Electronic Supplementary Information

High CO_2 Absorption Capacity by Chemisorption at Cations and Anions in Choline-Based Ionic Liquids

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Contents

1. Spectroscopic Characterization data:

[$N_{1,1,6,2O4}$][4-Triz] : light brown colour semi-solid; yield 83%; ^{1}H NMR (400 MHz, D_2O): δ 0.86-0.92 (m, 6H), 1.31-1.38 (m, 8H), 1.54-1.61 (m, 2H), 1.72-1.78 (m, 2H), 3.10 (s, 6H) 3.32-3.36 (m, 2H), 3.52-3.58 (m, 4H), 3.90 (bs, 2H), 8.09 (s, 2H); ^{13}C NMR (100.6 MHz, D_2O) δ 15.90, 16.03, 21.60, 24.55, 24.73, 27.98, 33.27, 33.57, 54.19, 65.63, 66.66, 68.28, 73.91, 153.45.

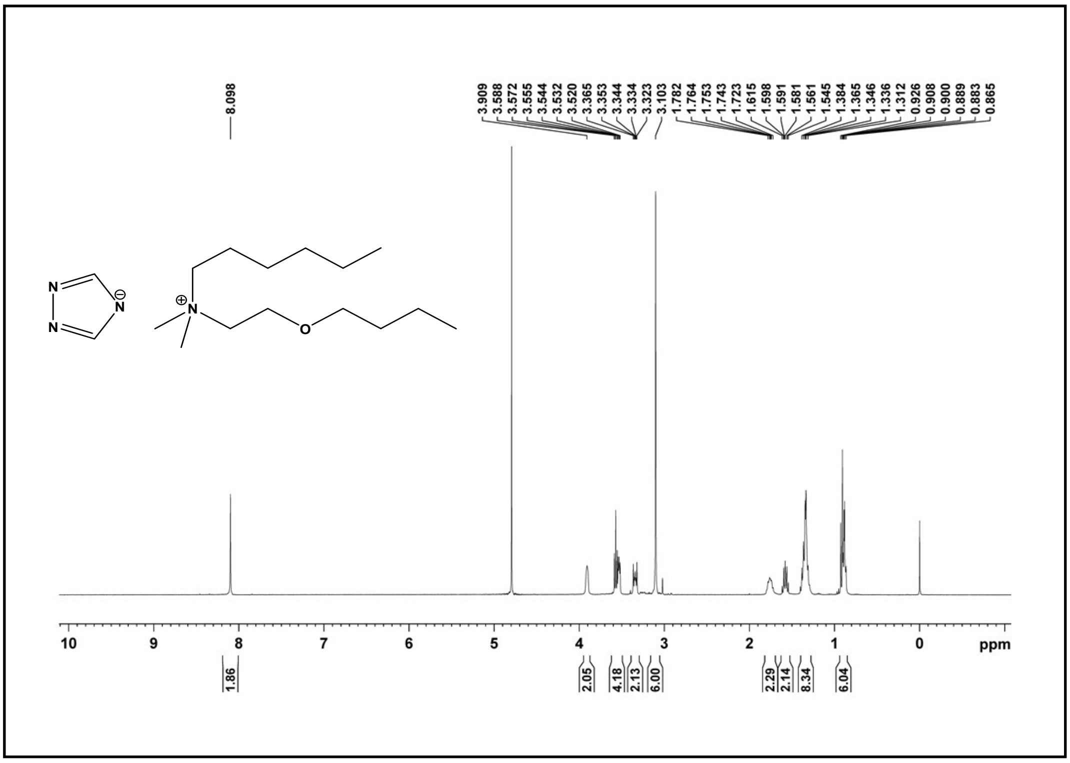
[$N_{1,1,6,2O4}$][Pyrz] : light brown colour solid; yield 81%; ^{1}H NMR (400 MHz, D_2O): δ 0.87-0.93 (m, 6H), 1.33-1.40 (m, 8H), 1.54-1.61 (m, 2H), 1.76 (bs, 2H), 3.10 (s, 6H) 3.32-3.36 (m, 2H), 3.52-3.59 (m, 4H), 3.91 (bs, 2H), 6.43 (s, 1H), 7.71 (s, 2H); ^{13}C NMR (100.6 MHz, D_2O) δ 15.78, 15.90, 21.47, 24.42, 24.60, 27.85, 33.14, 33.44, 54.07, 65.51, 66.53, 68.14, 73.78, 107.65, 137.33.

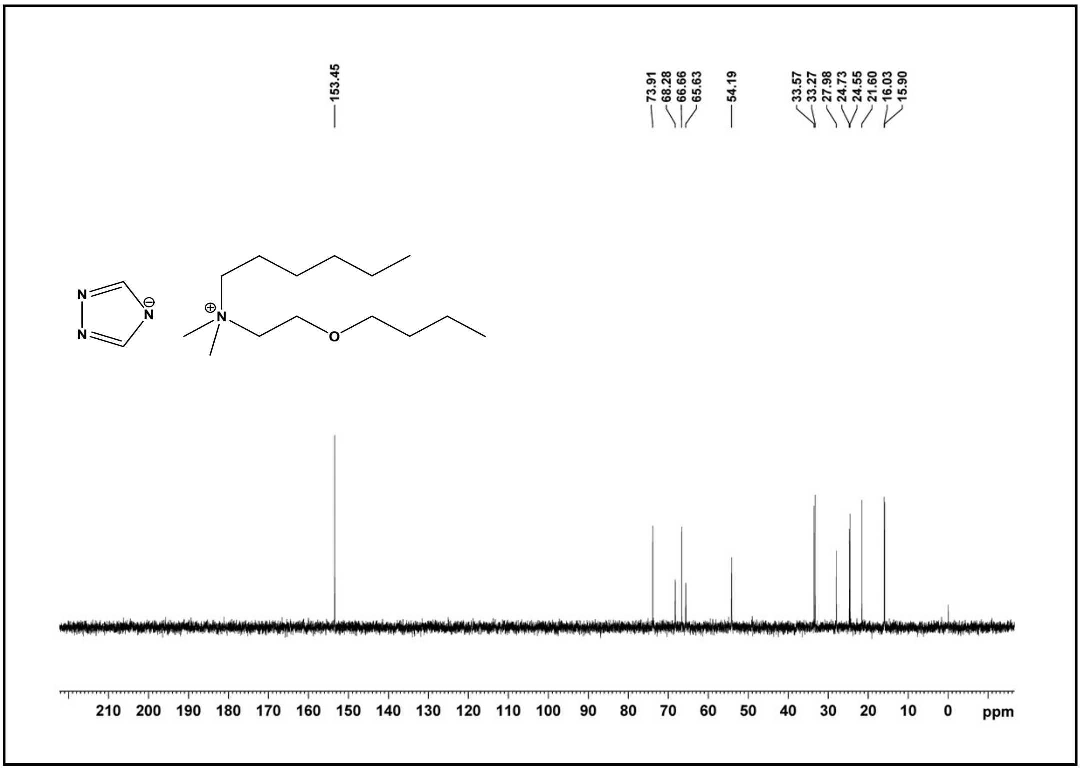
[$N_{1,1,6,2OH}$][4-Triz]: brown colour oil; yield 91%; ^{1}H NMR (400 MHz, D_2O): δ 0.88 (t, 3H, *J*= 6.8 Hz), 1.33 (s, 6H), 1.76-1.78 (m, 2H), 3.10 (s, 6H), 3.34 (t, 2H, *J*=8.4 Hz), 3.44-3.47 (m, 2H), 4.02 (s, 2H), 8.09 (s, 2H); ^{13}C NMR (100.6 MHz, D_2O) δ 153.42, 68.21, 67.52, 58.03, 53.99, 53.95, 33.09, 27.81, 24.52, 24.38, 15.87.

[$N_{1,1,6,2OH}$][Imi]: brown colour oil; yield 92%; ^{1}H NMR (400 MHz, D_2O): δ 0.87 (t, 3H, *J*= 6.8 Hz), 1.28-1.37 (m, 6H), 1.74-1.78 (m, 2H), 3.10 (s, 6H), 3.31-3.35 (m, 2H), 3.42 (t, 2H, *J*=5.2 Hz), 4.00 (s, 2H), 7.12 (s, 2H), 7.75 (s, 1H); ^{13}C NMR (100.6 MHz, D_2O) δ 15.87, 24.38, 24.53, 27.82, 33.09, 53.91, 53.94, 53.98, 58.08, 67.94, 68.15, 124.67, 139.13

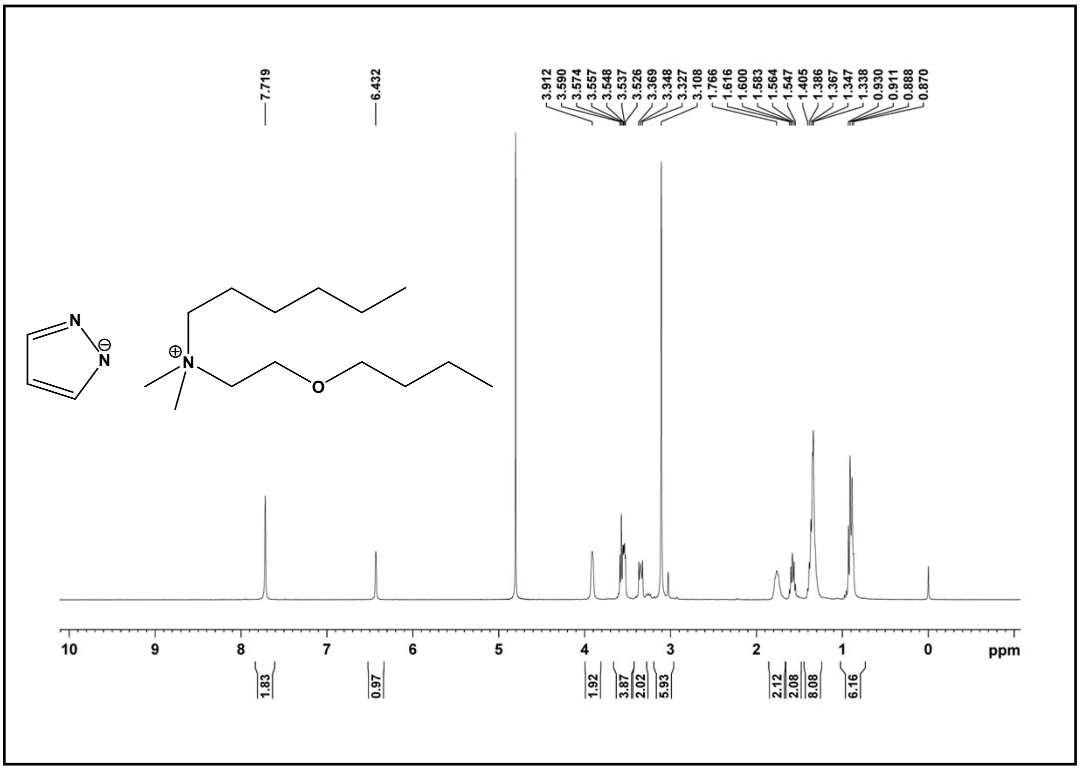
[$N_{1,1,6,2OH}$][Succ]: light brown colour viscous oil; yield 94%; ^{1}H NMR (400 MHz, D_2O): δ 0.89 (t, 3H, *J*= 6.8Hz), 1.30-1.39 (m, 6H), 1.77-1.82 (m, 2H), 2.44-2.53 (m, 4H) 3.13 (s, 6H), 3.35-3.39 (m, 2H), 3.48-3.50 (m, 2H), 4.04 (m, 2H); ^{13}C NMR (100.6 MHz, D_2O) δ 15.87, 24.38, 24.54, 27.82, 33.09, 34.41, 35.63, 54.01, 58.05, 67.52, 68.23, 181.69, 183.77.

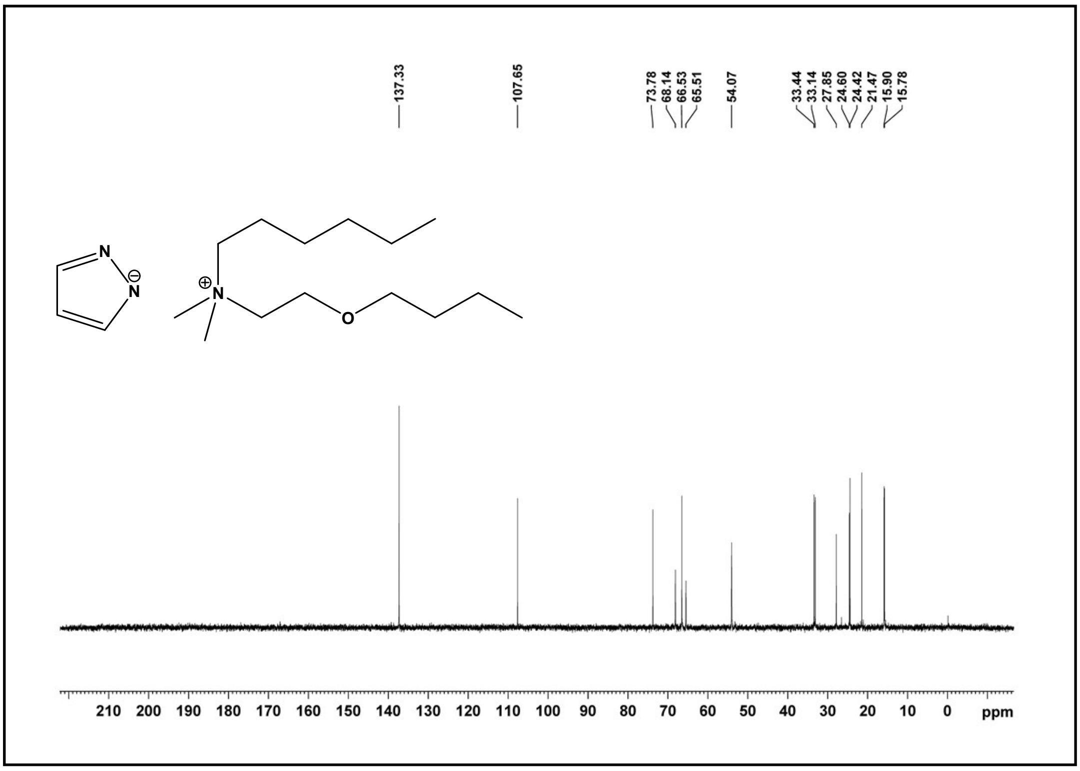
2. [1]H and [13]C NMR of all ILs



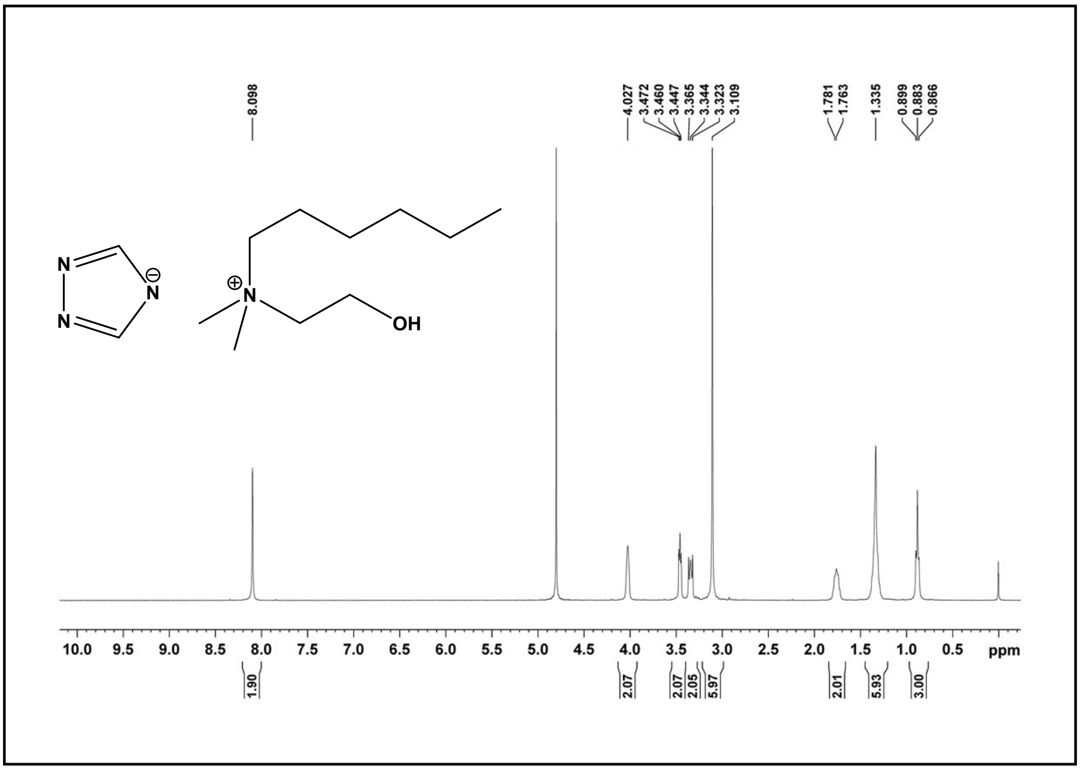


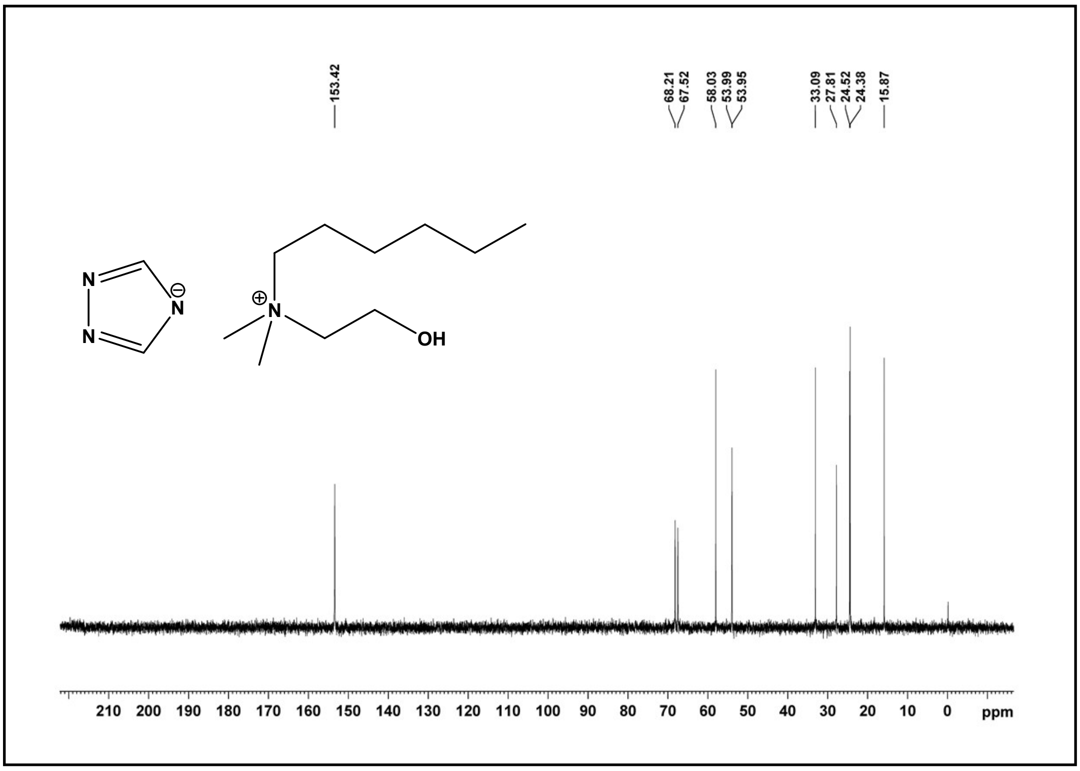
[1]H and [13]C NMR of $[N_{1,1,6,2O4}]$[4-Triz]



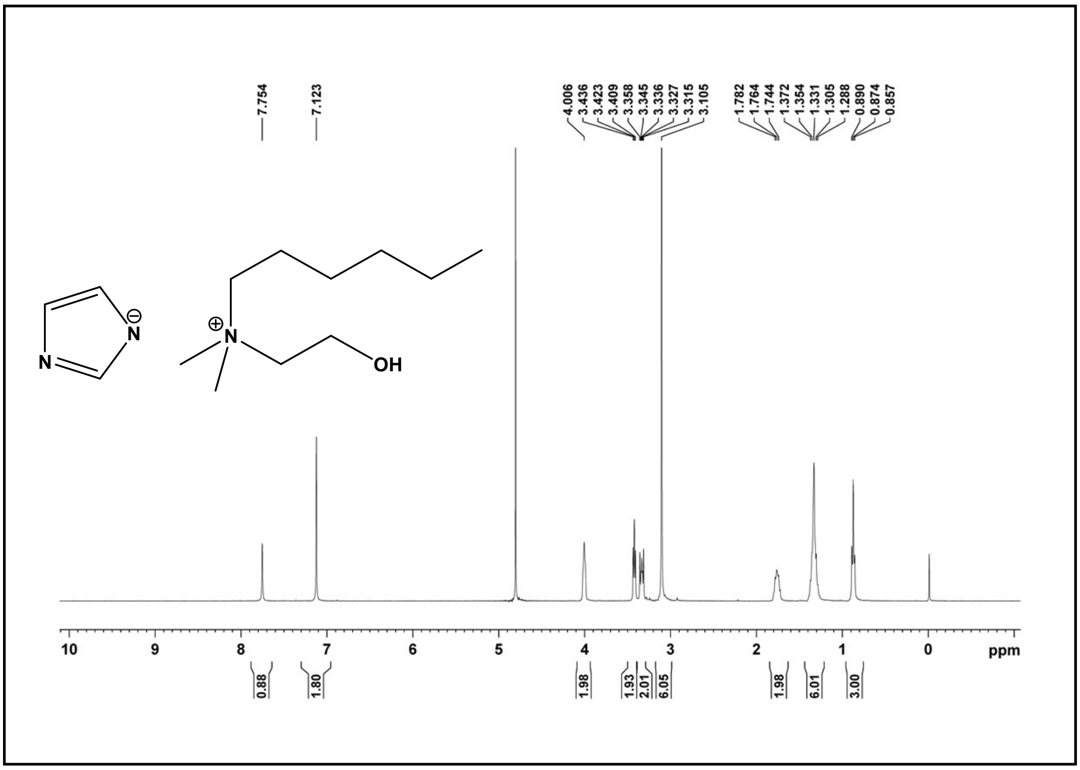


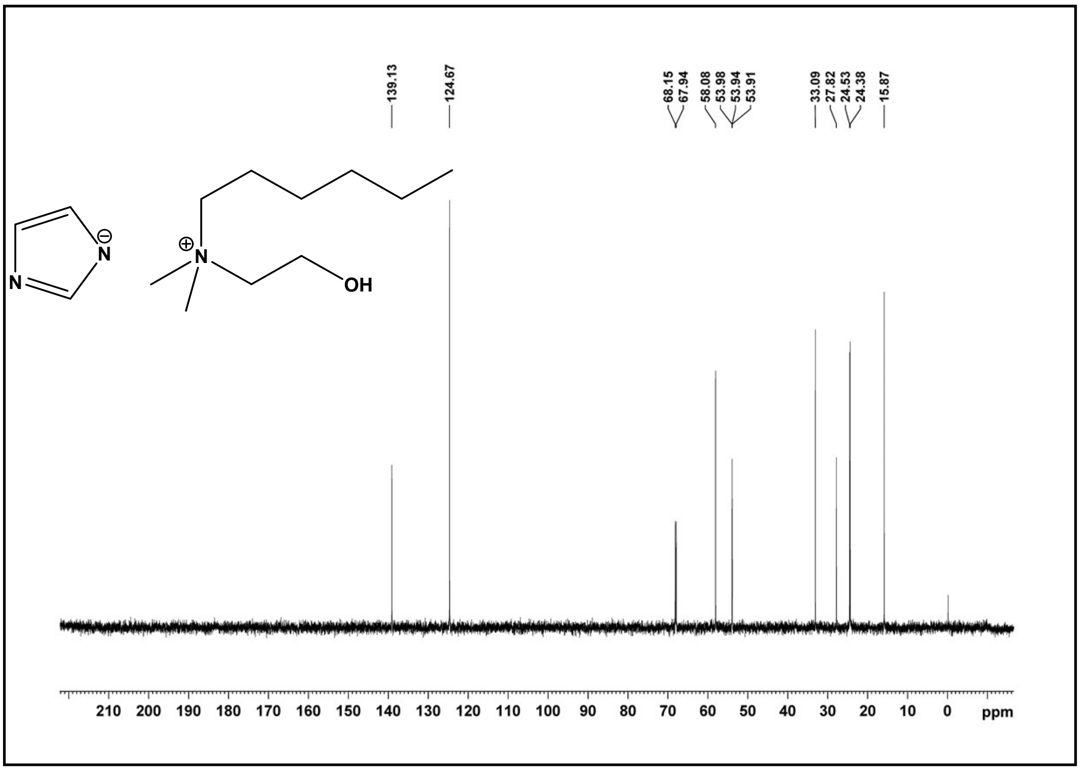
^{1}H and ^{13}C NMR of $[N_{1,1,6,2O4}]$[Pyrz]



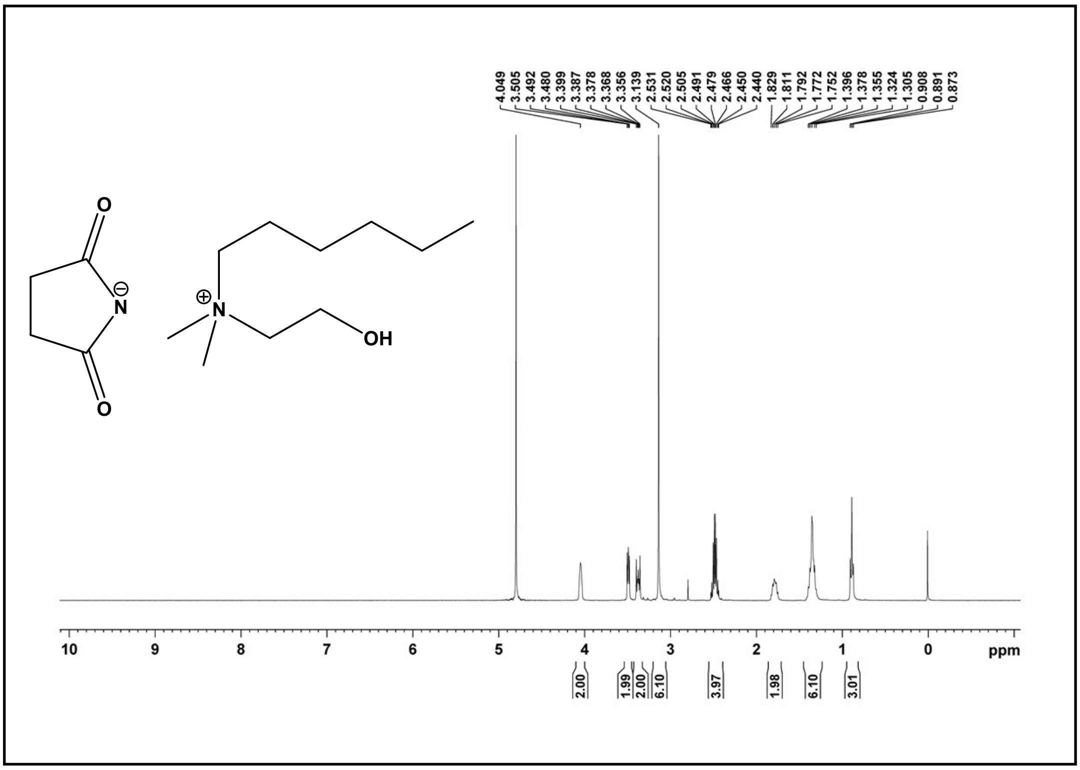


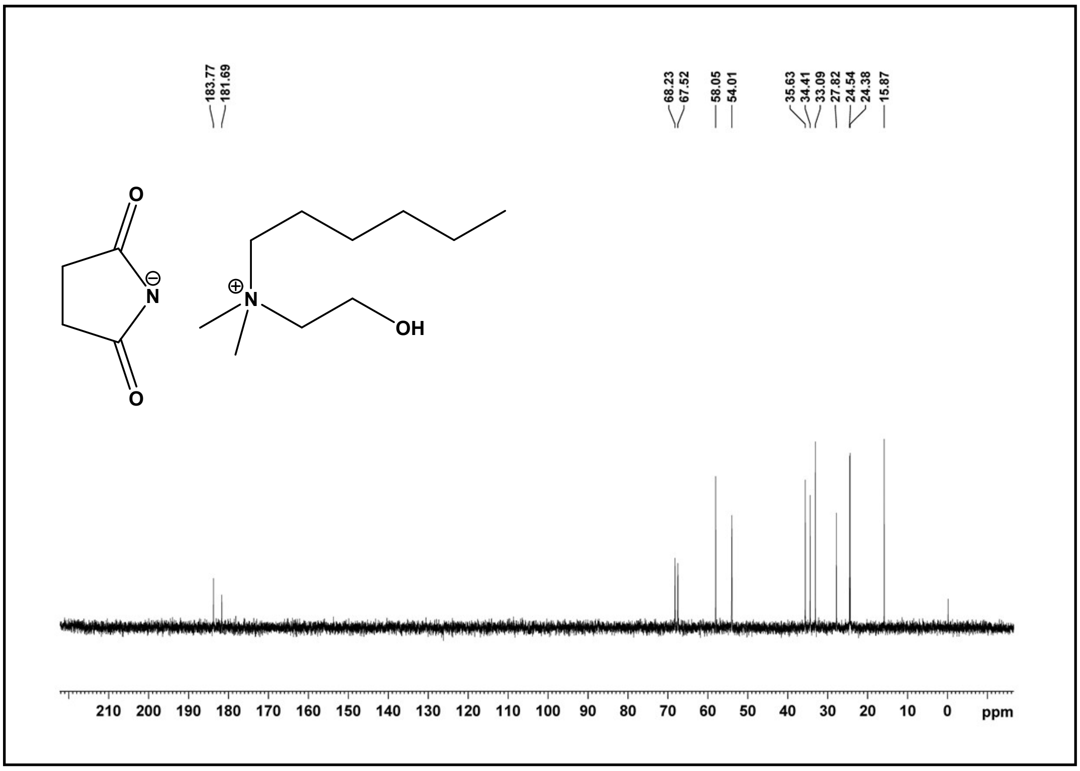
^{1}H and ^{13}C NMR of $[N_{1,1,6,2OH}]$[4-Triz]





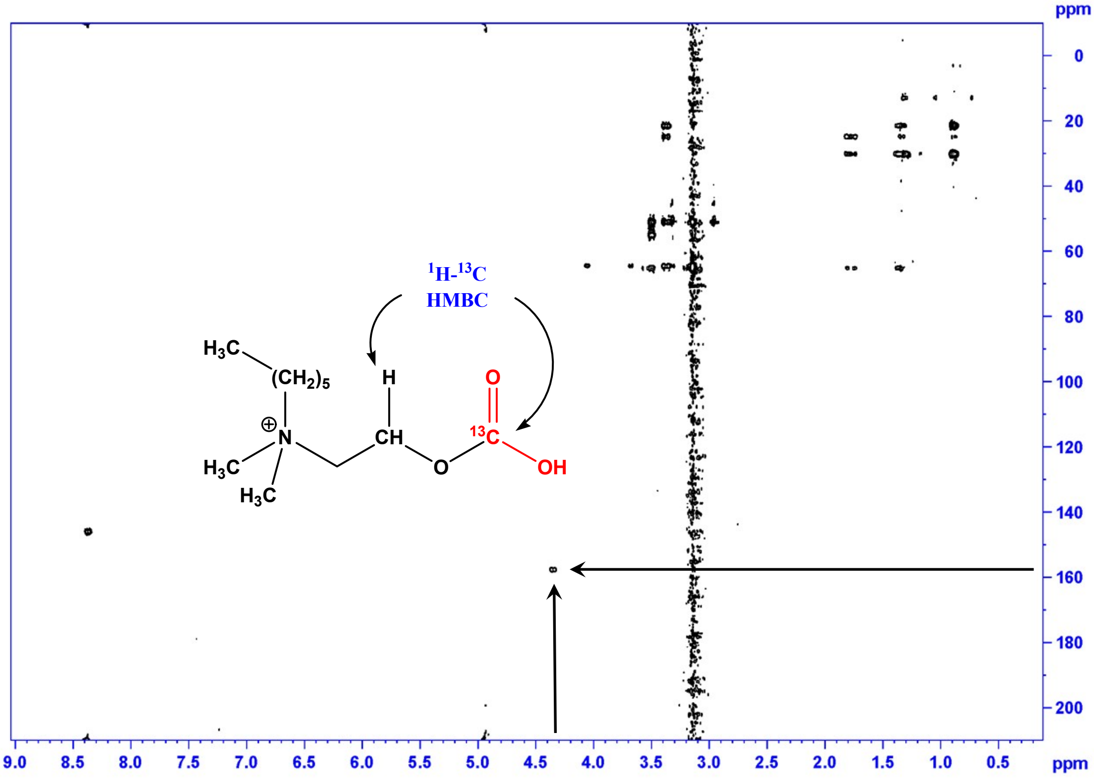
^{1}H and ^{13}C NMR of [$N_{1,1,6,2OH}$][Imi]



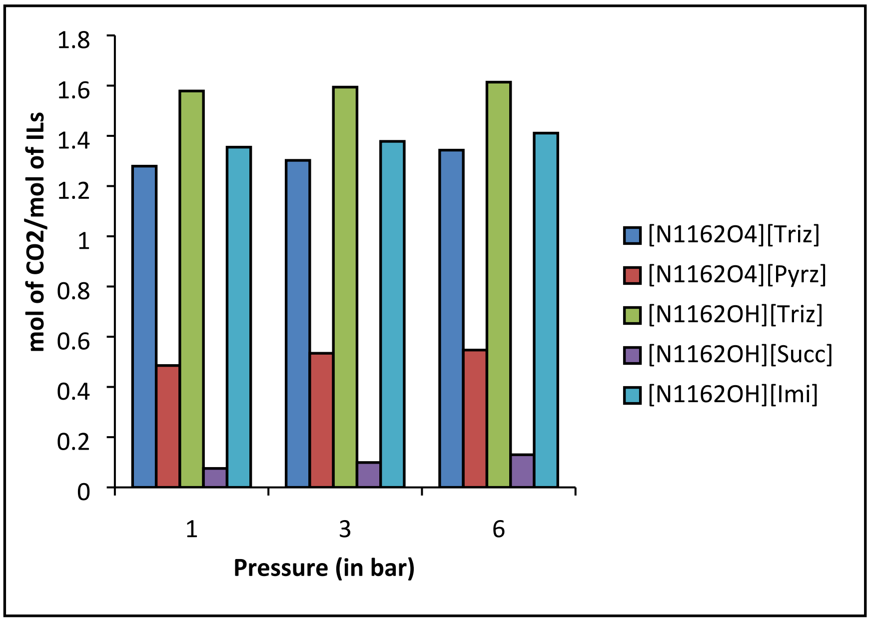


^{1}H and ^{13}C NMR of $[N_{1,1,6,2OH}][Succ]$

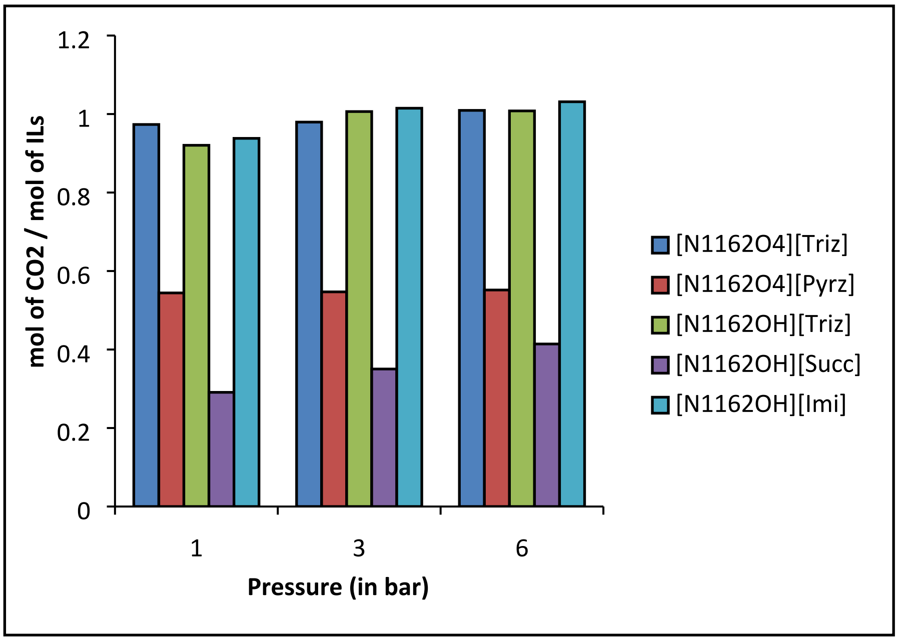
3. ^{1}H-^{13}C HMBC spectra of $[N_{1,1,6,2OH}][4\text{-}Triz]+^{13}CO_2$ in D_2O



4. CO_2 absorption capacities of Ionic Liquids

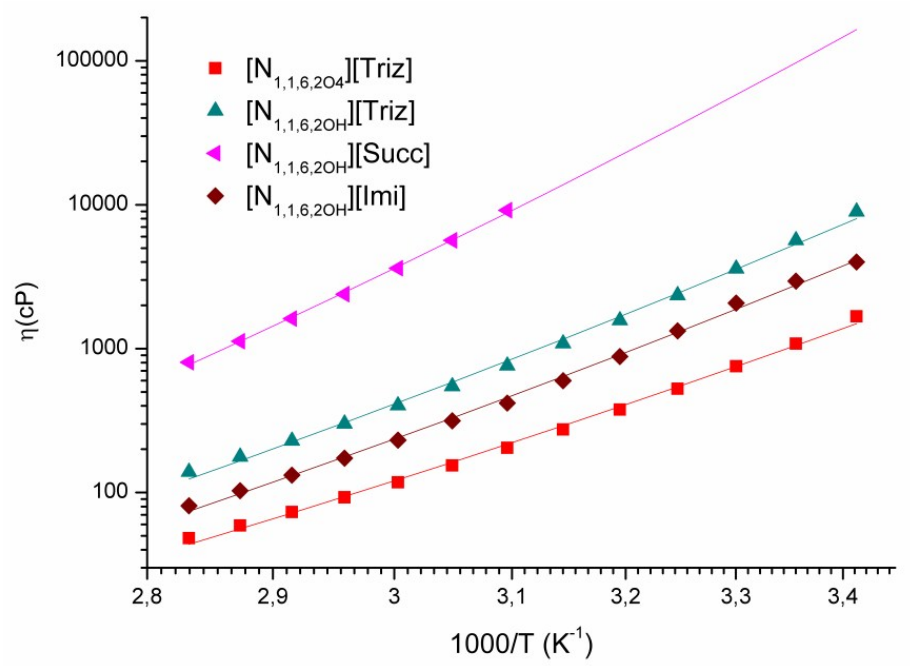


CO_2 capture capacity of ILs at 20°C

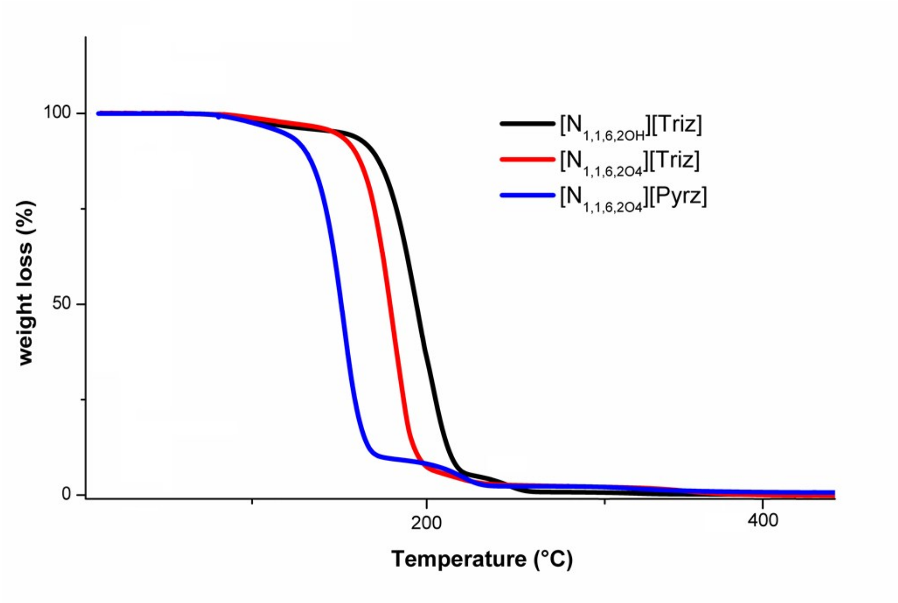


CO_2 capture capacity of ILs at 40°C

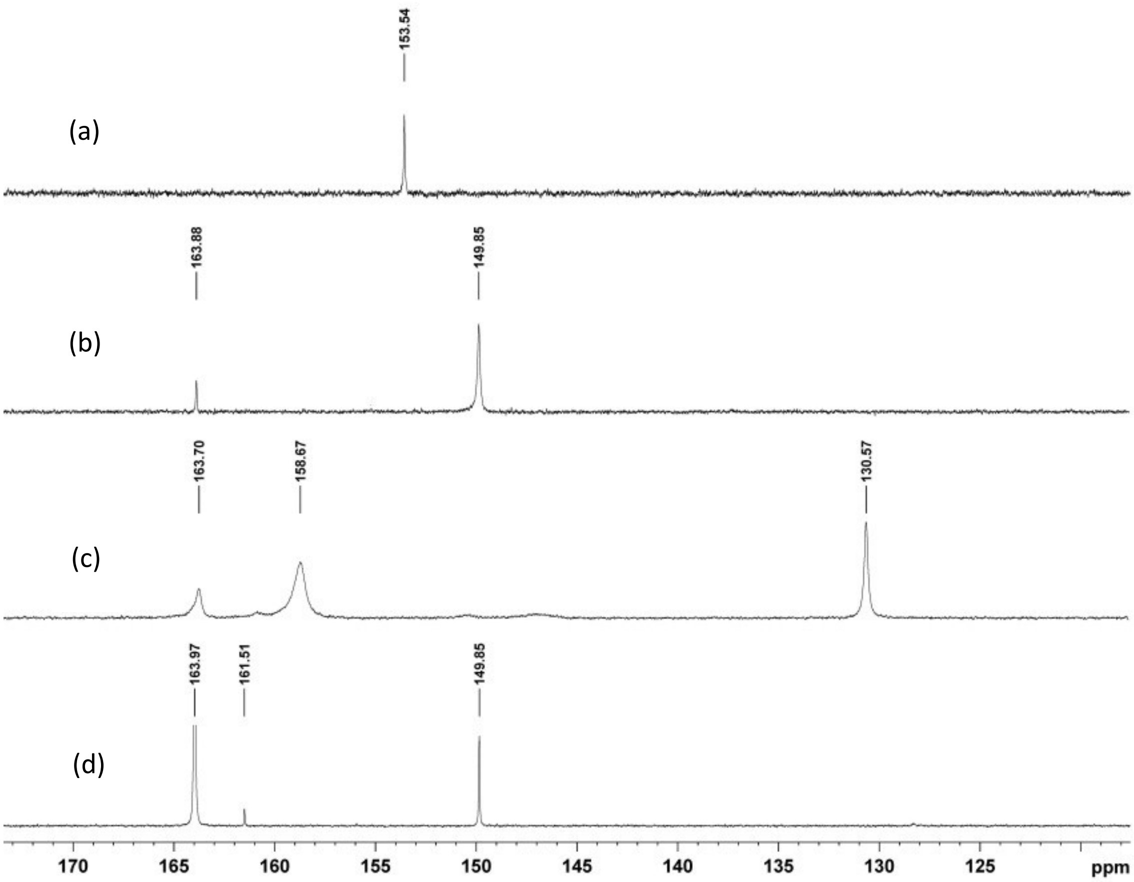
5. Viscosity of the synthesized choline based *N*-heterocyclic ionic liquids as a function of temperature



6. Thermogravimetric analysis (TGA) of [$N_{1,1,6,2OH}$][4-Triz], [$N_{1,1,6,2O4}$][4-Triz] and [$N_{1,1,6,2O4}$][Pyrz]

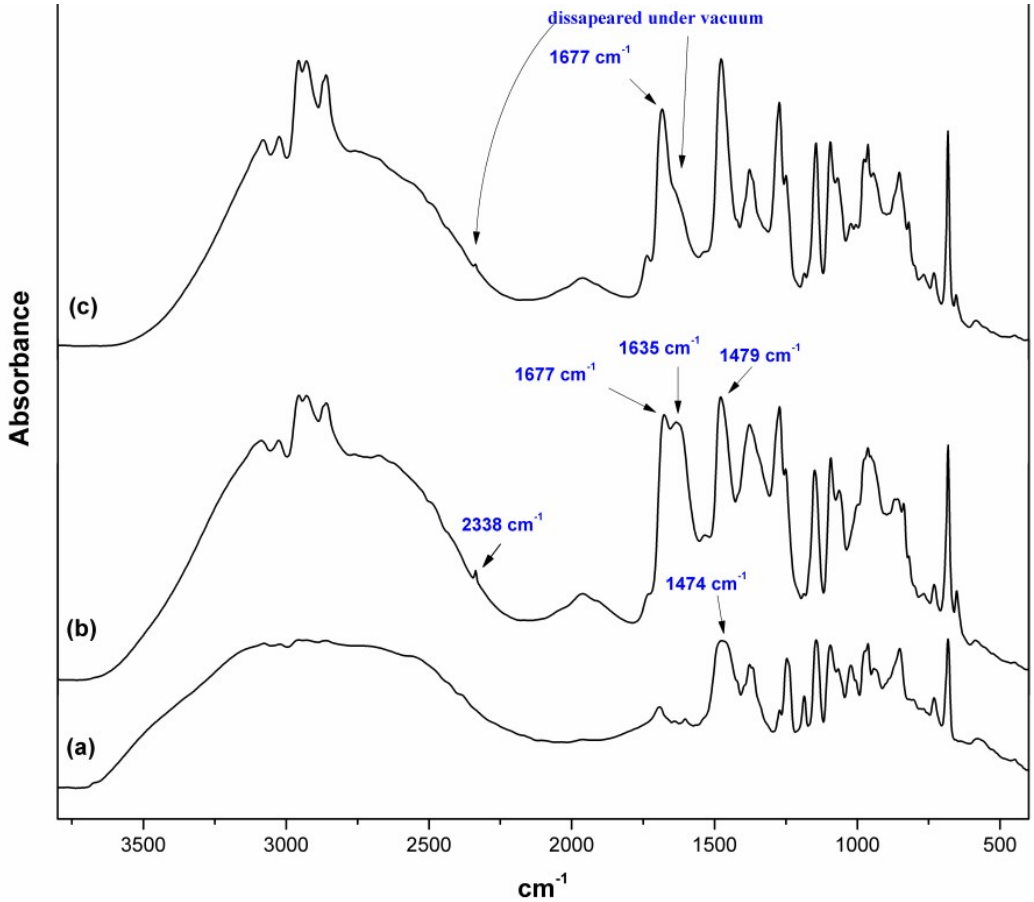


7. Comparative ^{13}C NMR data of $[N_{1,1,6,2OH}]$[4-Triz] and $[N_{1,1,6,2OH}]$[4-Triz]+CO_2 reaction



(a) IL before CO_2 absorption dissolved in D_2O, (b) IL after CO_2 absorption dissolved in D_2O, (c) neat IL after $^{13}CO_2$ absorption with D_2O as an external lock, and (c) IL after $^{13}CO_2$ absorption dissolved in D_2O.

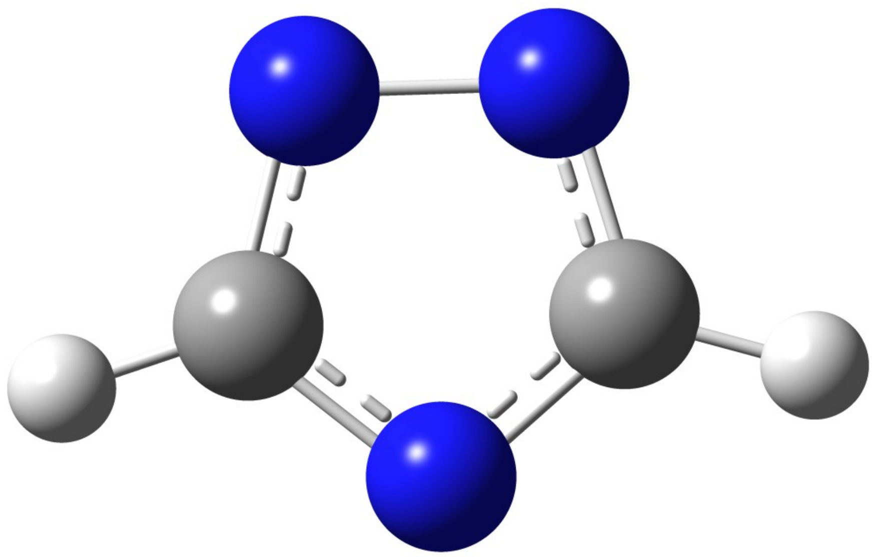
8. FT-IR spectra of $[N_{1,1,6,2OH}]$[4-Triz] and after CO_2 reaction



FT-IR spectra (under vacuum) of (a) IL $[N_{1,1,6,2OH}]$[4-Triz], (b) $[N_{1,1,6,2OH}]$[4-Triz]-CO_2, (c) $[N_{1,1,6,2OH}]$[4-Triz]-CO_2 after 5 minutes.

9. Computational data

B3LYP/6-311+G(d,p) optimized geometry of the 4-triazole, pyrazole and Imidazole anion as well as their carbamate anion with Cartesian coordinate.



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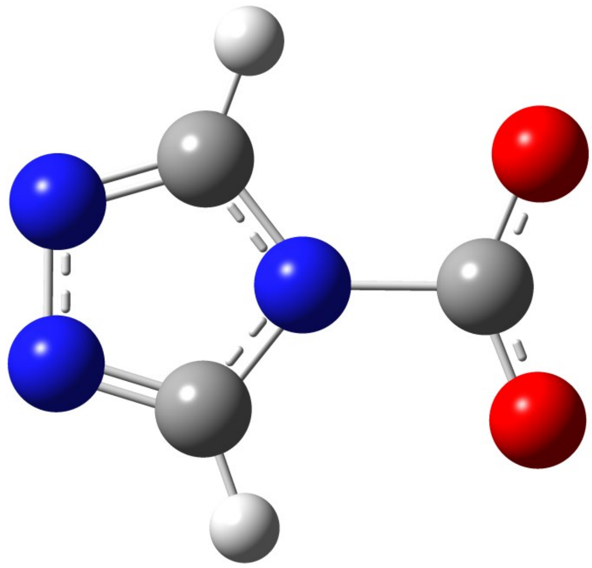
N	-0.94369400	0.71262800	0.00000000



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C	1.56270700	-0.03487800	0.00034000
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O	2.01255600	-1.17866300	0.00034400
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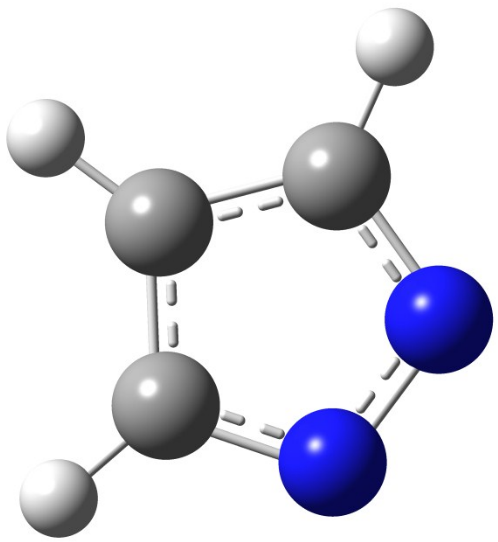

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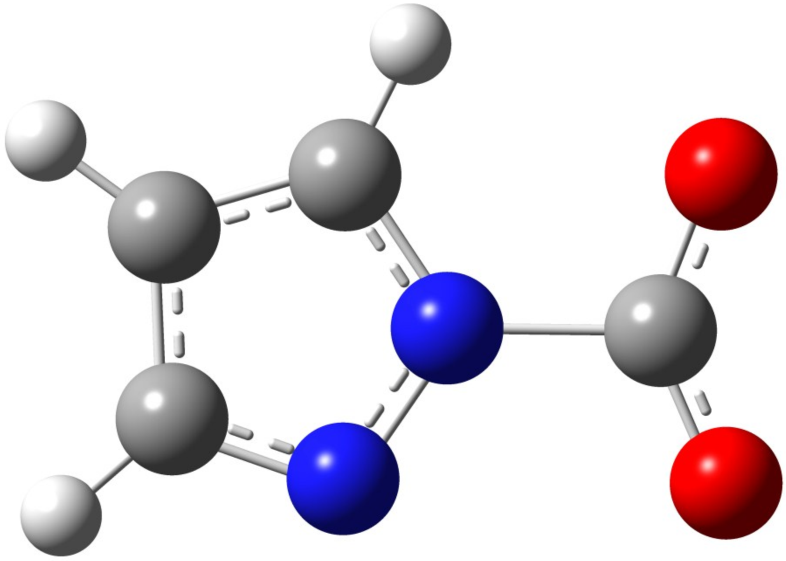

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H	-2.88363500	-1.38682300	-0.00064000
H	-2.99740100	1.37422000	-0.00045900
H	-0.31333300	2.08498000	0.00012000
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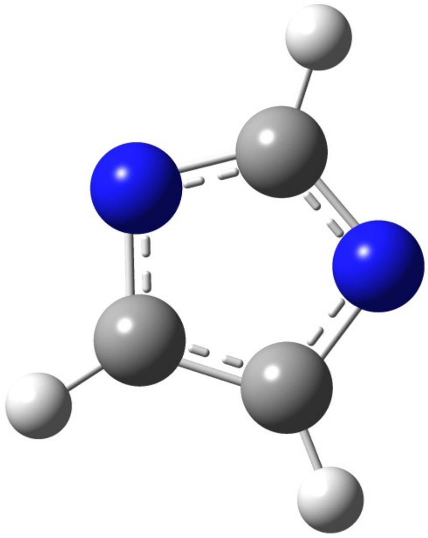

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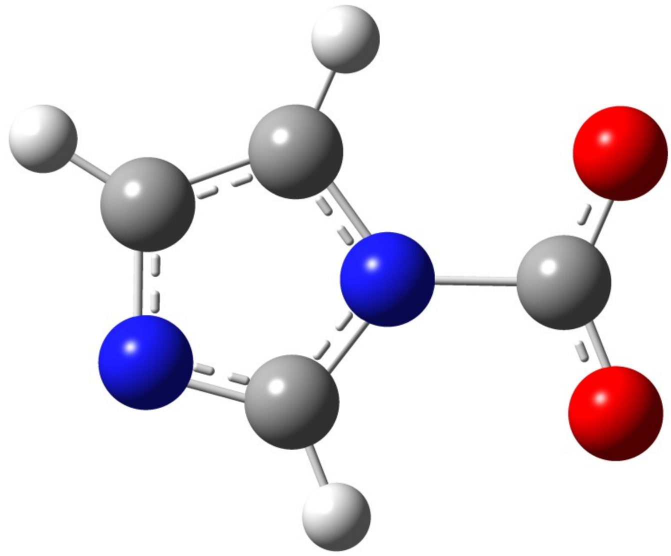

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N	-2.09462200	-0.70494500	-0.00043500