

Supporting Information

Novel diol functionalized dicationic ionic liquids: Synthesis, characterization and DFT calculations on H-bonding influence on thermophysical properties

Reza Fareghi - Alamdari^{*a}, Razieh Hatefipour^a, Mehdi Rakhshi^b, Negar Zekri^a

^a *Faculty of Chemistry and Chemical Engineering, Malek - Ashtar University of Technology, Tehran, I.R.Iran.*

^b *Department of Chemistry, University of Kashan, Kashan, I.R.Iran.*

* Corresponding authors: Fax: +98-21-77074772; Tel: +98-935-5999011.
E-mail: reza_fareghi@yahoo.com

1) FT-IR, ^1H NMR, ^{13}C -NMR spectrums for 2,2-Bis(1-(1-methylimidazolium)methylpropane-1,3-diol bromide [$\text{mim}_2\text{C}_3(\text{C}_1\text{OH})_2$][Br] $_2$ (**1a**))

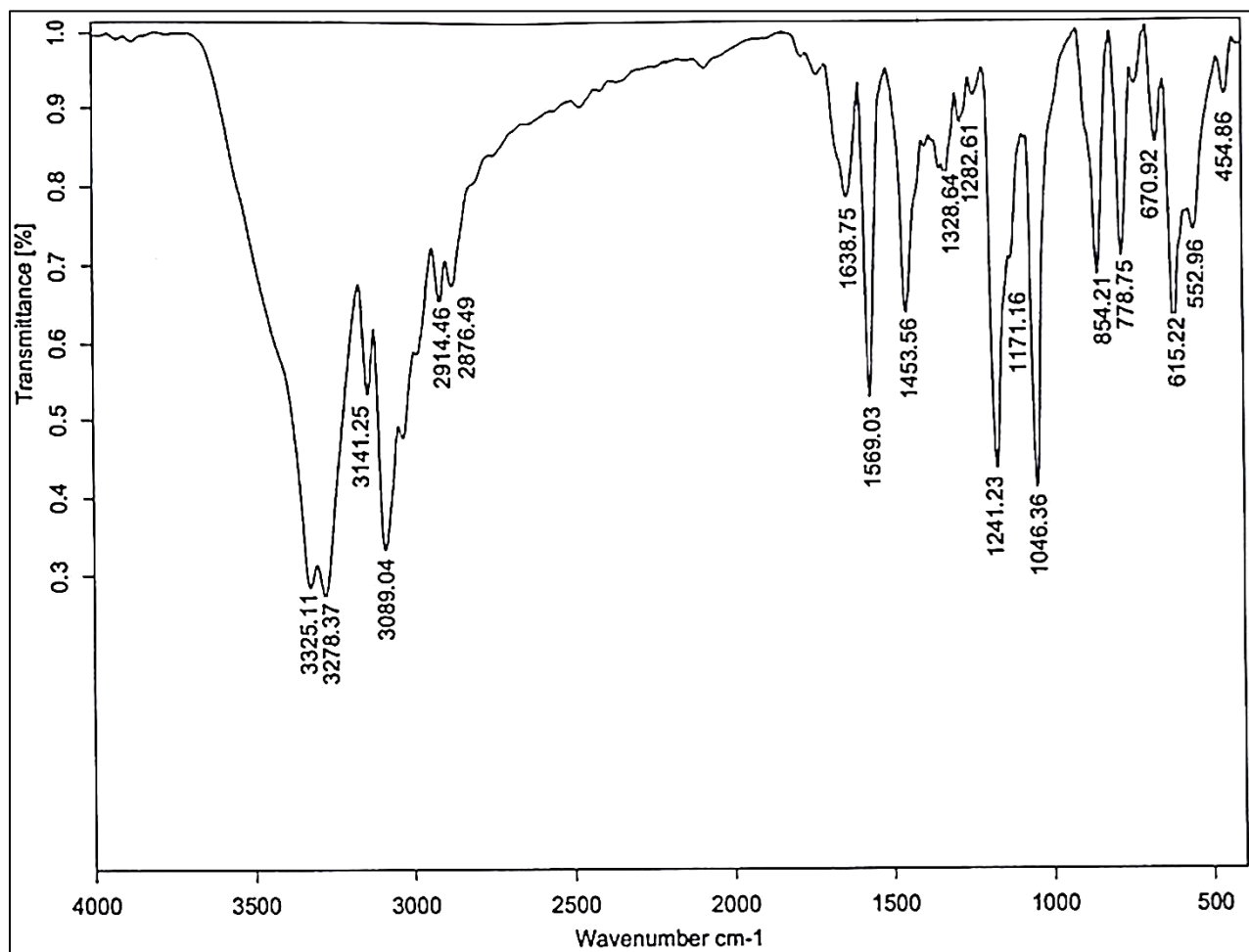


Figure S1. FT-IR spectrum of compound **1a**.

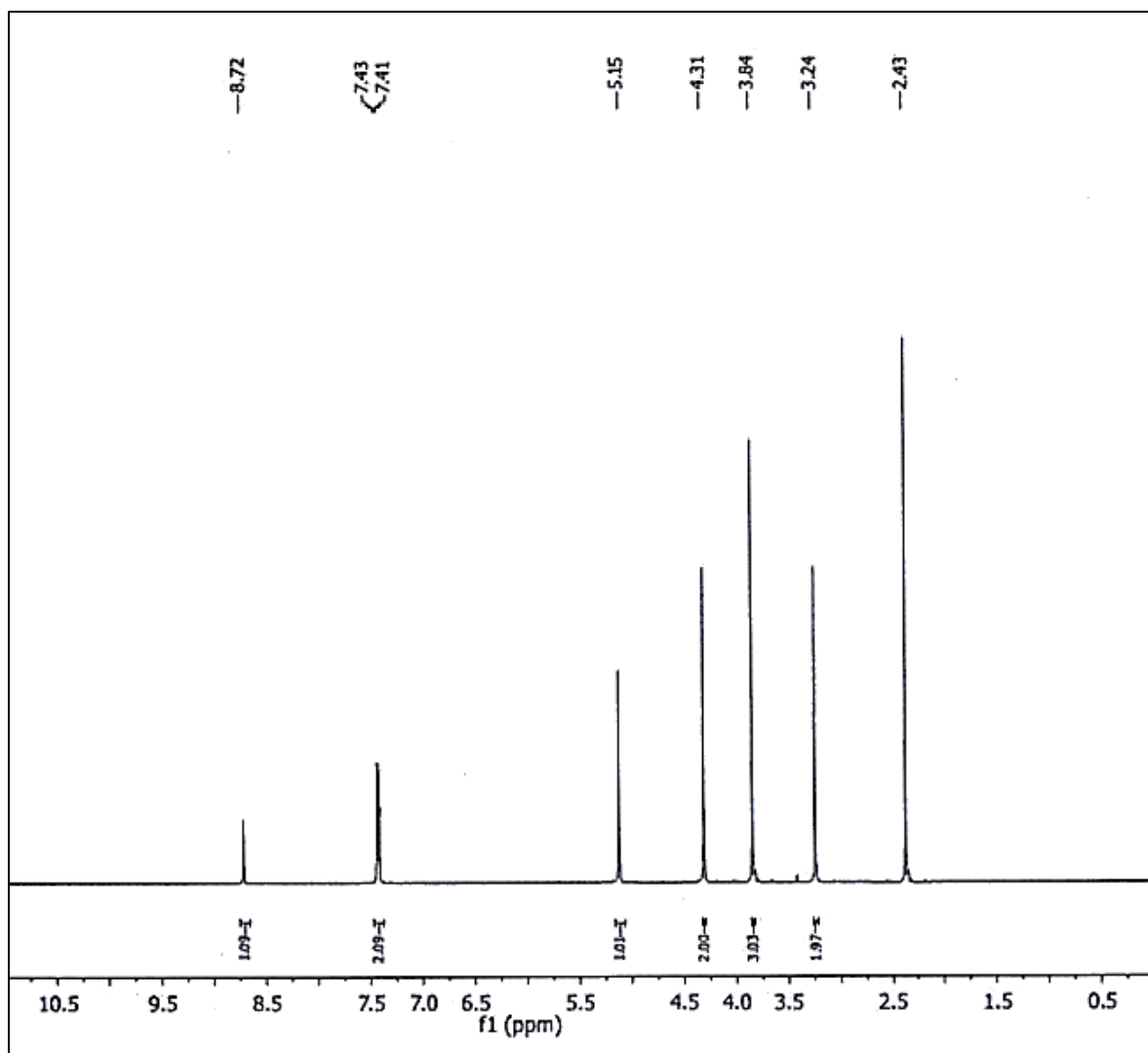


Figure S2. $^1\text{H-NMR}$ spectrum of compound **1a** (500 MHz, DMSO-d_6).

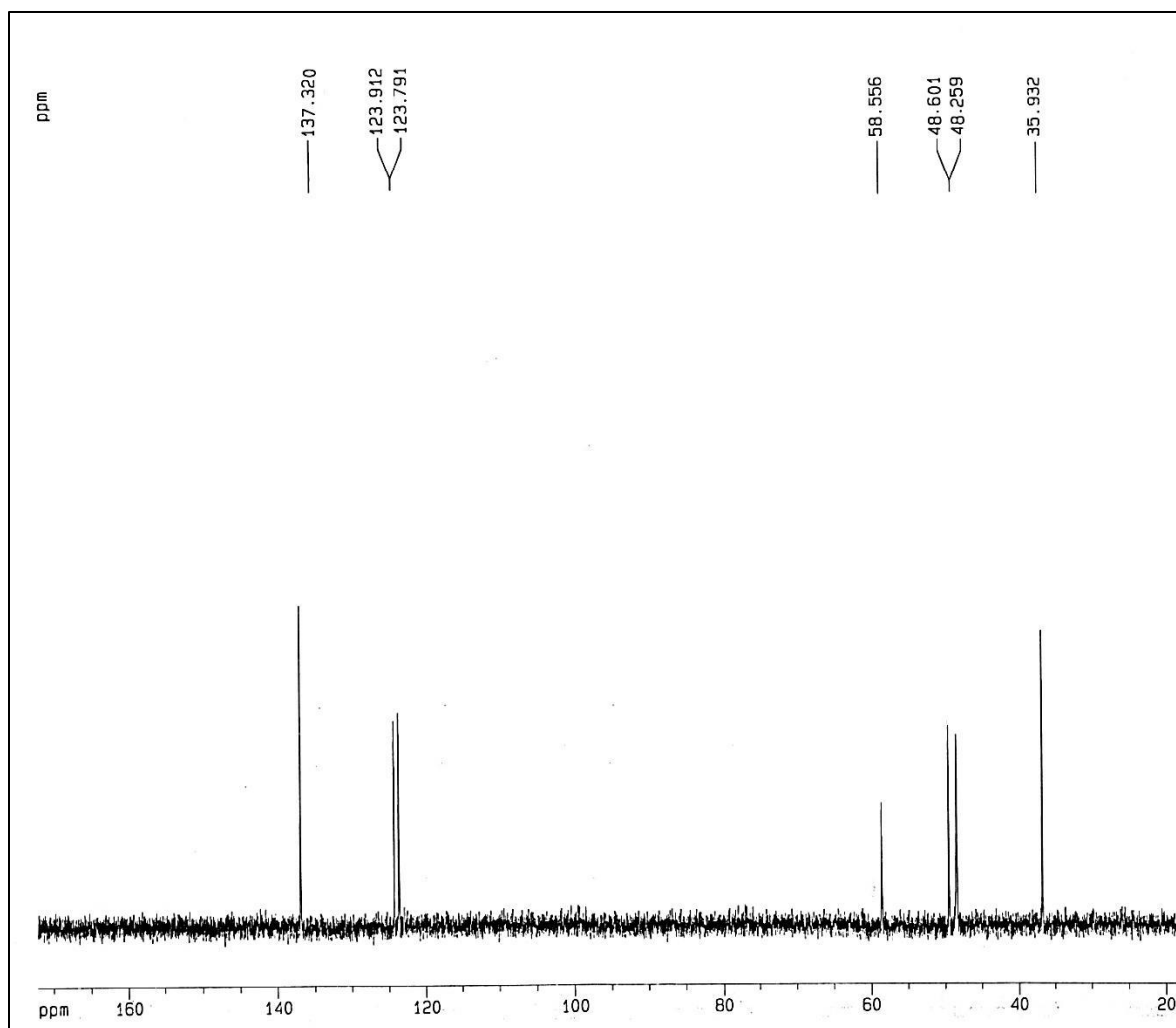


Figure S3. ^{13}C -NMR spectrum of compound **1a** (500 MHz, D_2O).

2) FT-IR, ^1H NMR, ^{13}C -NMR spectra for 2,2-Bis(1-(1-methylimidazolium)methylpropane-1,3-diol dicyanamide $[\text{mim}_2\text{C}_3(\text{C}_1\text{OH})_2][\text{DCA}]_2$ (**1b**)

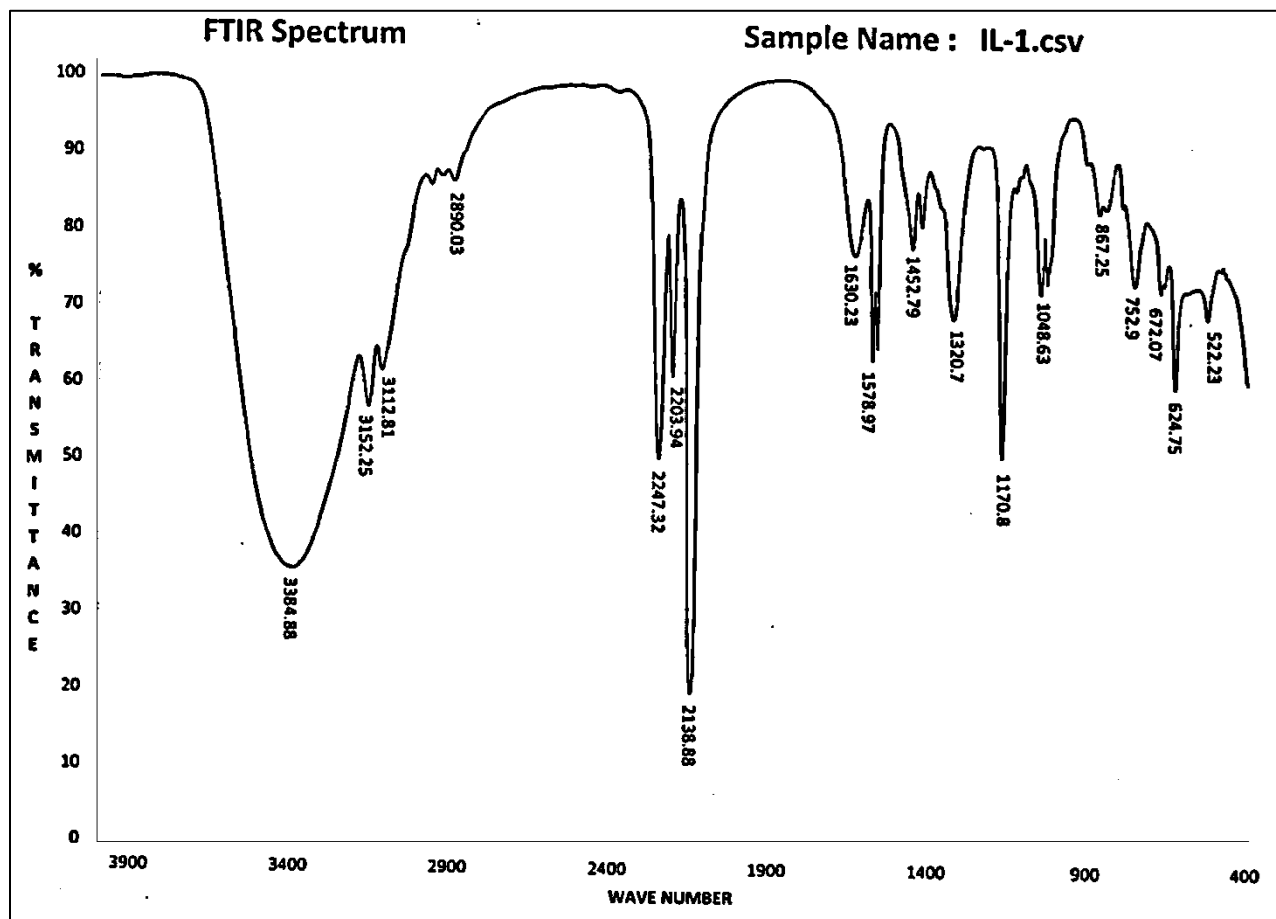


Figure S4. FT-IR spectrum of compound **1b**.

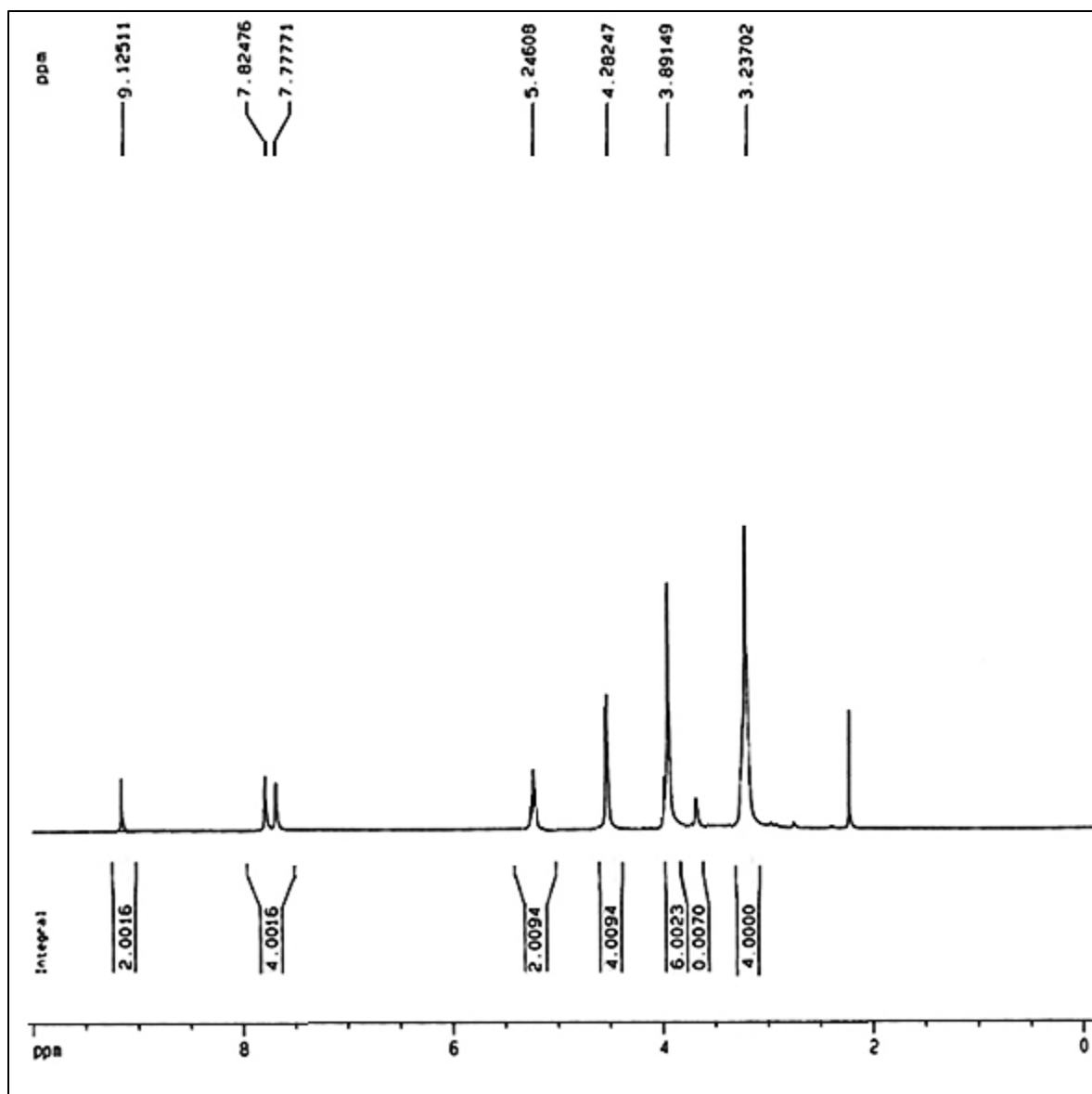


Figure S5. ¹H-NMR spectrum of compound **1b** (500 MHz, DMSO-d₆).

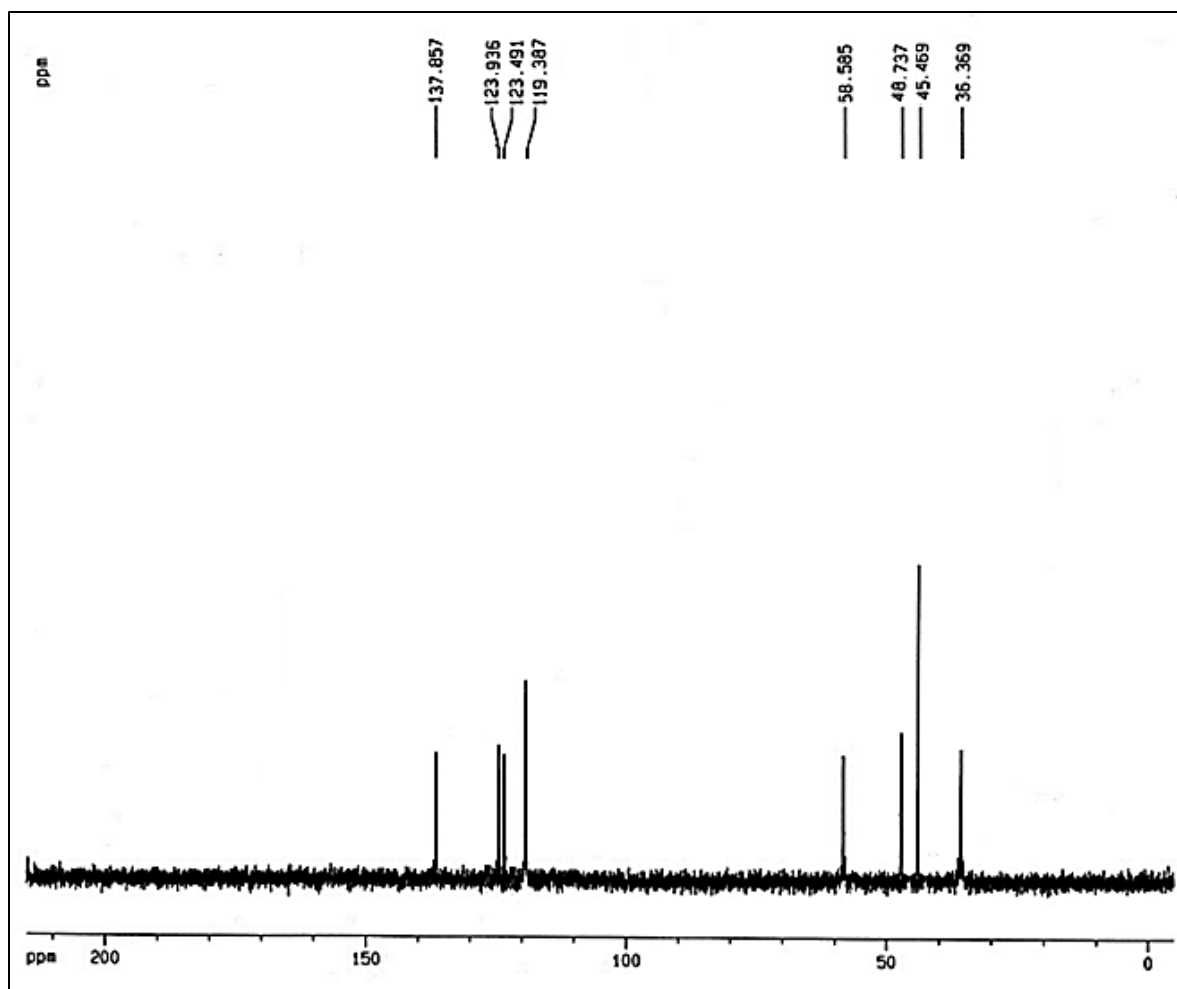


Figure S6. ^{13}C -NMR spectrum of compound **1b** (500 MHz, D_2O).

3) FT-IR, ^1H NMR, ^{13}C -NMR spectrums for 2,2-Bis(1-(1-vinylimidazolium)methylpropane-1,3-diol bromide [vim₂C₃(C₁OH)₂][Br]₂ (**2a**).

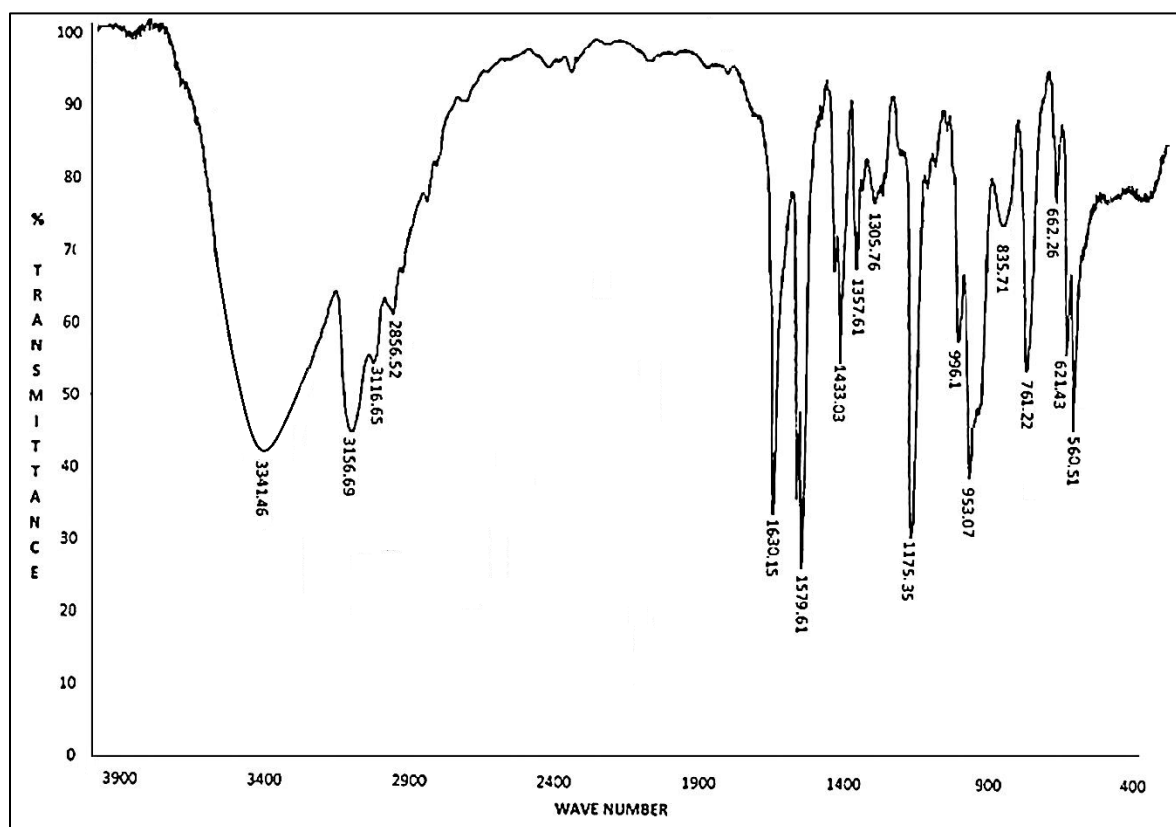


Figure S7. FT-IR spectrum of compound **2a**.

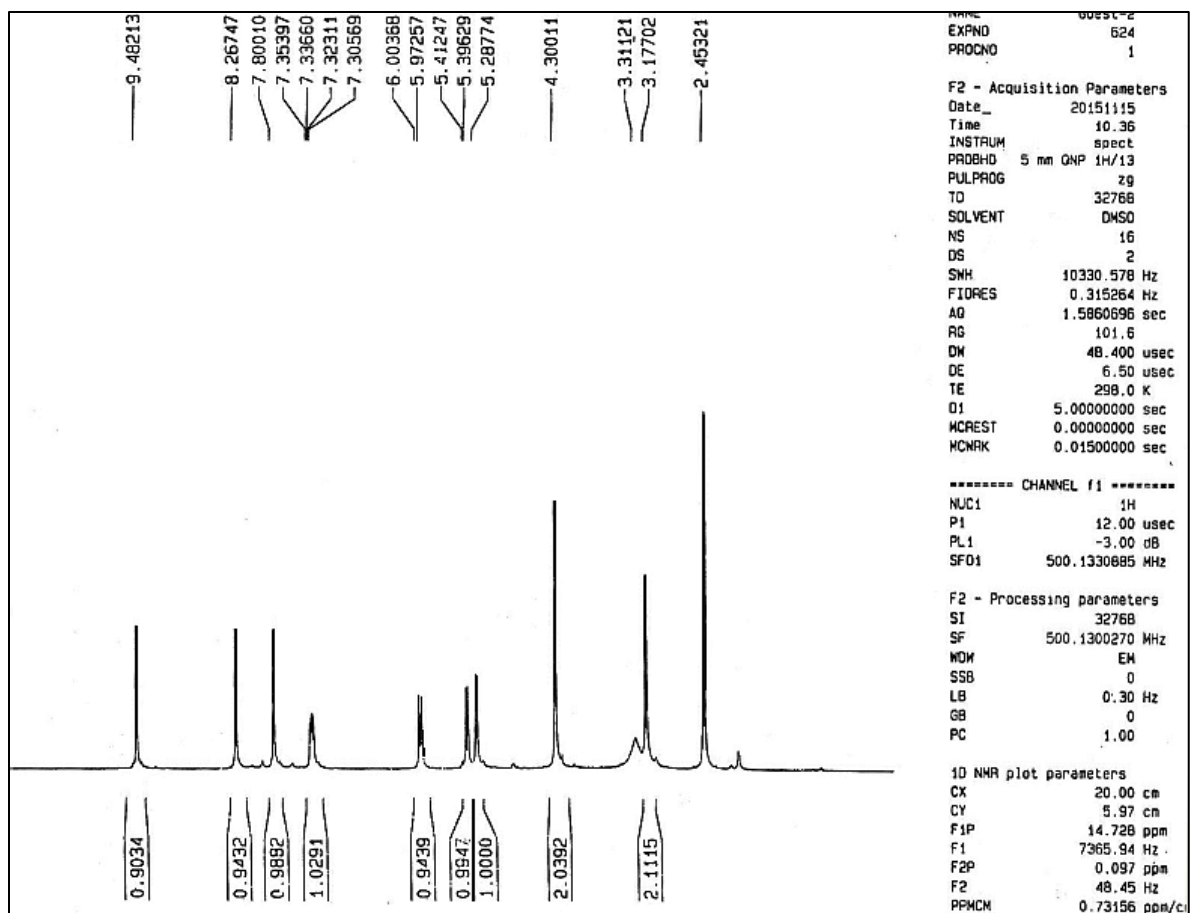


Figure S8. ^1H -NMR spectrum of compound **2a** (500 MHz, DMSO-d_6).

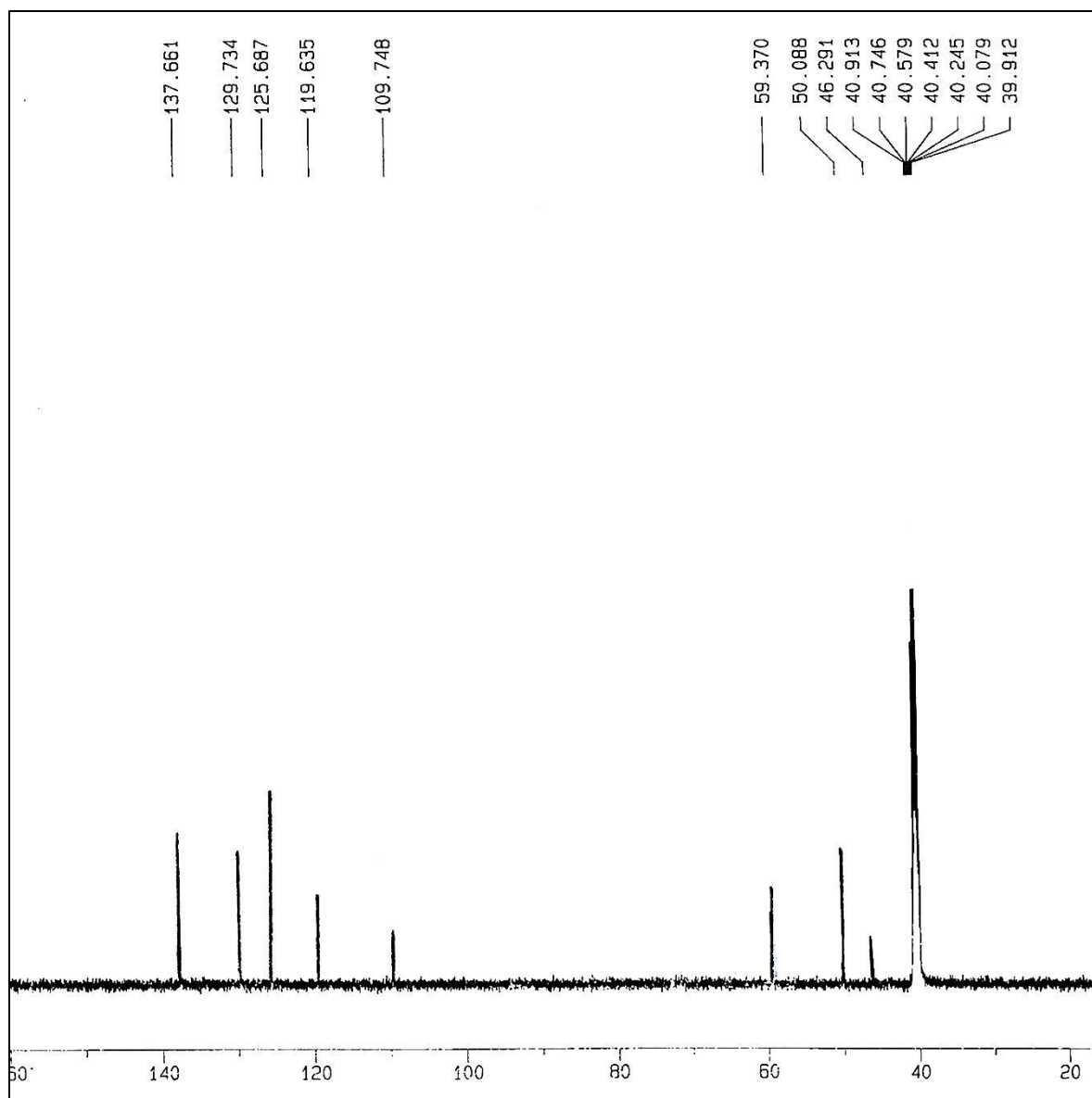


Figure S9. ^{13}C -NMR spectrum of compound **2a** (500 MHz, DMSO-d_6).

4) FT-IR, ^1H NMR, ^{13}C -NMR spectrums for 2,2-Bis(1-(1-vinylimidazolium)methylpropane-1,3-diol dicyanamide $[\text{vim}_2\text{C}_3(\text{C}_1\text{OH})_2][\text{DCA}]_2$ (**2b**):.

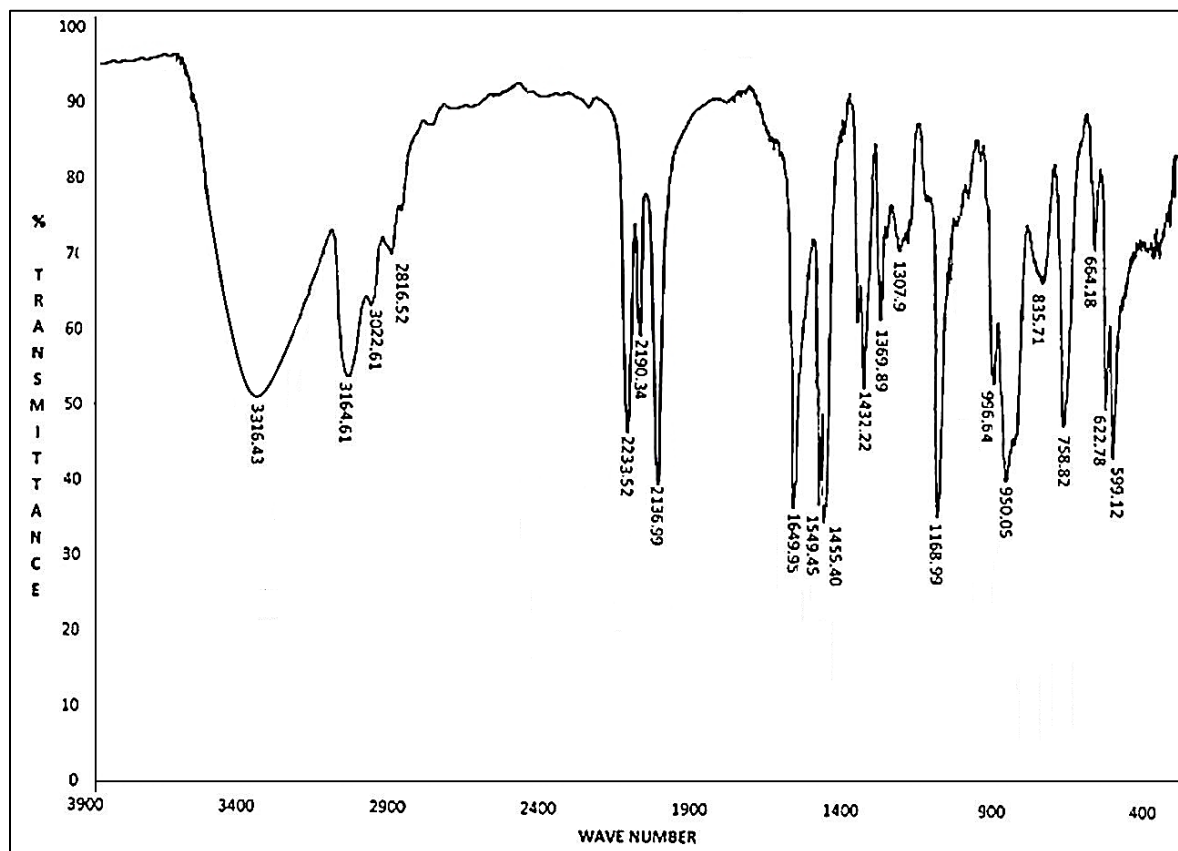


Figure S10. FT-IR spectrum of compound **2b**.

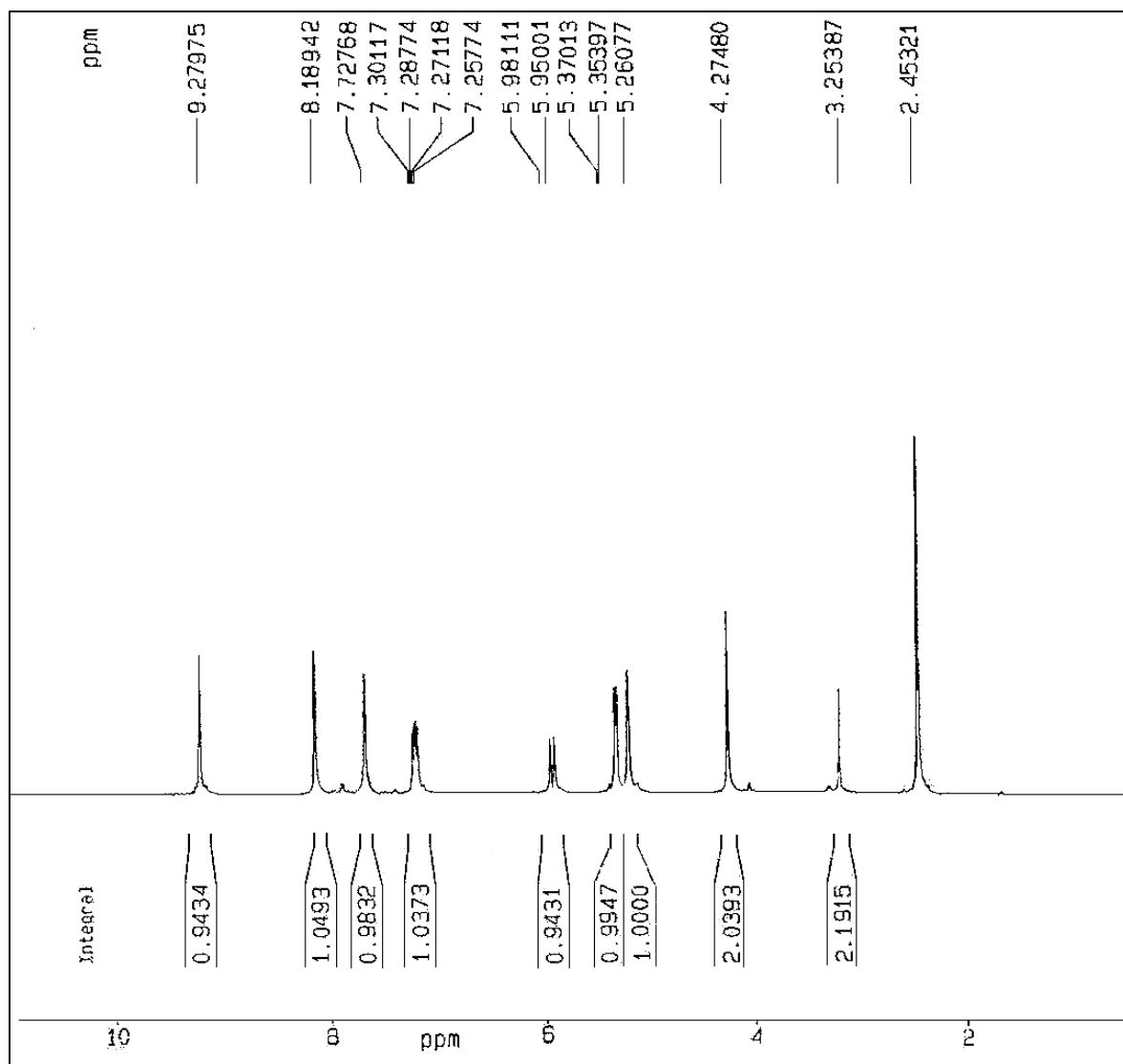


Figure S11. ¹H-NMR spectrum of compound **2b** (500 MHz, DMSO-d₆).

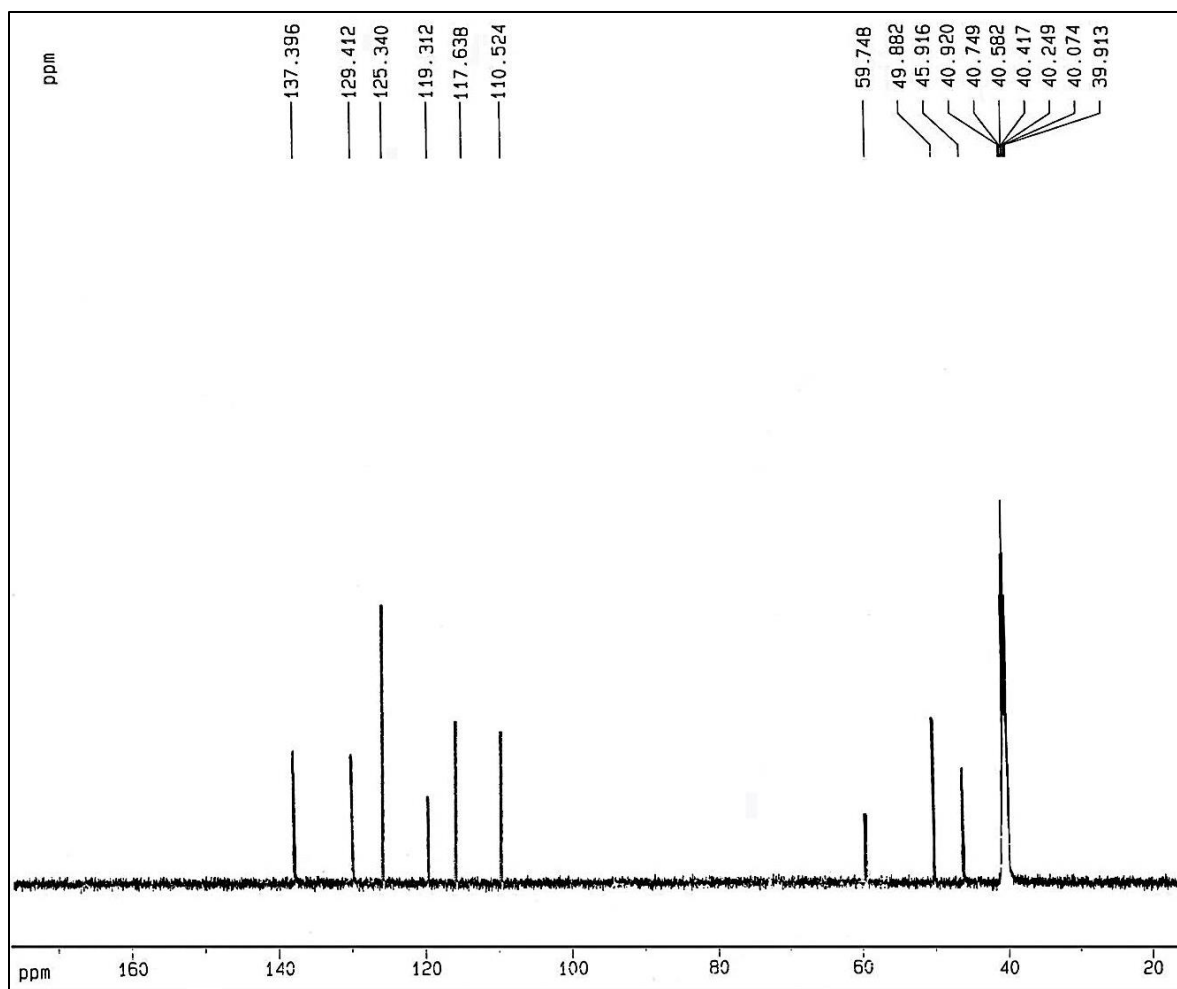


Figure S12. ^{13}C -NMR spectrum of compound **2b** (500 MHz, DMSO-d_6).

5) FT-IR, $^1\text{H-NMR}$, $^{13}\text{C-NMR}$ spectrums for 1,3-bis(3-methylimidazolium-1-yl)propane bromide $[\text{mim}_2\text{C}_3][\text{Br}]_2$ (**3a**)

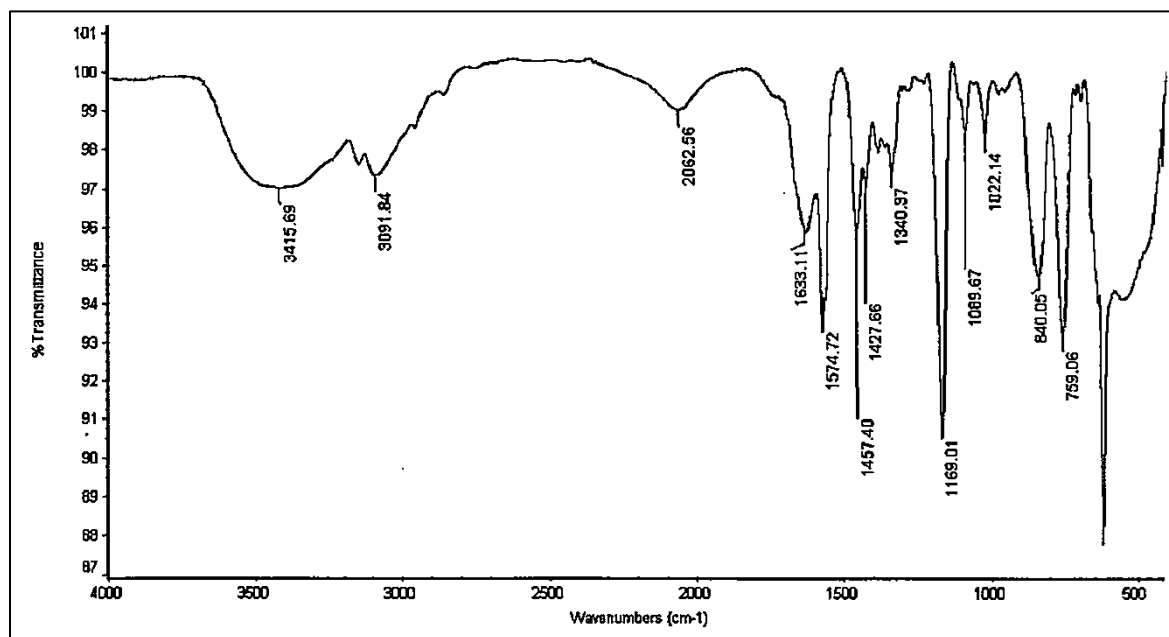


Figure S13. FT-IR spectrum of compound **3a**.

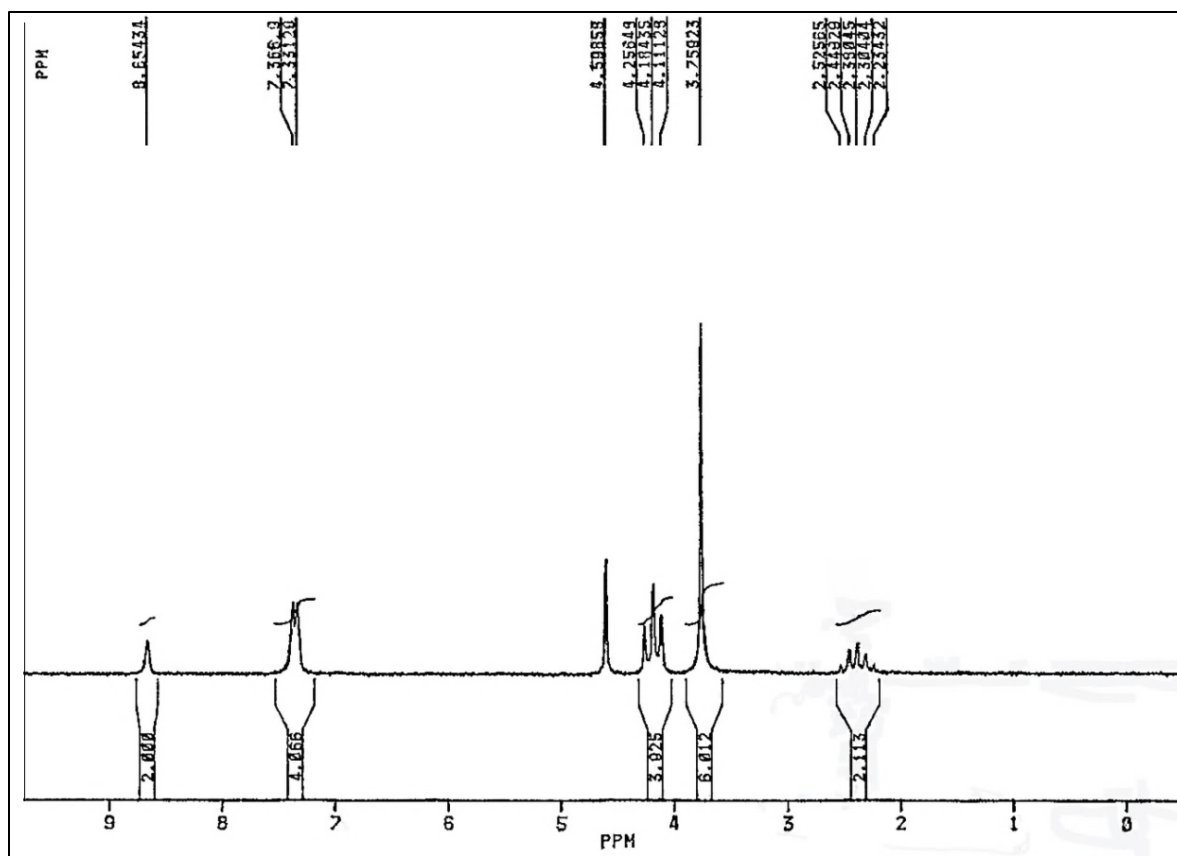


Figure S14. ¹H-NMR spectrum of compound **3a** (500 MHz, D₂O).

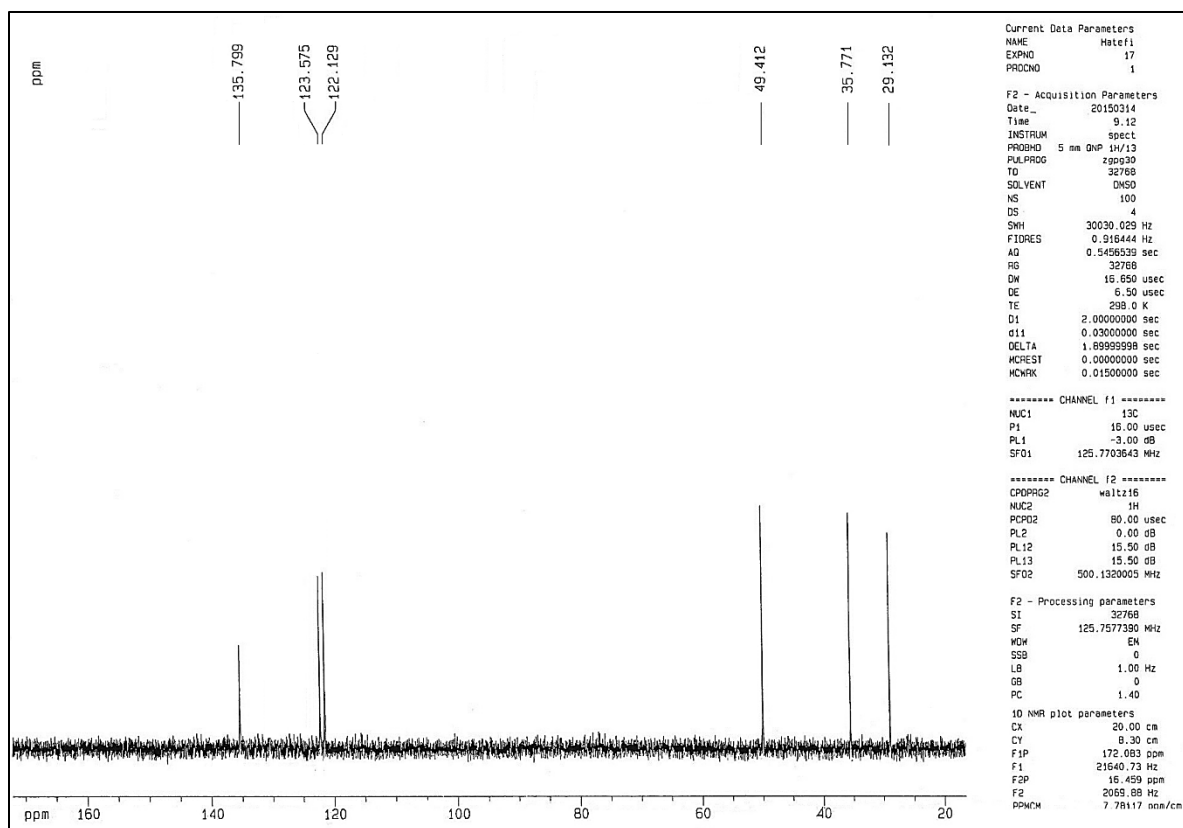


Figure S15. ^{13}C -NMR spectrum of compound **3a** (500 MHz, D_2O).

6) FT-IR, ^1H NMR, ^{13}C -NMR spectrums for 1,3-bis(3-methylimidazolium-1-yl)propane bromide [mim_2C_3][DCA] $_2$ (**3b**)

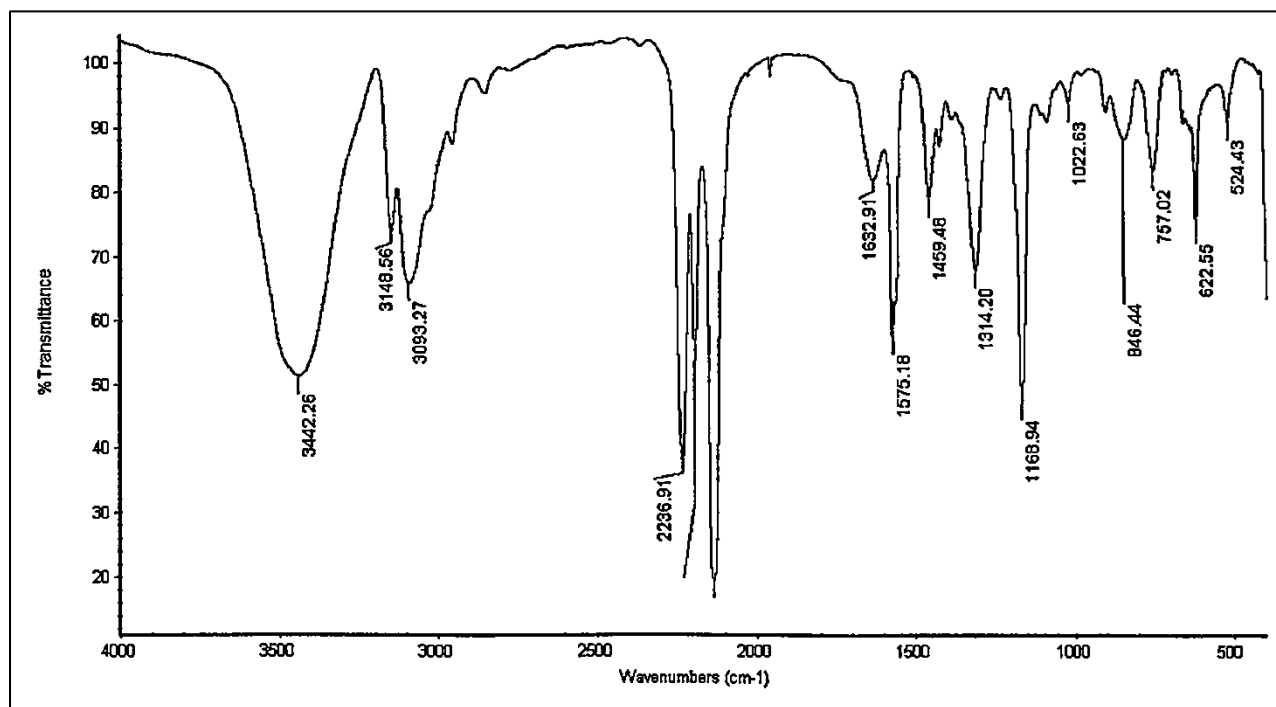


Figure S16. FT-IR spectrum of compound **3b**.

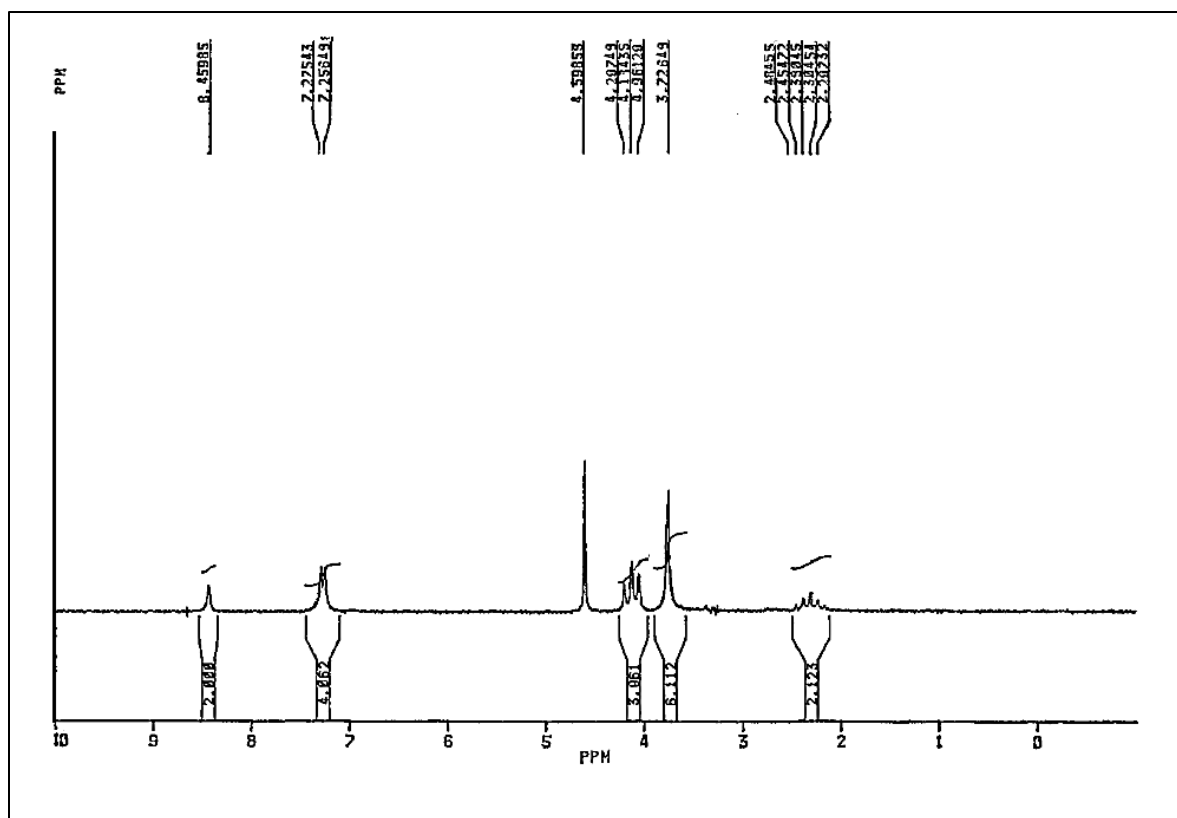


Figure S17. ¹H-NMR spectrum of compound **3b** (500 MHz, D₂O).

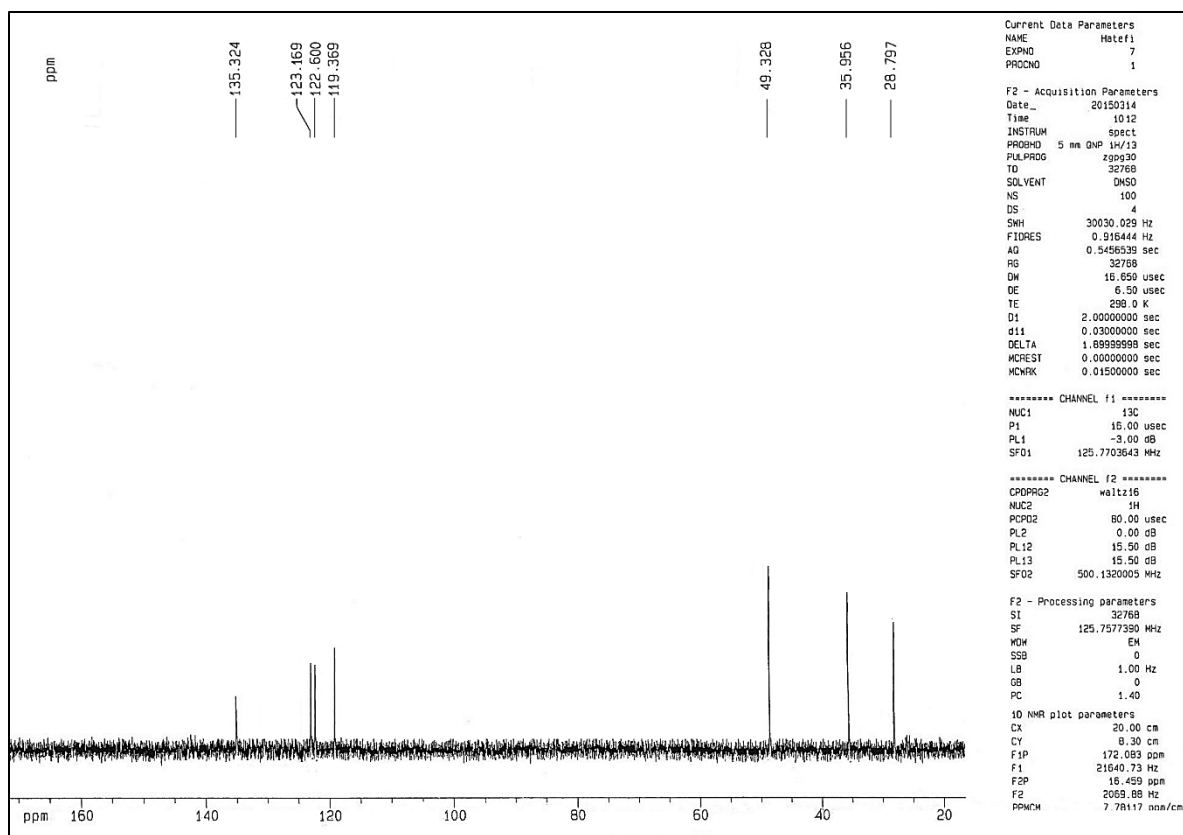


Figure S18. ^{13}C -NMR spectrum of compound **3b** (500 MHz, D_2O).

Table S1. Heat capacities of the synthesized dicationic ILs as a function of temperature

Temperature (K)	[mim ₂ C ₃ (C ₁ OH) ₂]DCA ₂		[vim ₂ C ₃ (C ₁ OH) ₂]DCA ₂		[mim ₂ C ₃]DCA ₂	
	J.g ⁻¹ .k ⁻¹	J.mol ⁻¹ .k ⁻¹	J.g ⁻¹ .k ⁻¹	J.mol ⁻¹ .k ⁻¹	J.g ⁻¹ .k ⁻¹	J.mol ⁻¹ .k ⁻¹
303	1.4	557.85	1.58	667.47	1.21	409.44
308	1.42	565.77	1.60	675.92	1.23	416.21
313	1.45	577.72	1.62	684.37	1.27	429.74
318	1.47	585.69	1.64	688.59	1.30	439.89
323	1.49	593.66	1.65	697.04	1.32	446.66
328	1.51	601.63	1.67	705.49	1.35	456.81
333	1.52	605.61	1.69	713.94	1.38	466.96
338	1.54	613.58	1.71	722.39	1.41	477.12
343	1.55	617.57	1.72	726.61	1.43	483.88
348	1.57	625.54	1.74	735.06	1.45	490.65
353	1.59	633.50	1.76	743.51	1.48	500.80
358	1.61	641.47	1.78	751.96	1.50	507.57
363	1.62	645.46	1.80	760.41	1.53	517.72
368	1.64	653.42	1.82	768.86	1.56	527.87
373	1.66	661.39	1.84	777.31	1.59	538.02
378	1.68	669.36	1.85	781.53	1.61	544.79
383	1.7	677.33	1.87	789.98	1.65	558.33
388	1.71	681.32	1.89	798.43	1.68	568.48
393	1.73	689.28	1.91	806.88	1.71	578.63