Supporting Information

For

Facile Synthesis of Binuclear Imidazole Based Poly(Ionic Liquid) via Monomer Self-polymerization: Unlocking High-Efficiency CO_2 Conversion to Cyclic Carbonate

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Catalyst characterization. ^{1}H NMR spectra and ^{13}C NMR spectra were performed on a Bruker DPX 500 spectrometer at ambient temperature by using D_2O and DMSO as the deuterium reagent. The infrared spectrum was obtained by using Beijing Rayleigh Fourier Transform infrared spectrometer WQF-510A, and the chemical functional groups and specific chemical bonds of the detected samples were analyzed. The wavelength range was 400-4000 cm^{-1}, and the scanning times were 32. Before the test, take a small amount of sample and potassium bromide (KBr) ground until evenly mixed, and dry under a drying lamp for use.The thermogravimetric analyzer STA449 was used to perform temperature programmed tests in the range of RT-800 ℃ under nitrogen (N_2) atmosphere at a temperature rate of 10 ℃·min^{-1}. The X-ray photoelectron spectrometer used was the Thermo Fisher Scientific ESCALAB 250. The correction was performed using a C 1s peak (284.8 eV). The basic morphologies of nitrogen-containing polymer precursors and their derived carbon materials were observed with a scanning electron microscope model Hitachi S4800. Before the test, a small amount of sample was added to anhydrous ethanol, dispersed evenly by ultrasound, and then dropped onto silicon wafers with capillary tubes for drying. Subsequently, the surface of the silicon wafer was sprayed with gold for about 90 s to eliminate the influence of the weak electrical conductivity of the material on the test process. N_2 adsorption-desorption tests were performed on samples at 77 K using the BELSORP MAX instrument. Before the test, samples were pre-treated at 100 ℃ under vacuum for 10 h. After the test, the specific surface area and pore volume of the sample were calculated using the Brunauer-Emmett-Teller (BET) method, and the pore size distribution of the sample was calculated and analyzed using the Barrett-Joyner-Halenda (BJH) method. The CO_2 adsorption isotherms of the samples at 25 ℃ were tested on the BELSORP-max physical adsorption instrument. Prior to the test, the samples were pretreated at 100 ℃ vacuum for 10 h.

Quantitative product analysis. Trace 1310 gas chromatography was used to detect and analyze the product, and the programmed heating process of the column box was as follows: The initial temperature was 50 ℃, reserved for 6 min, and was raised to

260 ℃ at the rate of 20 ℃·min^{-1}, reserved for 9.5 min. The reactants were quantitatively analyzed by gas chromatography.

Using n-butanol as the internal standard, mixed solutions of n-butanol and glycidol of different concentrations were prepared. The known mass of n-butanol and glycidol were m_s and m_i, and the peak areas of n-butanol and glycidol were obtained by gas chromatographic injection as A_s and A_i (as shown in **Figure S1**). The standard curves were obtained by linear regression:$A_i/A_s=2.2629m_i/m_s+0.0248$, relative deviation $R^2=0.9995$ (as shown in **Figure S2 (a)**); according to the same principle, the standard curve of glycerol carbonate is obtained:$A_i/A_s=5.3667m_i/m_s-0.0181$, relative deviation $R^2=0.9991$ (as shown in **Figure S2 (b)**).

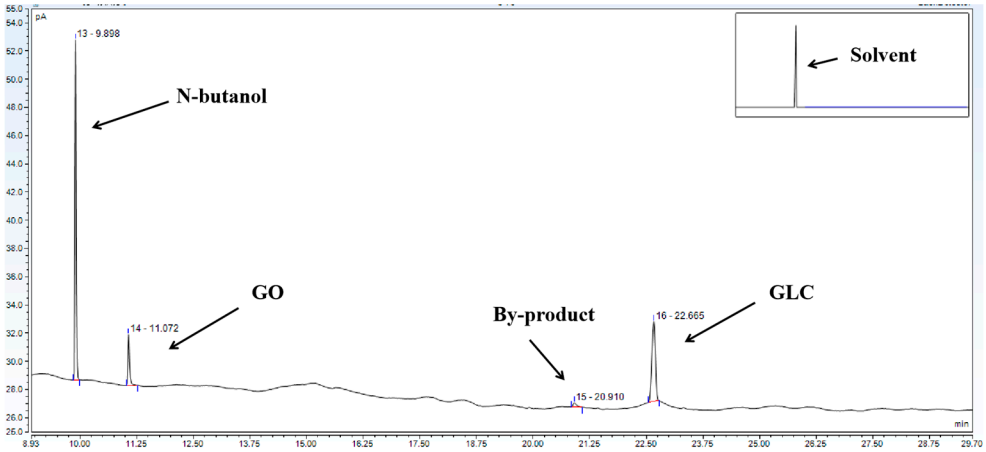


Figure S1 Schematic view of product peak position

(1) Calculation of GO conversion rate

The peak area ratio of GO and n-butanol could be obtained by gas chromatographic analysis of the reaction product mixed solution, and the ratio y was put into the GO linear regression equation: y=2.2629x+0.0248, in which the x was the mass ratio of GO and n-butanol. If the mass of n-butanol was known, the residual GO mass m_{ie} in the product could be obtained. If the initial addition amount of GO m_{iie} is known, then the calculation formula of GO conversion rate is in formula(1) as follows:

$$\text{GO conversion rate}/\%=(1-m_{ie}/m_{iie})\times 100\% \quad (1)$$

(2) Calculation of GLC yield

The peak area ratio of GLC and n-butanol could be obtained by gas chromatographic analysis of the reaction product mixed solution, and the ratio was put into the GLC linear regression equation:y=5.3667x-0.0181, in which the x was the mass ratio of GLC and n-butanol, the mass of n-butanol was known, the mass of the generated GLC was calculated as m_{ic}, and the theoretical mass of GLC was known as m_{iic}. The formula for calculating the GLC yield was shown in formula (2) as follows:

$$\text{GLC yield}/\% = m_{ic}/m_{iic} \times 100\% \quad (2)$$

(3) Calculation of Selectivity

The selectivity calculation formula shown in formula (3) as follows:

$$\text{Selectivity}/\% = \text{GLC yield/GO conversion rate} \quad (3)$$

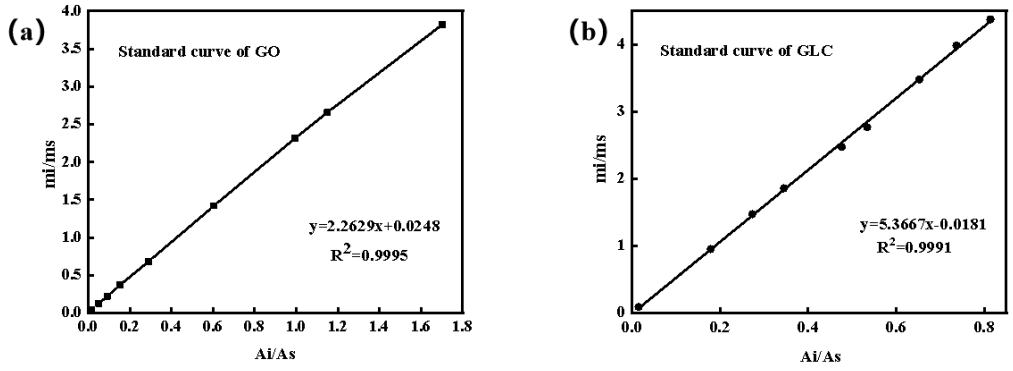


Figure S2 (a) Standard curve of GO; (b) Standard curve of GLC

CO_2 cycloaddition experiment. The CO_2 cycloaddition reaction was carried out in a 50 mL high-pressure reactor equipped with mechanical agitation. CO_2 gas was injected into the high-pressure reactor to flush the reactor three times and exhaust the air, and then adjusting the temperature to the set value. The catalyst and epoxide (10 mmol) were placed in a high-pressure reactor. After the reaction, when the temperature was cooled to room temperature, the unreacted low concentration CO_2 was slowly discharged. The internal standard n-butanol was dissolved in the reaction system, the solid catalyst was removed by filtration, and the collected liquid mixture was dissolved in 5 mL acetonitrile. The filtrate was analyzed by gas chromatography (Thermo Trace 1310), and the yield was determined by internal standard method. The

chromatography is equipped with a flame ionization detector (FID) and a capillary column (TG-5ms, 60 mm × 0.25 mm × 0.25 μm).

Computational method. The modeling of ionic liquid monomers and the associated DFT calculations were performed by Gaussian 16 software package. The B3lYP method and 6-31+g(d, p) basis set were used for the structural optimization of the reaction status, and the frequencies were calculated to ensure that the stable structures were obtained. The search for the transition state and the intrinsic reaction coordinate (IRC) analysis were performed at the same level. Subsequent energy calculations were performed using the M062X method and the 6-311+g(d, p) basis set. All structural optimization and energy calculations were corrected using BSSE dispersion [1,2]. The reaction sites of ionic liquids were determined by ionic localized chemical energy (ALIE), electrostatic potential (ESP), and dual-track weighted Fukui function analysis [3,4,5]. The interaction between ionic liquids, epoxides and CO_2 was investigated by interaction region indicator (IRI) analysis. All of the above analyses were performed by Multiwfn 3.8 and visualized by VMD 1.9.3 [6].

Table S1 Comparison of the performance of different catalysts.

Catalysts	Temperature (°C)	Pressure (MPa)	Time (h)	Yield (%)	Reference
PIM2 (0.2 mol%)	130	1	8	99[a]	7
PSIL(IMD)-1 (7.5 wt%)	130	2	5	98.5[b]	8
PIL-2 (5.4 wt%)	100	1	12	85.1[b]	9
PIL-DVB-IV (15.7 wt%)	110	2	6	95[b]	10
P-BVIMCl (6.7 wt%)	100	2	3	93.4[a]	This work
	120	2	4	93.7[b]	

a The substrate was GO. b The substrate was ECH.

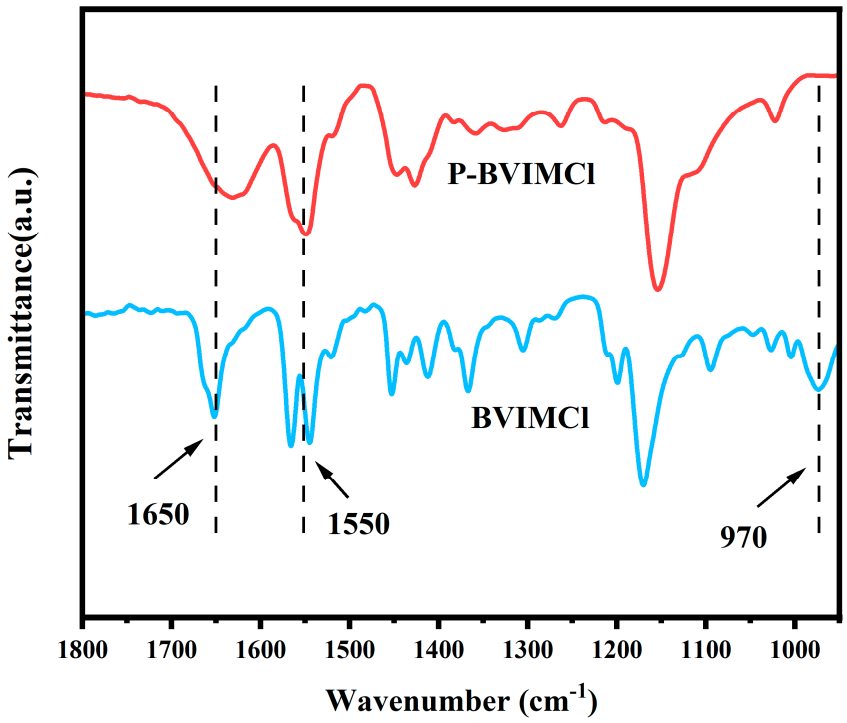


Figure S3 FT-IR spectra of P-BVIMCl and BVIMCl .

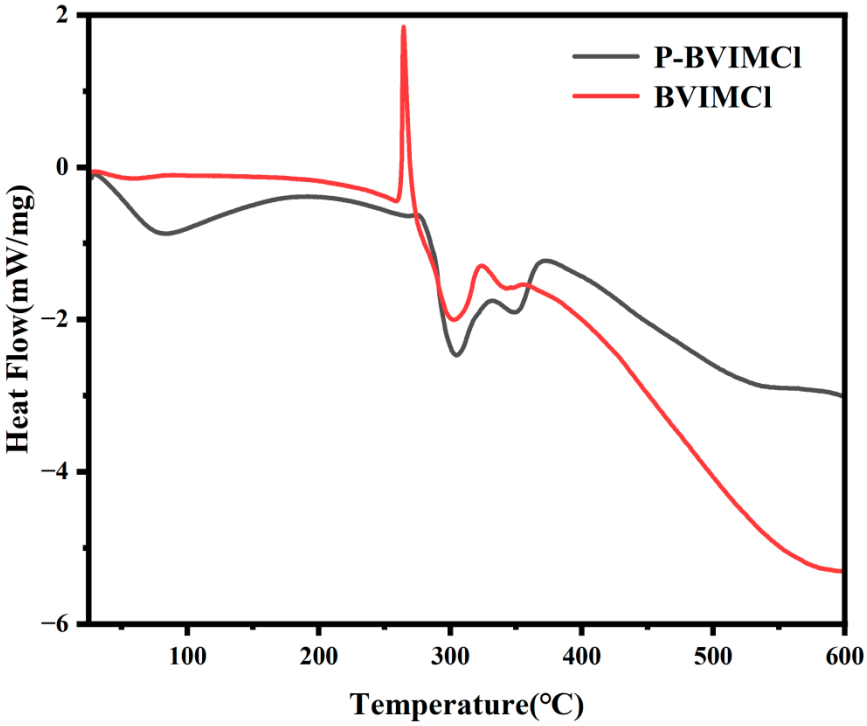


Figure S4 The DSC curves of P-BVIMCl and BVIMCl at temperature (25 to 600) °C.

References

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