Supporting Information

Novel hydroxyl functionalized ionic liquids as efficient catalysts for the conversion of CO_2 into cyclic carbonates under metal/halogen/cocatalyst/solvent-free conditions

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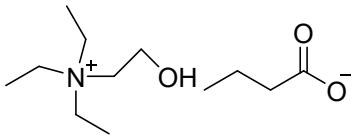
Characteristic data:

Ionic liquid 1:



(**1**) $[N_{2,2,2,2OH}][BA]$

$C_{12}H_{27}NO_3$(233). ^{1}H NMR (D_2O, 300MHz, RT): δ=3.91 (2H, s), 3.32 (8H, q), 2.08 (2H, t), 1.47 (2H, m), 1.21 (9H, t), 0.82 (3H, t); ^{13}C NMR (75.5MHz, D_2O): δ=184.05, 57.45, 54.81, 53.39, 39.69, 19.46, 13.32, 6.74; IR (KBr): v=1563 cm^{-1} (C=O).

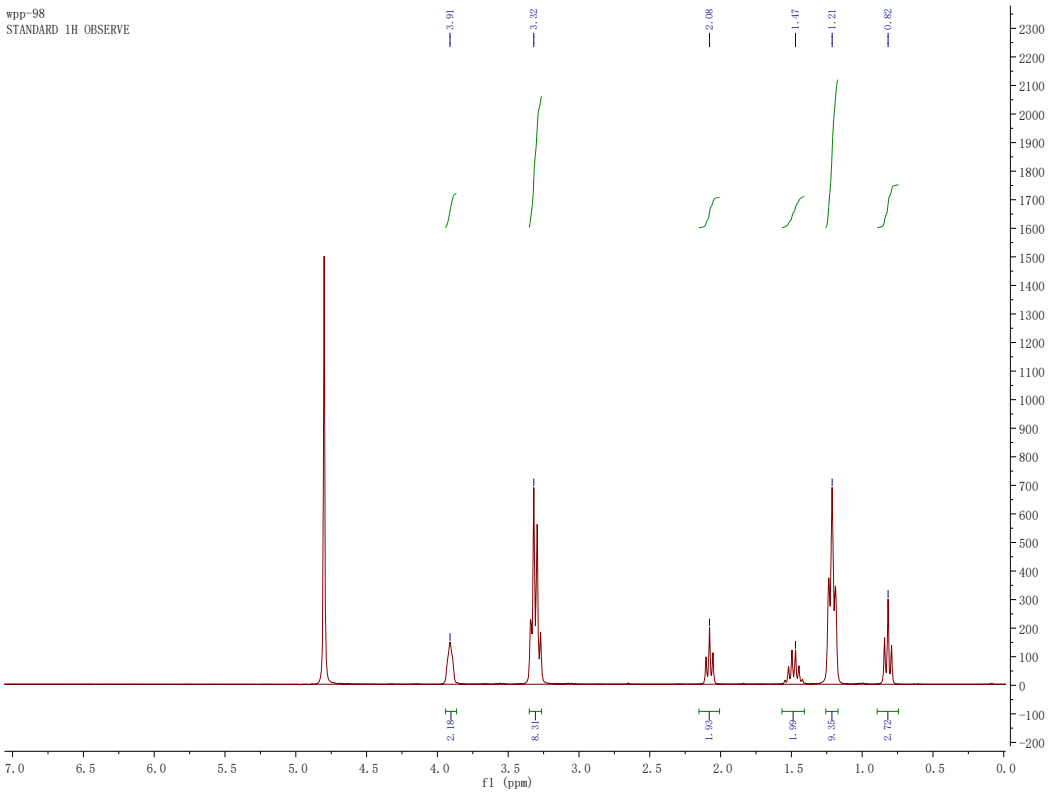


Figure S1-1. ^{1}H NMR spectrum of IL**1**

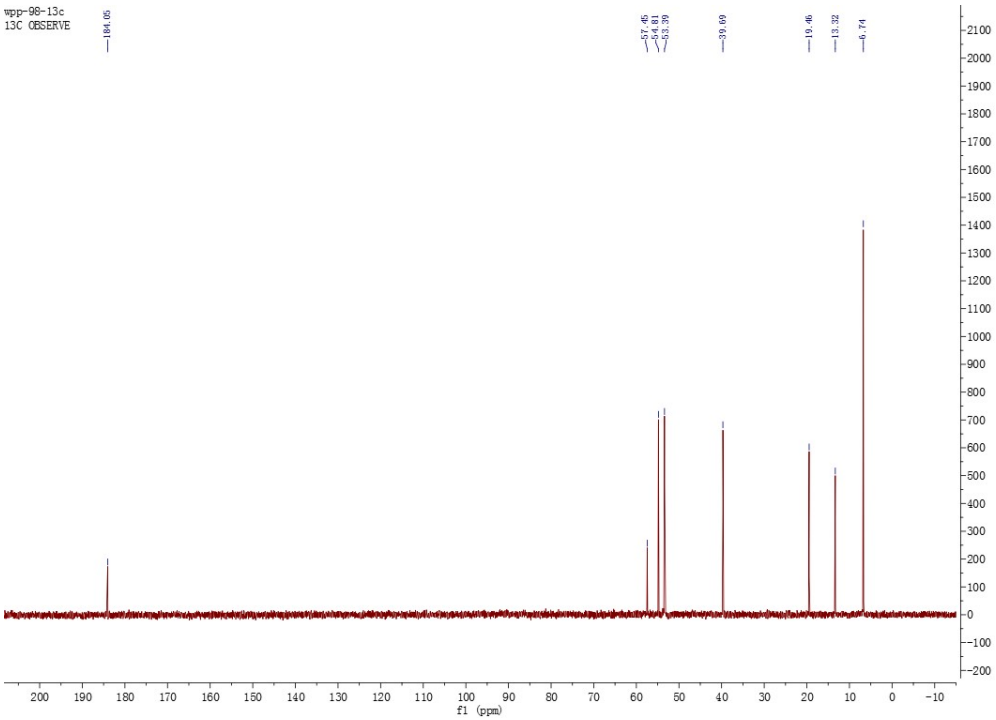


Figure S1-2. ^{13}C NMR spectrum of IL**1**

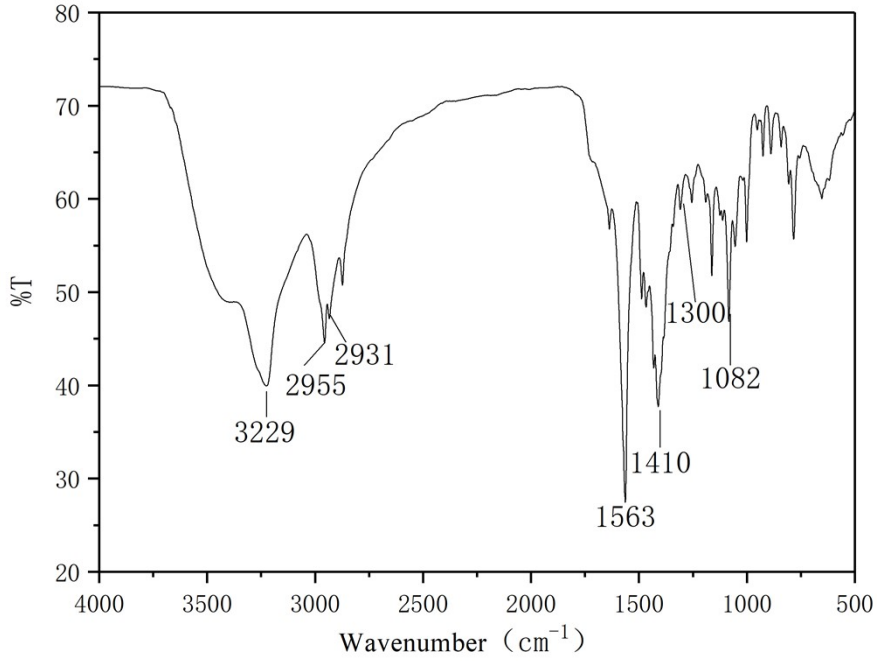
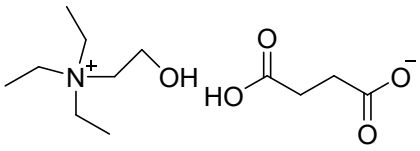


Figure S1-3. IR spectrum of IL **1**

Ionic liquid 2



(**2**) [$N_{2,2,2,2OH}$][SA]

$C_{12}H_{25}NO_5$(263). ^{1}H NMR (D_2O, 300MHz, RT): δ=3.90 (2H, s), 3.33 (8H, q), 2.44 (4H, t), 1.22 (9H, t); ^{13}C NMR (75.5MHz, D_2O): δ=180.08, 57.51, 54.87, 53.47, 32.03, 6.81; IR (KBr): v=1578 cm^{-1} (C=O).

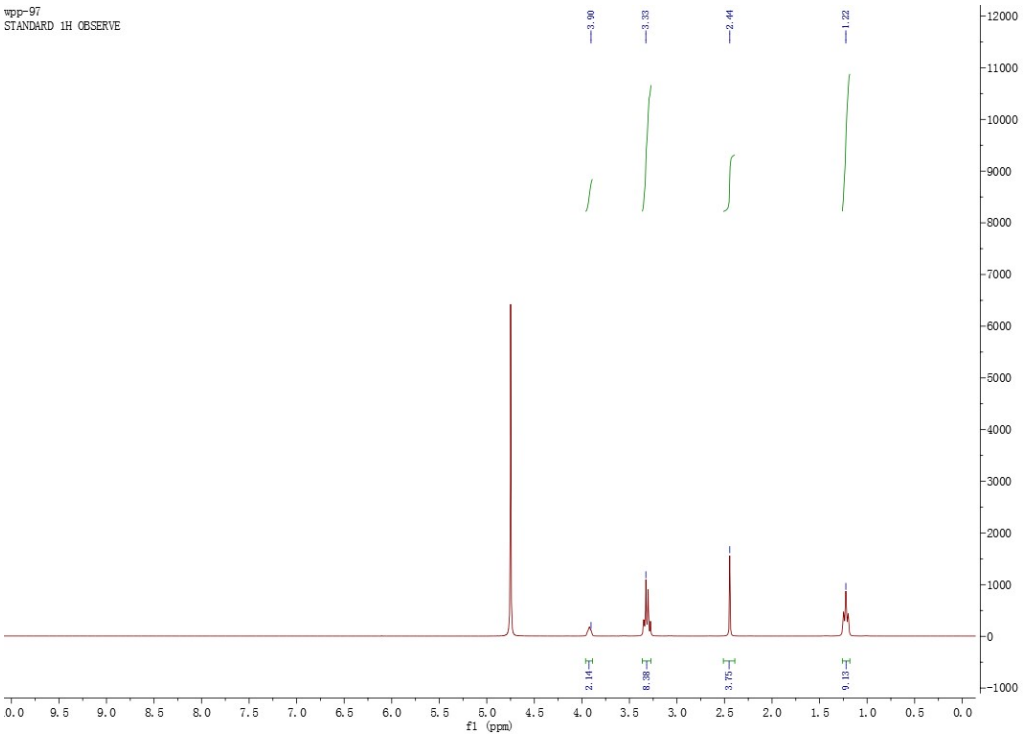


Figure S2-1. ^{1}H NMR spectrum of IL**2**

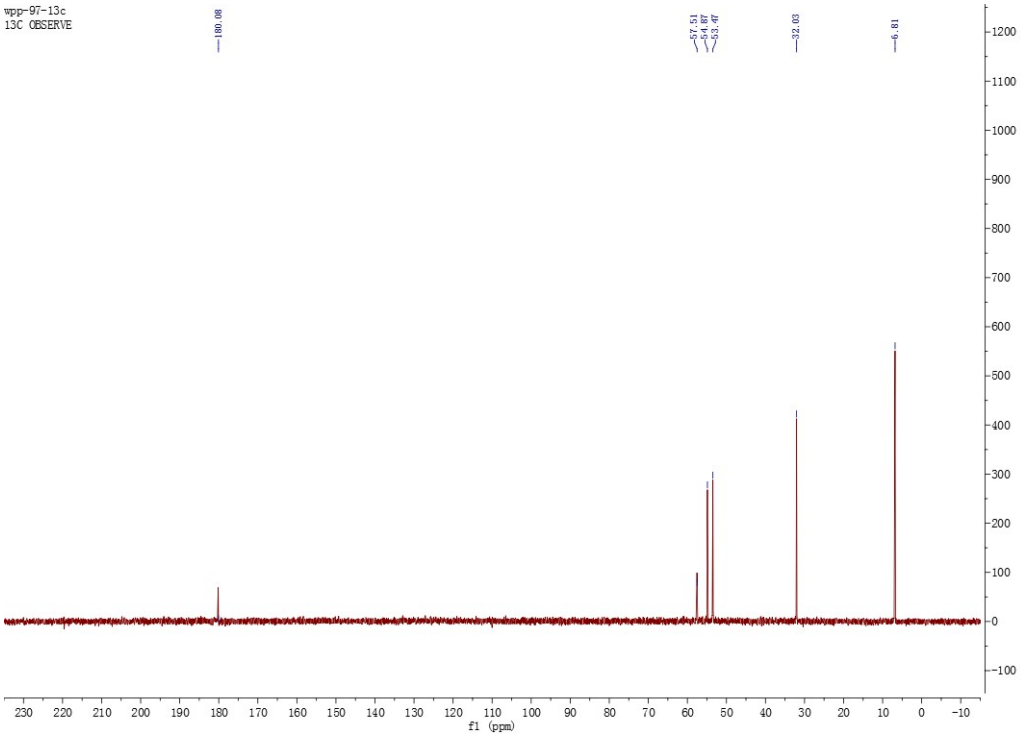


Figure S2-2. ^{13}C NMR spectrum of IL**2**

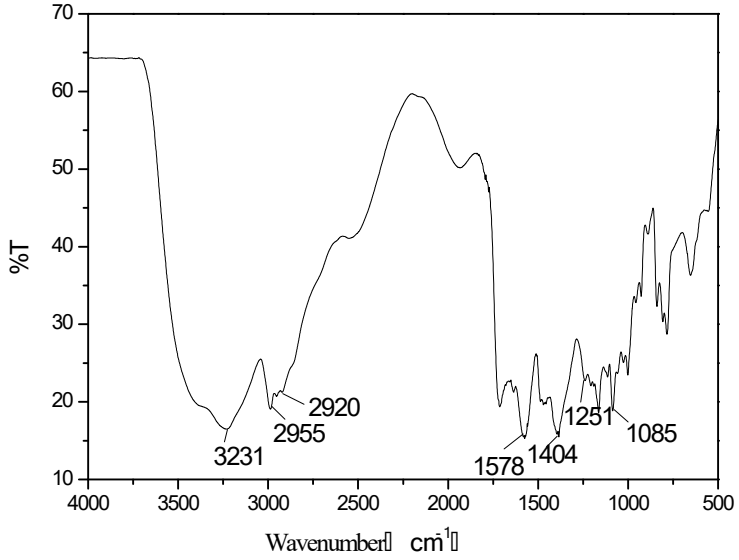
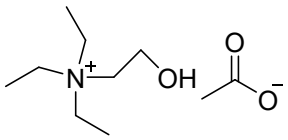


Figure S2-3. IR spectrum of IL **2**

Ionic liquid 3



(**3**) $[N_{2,2,2,2OH}][OAc]$

$C_{10}H_{23}NO_3$(205). ^{1}H NMR (D_2O, 300MHz, RT): δ=3.90 (2H, s), 3.30 (8H, q), 1.83 (3H, s), 1.20 (9H, t); ^{13}C NMR (75.5MHz, D_2O): δ=181.32, 62.62, 57.54, 54.87, 53.47, 23.38, 6.81; IR (KBr): ν=1581 cm^{-1} (C=O).

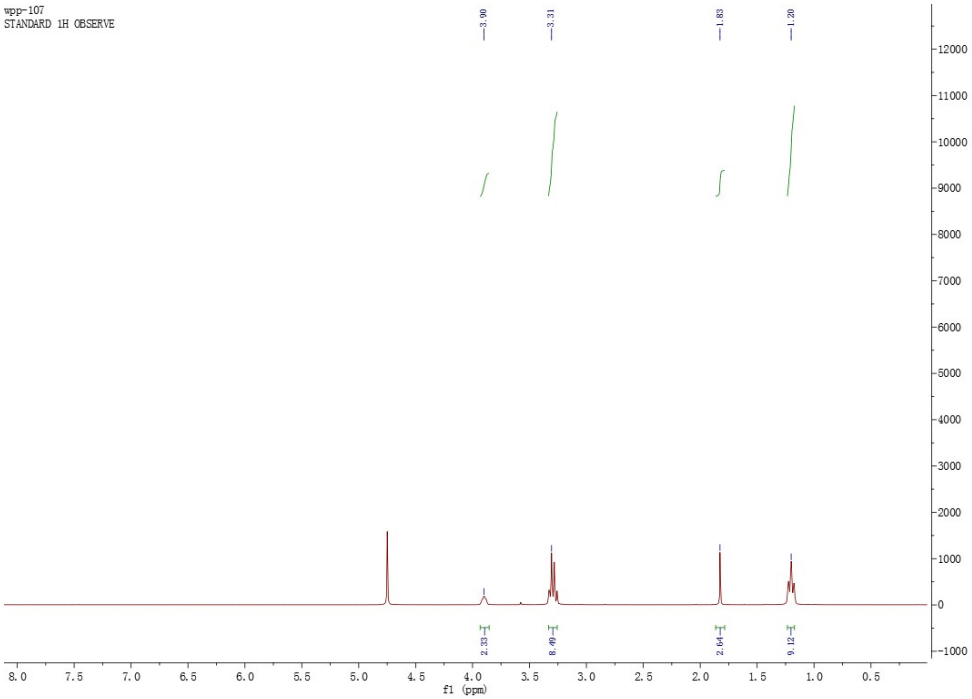


Figure S3-1. ^{1}H NMR spectrum of IL **3**

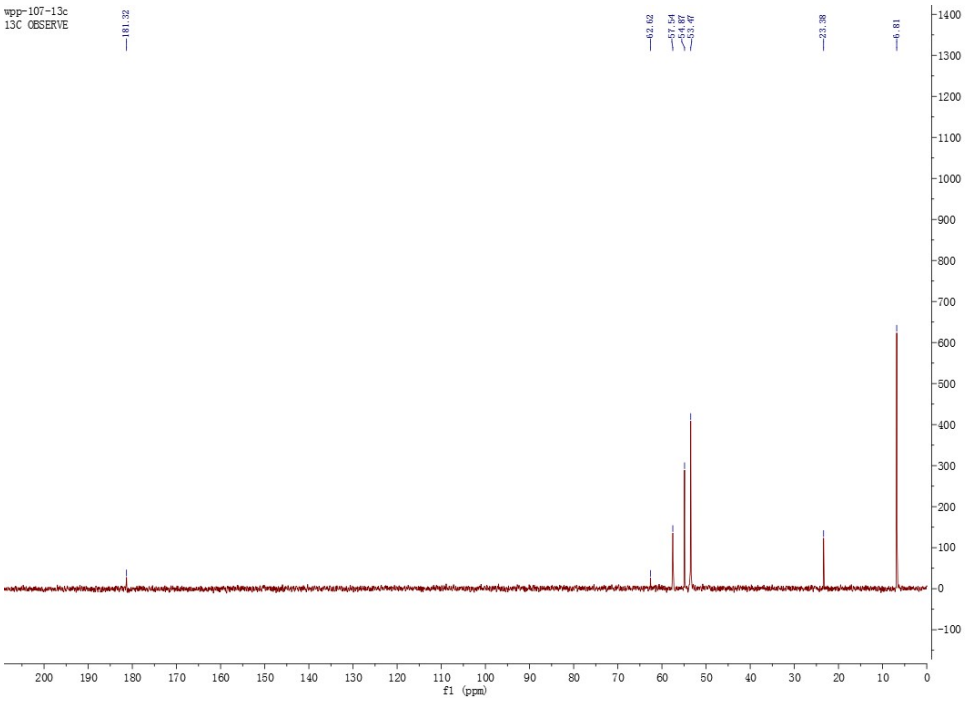


Figure S3-2. ^{13}C NMR spectrum of IL **3**

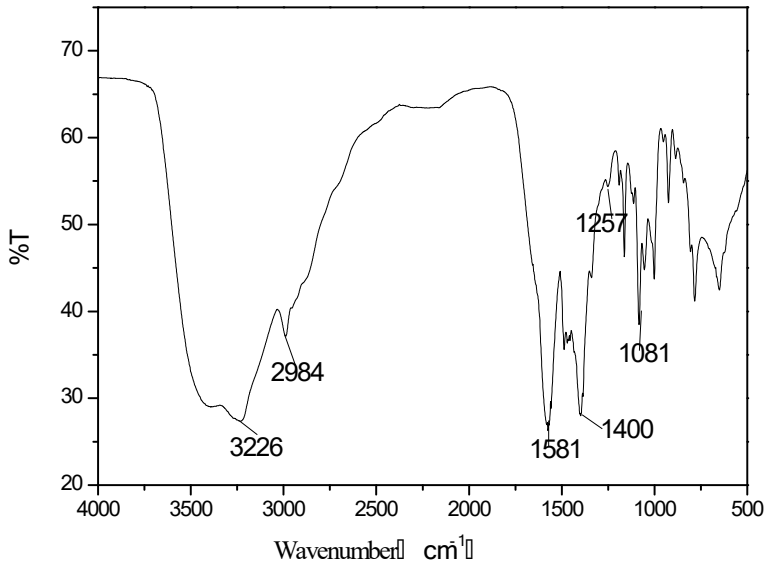
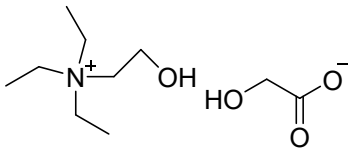


Figure S3-3. IR spectrum of IL **3**

Ionic liquid 4



(**4**) $[N_{2,2,2,2OH}][GA]$

$C_{10}H_{23}NO_4$(221). ^{1}H NMR (D_2O, 300MHz, RT): δ=3.85 (4H, d), 3.31 (8H, q), 1.21 (9H, t); ^{13}C NMR (75.5MHz, D_2O): δ=179.87, 61.30, 57.50, 54.87, 53.45, 6.79; IR (KBr): v=1600cm^{-1} (C=O).

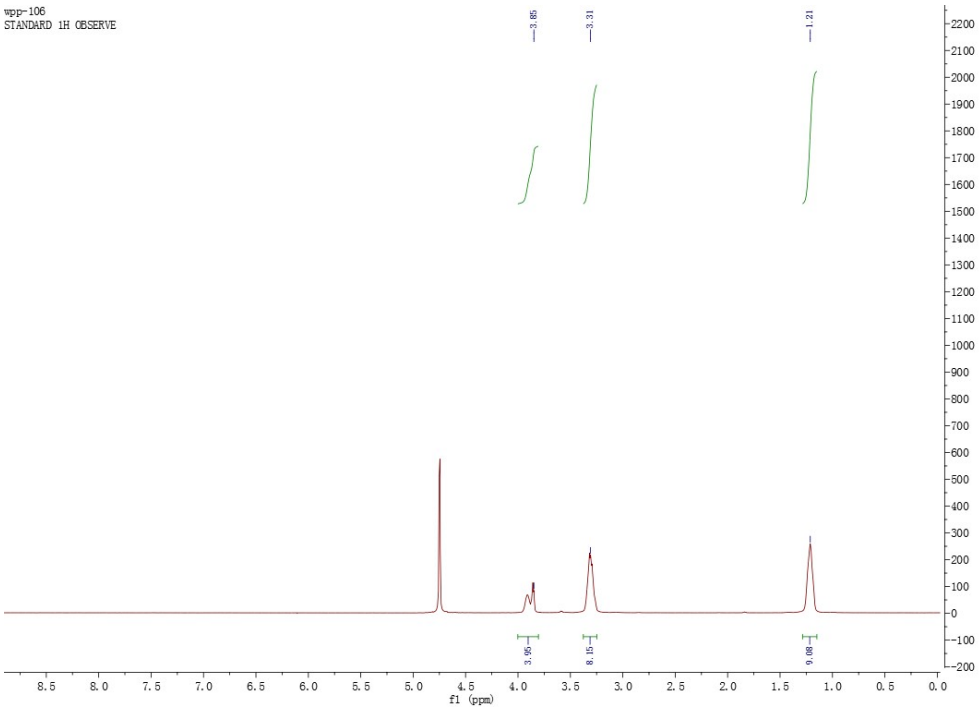


Figure S4-1. ^{1}H NMR spectrum of IL **4**

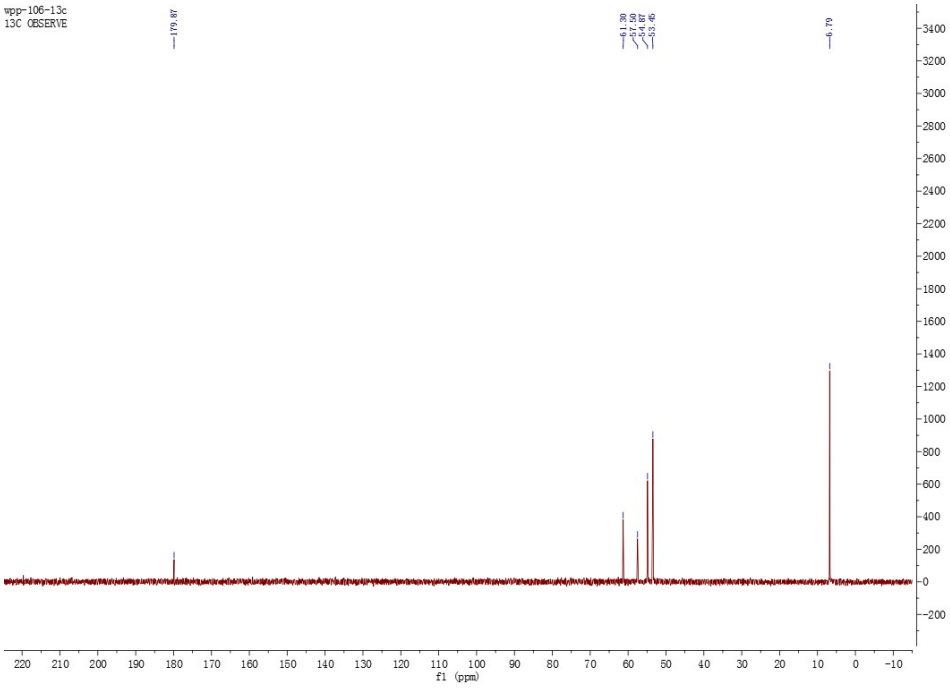


Figure S4-2. ^{13}C NMR spectrum of IL **4**

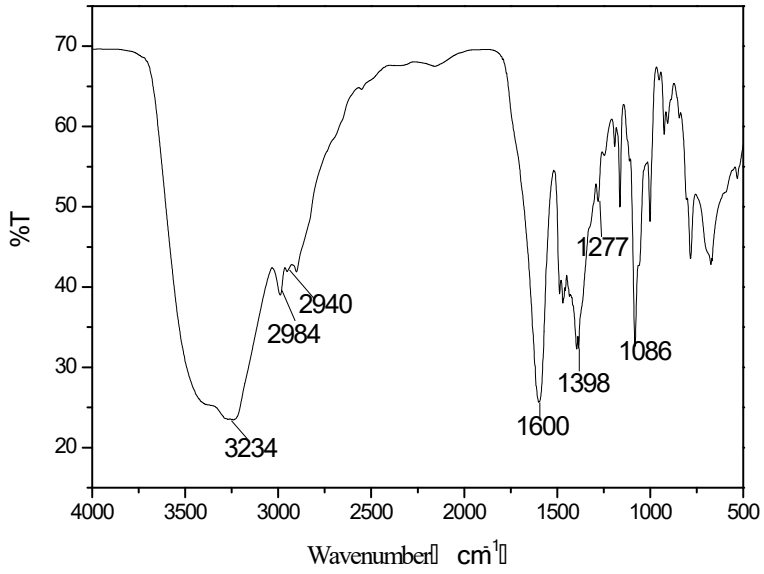
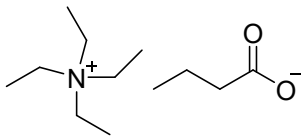


Figure S4-3. IR spectrum of IL **4**

Ionic liquid 5



(**5**) $[N_{2,2,2,2}][BA]$

$C_{12}H_{27}NO_2$(217). ^{1}H NMR (D_2O, 300 MHz, RT): δ =3.17 (8H, q), 2.08 (2H, m), 1.48 (2H, m), 1.18 (12H, m), 0.82 (3H, m); ^{13}C NMR (75 MHz, D_2O) δ =183.59, 52.07, 39.69, 19.58, 13.55, 6.82; IR (KBr): ν =1564 cm^{-1} (C=O).

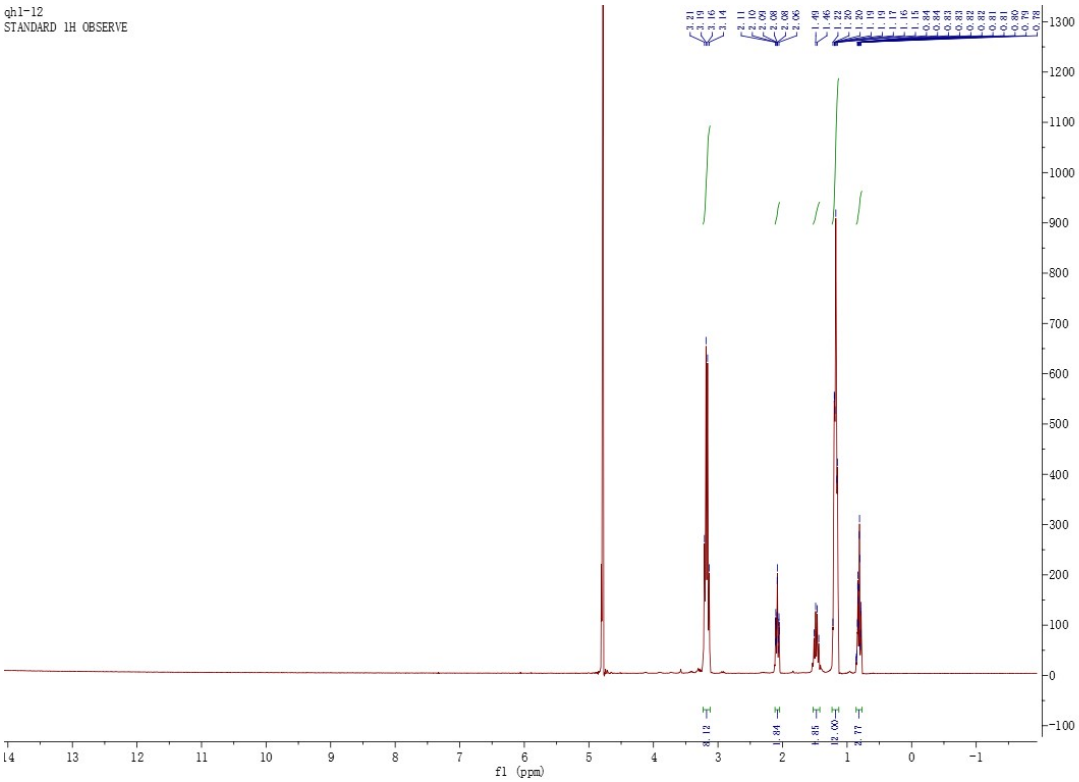


Figure S5-1. ^{1}H NMR spectrum of IL **5**

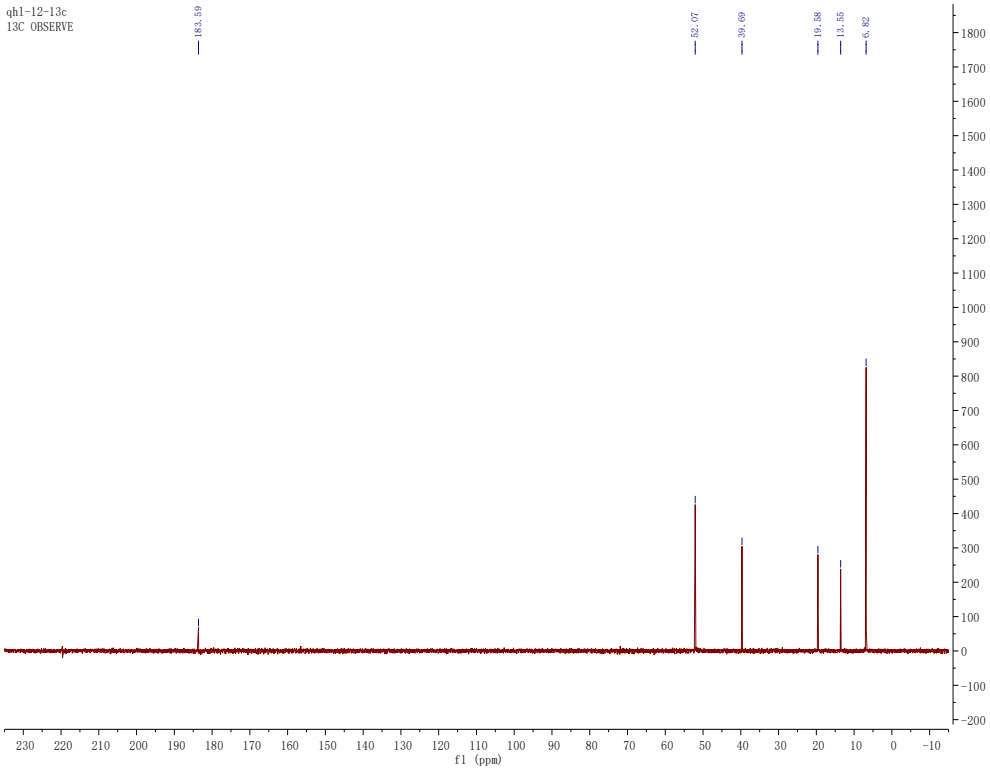


Figure S5-2. ^{13}C NMR spectrum of IL **5**

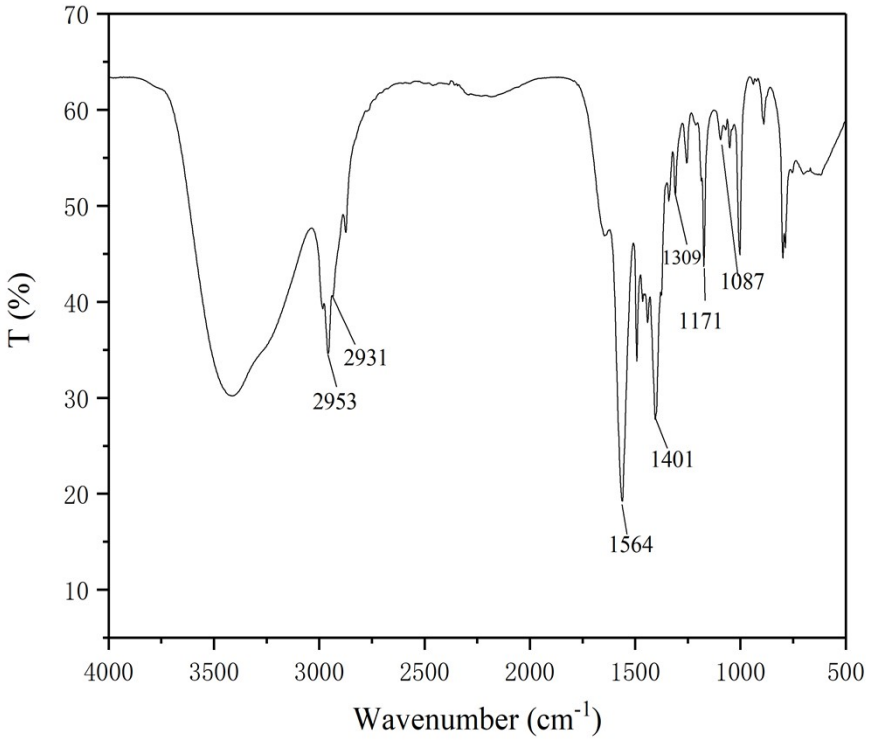


Figure S5-3. IR spectrum of IL **5**

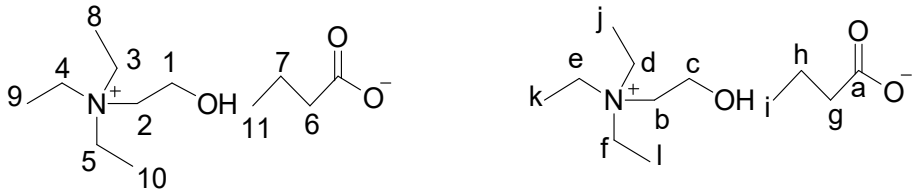


Figure S6. Distribution of ^{1}H NMR and ^{13}C NMR spectra of ionic liquid **1**.

Table S1

^{1}H NMR (D_2O) of IL **1** (δ, ppm).

H(1)	H(2,3,4,5)	H(6)	H(7)	H(8,9,10)	H(11)
3.91	3.32	2.08	1.47	1.21	0.82
(2H,s)	(8H,q)	(2H,t)	(2H,m)	(9H,t)	(3H,t)

^{13}C NMR (D_2O) of IL **1** (δ, ppm).

C^a	C^b	C^c	C^d	C^e	C^f	C^g, C^h, C^i	C^j, C^k, C^l
184.05	57.45	54.81	53.39	39.69	19.46	13.32	6.74

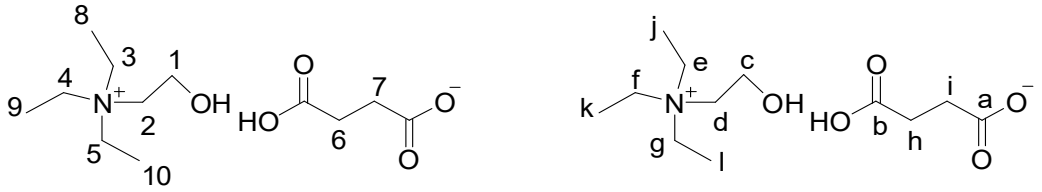


Figure S7. Distribution of ^{1}H NMR and ^{13}C NMR spectra of ionic liquid **2**.

Table S2

^{1}H NMR (D_2O) of IL **2** (δ, ppm).

H(1)	H(2,3,4,5)	H(6,7)	H(8,9,10)
3.90	3.33	2.44	1.22
(2H,s)	(8H,q)	(4H,t)	(9H,t)

^{13}C NMR (D_2O) of IL **2** (δ, ppm).

C^a,C^b	C^c	C^d	C^e, C^f, C^g	C^h, C^i	C^j, C^k, C^l
180.08	57.51	54.87	53.47	32.03	6.81

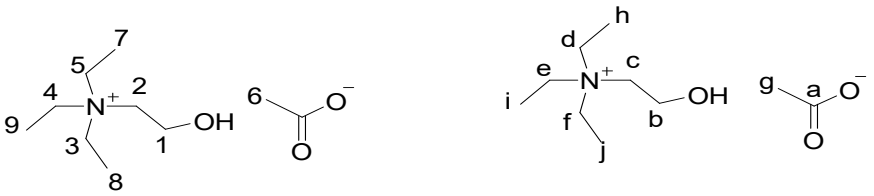


Figure S8. Distribution of ^{1}H NMR and ^{13}C NMR spectra of ionic liquid **3**.

Table S3

^{1}H NMR (D_2O) of IL **3** (δ, ppm).

H(1)	H(2,3,4,5)	H(6)	H(7,8,9)
3.90	3.30	1.83	1.20
(2H,s)	(8H,q)	(3H,s)	(9H,t)

^{13}C NMR (D_2O) of IL **3** (δ, ppm).

C^a	C^b	C^c	C^d	C^e, C^f	C^g	C^h, C^i, C^j
181.32	62.62	57.54	54.87	53.47	23.38	6.81

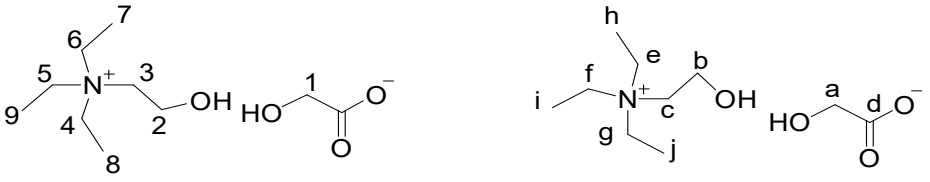


Figure S9. Distribution of ^{1}H NMR and ^{13}C NMR spectra of ionic liquid **4**.

Table S4

^{1}H NMR (D_2O) of IL **4** (δ, ppm).

H(1,2)	H(3,4,5,6)	H(7,8,9)
3.85	3.31	1.21
(4H,d)	(8H,q)	(9H,t)

^{13}C NMR (D_2O) of IL **4** (δ, ppm).

C^a	C^b	C^c	C^d	C^e, C^f, C^g	C^h, C^i, C^j
179.87	61.30	57.50	54.87	53.45	6.79

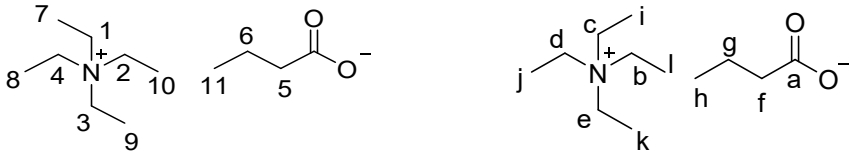


Figure S10. Distribution of ^{1}H NMR and ^{13}C NMR spectra of ionic liquid **5**.

Table S5

^{1}H NMR (D_2O) of IL **5** (δ, ppm).

H (1,2,3,4)	H(5)	H(6)	H(7,8,9,10)	H(11)
3.17	2.08	1.48	1.18	0.82
(8H,q)	(2H,m)	(2H,m)	(12H,m)	(3H,m)

^{13}C NMR (D_2O) of IL **5** (δ, ppm).

C^a	C^b ,C^c,C^d,C^e	C^f	C^g	C^h	C^i, C^j ,C^k, C^l
183.59	52.07	39.69	19.58	13.55	6.82

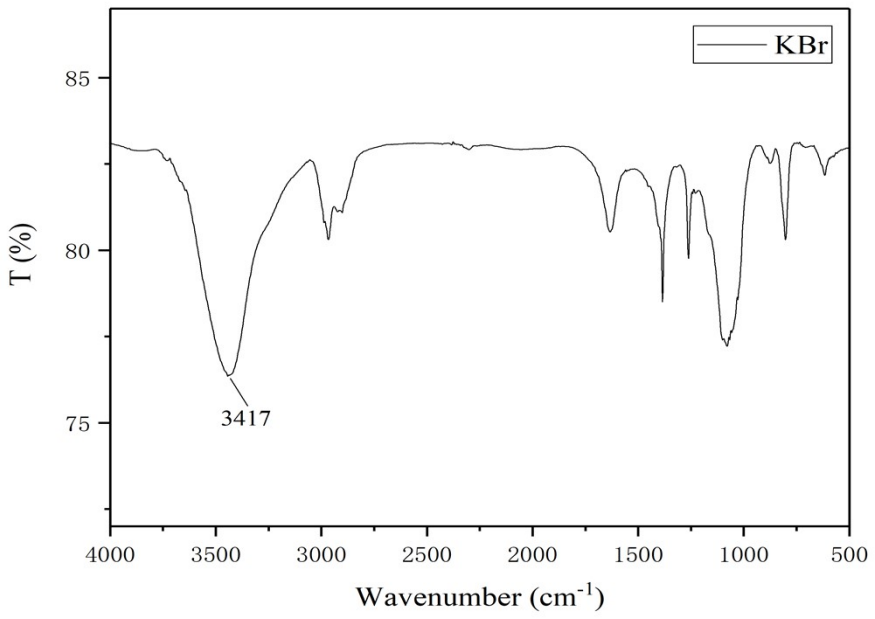


Figure S11. IR spectrum of IL KBr

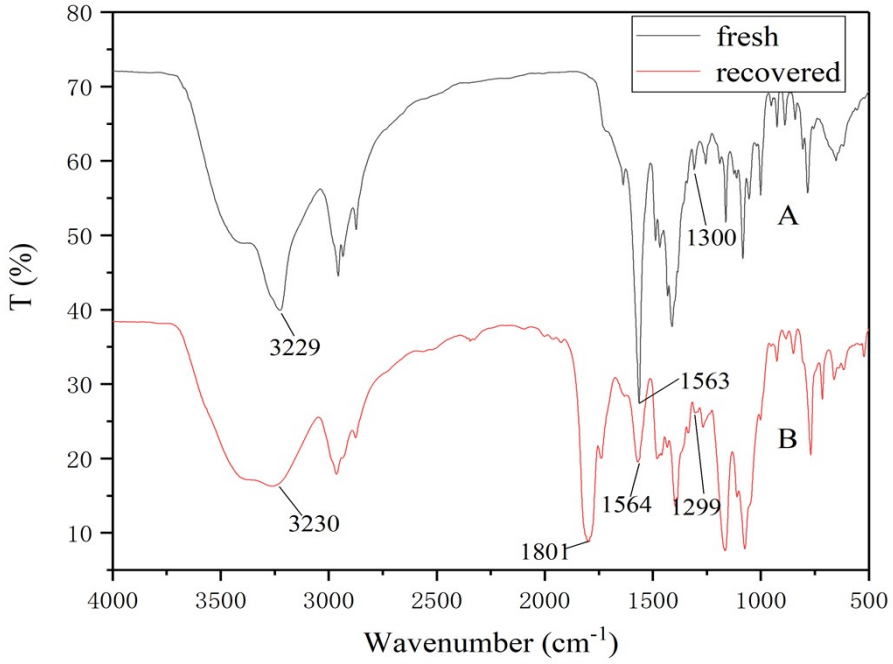


Figure S12. FT-IR spectra of catalyst: A: fresh, B: recovered.

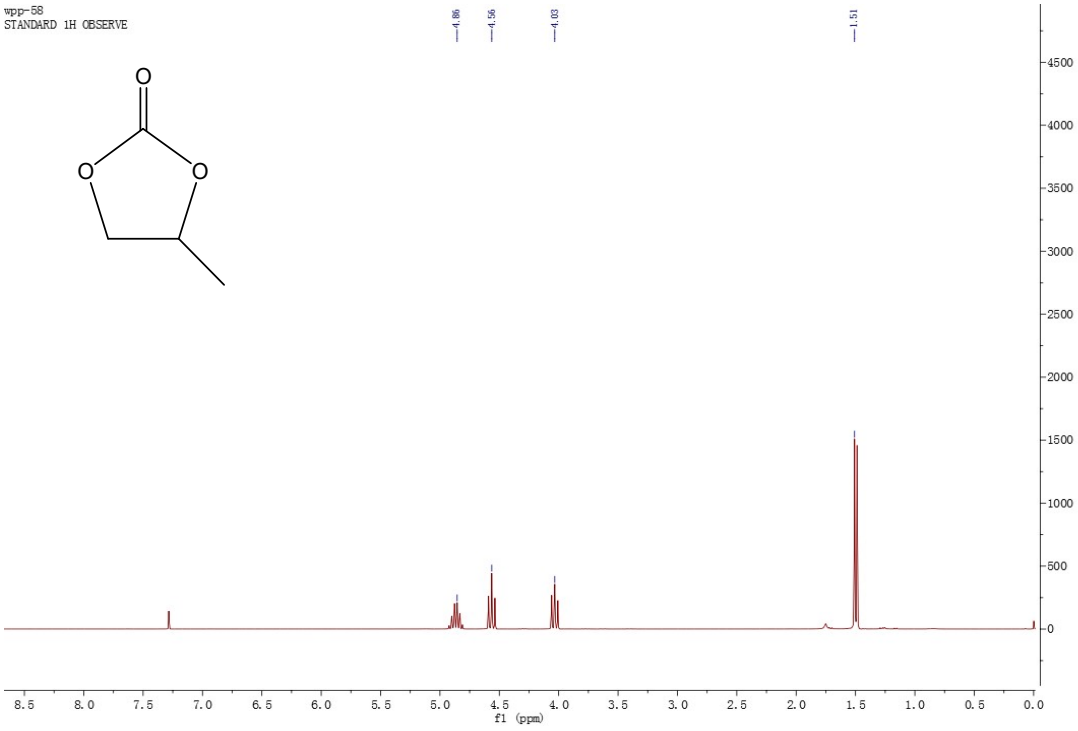


Figure S13. [1]H NMR spectrum of 4-methyl-1,3-dioxolan-2-one

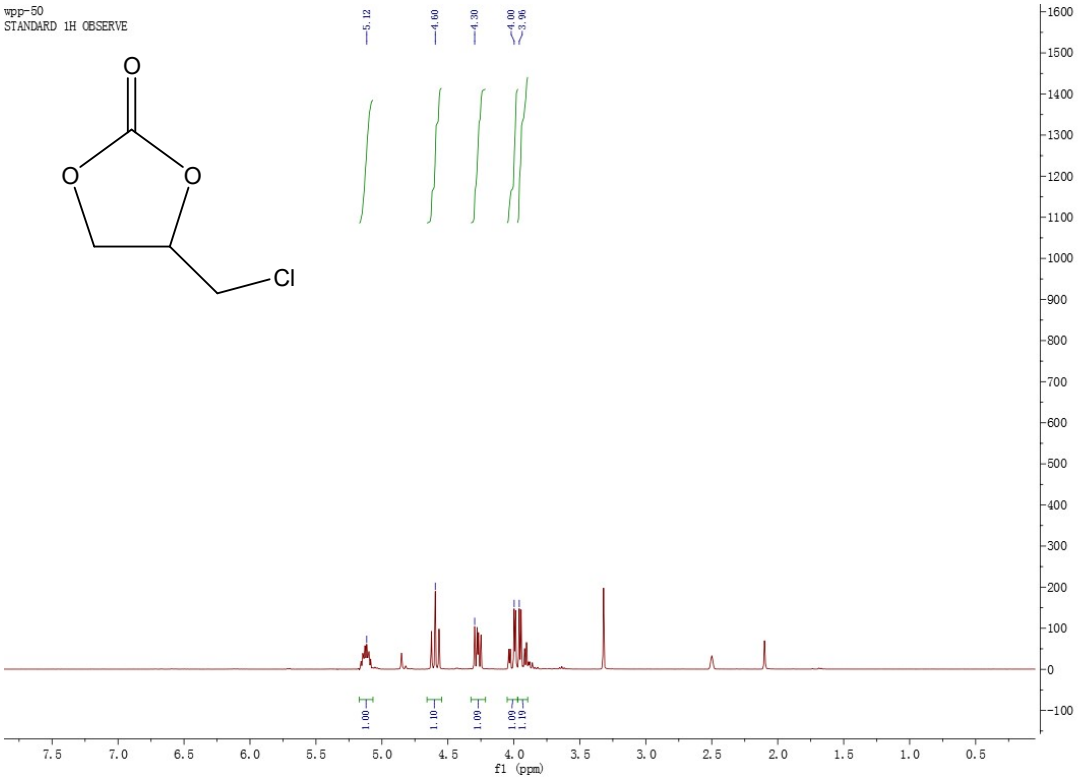


Figure S14. ^{1}H NMR spectrum of 4-(chloromethyl)-1,3-dioxolan-2-one

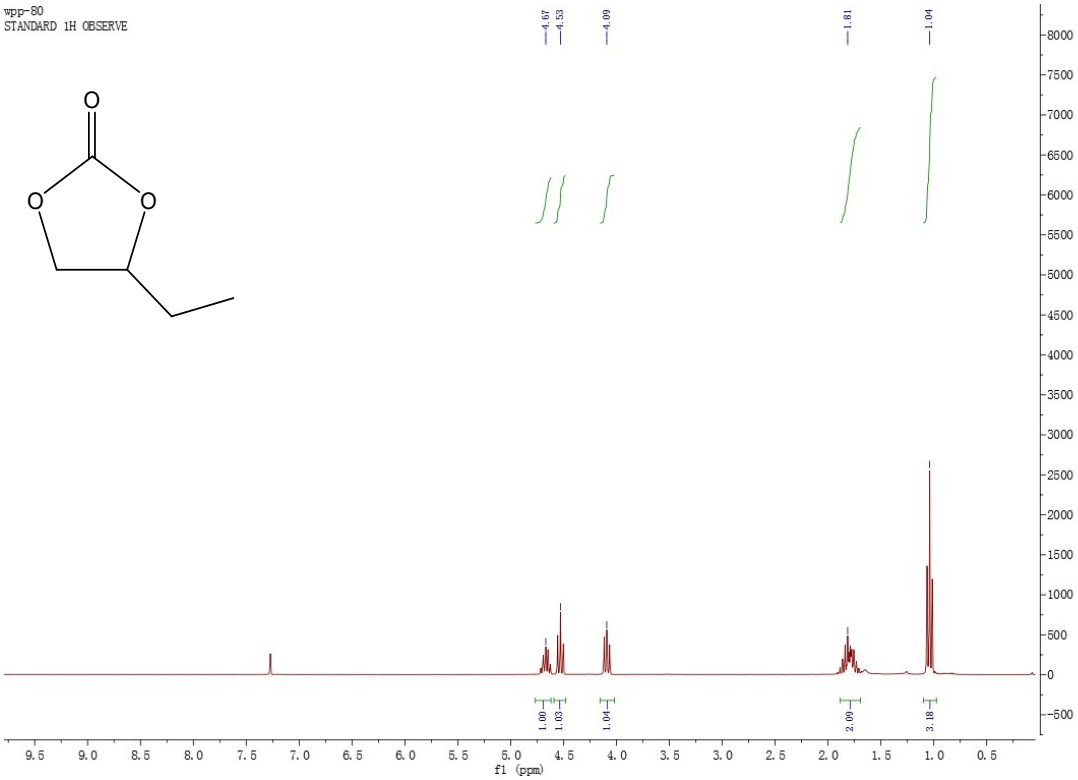


Figure S15. ^{1}H NMR spectrum of 4-ethyl-1,3-dioxolan-2-one

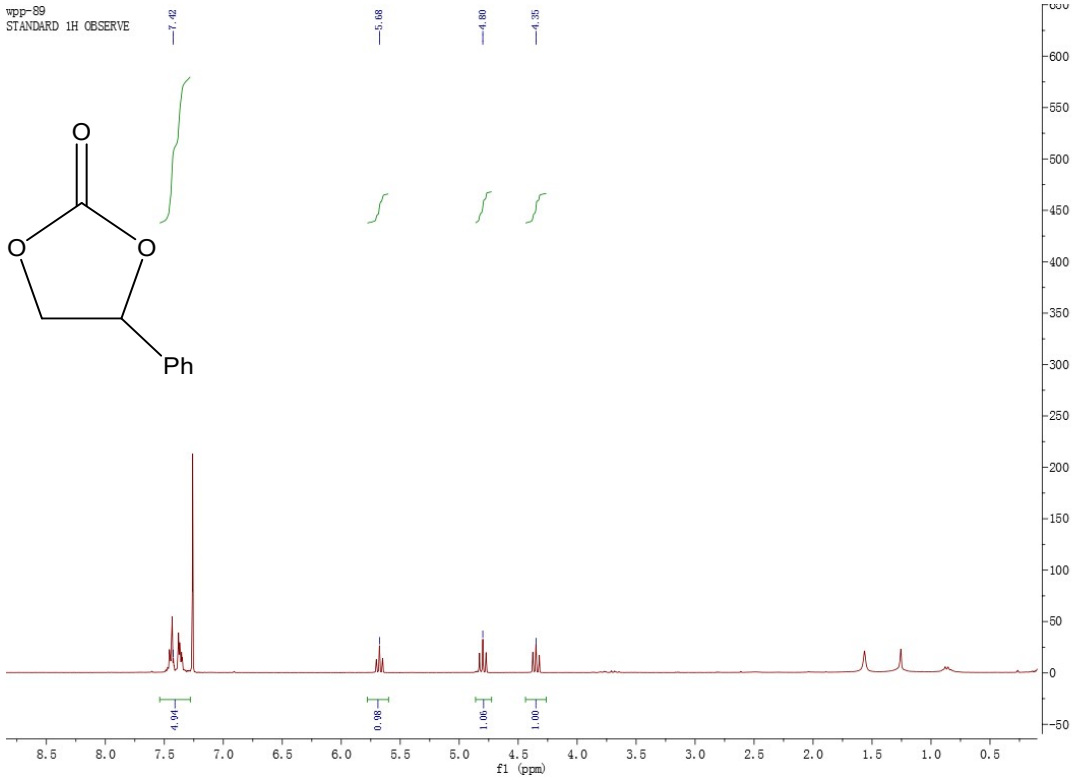


Figure S16. ^{1}H NMR spectrum of 4-phenyl-1,3-dioxolan-2-one

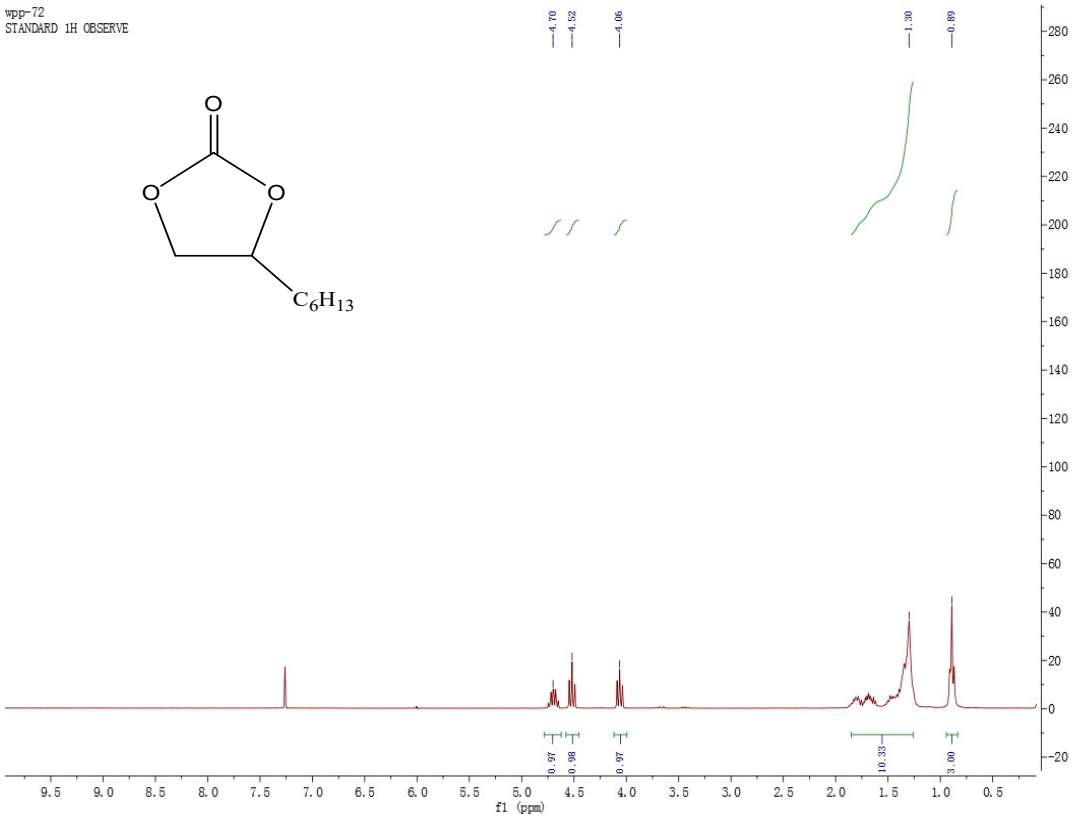


Figure. S17. ^{1}H NMR spectrum of 4-Hexyl-1,3-dioxolan-2-one

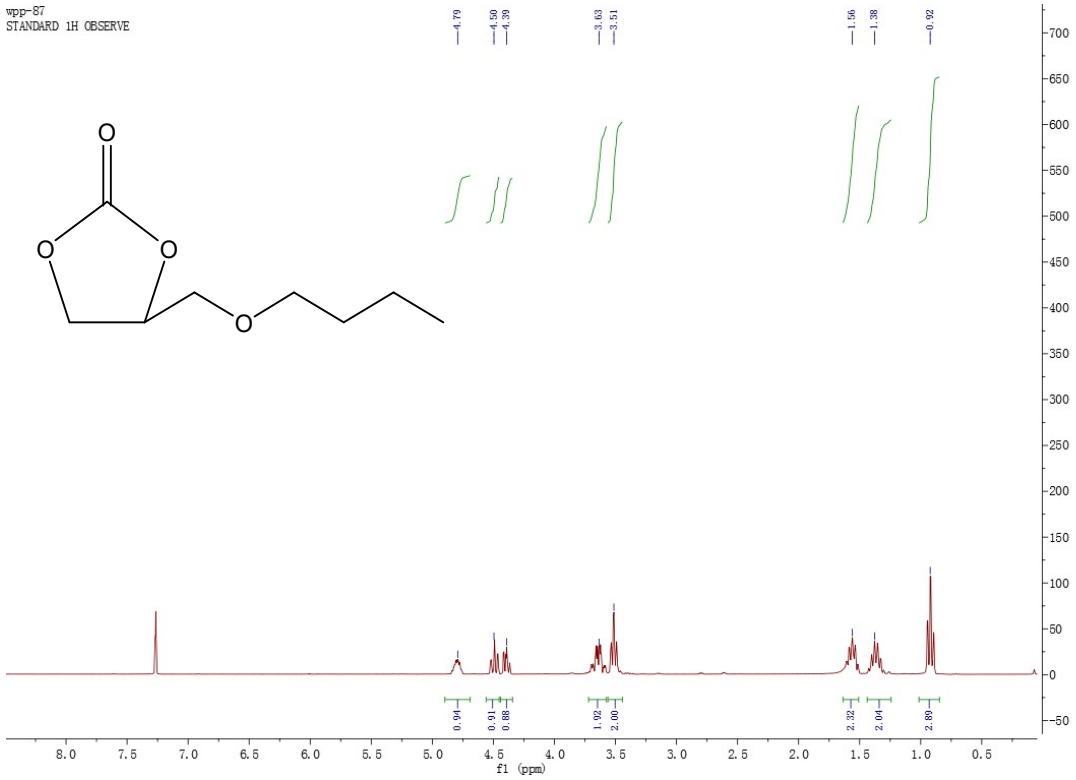


Figure S18. [1]H NMR spectrum of 4-butoxymethyl-1,3-dioxolan-2-one

Ionic liquid 1:

[1]H NMR (400 MHz, DMSO) δ 3.78 (s, 2H), 3.34 (m, 8H), 1.80 (d, *J* = 4.9 Hz, 2H), 1.40 (m, 2H), 1.17 (m, 9H), 0.80 (t, 3H).

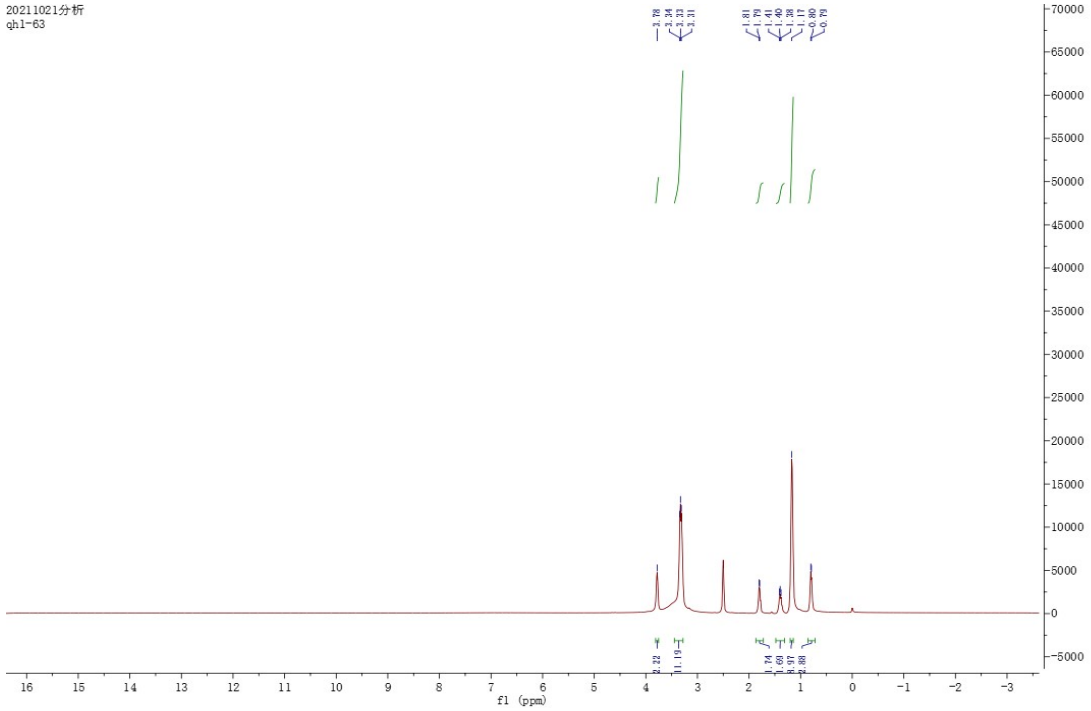


Figure S19-1. [1]H NMR spectrum of IL**1** in DMSO

^{1}H NMR (400 MHz, DMSO) δ3.79 (s, 3H), 3.34 (m, 8H), 1.80 (t, 2H), 1.40 (m, 2H), 1.17 (d, 9H), 0.80 (t, 3H). epichlorohydrin: 3.90 (m, 1H), 3.54 (m, 1H), 3.24 (m, 1H), 2.85 (m, 1H), 2.78 (m, 1H).

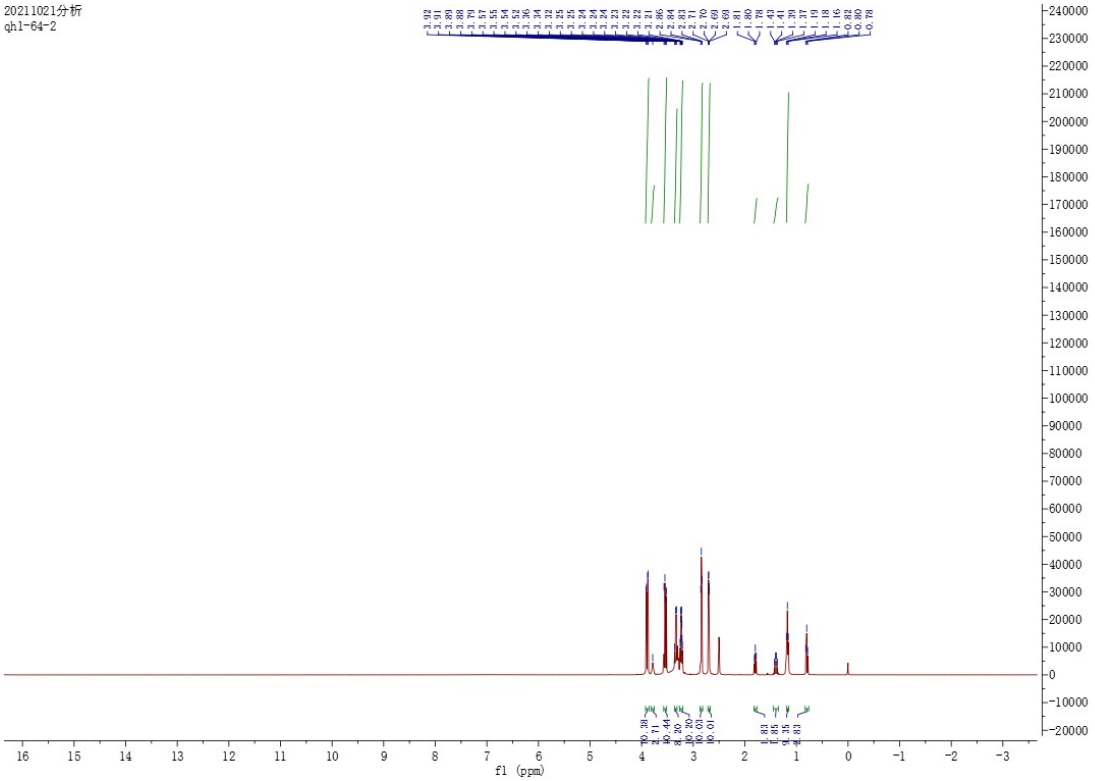


Figure S19-2 ^{1}H NMR spectrum for IL **1** + epichlorohydrin at 25 ℃ and t = 0.5 h in DMSO

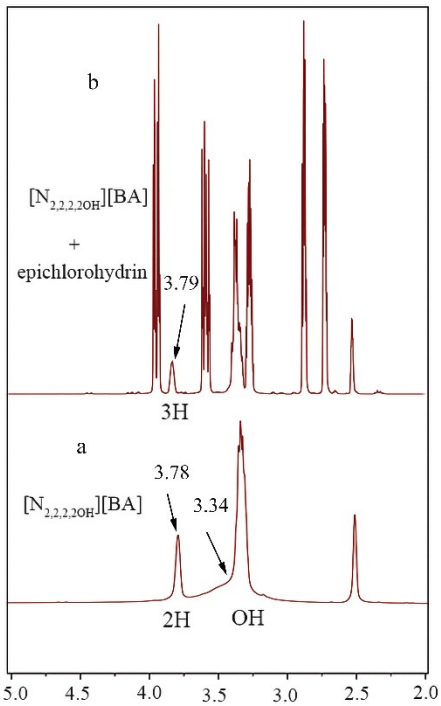


Figure S19-3. (a) ^{1}H-NMR spectrum for $[N_{2,2,2,2OH}][BA]$ in DMSO. (b) ^{1}H-NMR spectrum for $[N_{2,2,2,2OH}][BA]$ + epichlorohydrin at 25 ℃ and t = 0.5 h in DMSO.