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1-烷基-3-甲基咪唑氯化物焓变的热重分析

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Thermogravimetric Analysis of Enthalpy Variation of 1-Alkyl-3-methylimidazole chloride

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A 部分 ^{1}H NMR 谱
Section A ^{1}H NMR Spectra

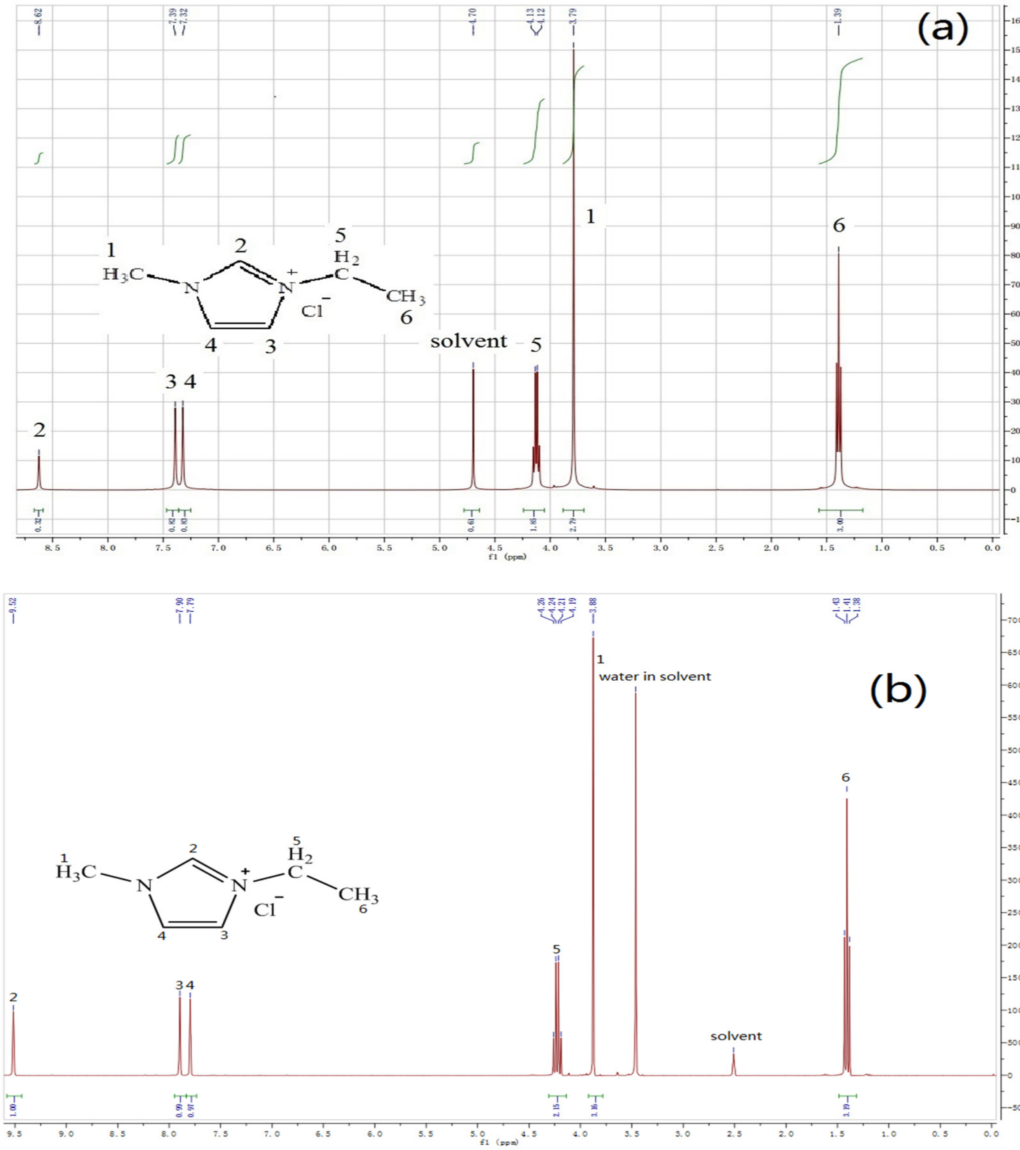

图 S1 (a)离子液体[C$_2$mim]Cl 的核磁共振氢谱；(b)离子液体[C$_2$mim]Cl 在 T = 503.15 K 蒸发后的残留物的核磁共振氢谱

Fig. S1 (a) ^{1}H NMR spectrum of IL [C$_2$mim]Cl; (b) ^{1}H NMR spectrum of residue after evaporation of IL [C$_2$mim]Cl at T = 503.15 K.

(a) ^{1}H NMR (300 MHz, DMSO) δ = 8.62 (s, 1H), 7.39 (d, 1H), 7.32 (d, 1H), 4.1 (m, 2H), 3.79 (s, 3H), 1.39 (t, 3H).

(b) ^{1}H NMR (300 MHz, DMSO) δ = 9.52 (s, 1H), 7.90 (d, 1H), 7.79 (d, 1H), 4.21 (m, 2H), 3.88 (s, 3H), 1.41 (t, 3H).

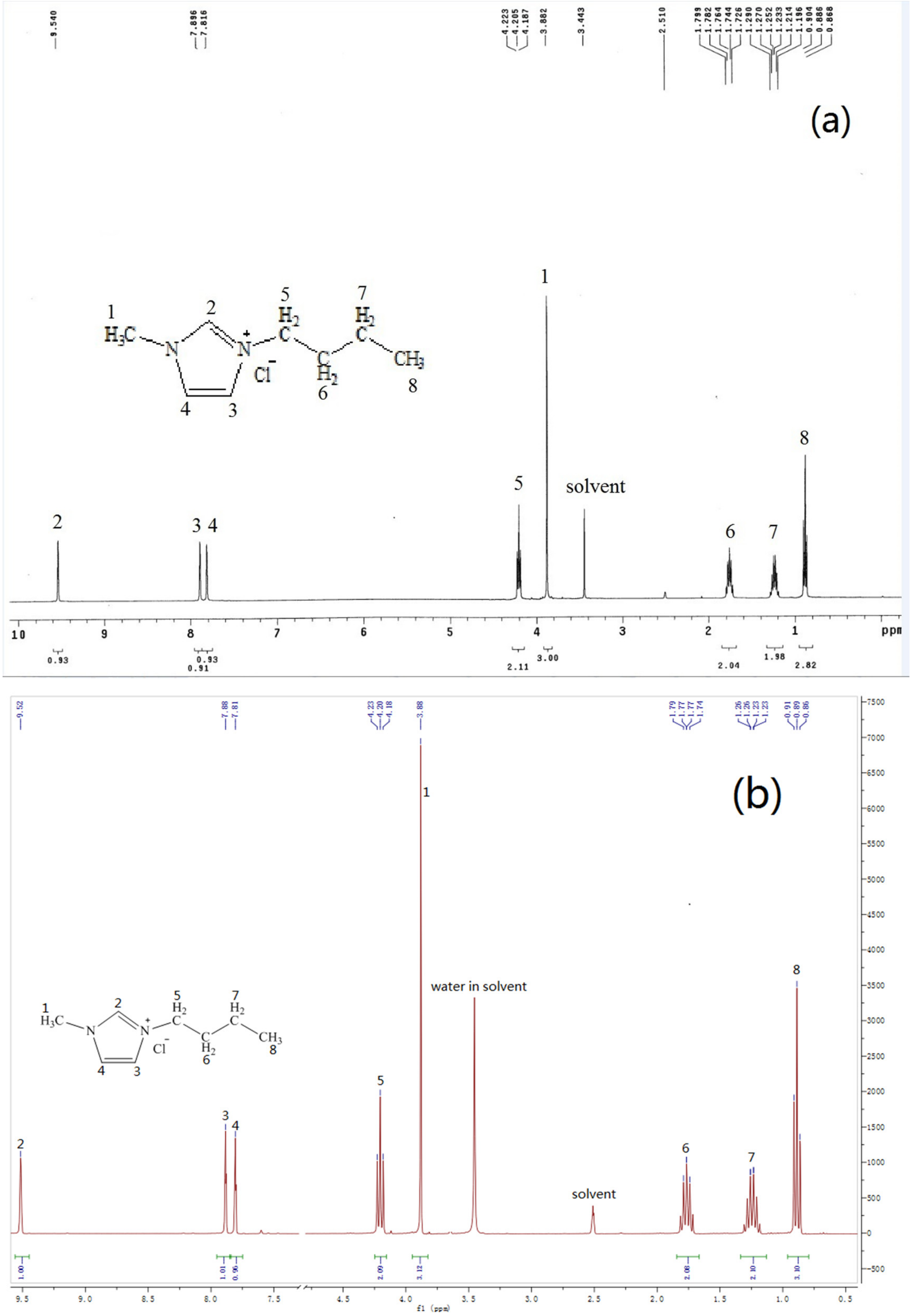

图 S2 (a)离子液体[C4mim]Cl 的核磁共振氢谱；(b)离子液体[C4mim]Cl 在 *T* = 503.15 K 蒸发后的残留物的核磁共振氢谱

Fig. S2 (a) ^{1}H NMR spectrum of IL [C4mim]Cl; (b) ^{1}H NMR spectrum of residue after evaporation of IL [C4mim]Cl at *T* = 503.15 K.

(a) ^{1}H NMR (300 MHz, DMSO) δ = 9.54 (s, 1H), 7.896 (d, 1H), 7.816 (d, 1H), 4.205 (t, 2H), 3.882 (s, 3H), 1.764 (m, 2H), 1.252 (m, 2H), 0.886 (t, 3H).

(b) ^{1}H NMR (300 MHz, DMSO) δ = 9.52 (s, 1H), 7.88 (d, 1H), 7.81 (d, 1H), 4.20 (t, 2H), 3.88 (s, 3H), 1.77 (m, 2H), 1.23 (m, 2H), 0.89 (t, 3H).

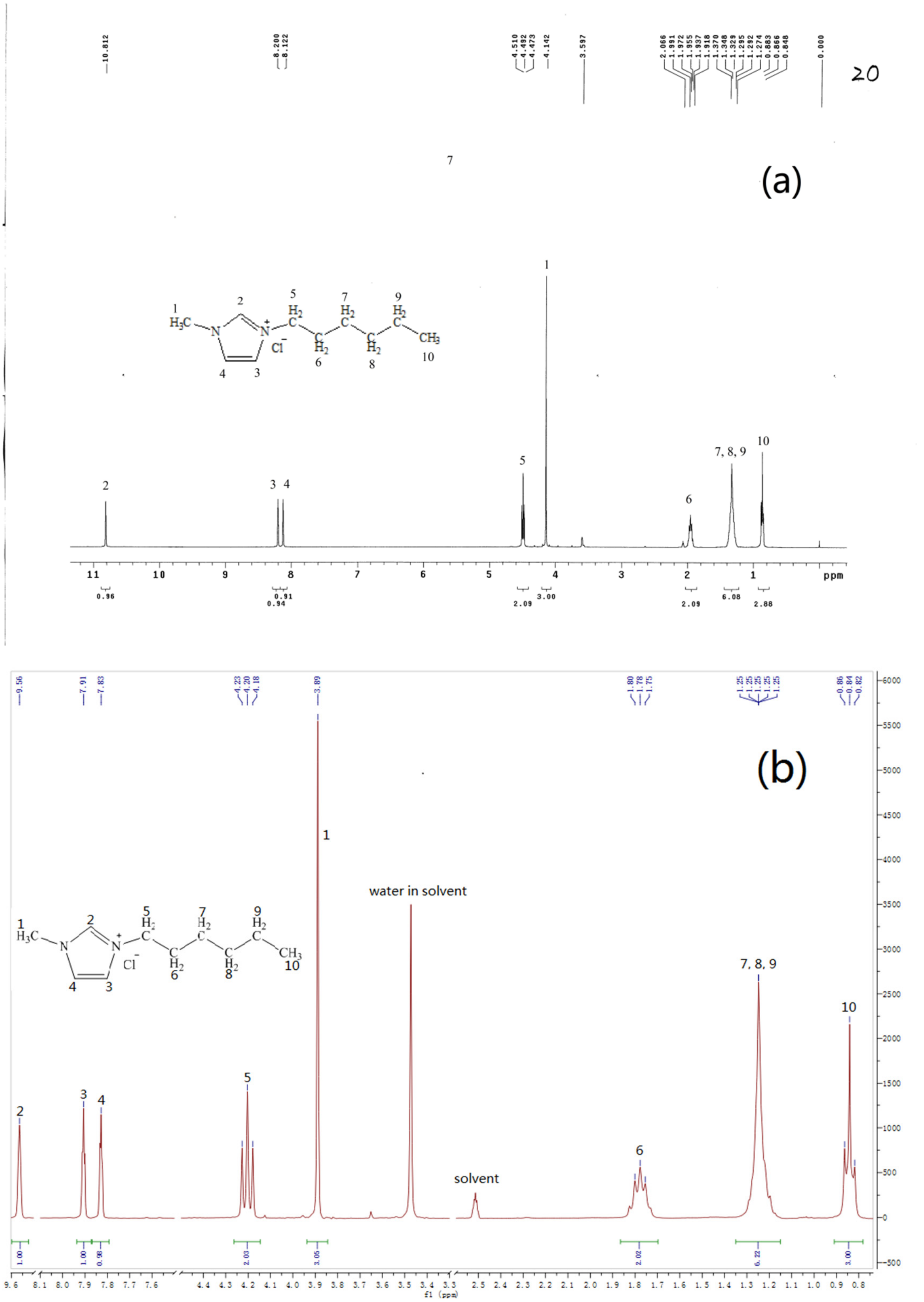

图 S3 (a)离子液体[C₆mim]Cl 的核磁共振氢谱；(b)离子液体[C₆mim]Cl 在 T = 503.15 K 蒸发后的残留物的核磁共振氢谱

Fig. S3 (a) ^{1}H NMR spectrum of IL [C_6mim]Cl; (b) ^{1}H NMR spectrum of residue after evaporation of IL [C_6mim]Cl at T = 503.15 K.

(a) ^{1}H NMR (300 MHz, DMSO) δ = 10.812 (s, 1H), 8.200 (d, 1H), 8.122 (d, 1H), 4.492 (t, 2H), 4.142 (s, 3H), 1.955 (m, 2H), 1.295 (m, 6H), 0.866 (t, 3H).

(b) ^{1}H NMR (300 MHz, DMSO) δ = 9.56 (s, 1H), 7.91 (d, 1H), 7.83 (d, 1H), 4.20 (t, 2H), 3.89 (s, 3H), 1.78 (m, 2H), 1.25 (m, 6H), 0.84 (t, 3H).

B 部分 ^{13}C NMR 谱

Section B ^{13}C NMR Spectra

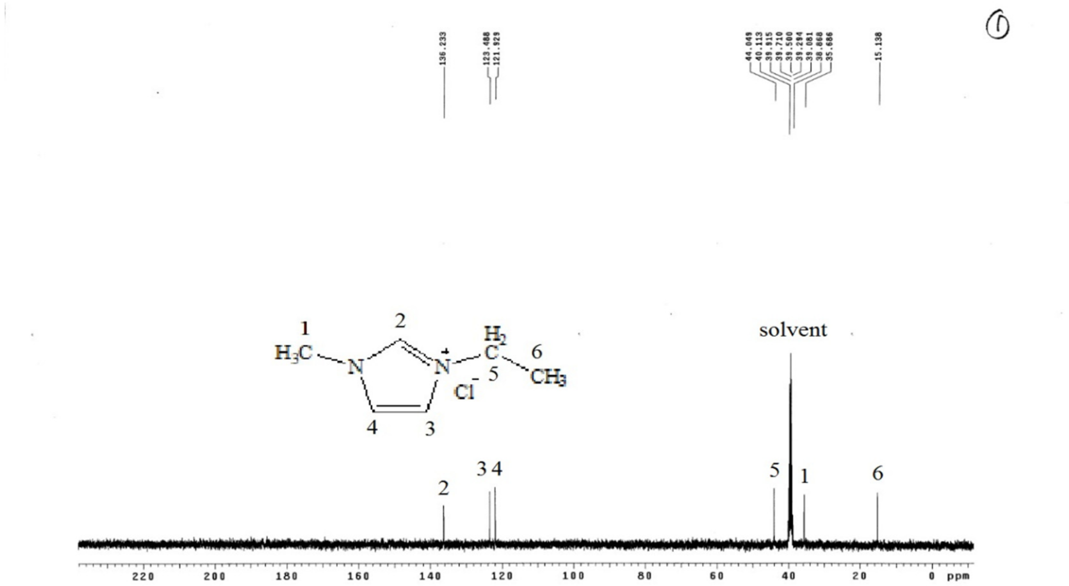

图 S4　离子液体[C_2mim]Cl 的核磁共振碳谱

Fig. S4　^{13}C NMR spectrum of IL [C_2mim]Cl.

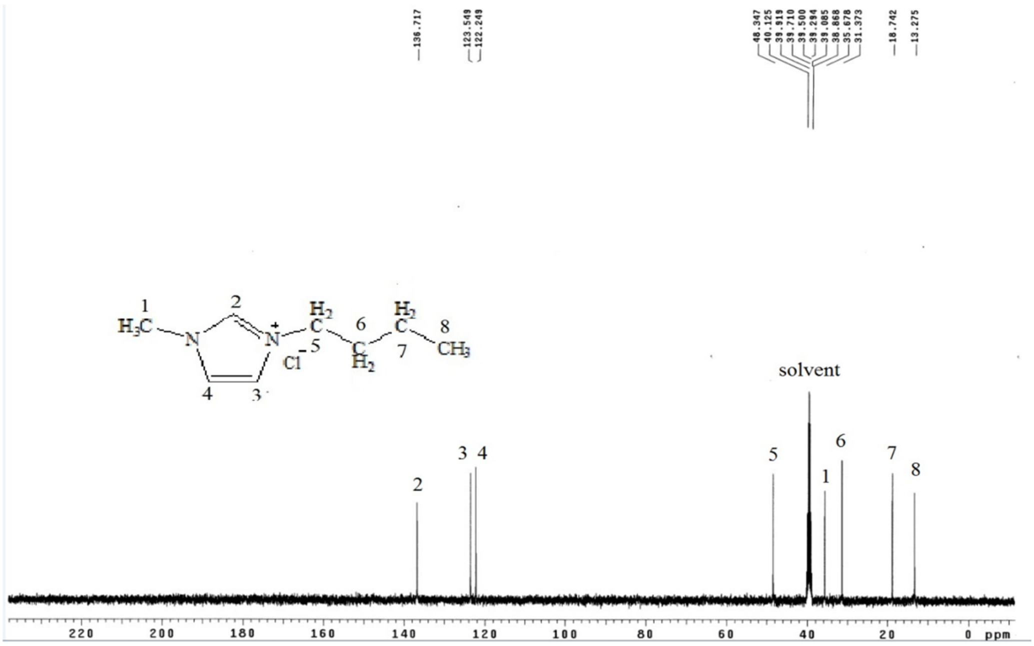

图 S5　离子液体[C_4mim]Cl 的核磁共振碳谱

Fig. S5　^{13}C NMR spectrum of IL [C_4mim]Cl.

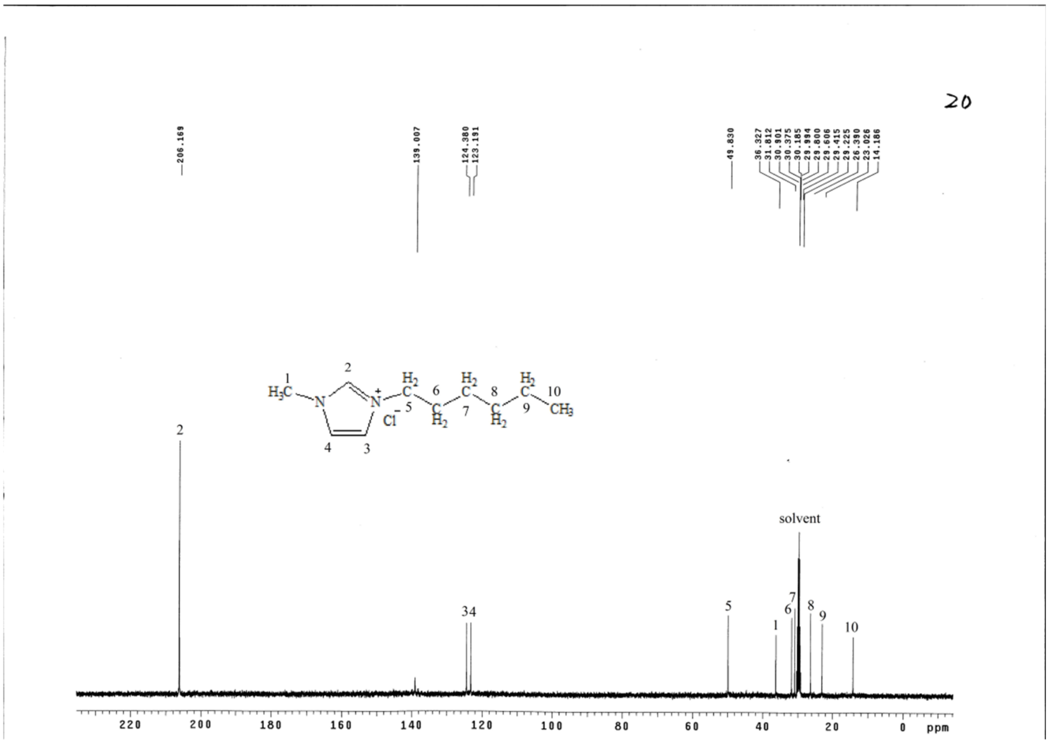

图 S6 离子液体[C_6mim]Cl 的核磁共振碳谱

Fig. S6 ^{13}C NMR spectrum of IL [C_6mim]Cl.

C 部分 热重分析

Section C Thermogravimetry Analysis

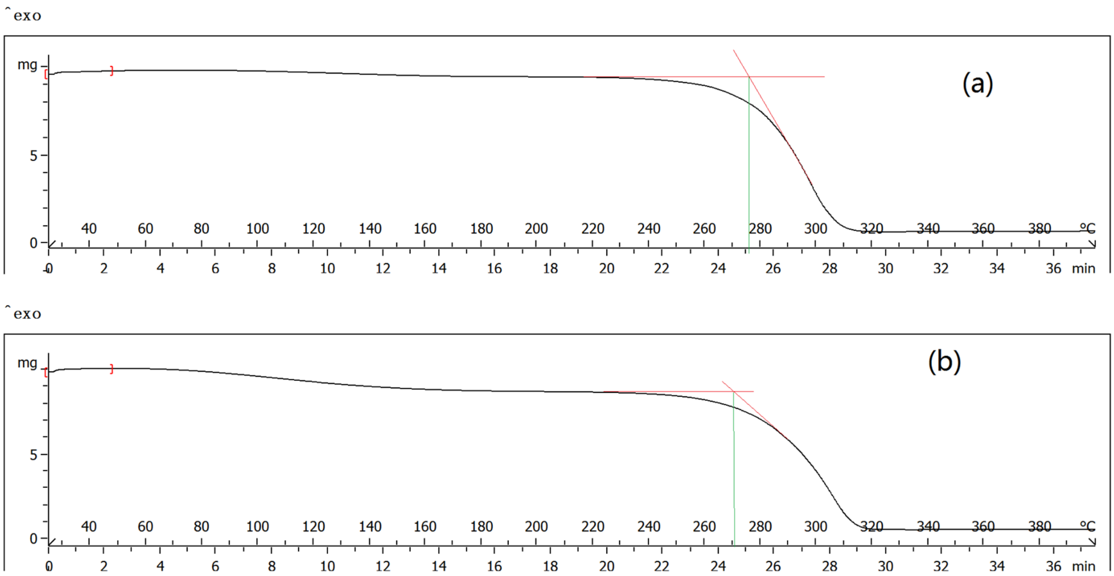

图 S7 (a)离子液体[C_2mim]Cl 的热重分析；(b)离子液体[C_2mim]Cl 在 T = 503.15 K 蒸发后的残留物的热重分析

Fig. S7 (a) Thermogravimetry analysis of IL [C_2mim]Cl; (b) thermogravimetry analysis of residue after evaporation of IL [C_2mim]Cl at T = 503.15 K.

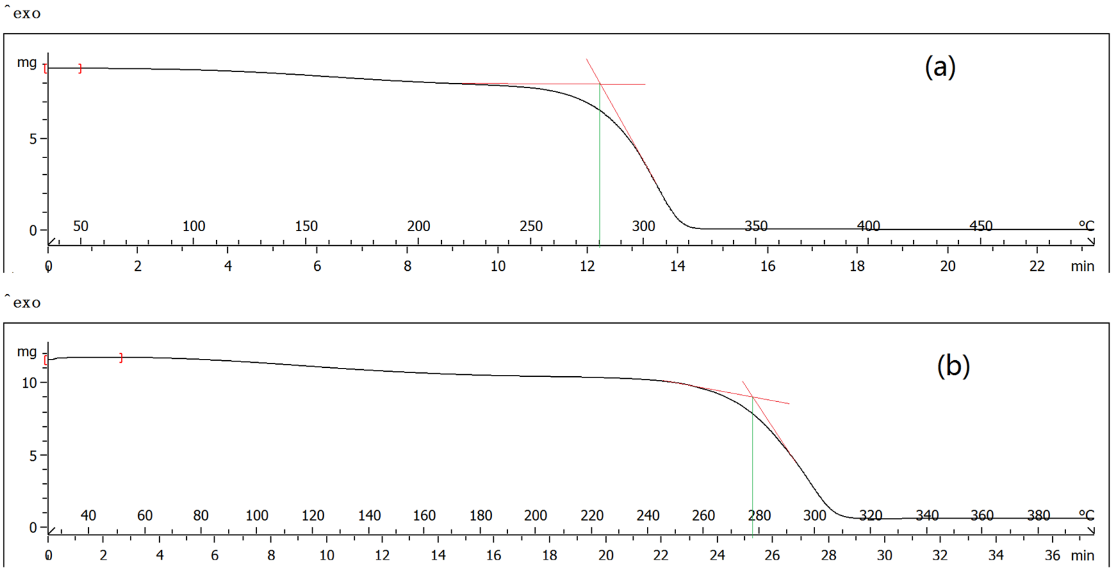

图 S8　(a)离子液体[C$_4$mim]Cl 的热重分析；(b)离子液体[C$_4$mim]Cl 在 T = 503.15 K 蒸发后的残留物的热重分析

Fig. S8　(a) Thermogravimetry analysis of IL [C$_4$mim]Cl; (b) thermogravimetry analysis of residue after evaporation of IL [C$_4$mim]Cl at T = 503.15 K.

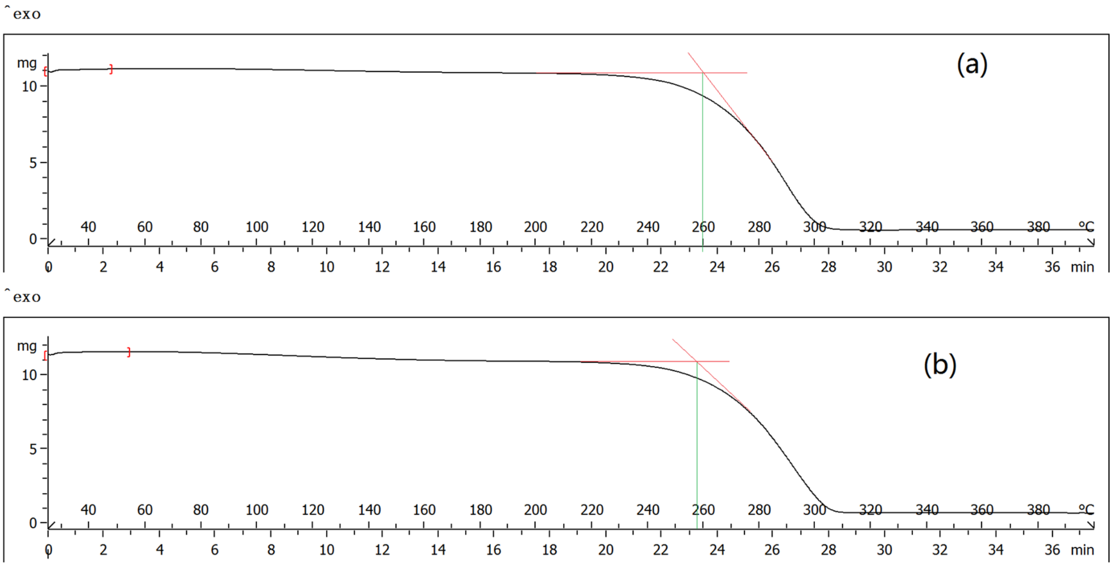

图 S9　(a)离子液体[C$_6$mim]Cl 的热重分析；(b)离子液体[C$_6$mim]Cl 在 T = 503.15 K 蒸发后的残留物的热重分析

Fig. S9　(a) Thermogravimetry analysis of IL [C$_6$mim]Cl; (b) thermogravimetry analysis of residue after evaporation of IL [C$_6$mim]Cl at T = 503.15 K.

表 S1 $\Delta H_{vap}(T_{av})$、$\Delta H_{vap}(298)$、ΔG_s 的计算值和计算[$C_n$mim]Cl (n = 2, 4, 6)的$\Delta^g{}_l C_p{}^{o}{}_m$ 所需要的相应数据

Table S1 The calculated values of $\Delta H_{vap}(T_{av})$, $\Delta H_{vap}(298)$, ΔG_s and the corresponding necessary data of calculating $\Delta^g{}_l C_p{}^{o}{}_m$ for [$C_n$mim]Cl (n = 2, 4, 6)

IL	$\Delta H_{vap}(298)$/(kJ·mol^{-1})	$\Delta H_{vap}(T_{av})$/(kJ·mol^{-1})	M/(kg·mol^{-1})	ρ/(kg·m^{-3})
[C_2mim]Cl	115.1	105.5	0.1466	1143.4[a]
[C_4mim]Cl	123.9	114.6	0.1707	1081.7[a]
[C_6mim]Cl	133.3	123.4	0.2027	1037.8[a]
IL	γ	$10^4 V_m$/(m^3·mol^{-1})	$10^4 \alpha_p$/(K^{-1})	$10^{10} \kappa_T$/(Pa^{-1})
[C_2mim]Cl	0.0653 [a]	1.2824	5.007	2.5248
[C_4mim]Cl	0.0503 [a]	1.5778	5.160	3.3889
[C_6mim]Cl	0.0397 [a]	1.9534	5.570	4.5096
IL	W/(m·s^{-1})	$C_p{}^{o}{}_m$ (l)/(J·K^{-1}·mol^{-1}) (Paulechka's)	$\Delta^g{}_l C_p{}^{o}{}_m$ /(J·K^{-1}·mol^{-1})	ΔG_s/(kJ·mol^{-1})
[C_2mim]Cl	2018.0	254.17	−54.6	14.023
[C_4mim]Cl	1759.6	310.75	−53.6	12.596
[C_6mim]Cl	1544.8	382.68	−56.7	11.287

[a] The data of density and surface tension at T = 298.15 K were obtained by using extrapolation method on values of density and surface tension in Ref. 39 at other temperature; α_p is the thermal expansion coefficient; κ_T is the isothermal compressibility, $\kappa_T = 1/\rho(1/W^2 + T\alpha_p{}^2 M/ C_p{}^{o}{}_m)$; $W(T, p)$ is the speed of the sound, $W = [\gamma/(6.3 \times 10^{-10}\rho)]^{2/3}$; $C_p{}^{o}{}_m$ (l) is heat capacity of the liquid state of the IL calculated by Paulechka's method; $\Delta^g{}_l C_p{}^{o}{}_m$ is the difference in heat capacity of the gaseous and liquid state of the IL at constant pressure, $\Delta^g{}_l C_p{}^{o}{}_m = C_p{}^{o}{}_g - C_p{}^{o}{}_l = (3/2)R + (3/2)R + R - 3R - 3R - (C_p{}^{o}{}_m - C_V{}^{o}{}_m)_l = -2R - (C_p{}^{o}{}_m - C_V{}^{o}{}_m)_l$.