Supplementary Information:

Green synthesis of polyureas from CO_2 and diamines with a functional ionic liquid as the catalyst

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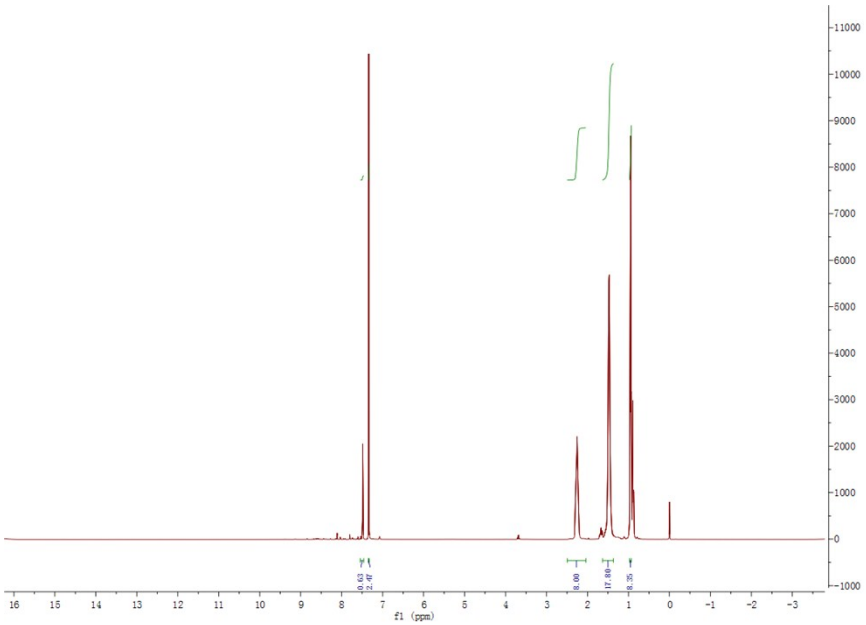
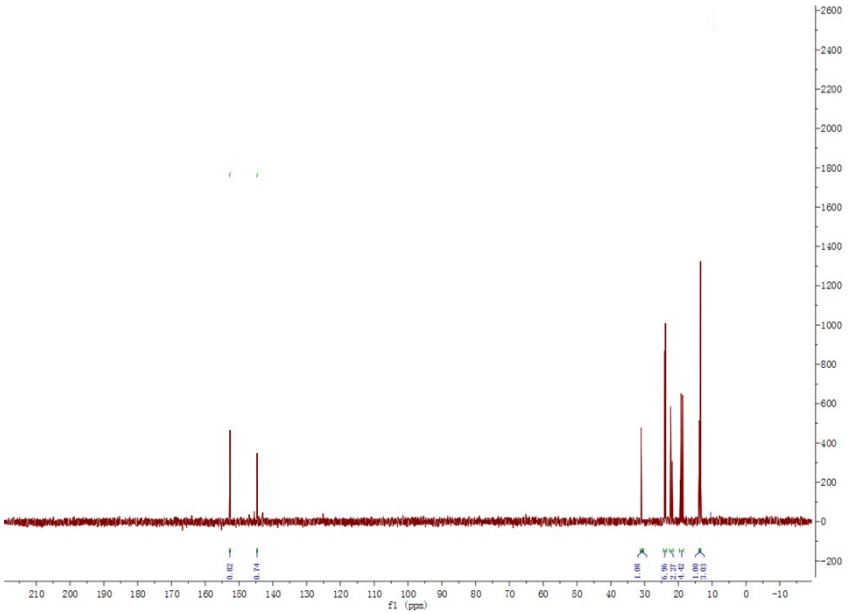
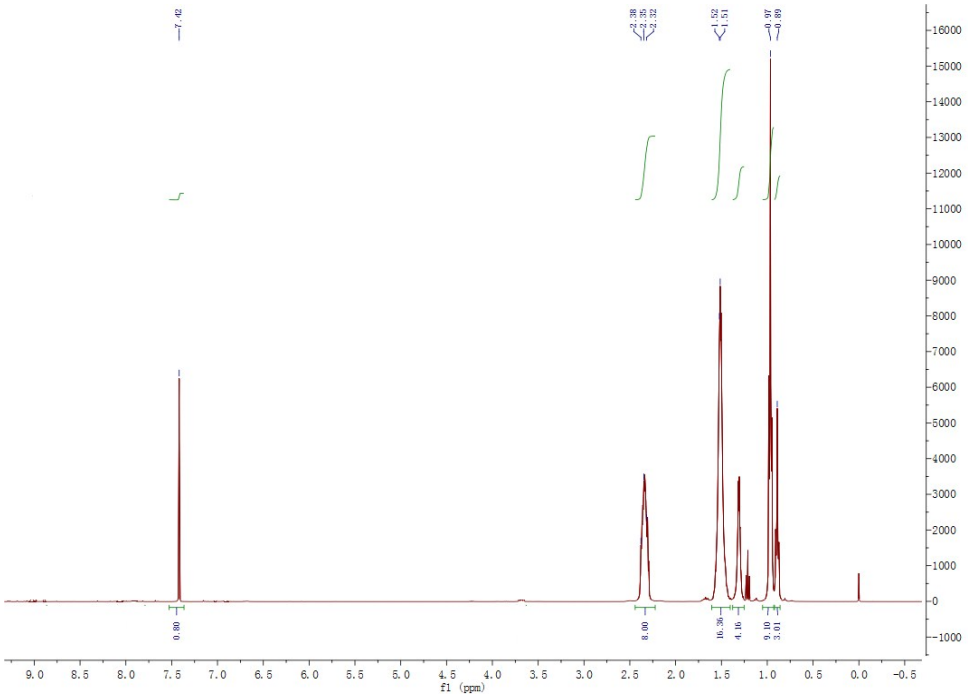
Hexyltributylphosphonium triazole ($P_{4,4,4,6}$Triz) and hexyltributylphosphonium aminotriazole ($P_{4,4,4,6}$ATriz) were prepared by the neutralization of hexyltributylphosphonium hydroxide ($P_{4,4,4,6}$OH) and 1,2,4-triazole or 3-amino-1,2,4-triazole according to literature methods.[26-27] Typically, a solution of $P_{4,4,4,6}$OH in ethanol was first prepared from $P_{4,4,4,6}$Br using the anion-exchange resin method. Second, equimolar 1,2,4-triazole or 3-amino-1,2,4-triazole was added to the $P_{4,4,4,6}$OH solution in ethanol. Next, the mixture was stirred at room temperature for 12 h. Subsequently, ethanol and water were removed by distillation at 60°C under reduced pressure. The obtained ILs were dried under high vacuum at 80 °C for 8 h. The structures of these ILs were confirmed by NMR spectroscopy. ^{1}H NMR and ^{13}C NMR spectra were recorded on a Bruker AMX FT 400 MHz NMR spectrometer (Fig. S1).



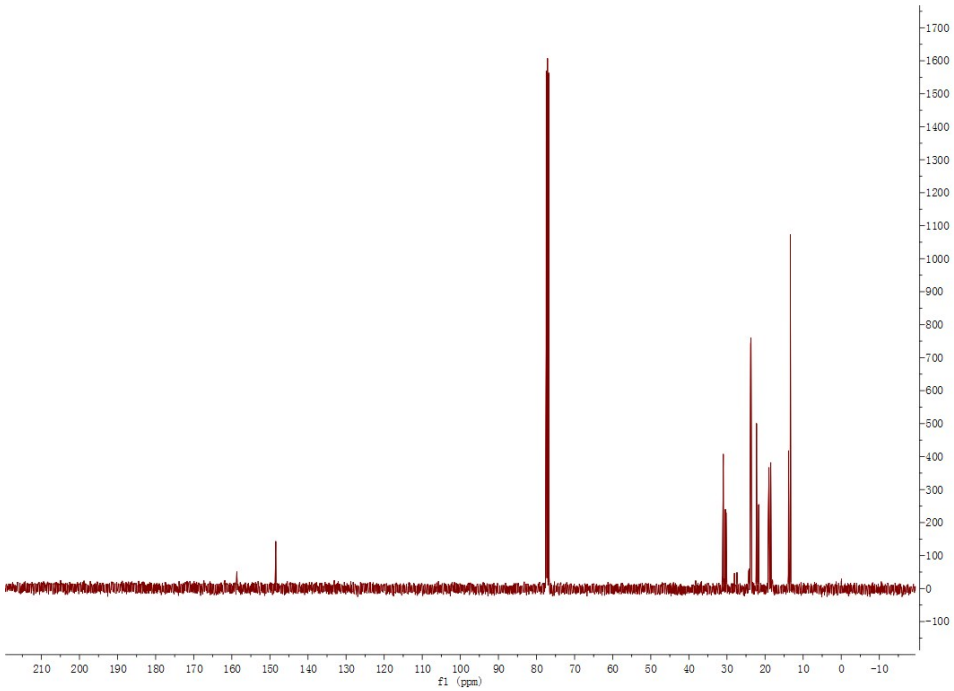
$P_{4,4,4,6}$Triz ^{1}H NMR ($CDCl_3$) 0.95 (m, 12H, CH_3), 1.30–1.52 (m, 20H, CH_2), 2.29–2.38 (m, 8H, PCH_2), 8.07 ppm (s, 2H, Triz C_2 and C_5);



$P_{4,4,4,6}$Triz ^{13}C NMR ($CDCl_3$) 13.3, 13.8, 18.5, 19.0, 21.7, 22.2, 23.7, 23.9, 30.3, 30.9, 148.8, 152.5 ppm.



$P_{4,4,4,6}$ATriz ^{1}H NMR ($CDCl_3$) 0.94 (m, 12H, CH_3), 1.29–1.50 (m, 20H, CH_2), 2.21–2.29 (m, 8H, PCH_2), 7.34 (s, 2H, Triz-NH_2), 7.49 ppm (s, H, Triz C5);



$P_{4,4,4,6}$ATriz 13C NMR (CDCl3) 13.4, 13.8, 18.5, 19.1, 21.7, 22.2, 23.6, 23.9, 30.4, 30.9, 148.6, 158.9 ppm.

Fig. S1 NMR spectrum of the $P_{4,4,4,6}$Triz and $P_{4,4,4,6}$ATriz.

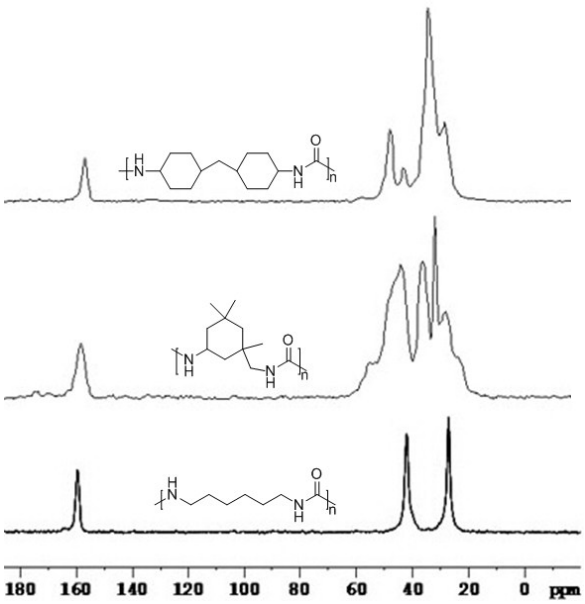


Fig. S2 CP/MAS ^{13}C NMR spectrum of the solid products of diamines reaction with CO_2.

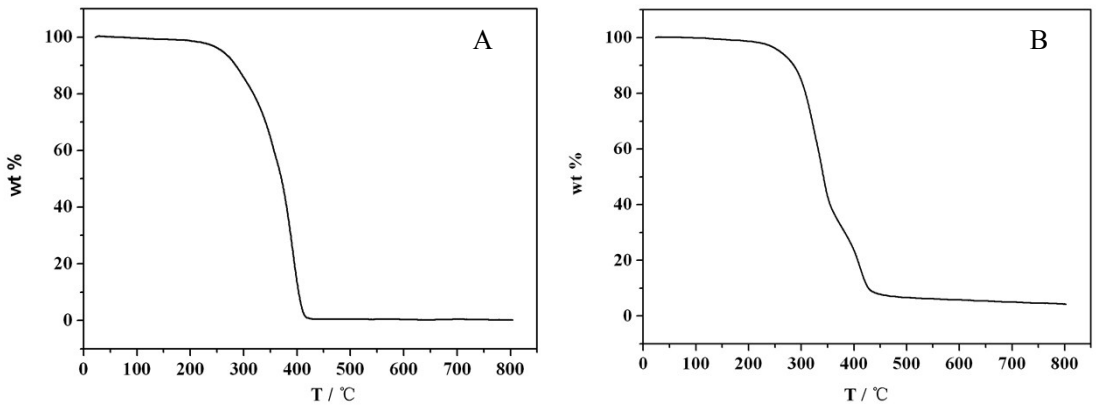


Fig .S3 TGA traces of $P_{4,4,4,6}$Triz; (B) TGA traces of $P_{4,4,4,6}$ATriz.

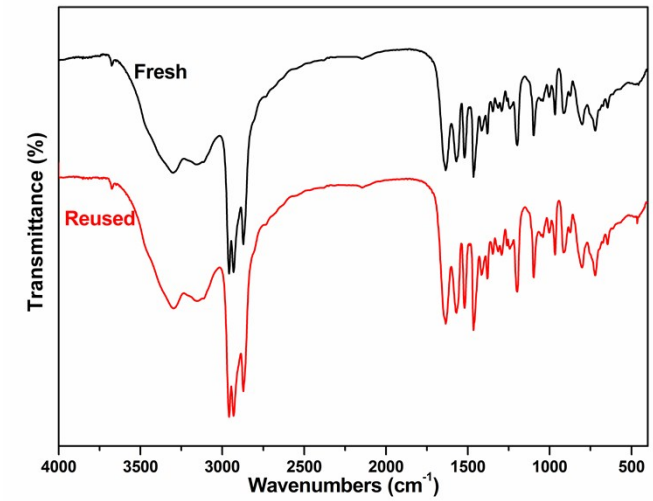


Fig. S4 FT-IR spectra of $P_{4,4,4,6}$ATriz before and after use.

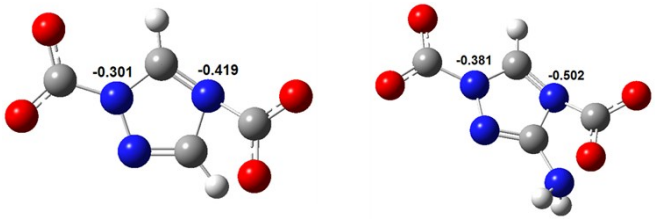


Fig. S5 Optimized structures of anion–$2CO_2$ complexes at the B3LYP/6-31+G (d, p) level

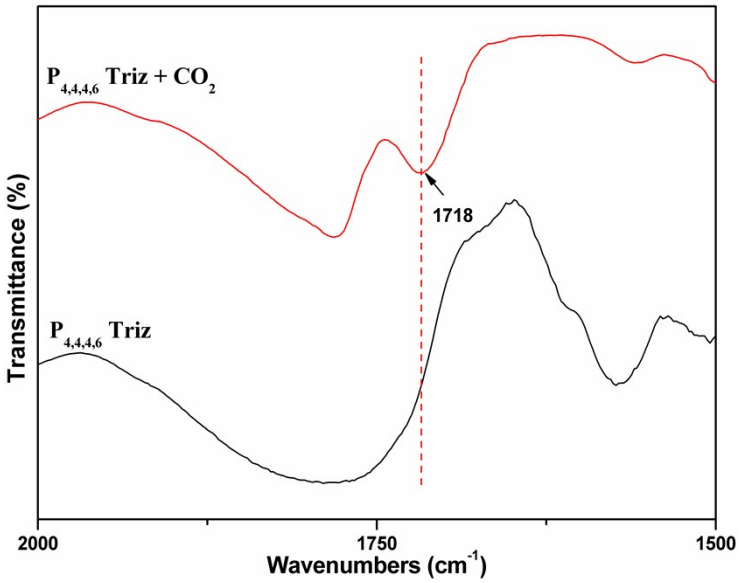


Fig. S6 FT-IR spectra of $P_{4,4,4,6}$Triz before and after absorption of CO_2.