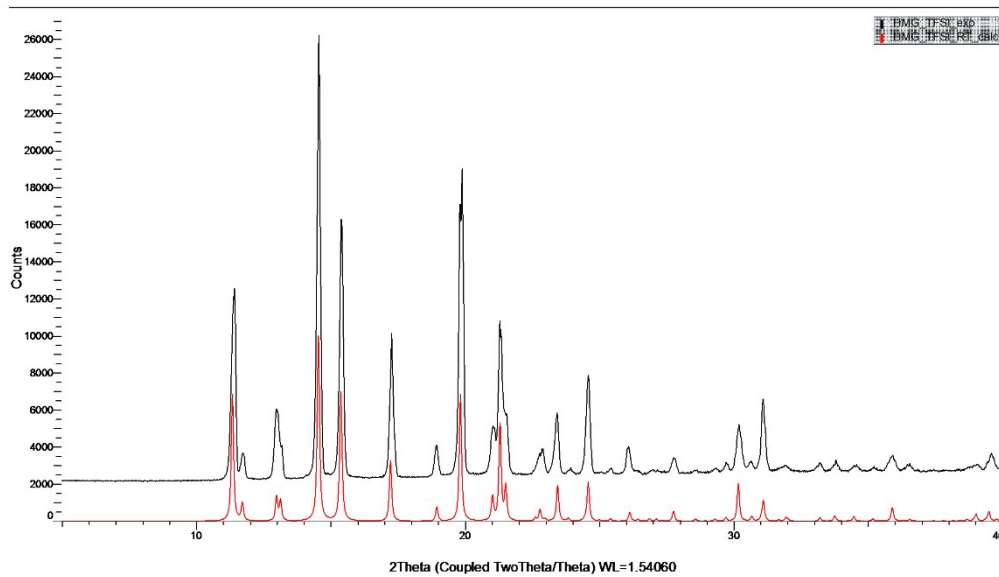


Figure S19; Experimental (black) and calculated (red) PXRD for [HMG][TFSI].

HMG BF4 (Coupled TwoTheta/Theta)

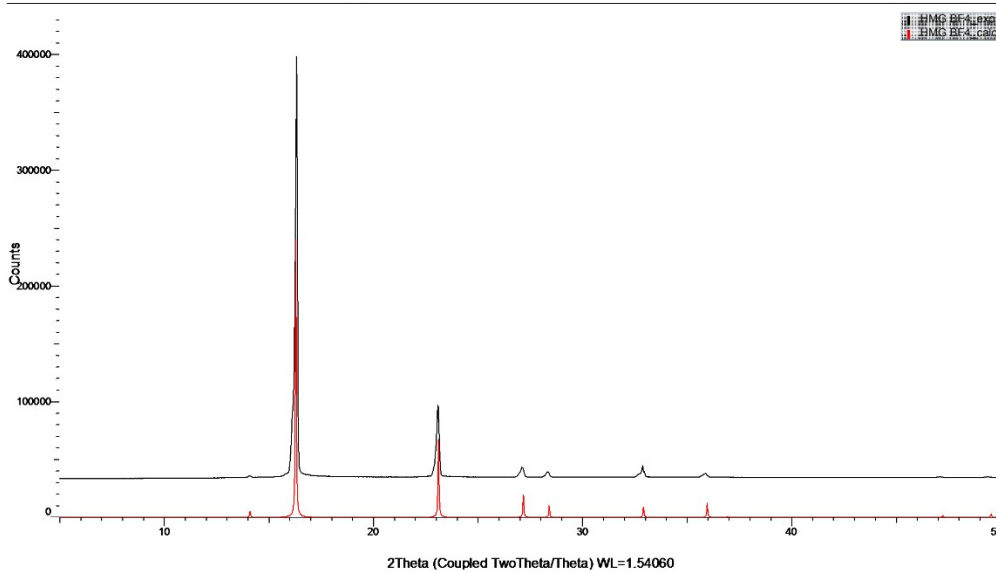


Figure S20; Experimental (black) and calculated (red) PXRD for [HMG][BF₄].

PALS Data

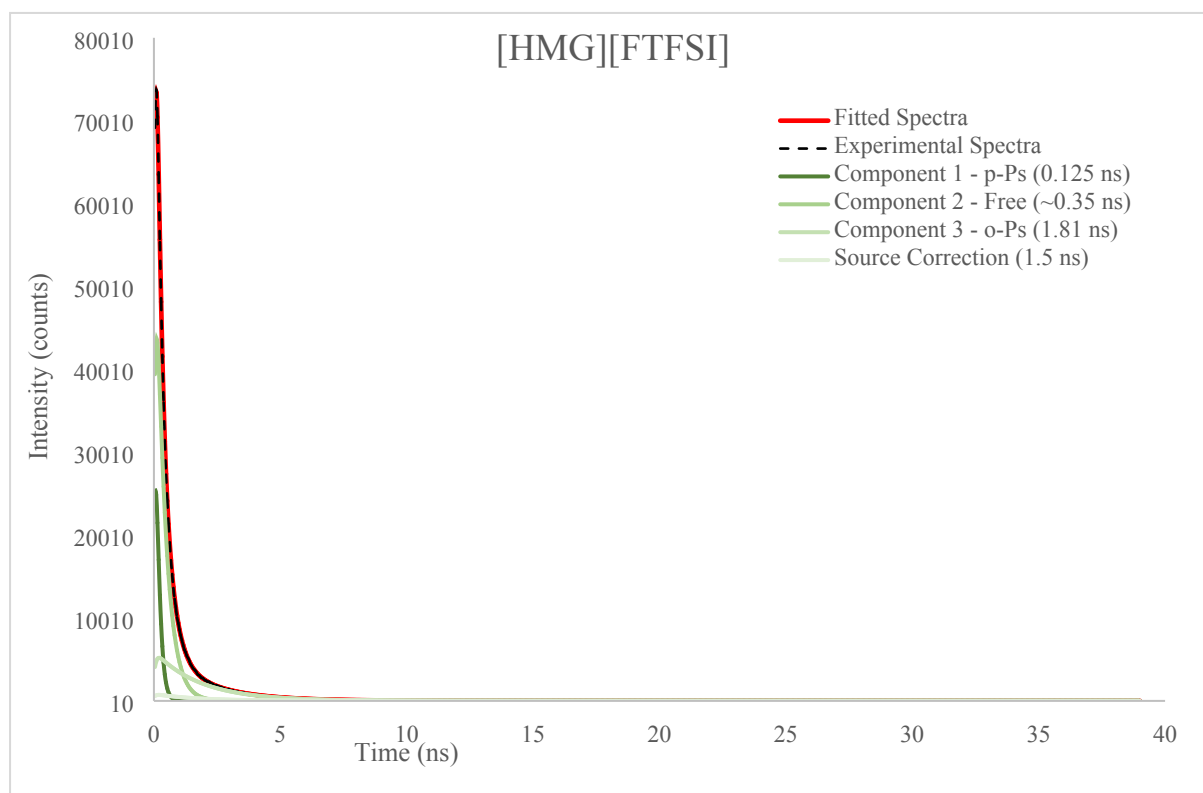


Figure S21. Fitted Positron Annihilation Lifetime spectra of [HMG][FTFSI] using LT-9 software.

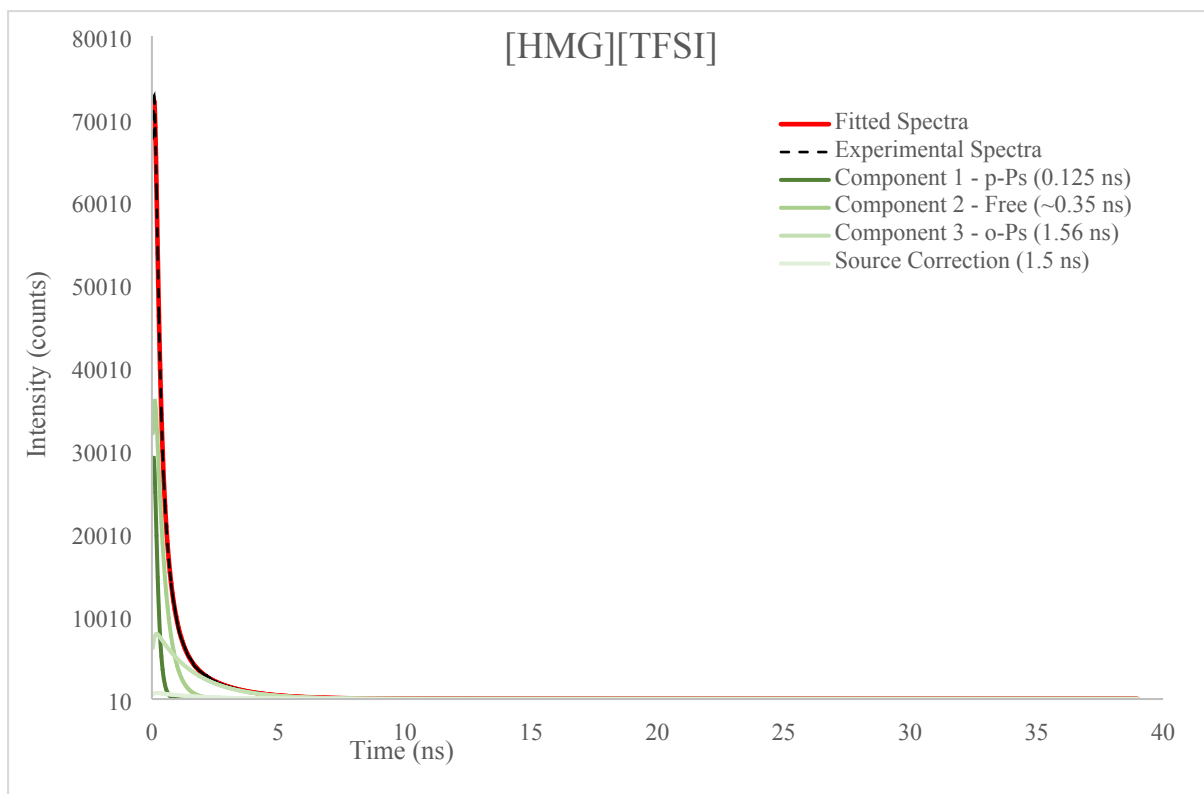


Figure S22. Fitted Positron Annihilation Lifetime spectra of [HMG][TFSI] using LT-9 software.

[HMG][FSI]

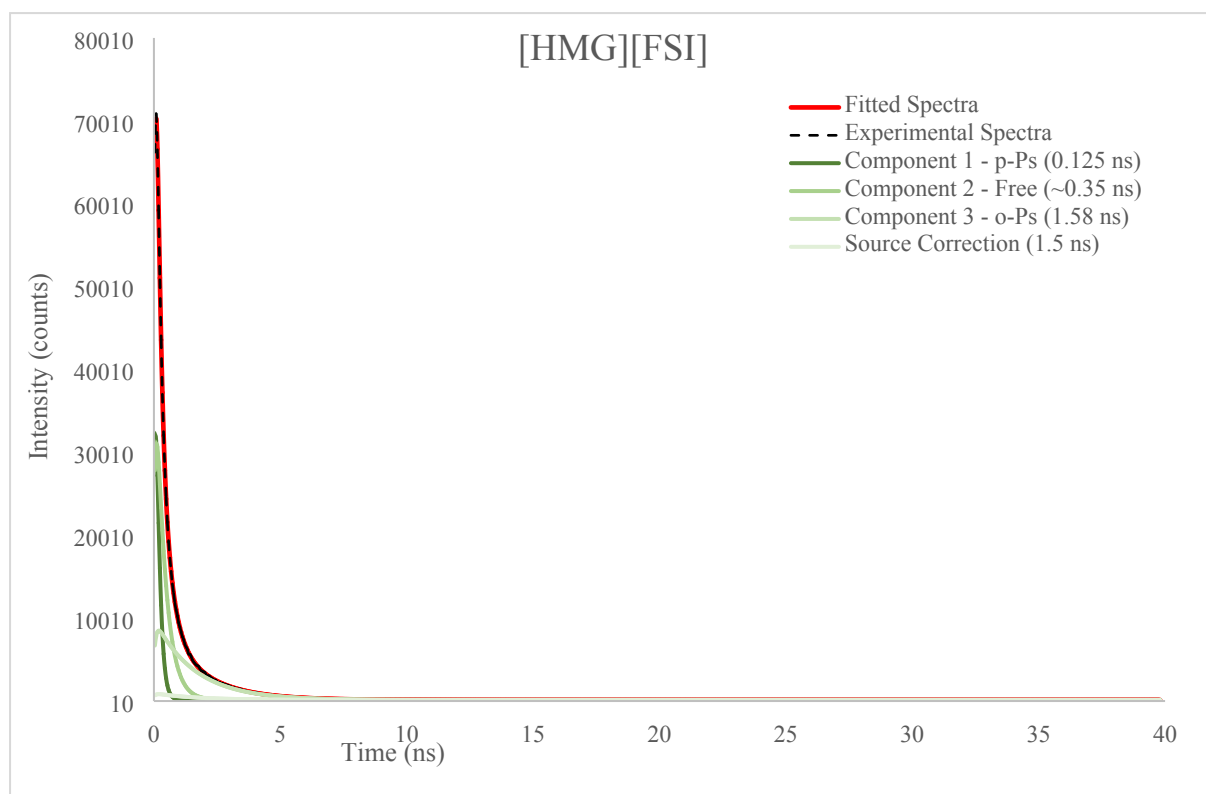


Figure S23. Fitted Positron Annihilation Lifetime spectra of [HMG][FSI] using LT-9 software.

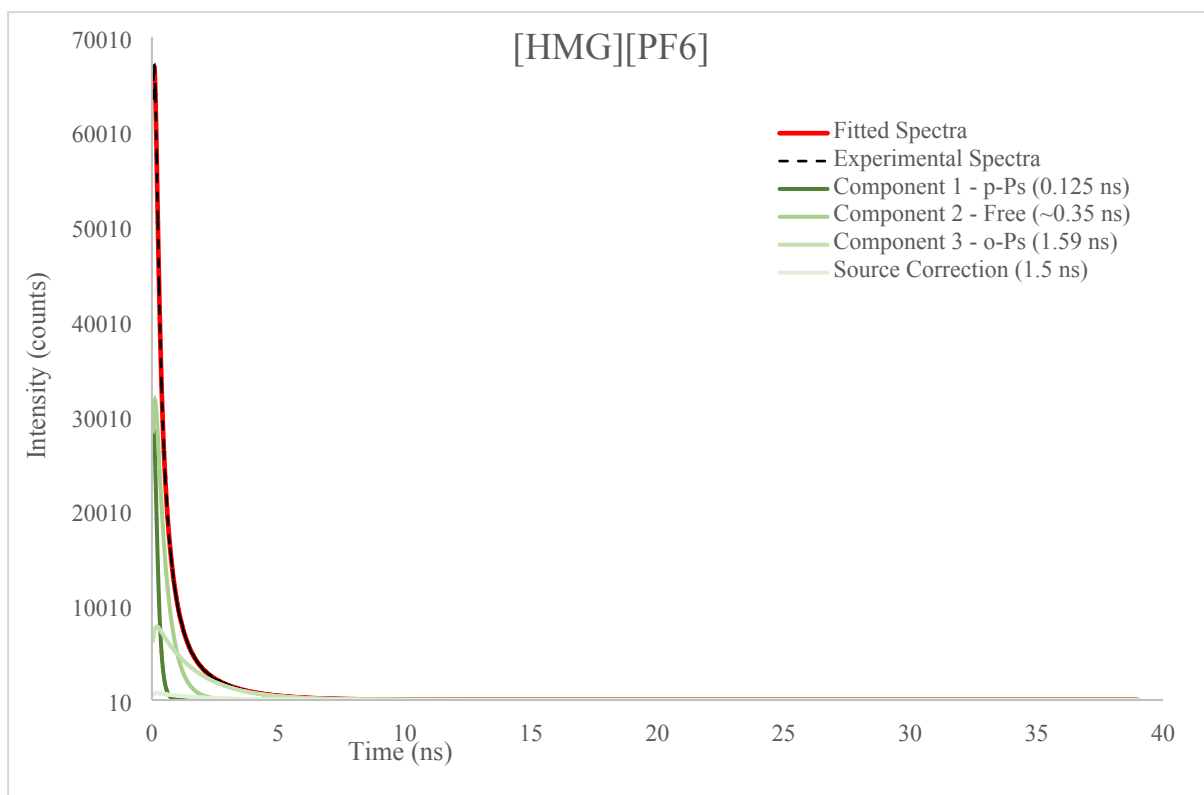


Figure S24. Fitted Positron Annihilation Lifetime spectra of [HMG][PF6] using LT-9 software.

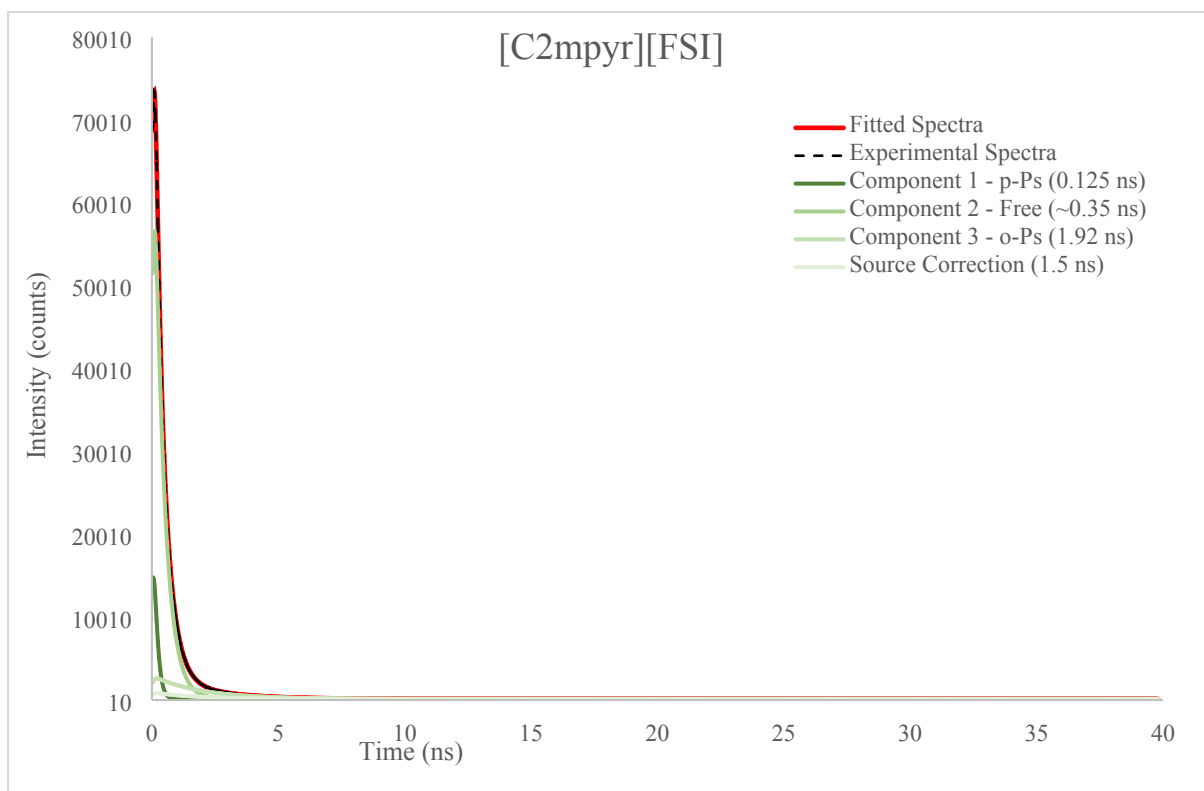


Figure S25. Fitted Positron Annihilation Lifetime spectra of [C₂mpyr][FSI] using LT-9 software.

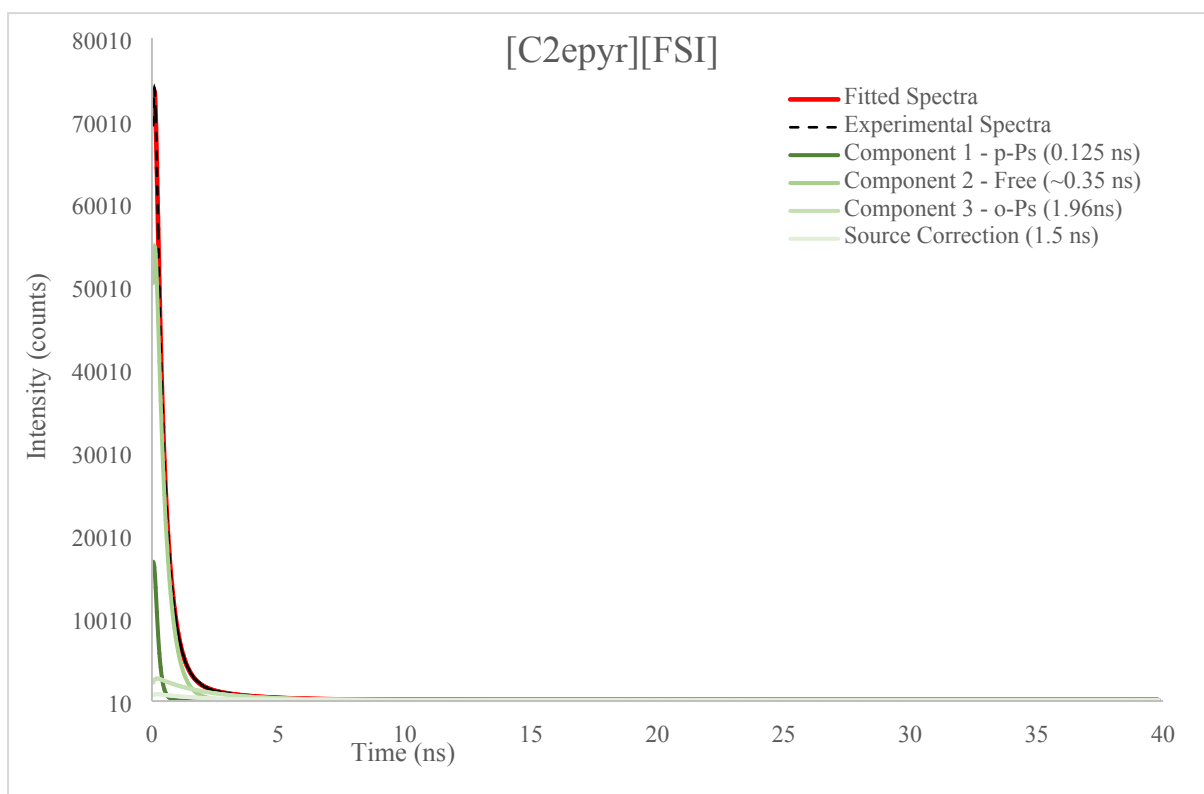


Figure S26. Fitted Positron Annihilation Lifetime spectra of [C₂epyr][FSI] using LT-9 software.

Table S1. Summary of fitted PALS Data

	Lifetimes τ_1 (ns)	Intensities I_1 (%)	Lifetimes τ_2 (ns)	Intensities I_2 (%)	Lifetimes τ_3 (ns)	Intensities I_3 (%)
[HMG][FTFSI]	0.125	91.2 ± 1.8	0.365 ± 0.004	57.4 ± 1.6	1.806 ± 0.01	23.3 ± 0.2
[HMG][TFSI]	0.125	22.4 ± 0.8	0.371 ± 0.004	46.7 ± 0.6	1.564 ± 0.01	31.0 ± 0.3
[HMG][FSI]	0.125	24.3 ± 0.5	0.359 ± 0.006	41.8 ± 0.4	1.581 ± 0.012	34.0 ± 0.3
[HMG][PF ₆]	0.125	21.7 ± 0.8	0.433 ± 0.004	47.1 ± 0.8	1.592 ± 0.01	31.1 ± 0.1
[C ₂ mpyr][FSI]	0.125	13.0 ± 1.2	0.384 ± 0.003	75.8 ± 1.2	1.921 ± 0.013	11.2 ± 0.1
[C ₂ epyr][FSI]	0.125	11.6 ± 1.1	0.376 ± 0.001	76.4 ± 1.1	1.956 ± 0.019	12.0 ± 0.1