10.1071/CH17656_AC

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Supplementary Material

Amino-functional ionic liquids as efficient catalysts for the cycloaddition of carbon dioxide to cyclic carbonate: Catalytic and kinetic investigation

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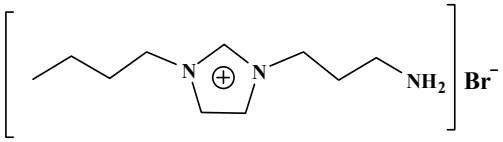
Characteristic data:

Ionic liquid 1:



[APbim]Br: ^{1}H NMR (600 MHz, D_2O): δ(ppm) 8.90(1H, s), 7.58(2H, s), 4.37(2H, t), 4.24 (2H, m), 3.11(2H, t), 2.32(2H, m), 1.88(2H, m), 1.36(2H, m), 0.95(3H, t) ; IR(KBr): ν(=C–H) 3093.81 cm^{-1}, ν(RC–H) 2954.91 cm^{-1},ν(C=C) 1622.86 cm^{-1}, δ(C–H) 1457.51 cm^{-1}, ν(C–N) 1387.91 cm^{-1}, ν(C–C) 1133.05 cm^{-1}; TOF-MS m/z: $[APbim]^+$=182.1.

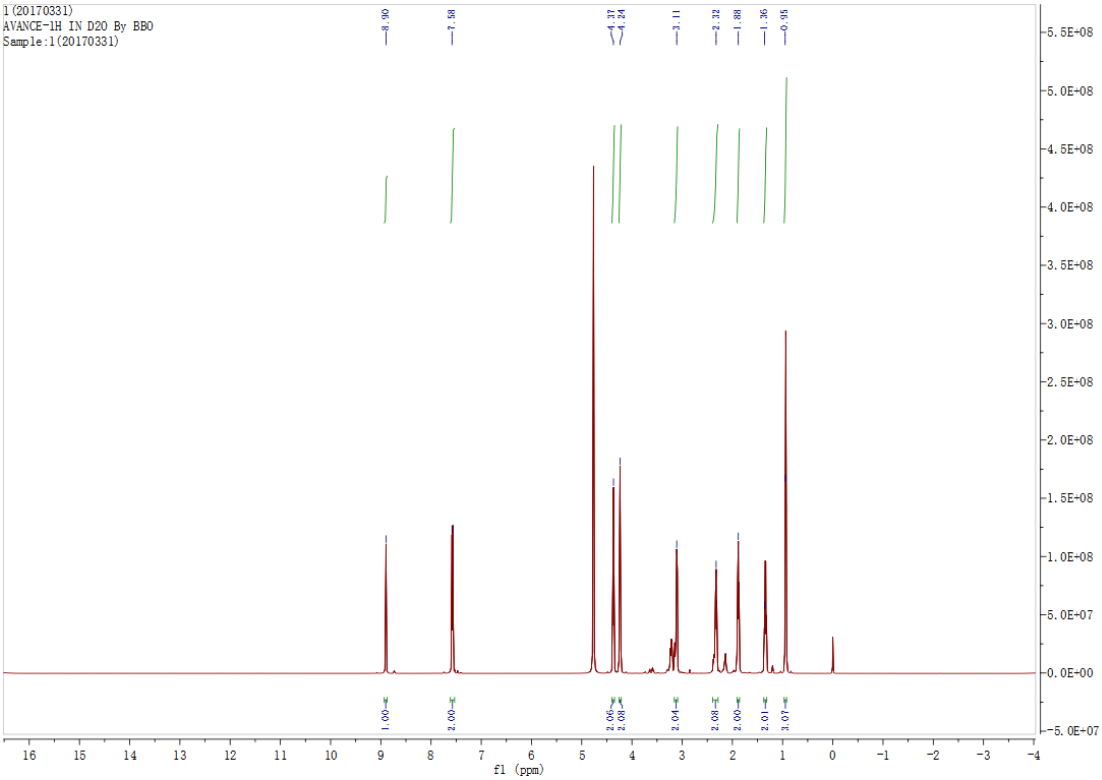


Figure S1-1 ^{1}H NMR spectrum of [APbim]Br

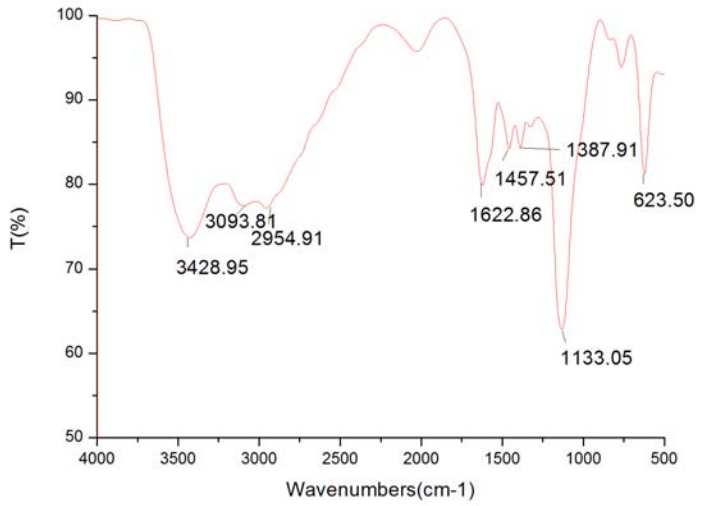
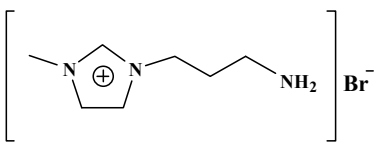


Figure S1-2 IR spectrum of [APbim]Br

Ionic liquid 2:



[APmim]Br: ^{1}H NMR (300 MHz, DMSO): δ(ppm) 9.21(1H, s), 7.83(1H, s), 7.76(1H, s),

4.31(2H, t), 3.87(3H, s), 2.82(2H, t), 2.11(2H, m); IR(KBr):ν(=C–H) 3036.74 cm^{-1}, ν(RC–H) 2944.47 cm^{-1}, ν(C=C) 1578.68 cm^{-1}, δ(C–H) 1456.32 cm^{-1}, ν(C–N) 1392.81 cm^{-1}; TOF-MS m/z: $[APmim]^+$=140.1.

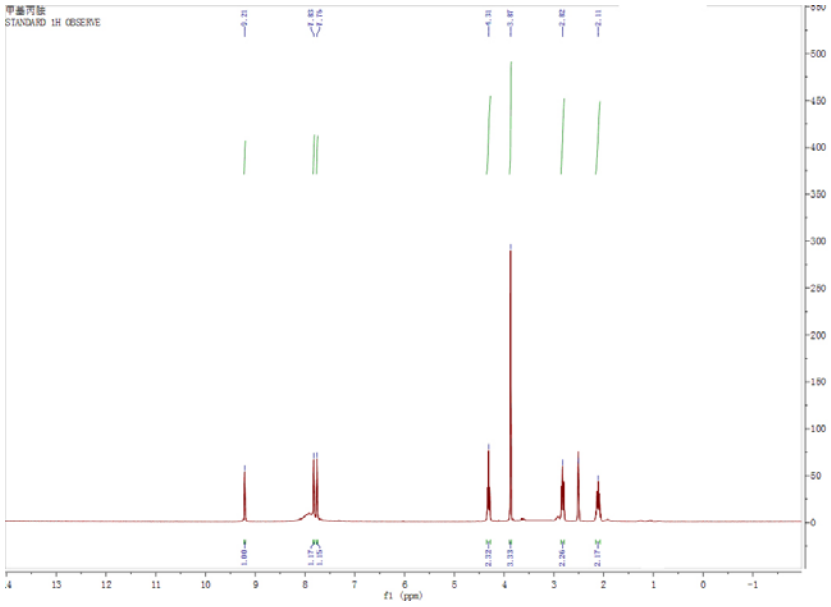


Figure S2-1 ^{1}H NMR spectrum of [APmim]Br

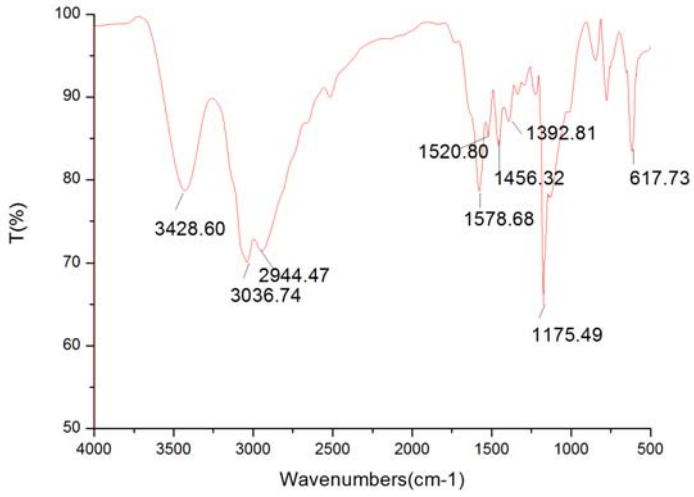
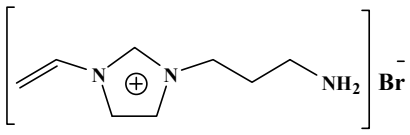


Figure S2-2 IR spectrum of [APmim]Br

Ionic liquid 3:



[APeim]Br: ^{1}H NMR(300 MHz, DMSO): δ(ppm) 9.66(1H, s), 8.28(1H, s), 8.01(1H, s)

, 7.34(1H, m), 6.02(1H, d), 5.42(1H, d), 4.37(2H, s), 2.86(2H, t), 2.17(2H, t); IR(KBr): ν(RC–H) 2973.65 cm^{-1}, ν(C=N) 1655.89 cm^{-1}, ν(C=C) 1602.91 cm^{-1}, δ(C–H) 1566.87 cm^{-1}, 1546.77 cm^{-1}, ν(C–N) 1465.01 cm^{-1}, ν(C–C) 1160.56 cm^{-1}; TOF-MS m/z: [APeim]$^{+}$=152.12.

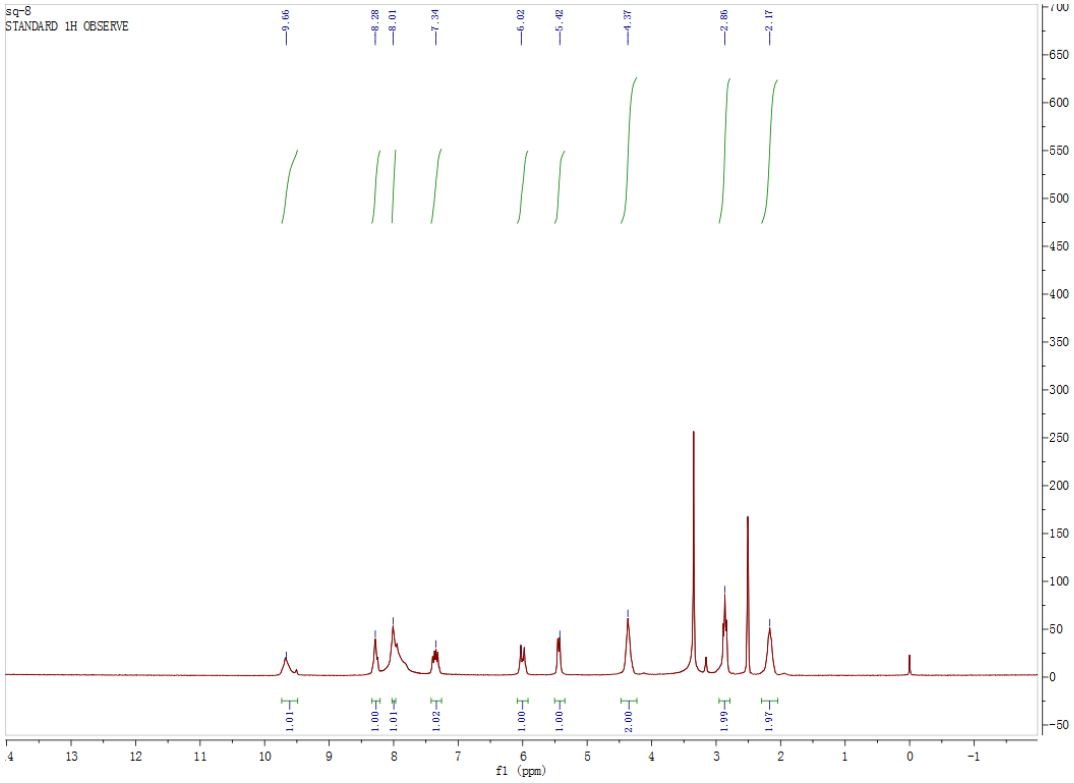


Figure S3-1 ^{1}H NMR spectrum of [APeim]Br

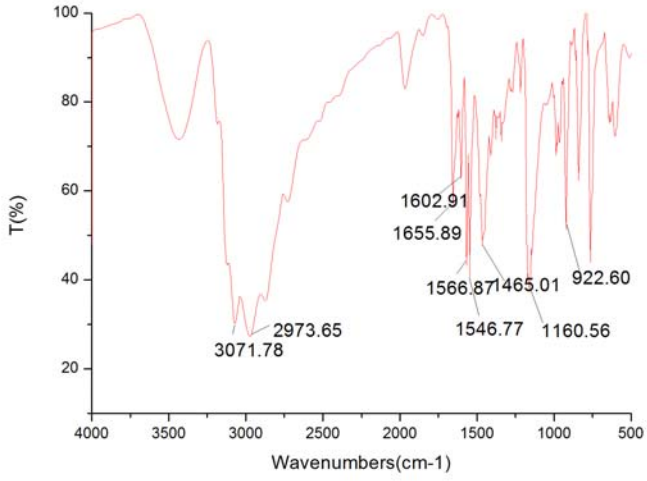
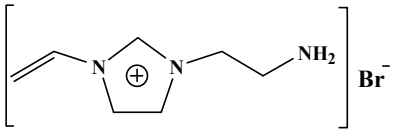


Figure S3-2 IR spectrum of [APeim]Br

Ionic liquid 4:



[AEeim]Br: ^{1}H NMR (300 MHz, DMSO): δ(ppm) 9.60(1H, s), 8.28(1H, s), 7.97(1H, m), 7.37(1H, s), 5.98(1H, m), 5.44(1H, m), 4.47(2H, t), 3.36(2H, t); IR(KBr): ν(RC–H) 2939.41 cm^{-1}, 2858.63 cm^{-1}, ν(C=C) 1639.51 cm^{-1}, δ(C–H) 1557.51 cm^{-1}, ν(C–N) 1477.59 cm^{-1}, ν(C–C) 1174.75 cm^{-1},1105.96 cm^{-1}; TOF-MS m/z: [AEeim]$^+$=140.12.

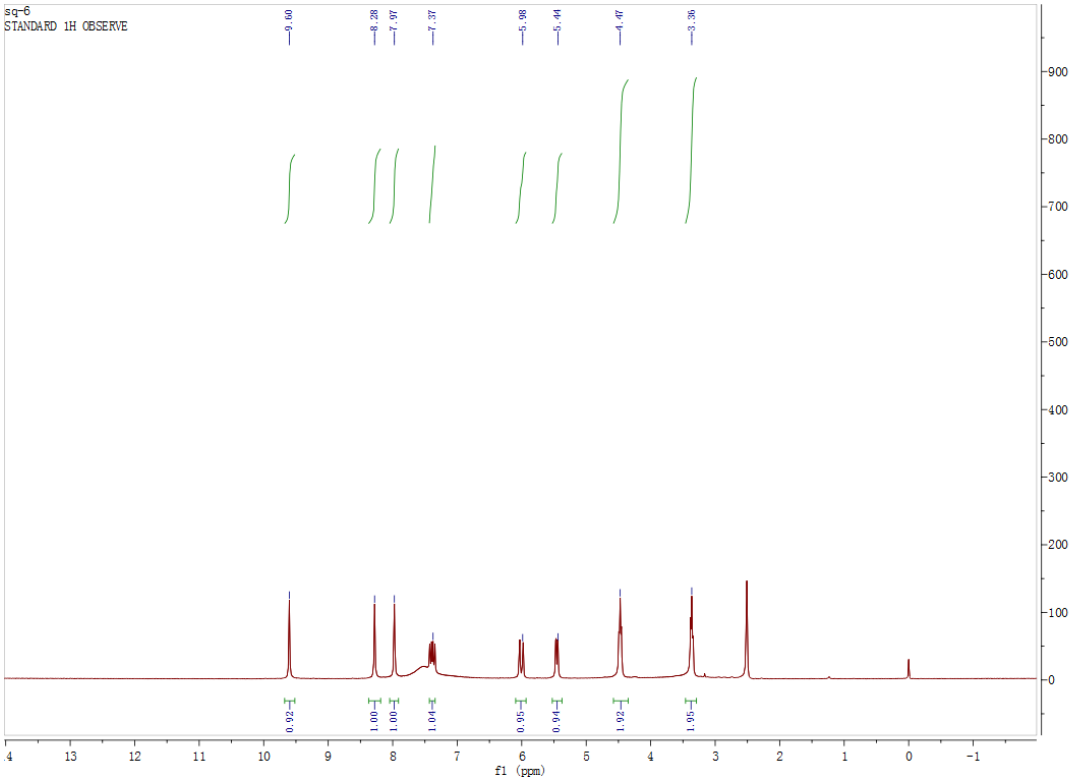


Figure S4-1^{1}H NMR spectrum of [AEeim]Br

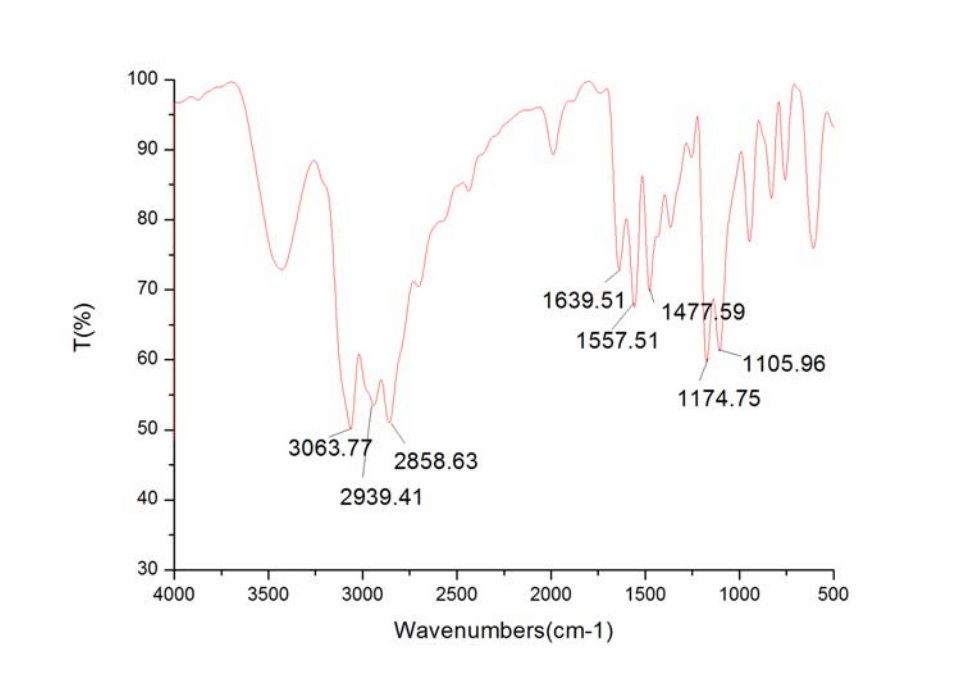


Figure S4-2 IR spectrum of [AEeim]Br

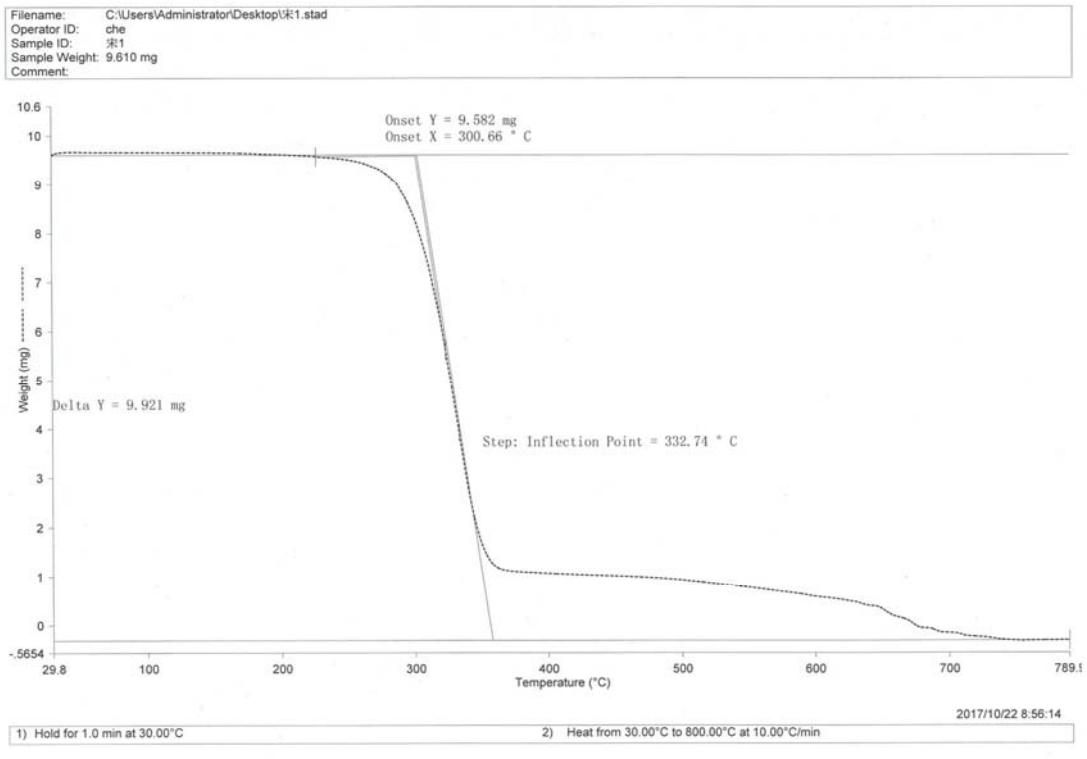


Figure S7. TG curve of [APbim]Br.

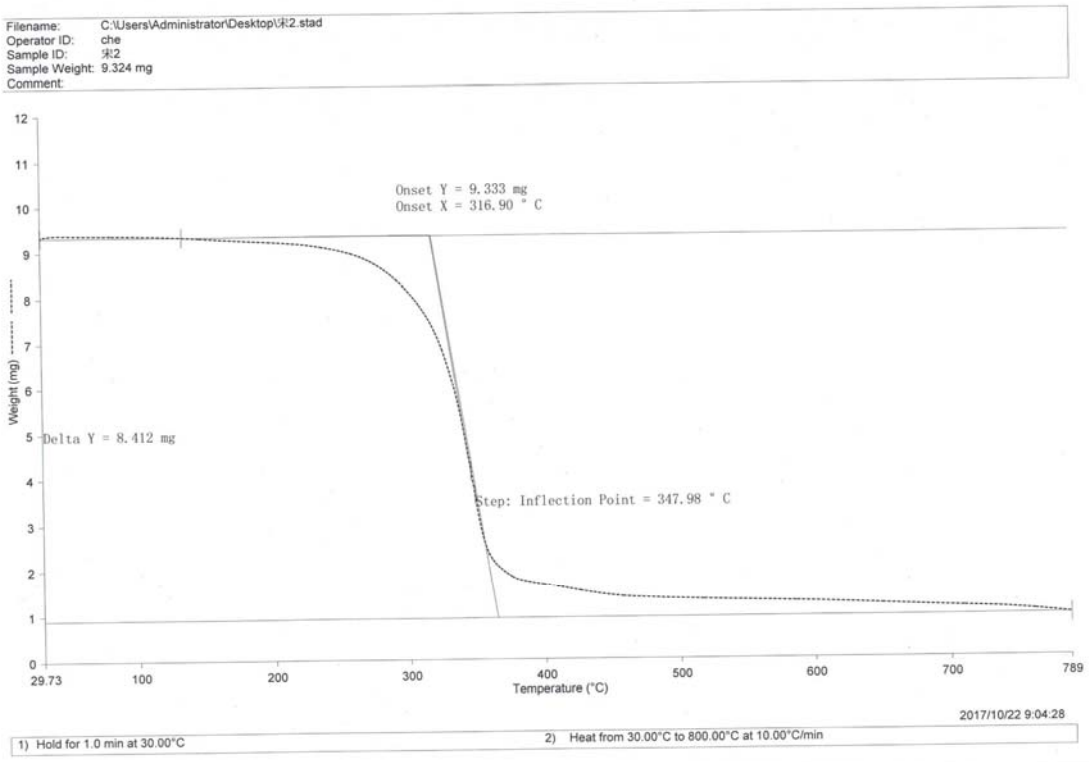


Figure S8. TG curve of [APmim]Br.

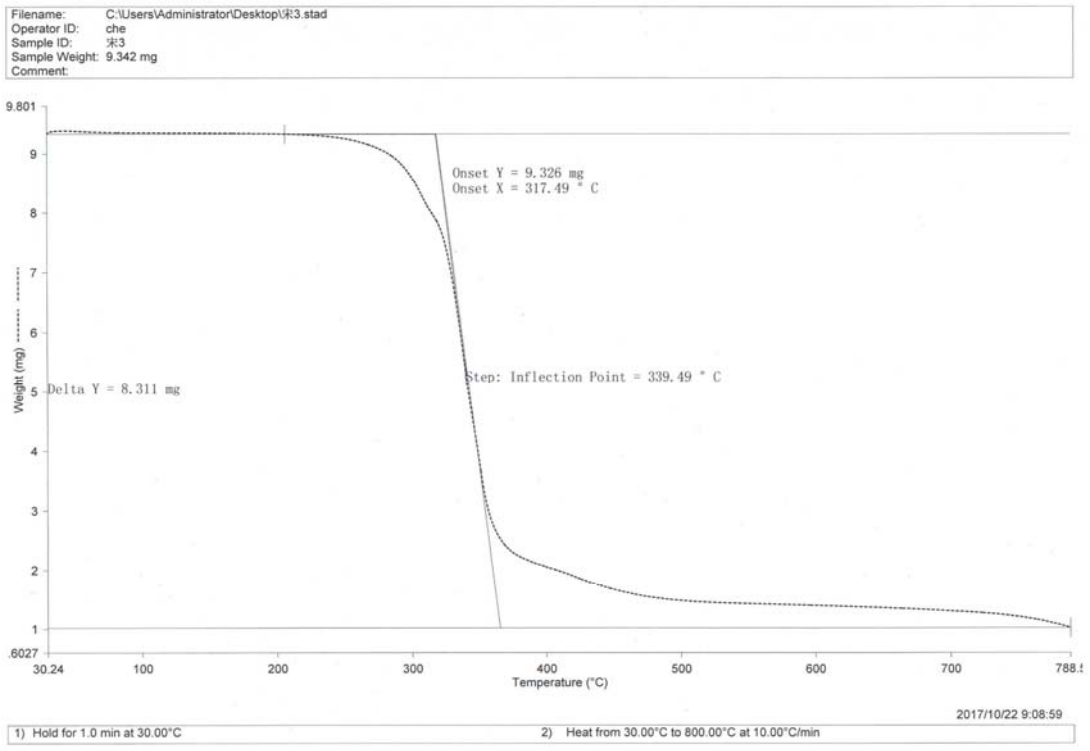


Figure S9. TG curve of [APeim]Br.

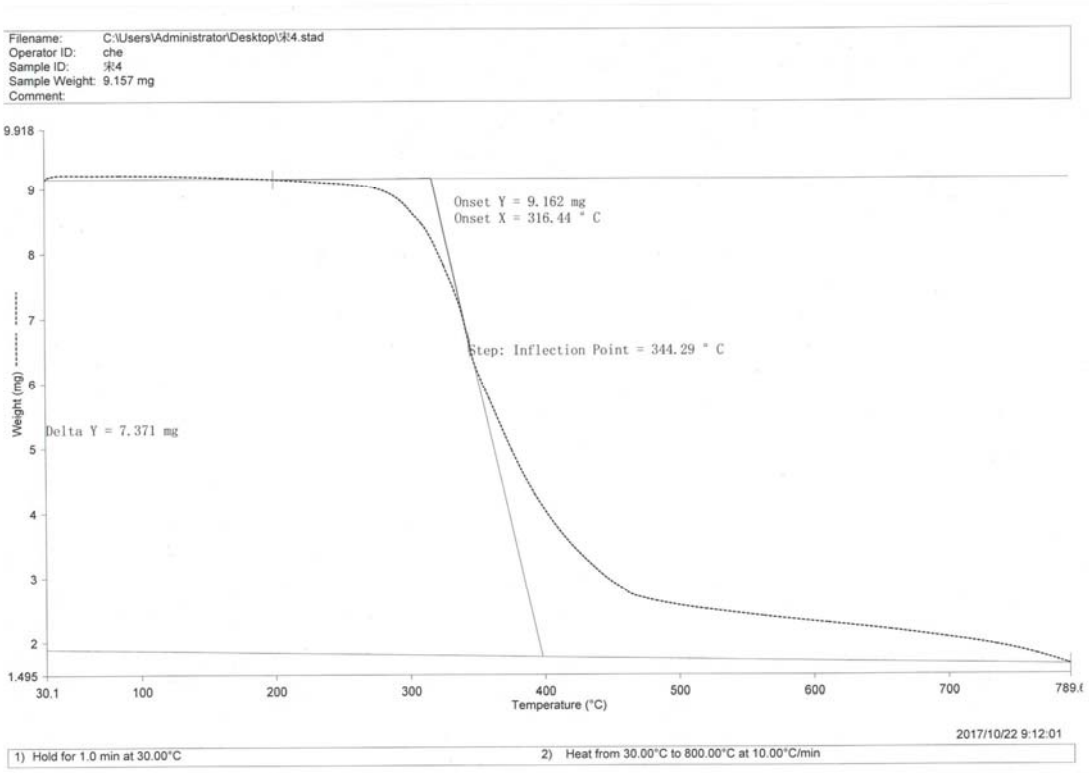


Figure S10. TG curve of [AEeim]Br.

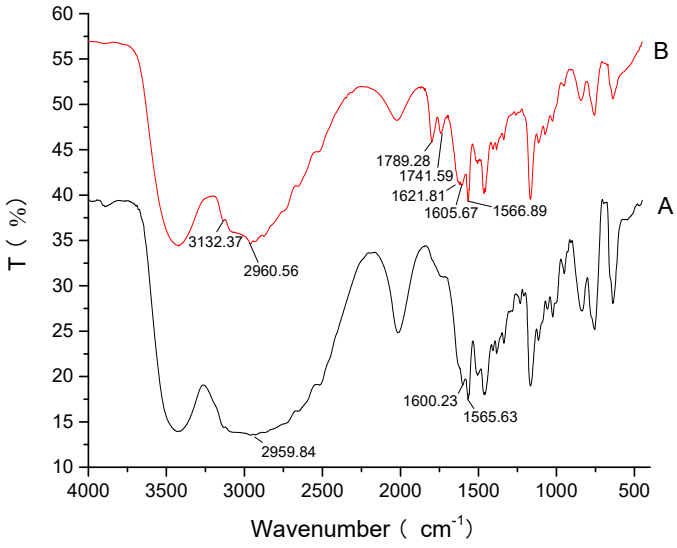


Figure S6. FT-IR spectra of catalyst: A fresh ([APbim]Br), B recovered ([APbim]Br).

Table S1 Kinetic Equations and Kinetic Parameters at Different Temperature

T/(℃)	Kinetic equation	R’	*k* (min^{-1})	1/*T* (K^{-1})	In *k*
100	$y = 0.0152x+0.024$	0.9990	0.0152	0.00268	-4.1864
110	$y = 0.0252x-0.072$	0.9939	0.0252	0.00261	-3.7636

120	$y = 0.0352x-0.172$	0.9937	0.0352	0.00254	-3.3467
130	$y = 0.0452x-0.272$	0.9934	0.0452	0.00248	-3.0966

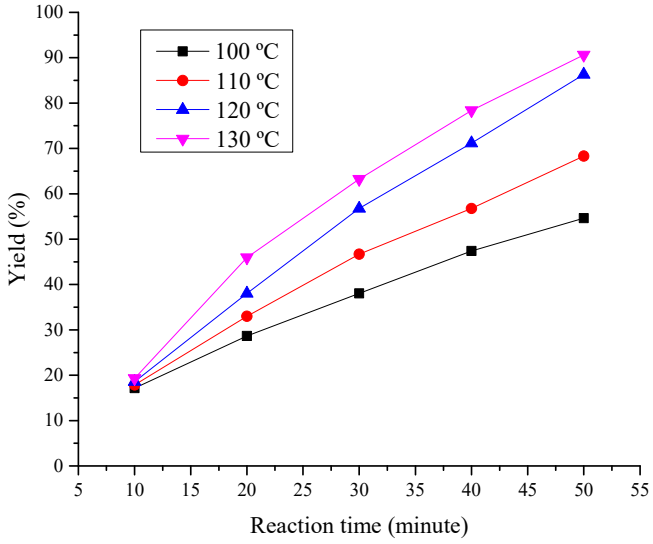


Figure S5. The chloropropene carbonate yield-time profile at different temperatures catalyzed by IL **1** as catalyst. Reaction conditions: n[epichlorohydrin] = 0.06 mol, CO_2 1.0 MPa, IL**1** 0.6 mol%.

Table S2. The loss rate of IL**1** in every run.

Run	loss rate (%)
1	1.41
2	1.39
3	1.38
4	1.40
5	1.37
6	1.42
7	1.37
8	1.38

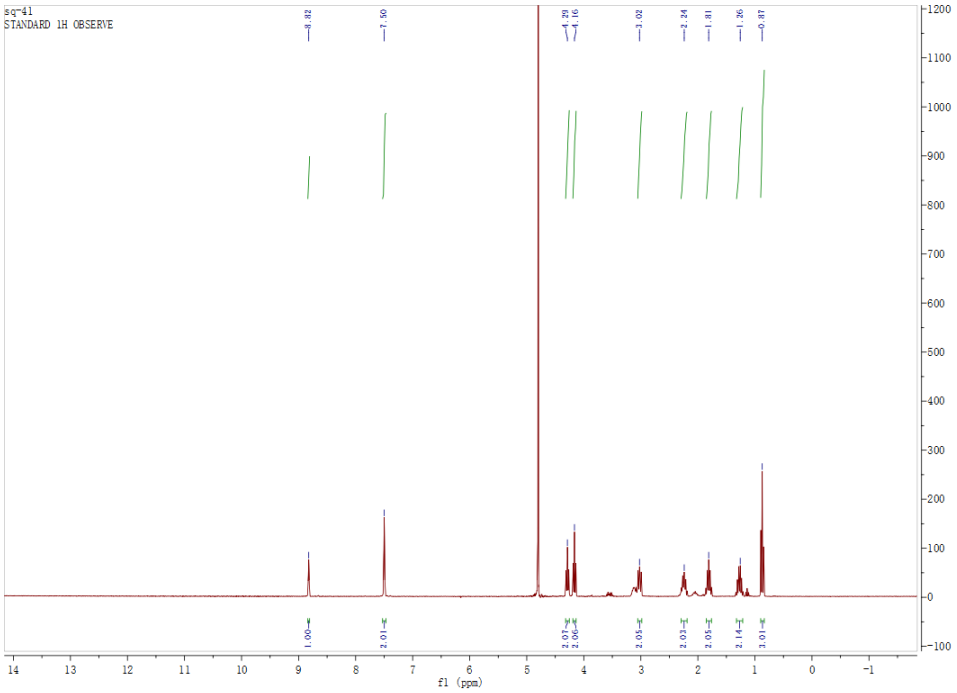
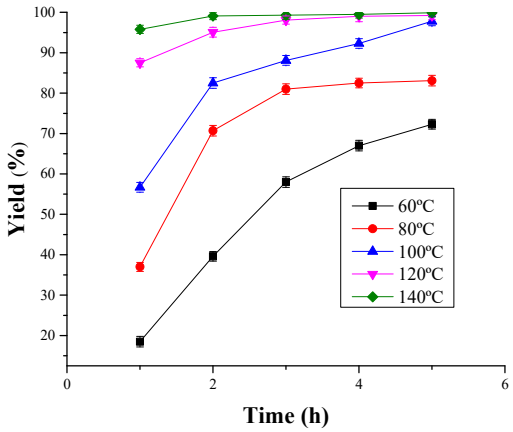


Figure S11. ^{1}H NMR spectrum of [APbim]Br after cyclic experiment



FigureS12. Effect of the reaction temperature and time on the yield of chloropropene carbonate. Reaction conditions: epichlorohydrin 5.0 mL (0.0638 mol), catalyst [APbim]Br 1.0 mol%, p(CO_2)= 1.0 MPa. Error bars show the standard deviation (n =3).

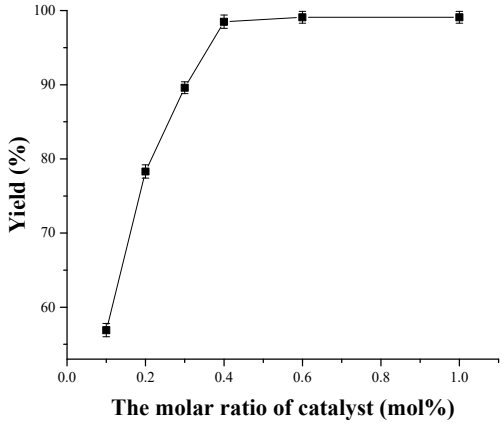


Figure S13. Effect of the catalyst amount on the yield of chloropropene carbonate. Reaction conditions: epichlorohydrin 5.0 mL (0.0638 mol), p(CO_2)= 1.0 MPa, T=120 ℃, t=2.0 h. Error bars show the standard deviation (n =3).

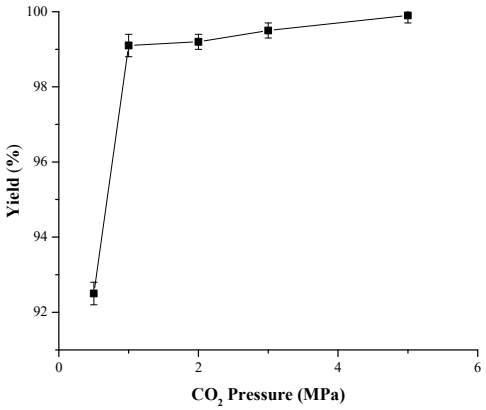


Figure S14. Effect of CO_2 pressure on the yield of chloropropene carbonate. Reaction conditions: epichlorohydrin 5.0 mL (0.0638 mol), catalyst [APbim]Br 1.0 mol%, 120 ℃, t=2.0 h. Error bars show the standard deviation (n =3).