

Supplementary Material

Solubility of carbon dioxide in some imidazolium and pyridinium-based ionic liquids and correlation with NRTL model

Narmin Noorani^{A,} and Abbas Mehrdad^A*

^ADepartment of Physical Chemistry, Faculty of Chemistry, University of Tabriz, Tabriz, Iran

*Correspondence to: Email: nnorani1@yahoo.com

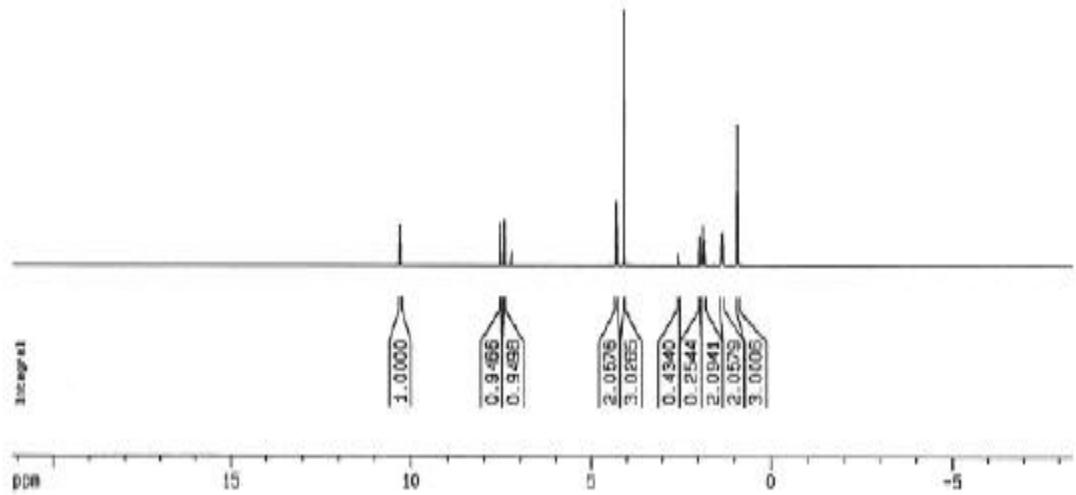


Figure S1. ^1H NMR data of 1-butyl-3-methyl imidazolium bromide: ^1H NMR (400 MHz: CDCl_3 ; δ/ppm relative to TMS): 0.91 (3H, but-CH₃), 1.34 (2H, CH₂), 1.86 (2H, CH₂), 4.08 (3H, NCH₃), 4.29 (2H, NCH₂), 7.46(1H, NCH), 7.58 (1H, NCH), 10.30 (1H, NCHN).

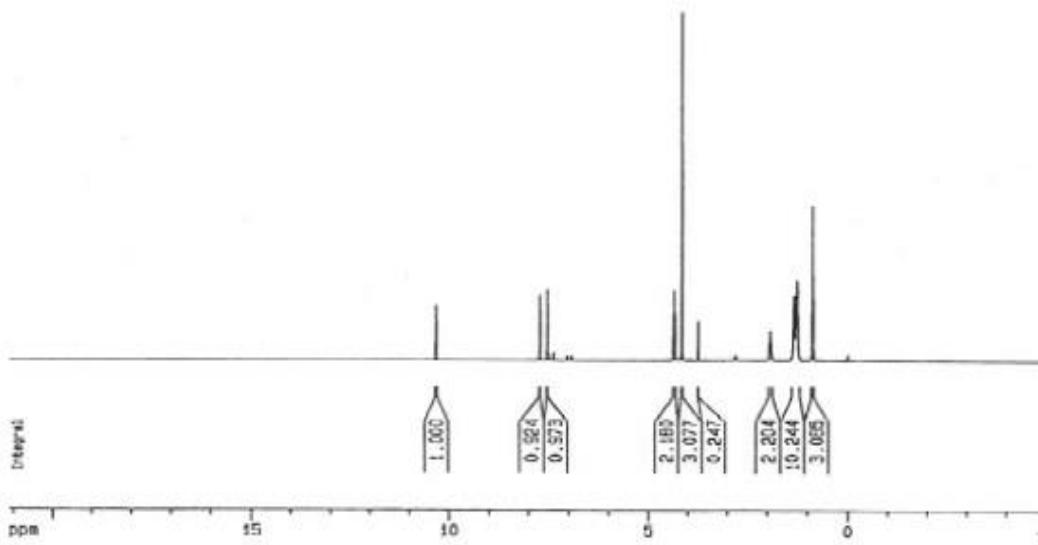


Fig. S2. ^1H NMR data of 1-octyl-3-methylimidazolium bromide: ^1H NMR (400 MHz; CDCl_3 ; δ/ppm relative to TMS): 0.87 (3H, oct- CH_3), 1.30 (10H, CH_2), 1.92 (2H, CH_2), 4.14 (3H, NCH_3), 4.34 (2H, NCH_2), 7.55(1H, NCH), 7.73 (1H, NCH), 10.32 (1H, NCHN).

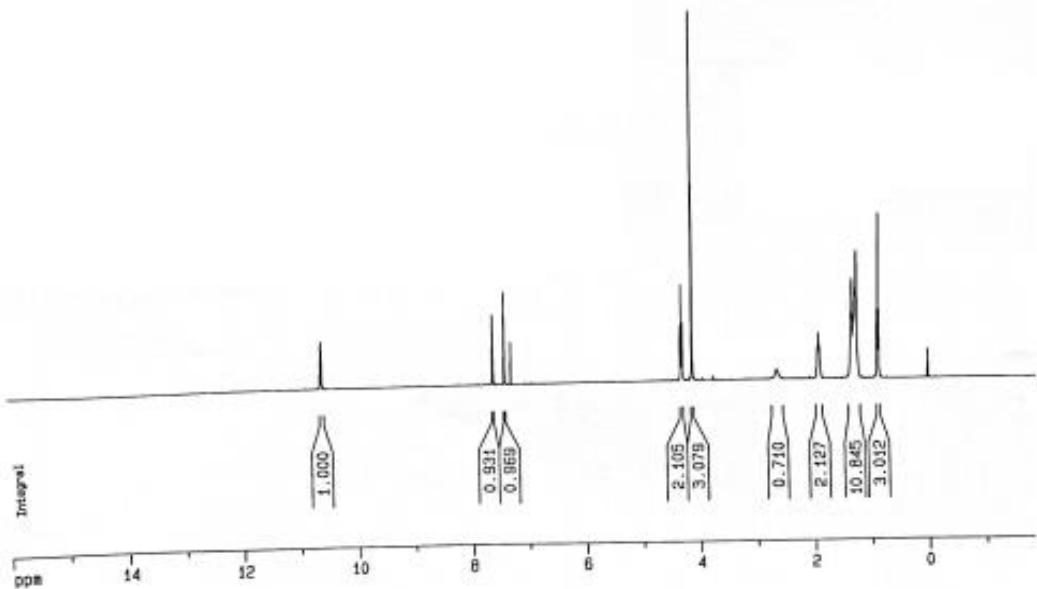


Figure S3. ^1H NMR data of 1-octyl-3-methyl imidazolium chloride: ^1H NMR (400 MHz: CDCl_3 ; δ/ppm relative to TMS): 0.856 (3H, oct- CH_3), 1.28 (10H, CH_2), 1.92 (2H, CH_2), 4.32 (3H, NCH_3), 7.43 (1H, NCH), 7.64 (1H, NCH), 10.63 (1H, NCHN).

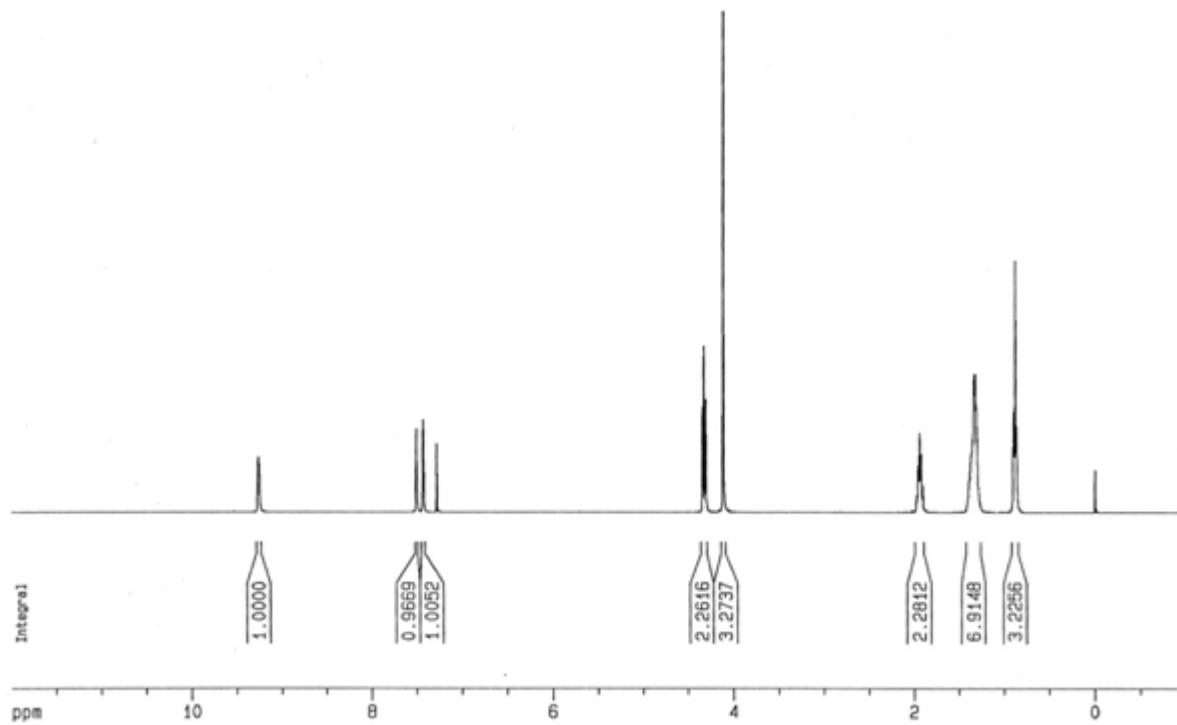


Fig. S4. ^1H NMR data of 1-hexyl-3-methylimidazolium thiocyanate: ^1H NMR (400 MHz: CDCl_3 ; δ/ppm relative to TMS): 0.88 (3H, hex- CH_3), 1.33 (6H, CH_2), 1.94 (2H, CH_2), 4.11 (3H, NCH_3), 4.33 (2H, NCH_2), 7.29 (1H, NCH), 7.48 (1H, NCH), 9.26 (1H, NCHN).

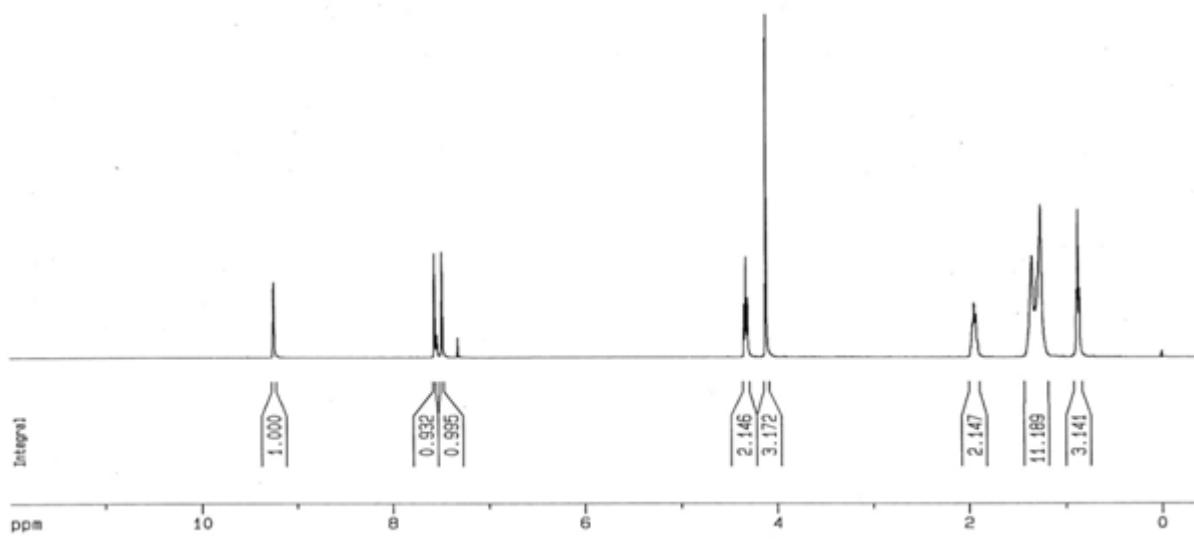


Fig S5: ^1H NMR data of 1-octyl-3-methylimidazolium thiocyanate: ^1H NMR (400 MHz; CDCl_3 ; δ/ppm relative to TMS): 0.871 (3H, oct- CH_3), 1.31 (10H, CH_2), 1.96 (2H, CH_2), 4.09 (3H, NCH_3), 4.33 (2H, NCH_2), 7.48 (1H, NCH), 7.56 (1H, NCH), 9.24 (1H, NCHN).

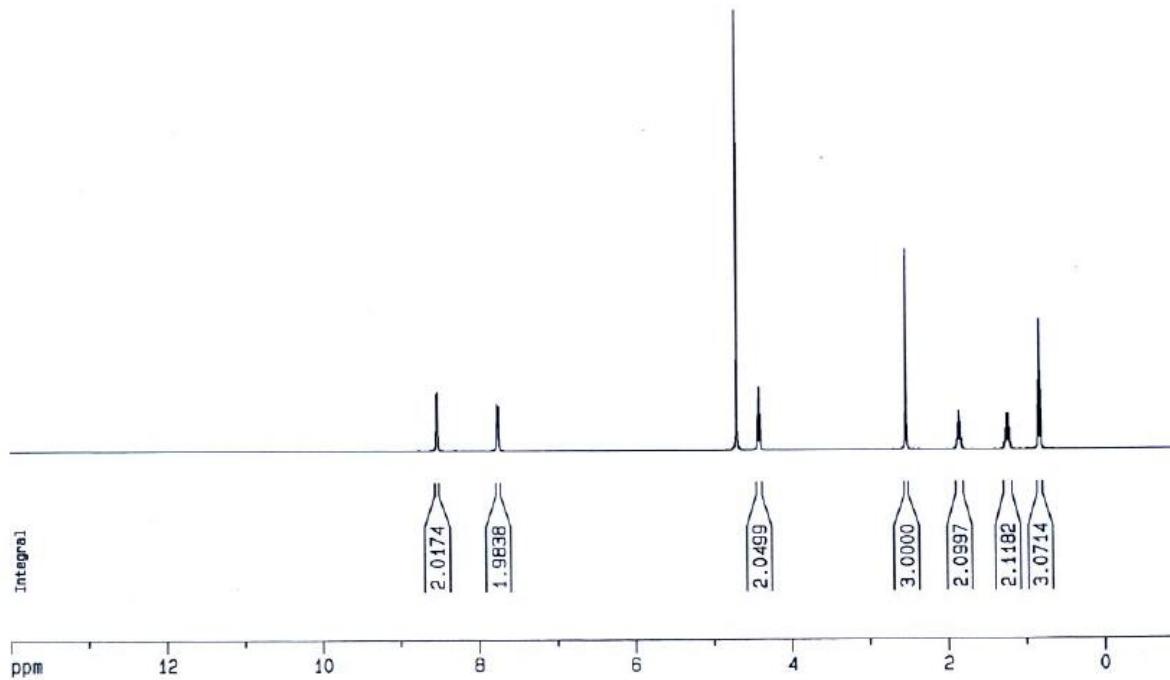


Fig. S6. ¹H-NMR data of 1-butyl-4-methylpyridinium bromide: ¹H-NMR (400 MHz: D₂O; δ/ppm relative to TMS): 0.81 (3H, but-CH₃), 1.24 (2H, CH₂), 1.85 (2H, CH₂), 2.53 (3H, C-CH₃), 4.42 (2H, N-CH₂), 7.75(2H, CH), 8.53 (2H, N-CH).

Additionally, the spectrum shows a signal at 4.7 ppm (D₂O, HDO).

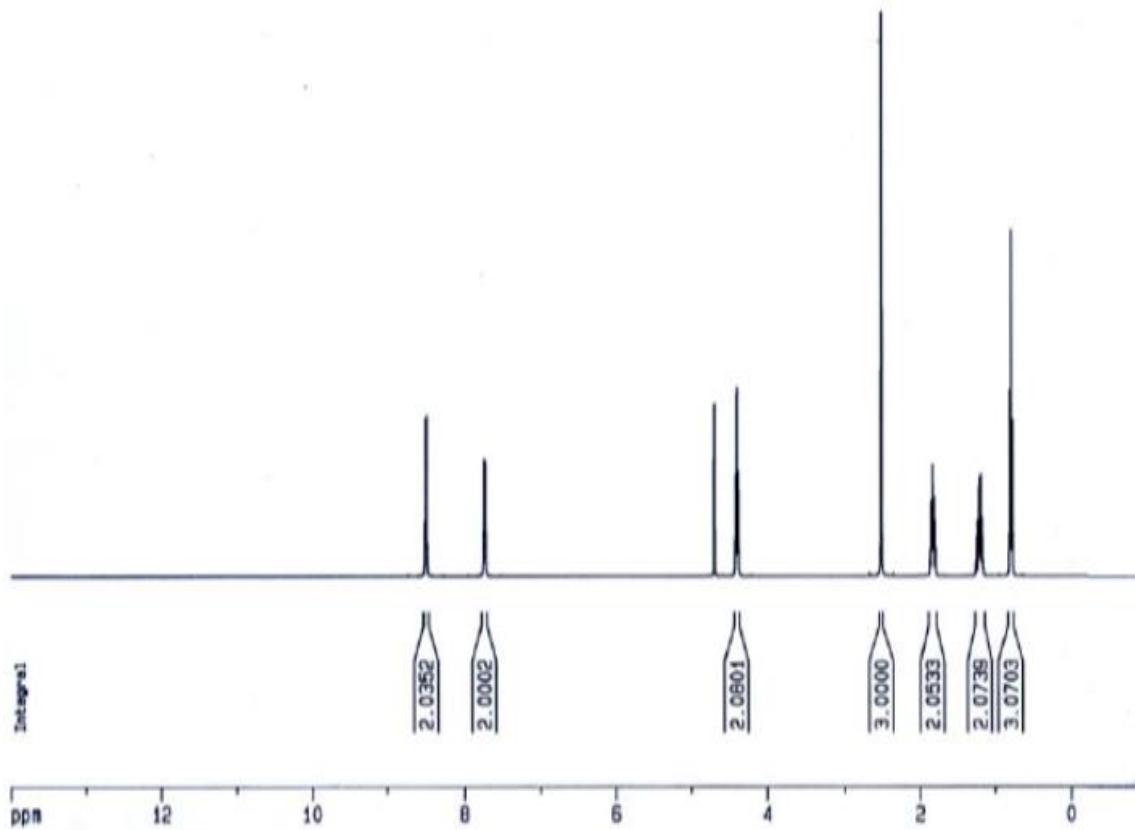


Fig. S 7. ^1H NMR data of 1-butyl-4-methylpyridinium chloride: ^1H NMR (400 MHz; D_2O ; δ /ppm relative to TMS): 0.79 (3H, but- CH_3), 1.22 (2H, CH_2), 1.82 (2H, CH_2), 2.51 (3H, C- CH_3), 4.40 (2H, N- CH_2), 7.73 (2H, CH), 8.51 (2H, N-CH).

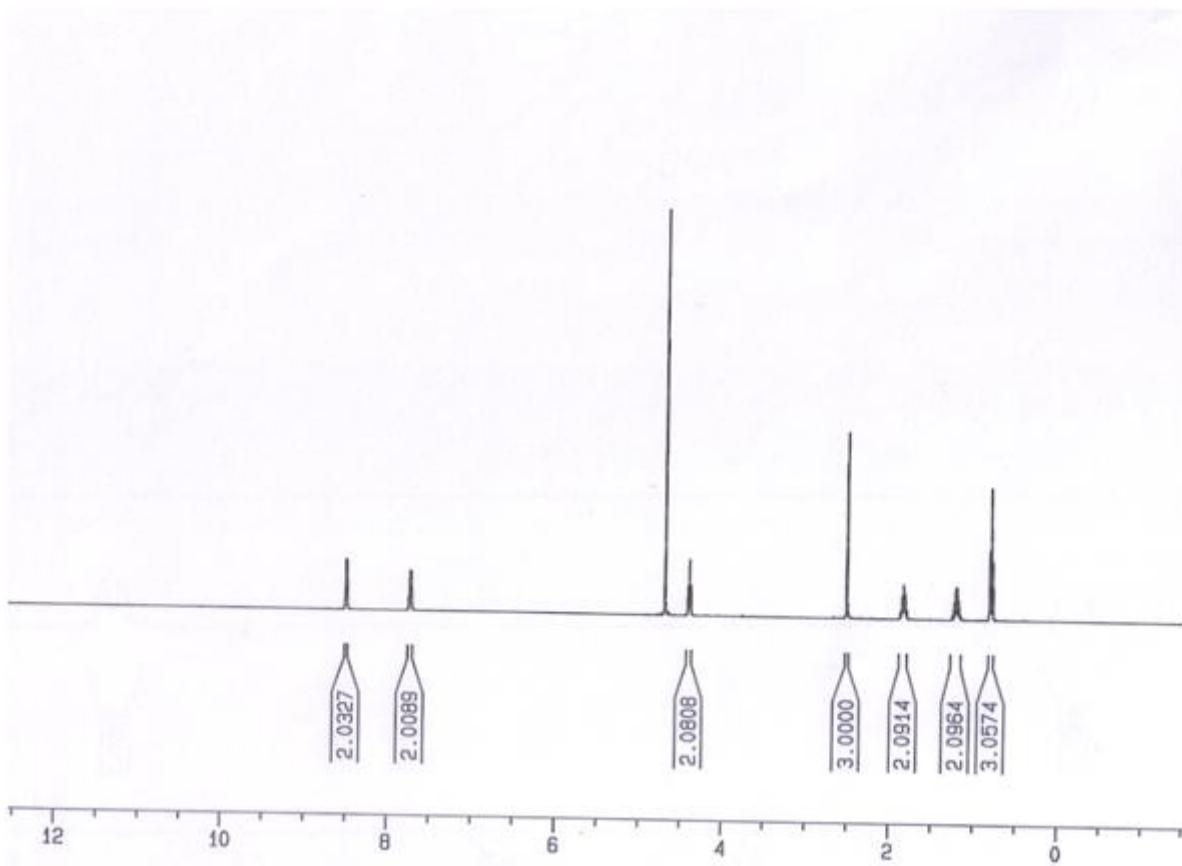


Fig. S8. ^1H NMR data of 1-butyl-4-methylpyridinium thiocyanate: ^1H NMR (400 MHz; D_2O ; δ / ppm relative to TMS): 0.80 (3H, but- CH_3), 1.22 (2H, CH_2), 1.84 (2H, CH_2), 2.51 (3H, C- CH_3), 4.70 (2H, N- CH_2), 7.73 (2H, CH), 8.51 (2H, N-CH).

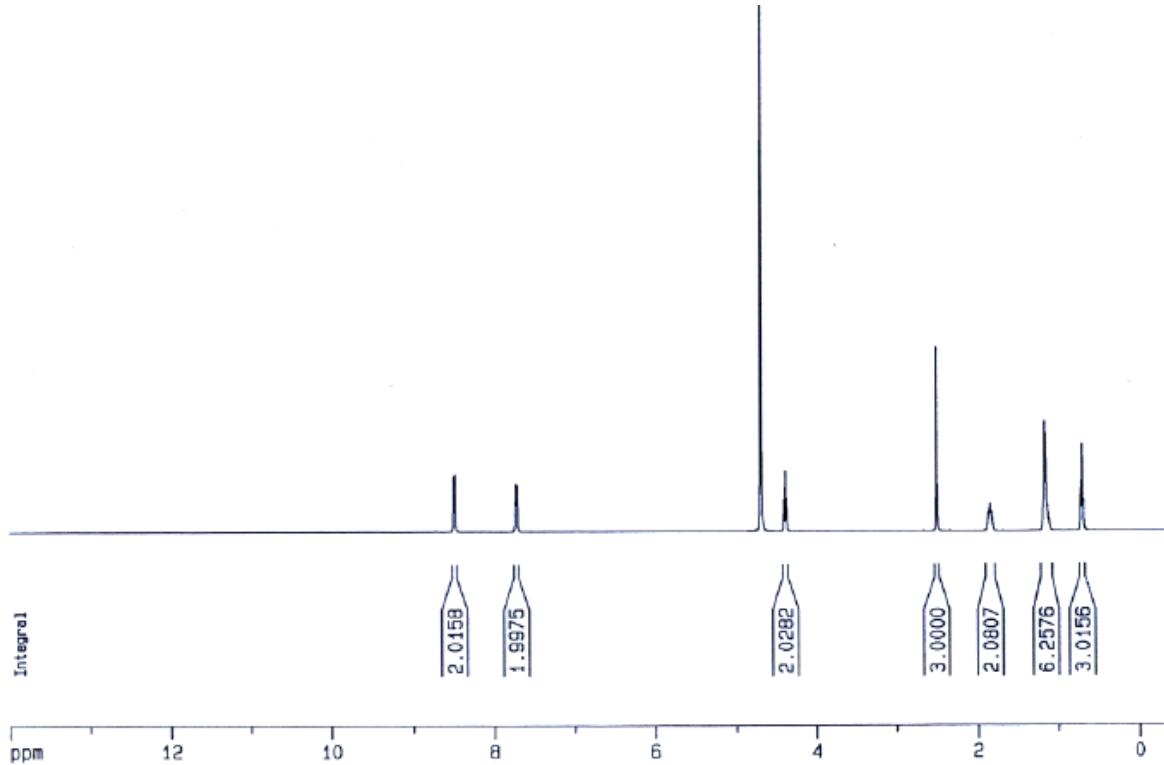


Figure S9. ^1H -NMR data of 1-hexyl-4-methylpyridinium bromide: ^1H -NMR (400 MHz: D_2O ; δ/ppm relative to TMS): 0.71 (3H, hex- CH_3), 1.15 (6H, CH_2), 1.85 (2H, CH_2), 2.51 (3H, $\text{C}-\text{CH}_3$), 4.39 (2H, $\text{N}-\text{CH}_2$), 7.73 (2H, CH), 8.50 (2H, $\text{N}-\text{CH}$).

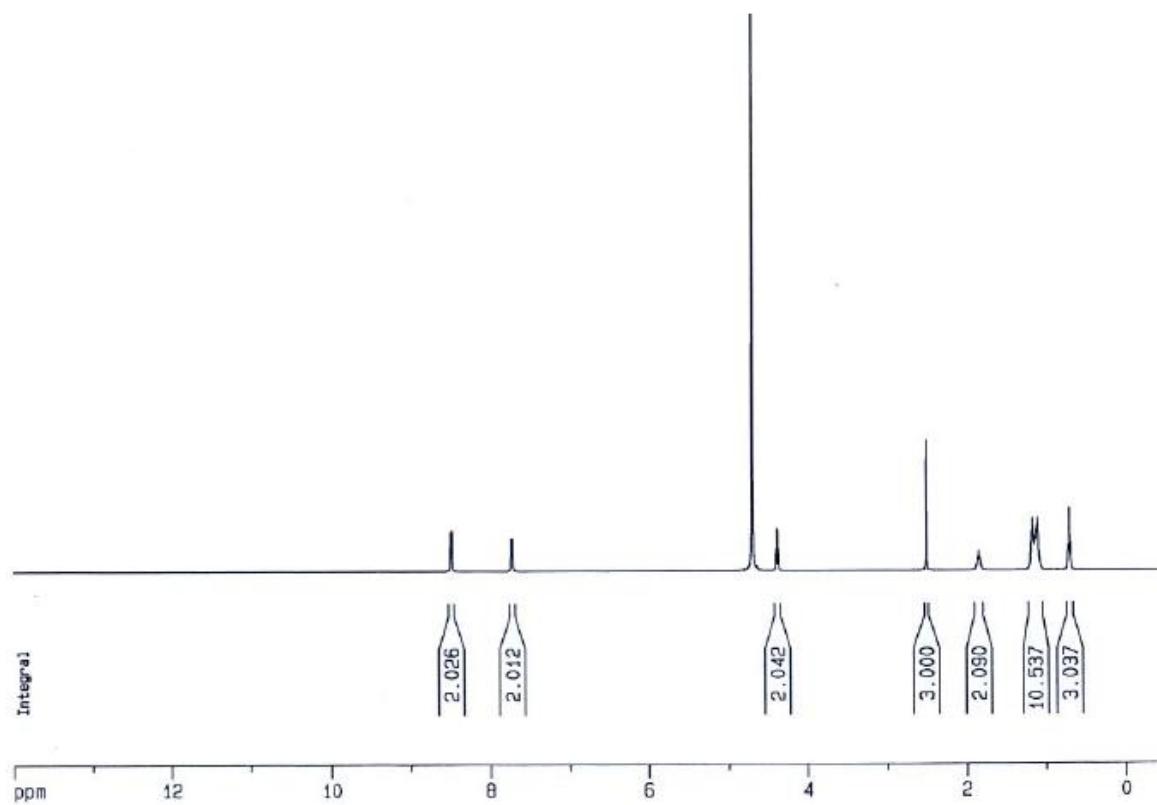


Figure S10. ^1H -NMR data of 1-octyl-4-methylpyridinium bromide: ^1H -NMR (400 MHz: D_2O ; δ /ppm relative to TMS): 0.71 (3H, oct- CH_3), 1.14 (10H, CH_2), 1.85 (2H, CH_2), 2.51 (3H, C- CH_3), 4.39 (2H, N- CH_2), 7.73 (2H, CH), 8.50 (2H, N-CH).