

Electronic Supplementary Information

Efficient absorption of ammonia with dialkylphosphate-based ionic liquids

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Table S1 The water contents of the ILs

IL	[C ₄ C ₁ im] [DBP]	[C ₄ C ₁ im] [DMP]	[C ₂ C ₁ im] [DEP]	[C ₂ C ₁ im] [DMP]	[C ₁ C ₁ im] [DMP]
H ₂ O /ppm	276	232	353	259	388

Table S2 The density ρ and viscosity η of dialkylphosphate-based ILs at 298.15 K and 0.1 MPa

Component	$\rho/(\text{g}\cdot\text{cm}^{-3})$		$\eta/(\text{mPa}\cdot\text{s})$	
	Exp.	Lit.	Exp.	Lit.
[bmim][DMP]	1.1645	1.1619 ^a	543.01	584.74 ^a
[emim][DMP]	1.2242	1.22 ^a	249.67	269.872 ^a
[emim][DEP]	1.1466	1.146 ^b	419.29	410 ^c
[mmim][DMP]	1.2616	1.2587 ^d	290.32	271.86 ^d
[bmim][DBP]	1.0454	<i>NA</i>	1741.1	<i>NA</i>

Reference

^a Y H. Gong, C. Shen, Y.Z. Lu, H. Meng, C.X. Li, J. Chem. Eng. Data., 57 (2012) 33-39.

^b W.M.D.W. Normazlan, N. A.Sairi, Y. Alias, A.F. Udaiyappan, A. Jouyban, M. Khoubnasabjafari, J. Chem. Eng. Data., 59 (2014) 2337-2348.

^c C. M. Tenney, M. Massel, J. M. Mayes, M. Sen, J. F. Brennecke, E. J. A. Marginn, J. Chem. Eng. Data., 59 (2014) 391-399.

^d Z.B. He, Z.C. Zhao, X.D. Zhang, H. Feng, Fluid Phase Equilibr., 298 (2010) 83-91.

Table S3 The comparison of density and volume before and after CO₂ absorption at 303.15 K

IL	$\rho(\text{IL})$ /g·cm ⁻³	$V(\text{IL})$ /cm ³	$\rho(\text{IL}+\text{CO}_2)$ /g·cm ⁻³	$V(\text{IL}+\text{CO}_2)$ /cm ³	$\Delta V/\%$
[C ₄ C ₁ im][DBP]	1.0392	11.503	1.0445	11.746	2.11
[C ₄ C ₁ im][DMP]	1.1537	11.260	1.1542	11.559	2.65
[C ₂ C ₁ im][DEP]	1.1403	10.104	1.1426	10.337	2.31
[C ₂ C ₁ im][DMP]	1.2141	9.971	1.2079	10.350	3.79
[C ₁ C ₁ im][DMP]	1.2562	9.483	1.2527	9.783	3.15

Table S4 Uncertainties of the used instruments in measurements

Measurements	Uncertainties
Density/ ($\text{g} \cdot \text{cm}^{-3}$)	0.002
Viscosity/ $\text{mPa} \cdot \text{s}$	0.05
Solubility	0.005
Temperatures of water bath/K	0.05
Pressure transmitter /kPa	0.1
Mass of ILs /g	0.001

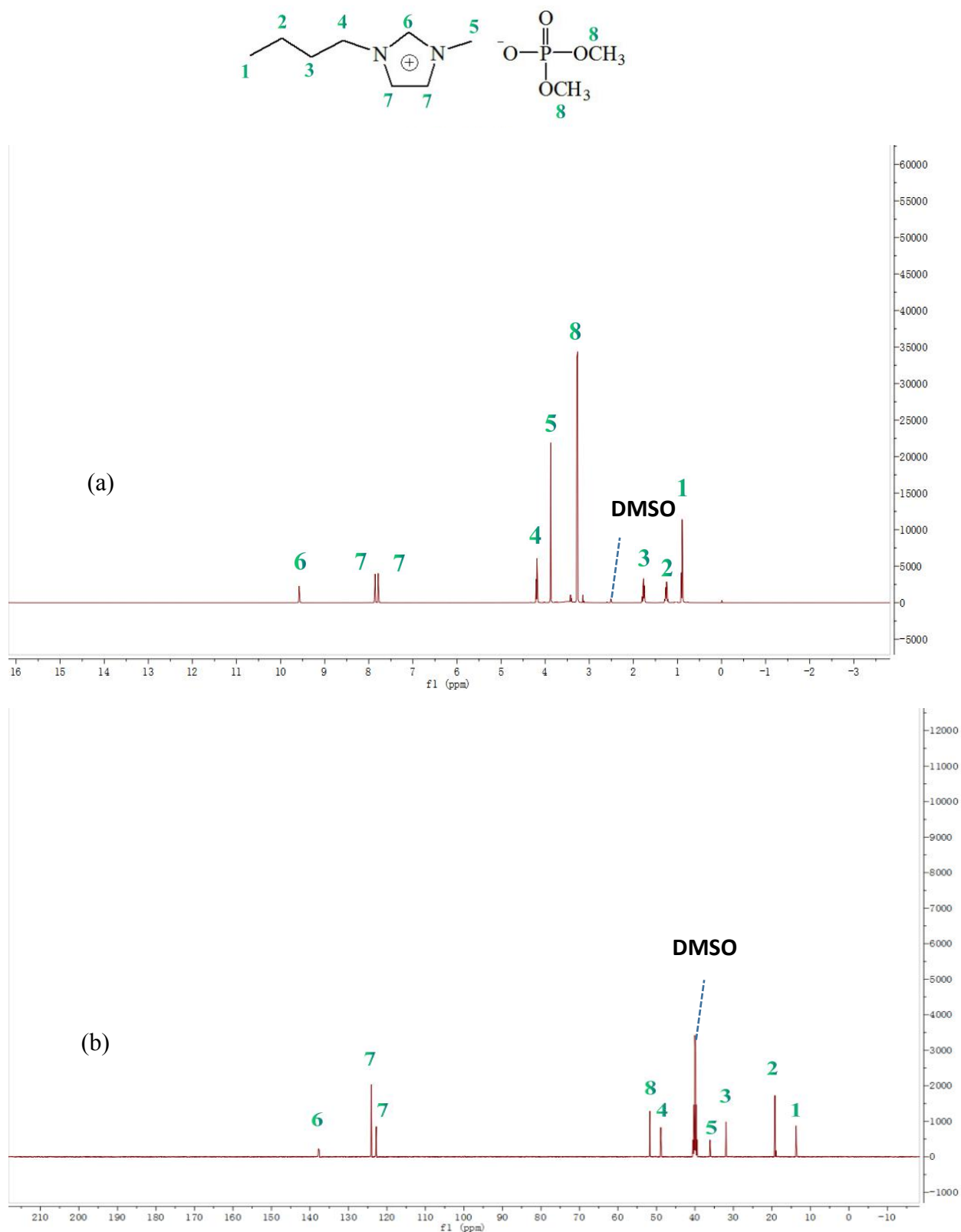


Figure S1 NMR spectra for [C₄C₁im][DMP] (1-butyl-3-methylimidazolium dimethylphosphate) in DMSO-d₆ with tetramethylsilane (TMS) as the internal standard: (a) ¹H NMR and (b) ¹³C NMR.

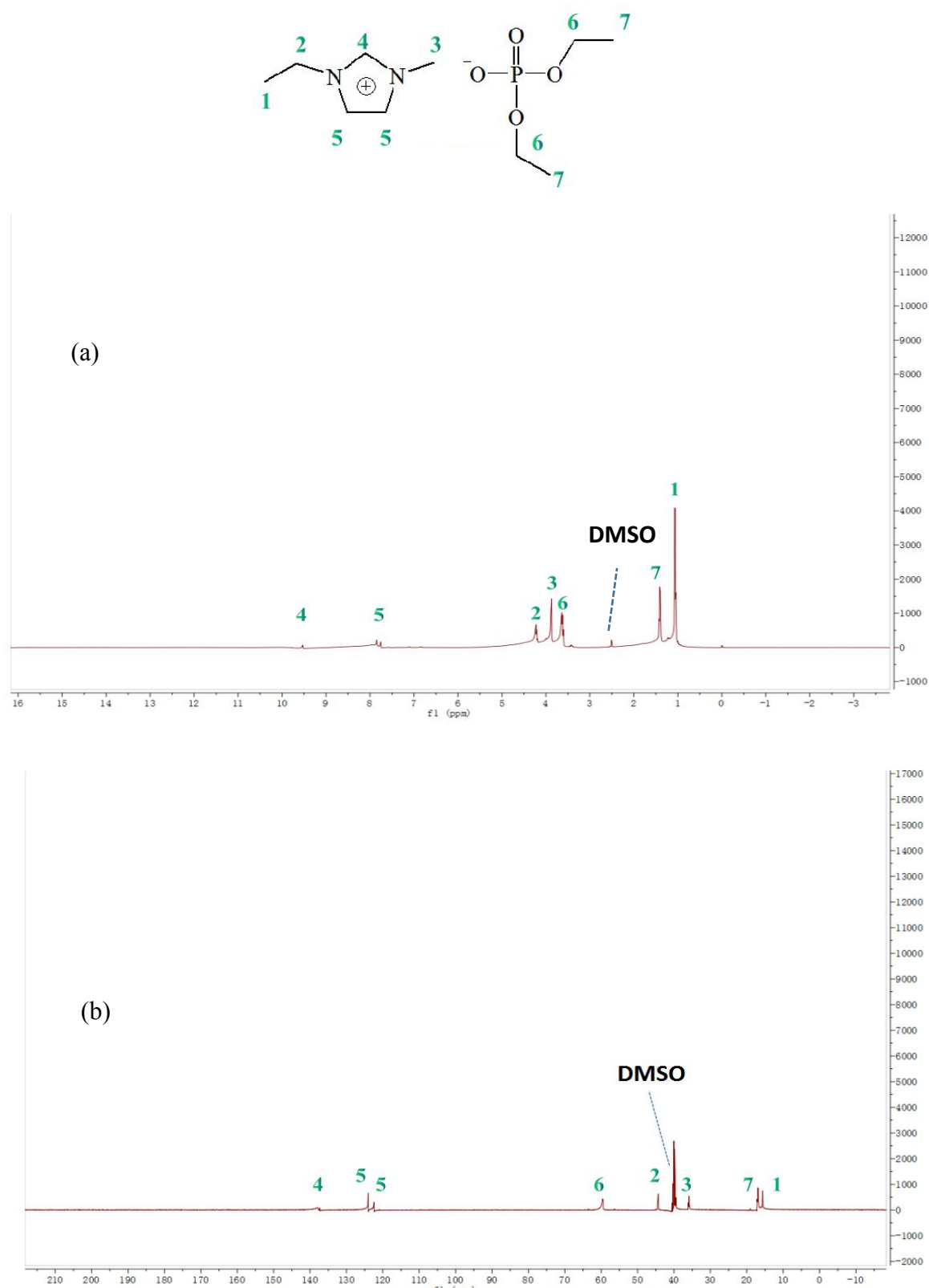


Figure S2 NMR spectra for [C₂C₁im][DEP] (1-ethyl-3-methylimidazolium diethylphosphate) in DMSO-d₆ with tetramethylsilane (TMS) as the internal standard: (a) ¹H NMR and (b) ¹³C NMR.

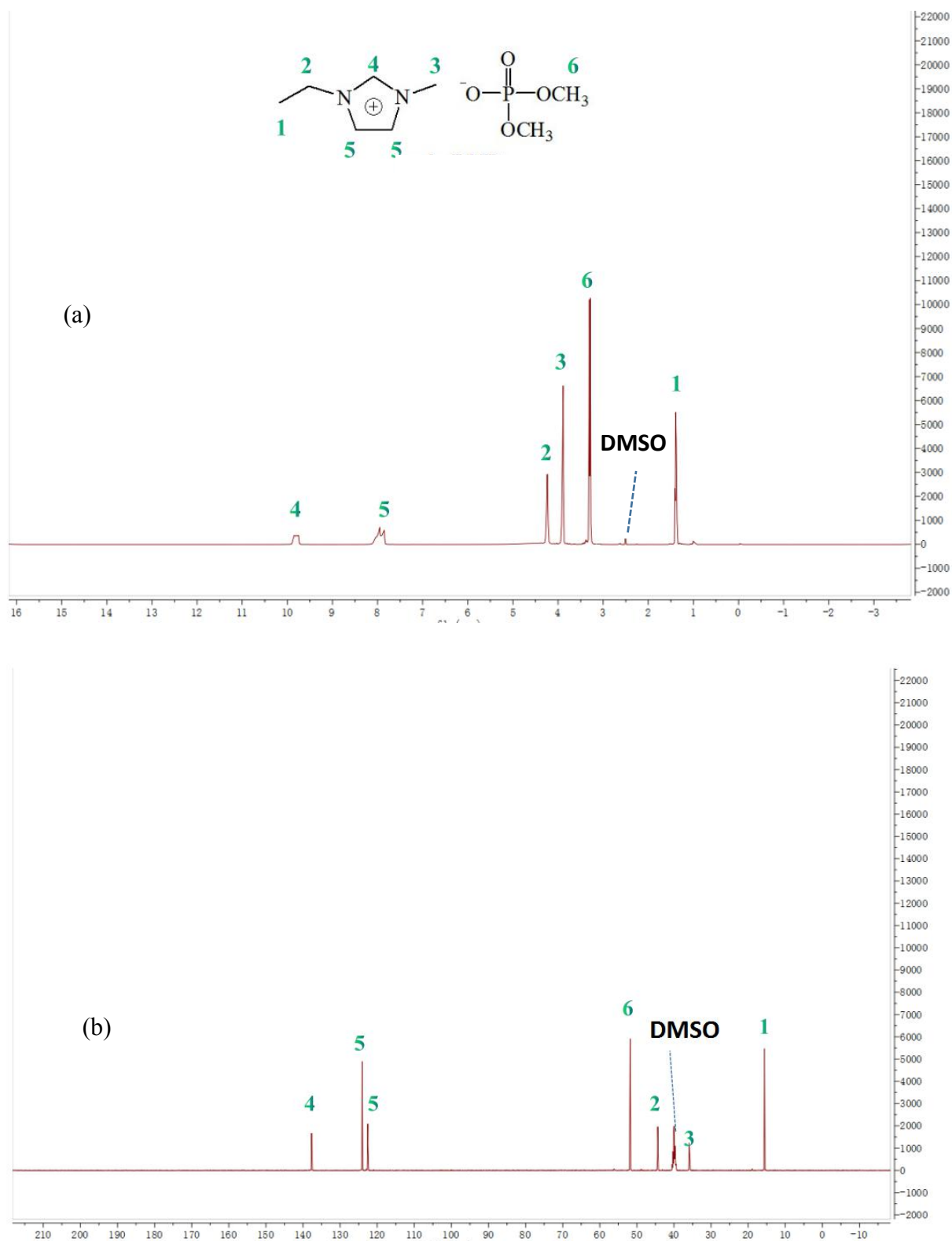


Figure S3 NMR spectra for [C₂C₁im][DMP] (1-ethyl-3-methylimidazolium dimethylphosphate) in DMSO-d₆ with tetramethylsilane (TMS) as the internal standard: (a) ¹H NMR and (b) ¹³C NMR.

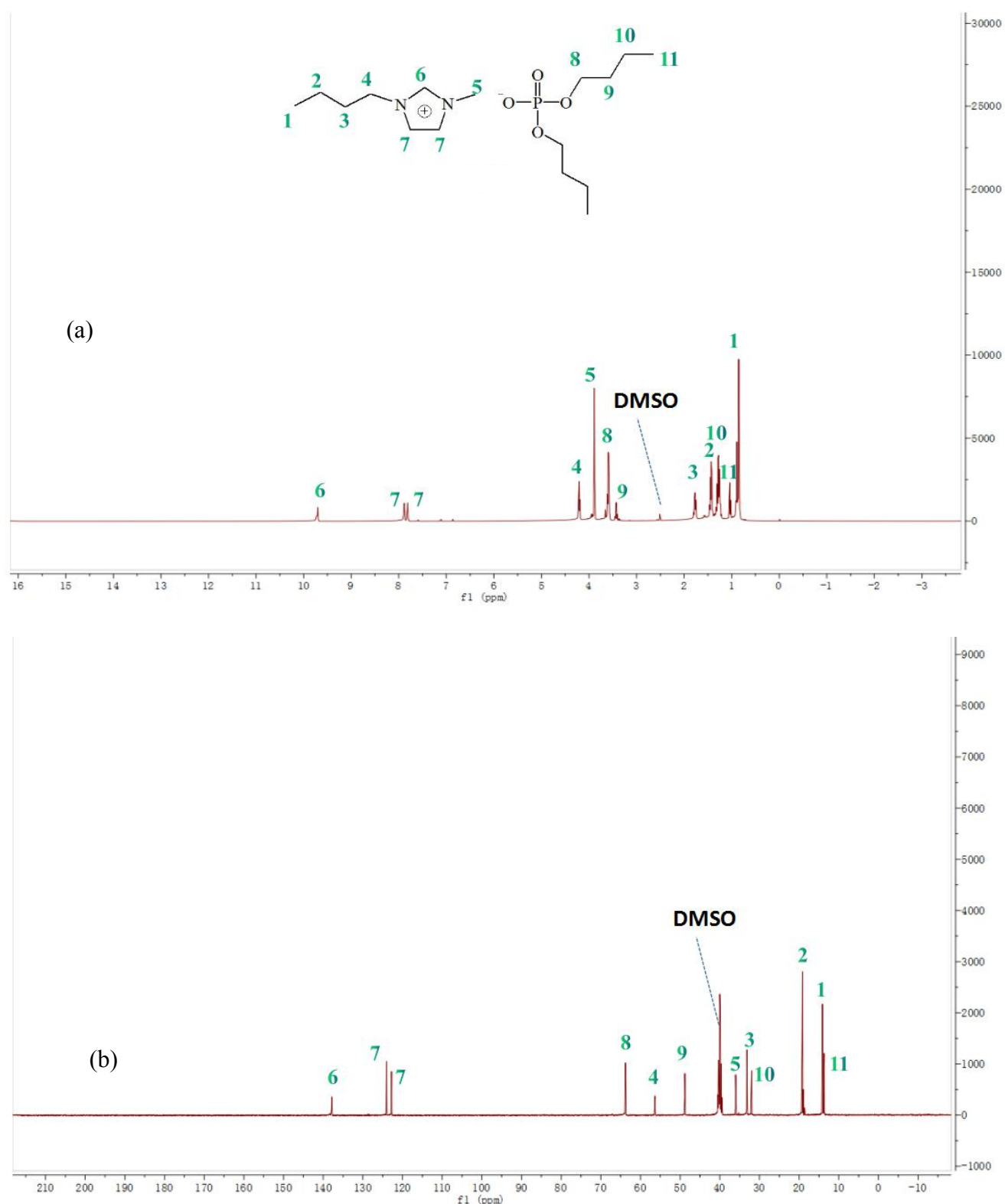


Figure S4 NMR spectra for [C₄C₁im][DBP] (1-butyl-3-methylimidazolium dibutylphosphate) in DMSO-d₆ with tetramethylsilane (TMS) as the internal standard: (a) ¹H NMR and (b) ¹³C NMR.

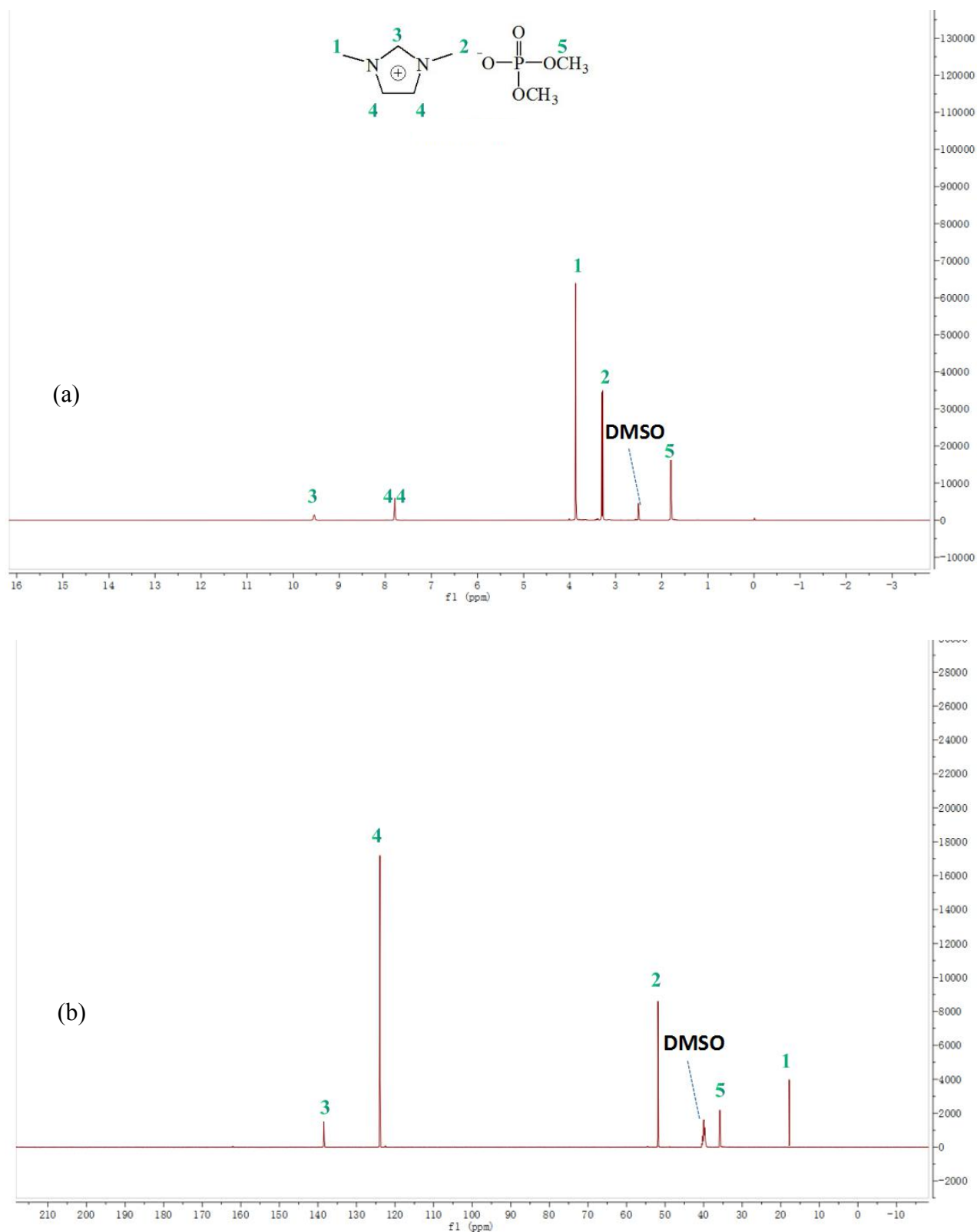


Figure S5 NMR spectra for $[C_1C_1im][DMP]$ (1,3-dimethylimidazolium dimethylphosphate) in $DMSO-d_6$ with tetramethylsilane (TMS) as the internal standard: (a) 1H NMR and (b) ^{13}C NMR.

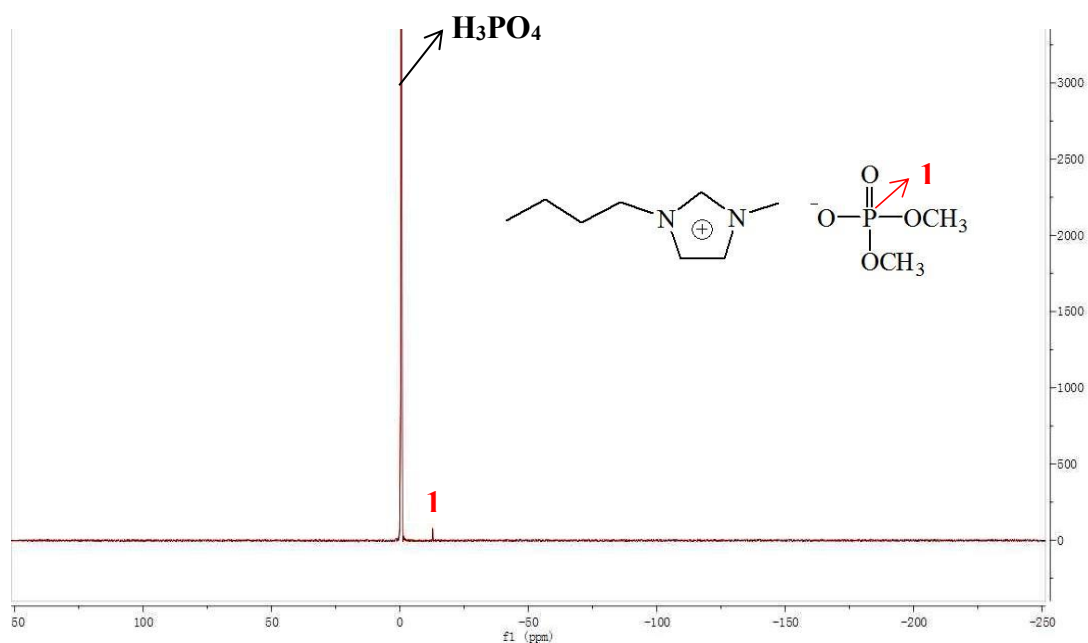


Figure S6 ^{31}P NMR spectra for $[\text{C}_4\text{C}_1\text{im}][\text{DMP}]$ (1-butyl-3-methylimidazolium dimethylphosphate) in phosphoric acid as the internal standard.

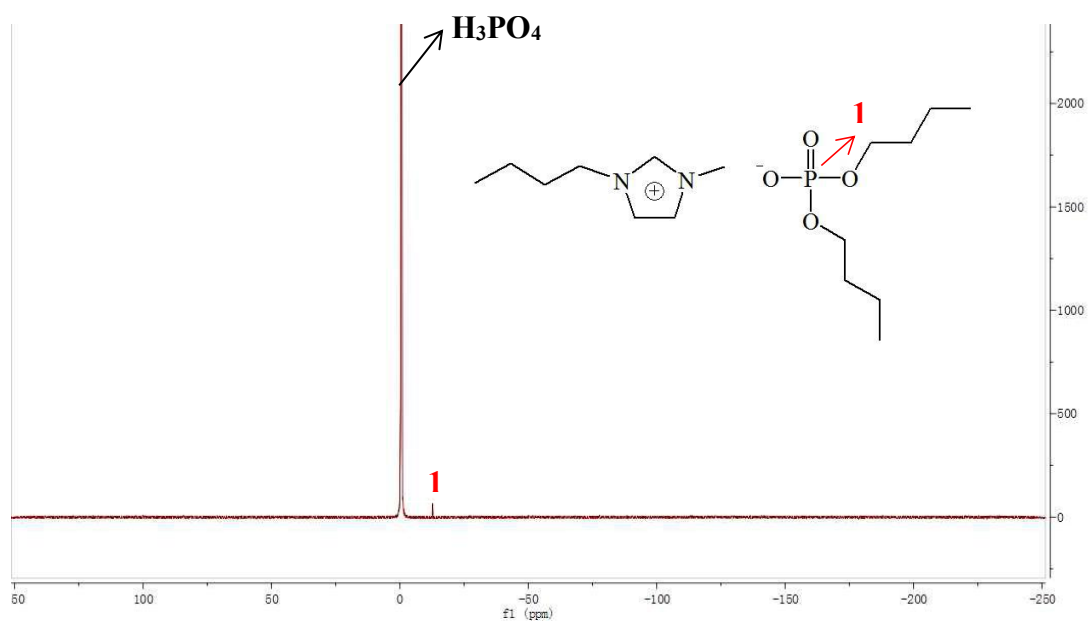


Figure S7 ^{31}P NMR spectra for $[\text{C}_4\text{C}_1\text{im}][\text{DBP}]$ (1-butyl-3-methylimidazolium dibutylphosphate) in phosphoric acid as the internal standard.

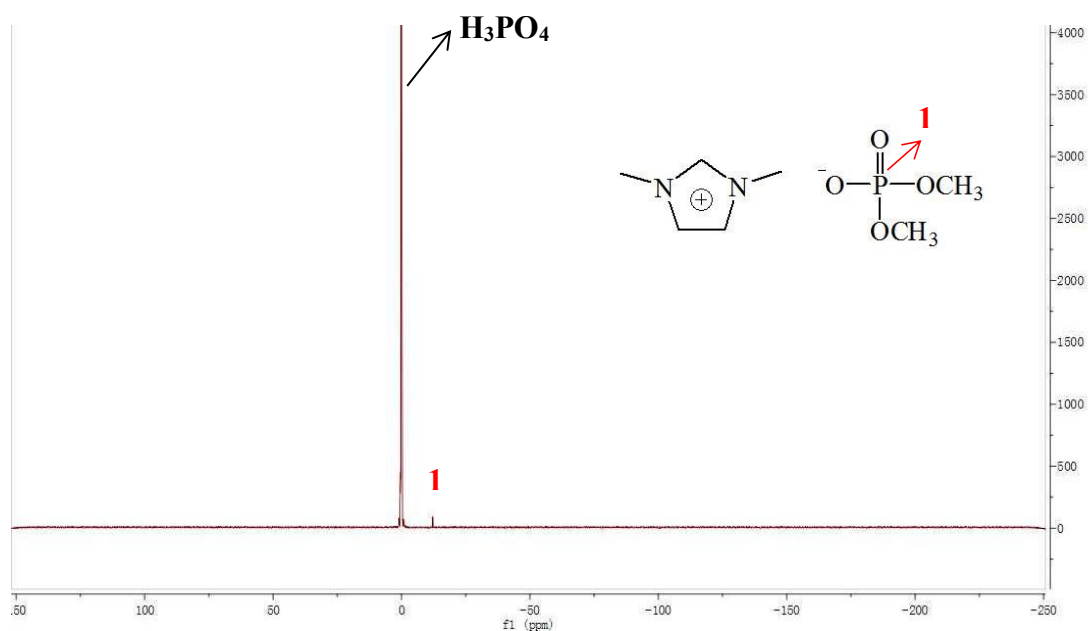


Figure S8 ^{31}P NMR spectra for $[\text{C}_1\text{C}_1\text{im}][\text{DMP}]$ (1,3-dimethylimidazolium dimethylphosphate) in phosphoric acid as the internal standard.

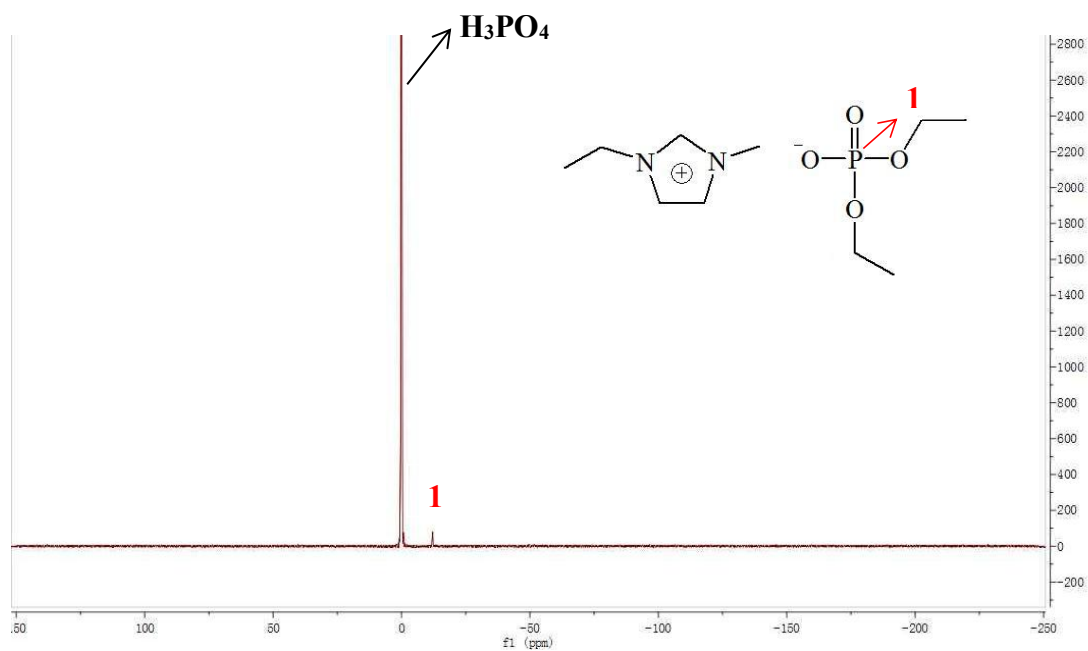


Figure S9 ^{31}P NMR spectra for $[\text{C}_2\text{C}_1\text{im}][\text{DEP}]$ (1-ethyl-3-methylimidazolium diethylphosphate) in phosphoric acid as the internal standard.

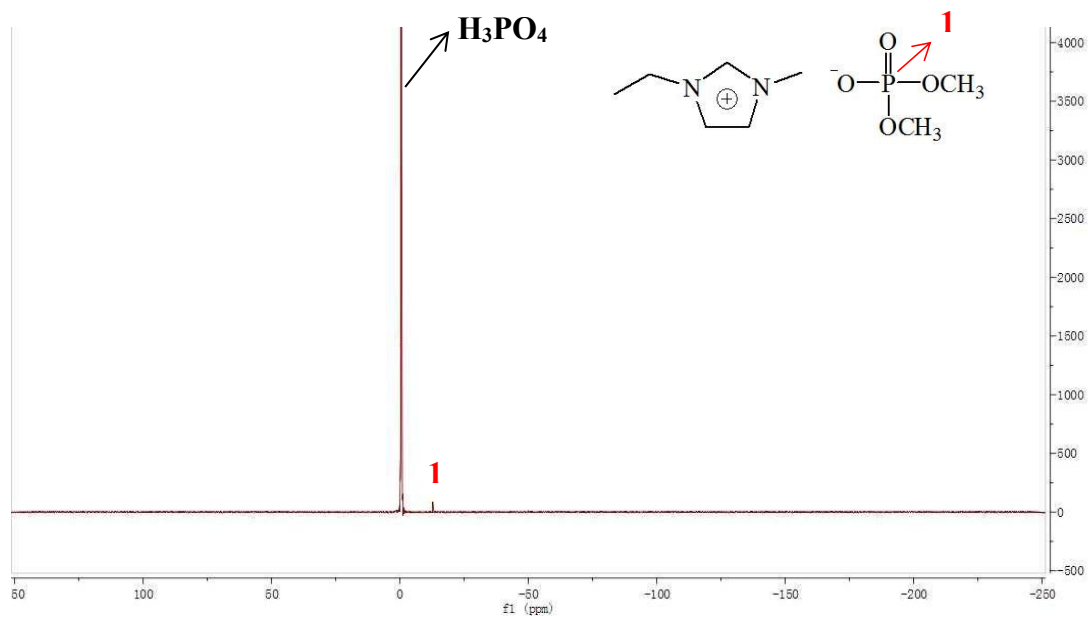


Figure S10 ^{31}P NMR spectra for $[\text{C}_2\text{C}_1\text{im}][\text{DMP}]$ (1-ethyl-3-methylimidazolium dimethylphosphate) in phosphoric acid as the internal standard.

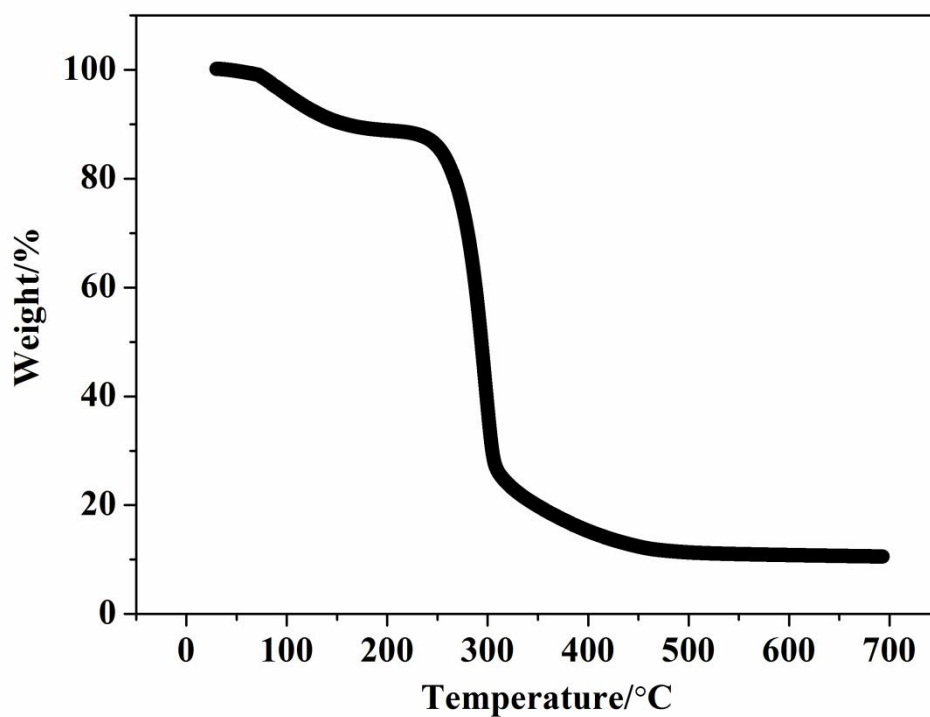


Figure S11. Scanning TGA results for $[\text{C}_4\text{C}_1\text{im}][\text{DBP}]$ from room temperature with a $10\text{ }^\circ\text{C}/\text{min}$ temperature ramping rate to $700\text{ }^\circ\text{C}$.

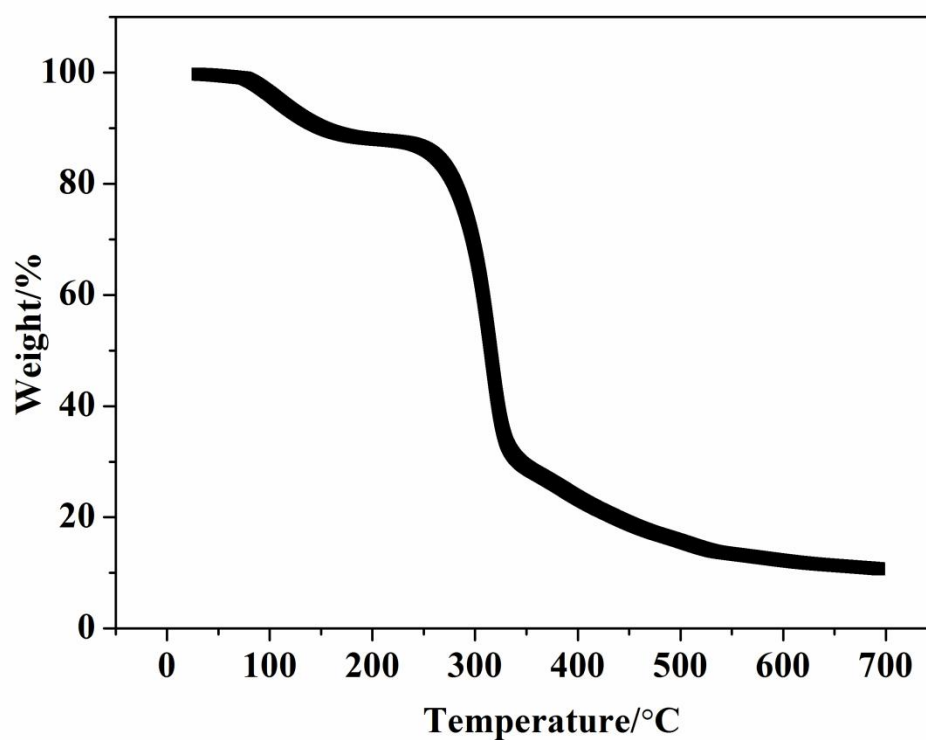


Figure S12. Scanning TGA results for [C₄C₁im][DMP] from room temperature with a 10 °C/min temperature ramping rate to 700 °C.

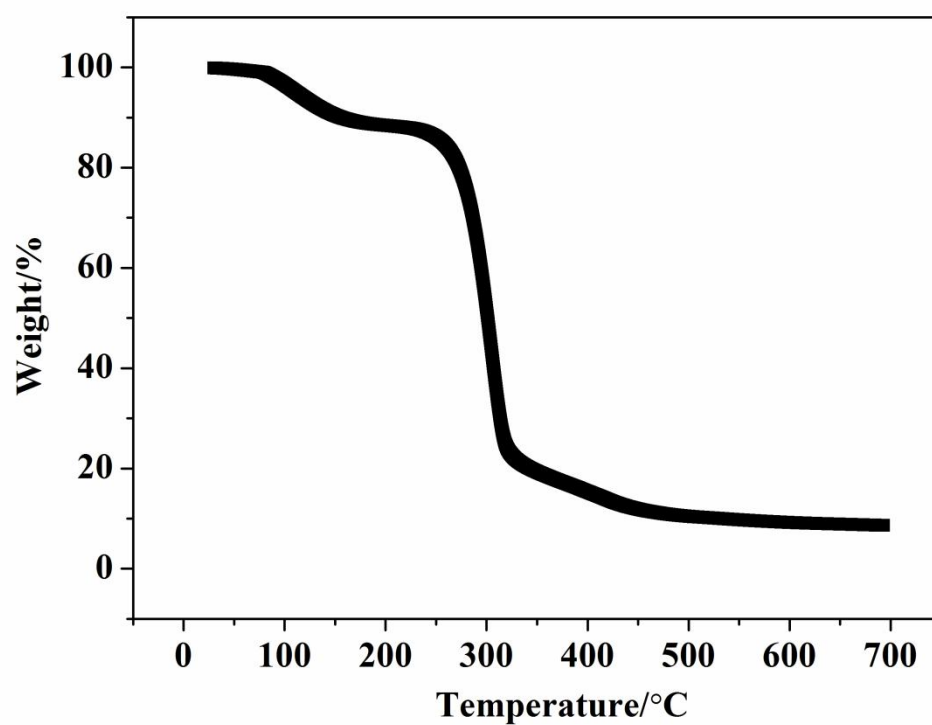


Figure S13. Scanning TGA results for [C₂C₁im][DEP] from room temperature with a 10 °C/min temperature ramping rate to 700 °C.

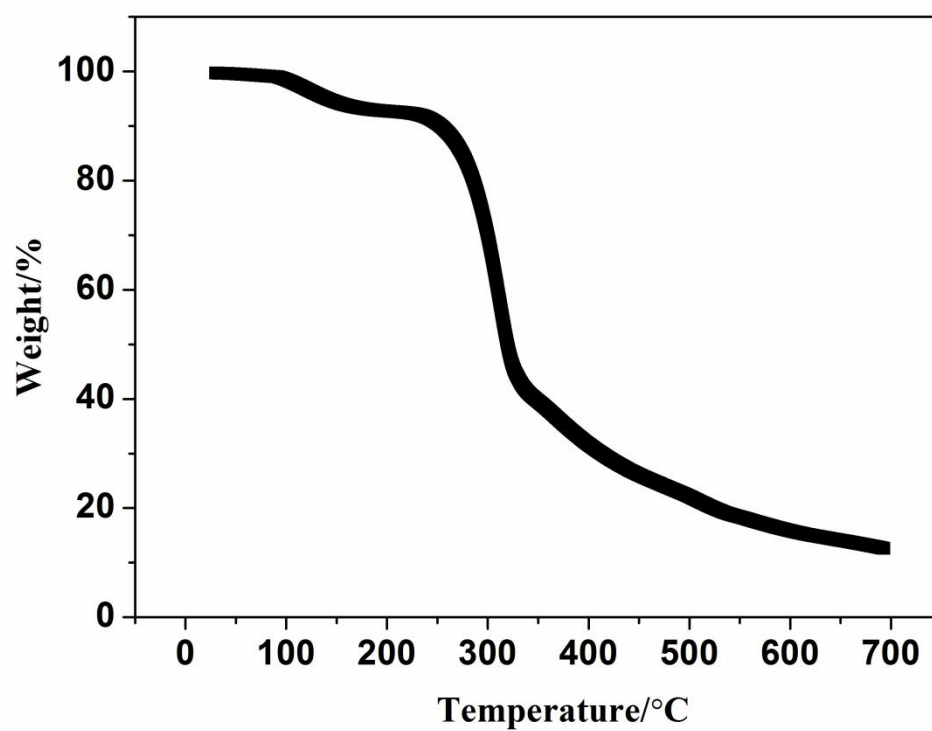


Figure S14. Scanning TGA results for [C₂C₁im][DMP] from room temperature with a 10 °C/min temperature ramping rate to 700 °C.

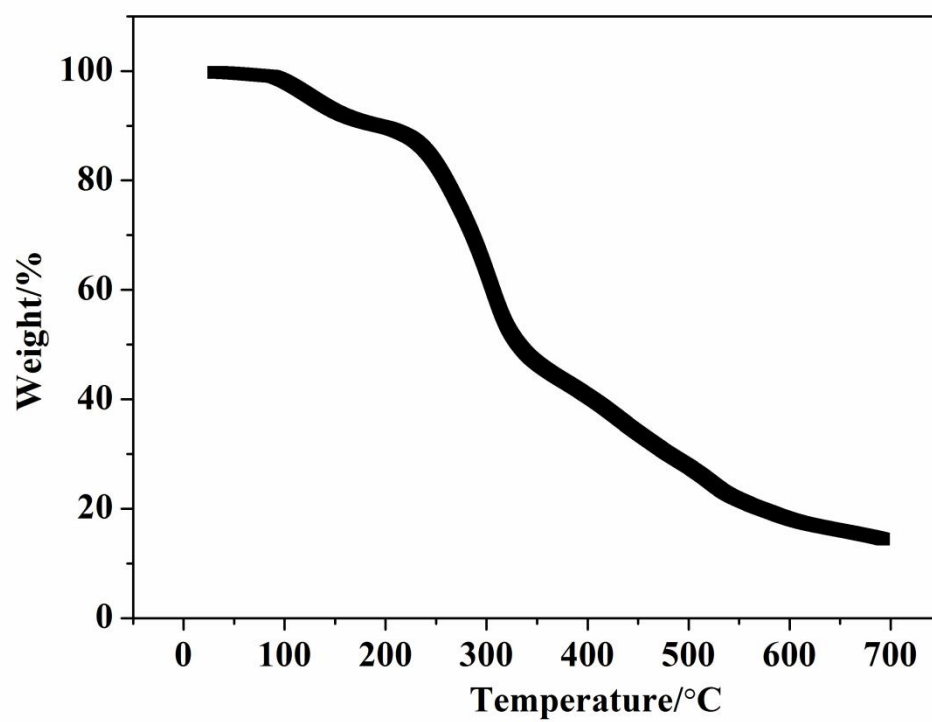


Figure S15. Scanning TGA results for [C₁C₁im][DMP] from room temperature with a 10 °C/min temperature ramping rate to 700 °C.

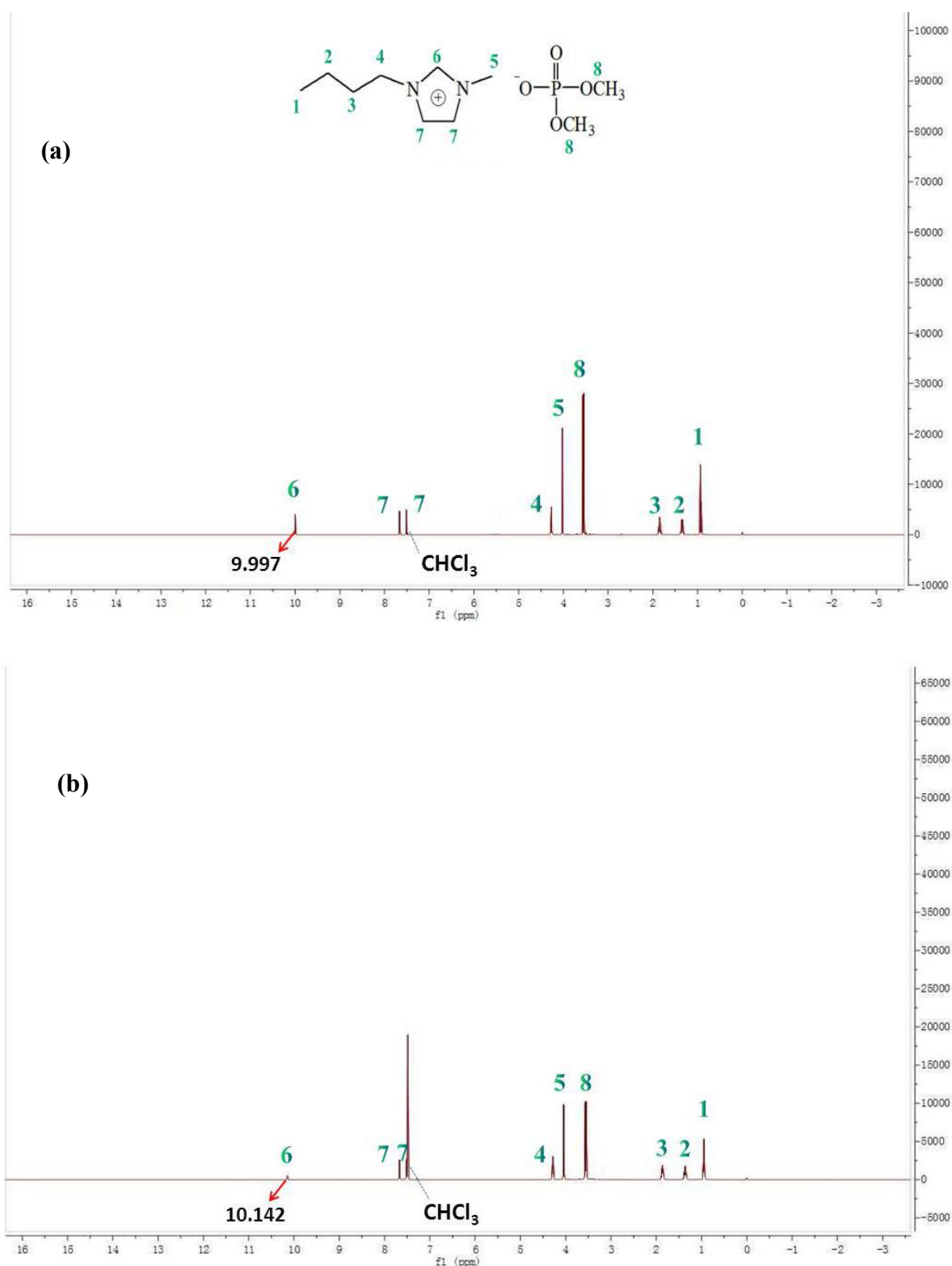


Figure S16 ^1H NMR spectra for $[\text{C}_4\text{C}_{1\text{im}}][\text{DMP}]$ (1-butyl-3-methylimidazolium dimethylphosphate) in CDCl_3 with tetramethylsilane (TMS) as the internal standard: (a) fresh ionic liquid; (b) ionic liquid+ NH_3 .

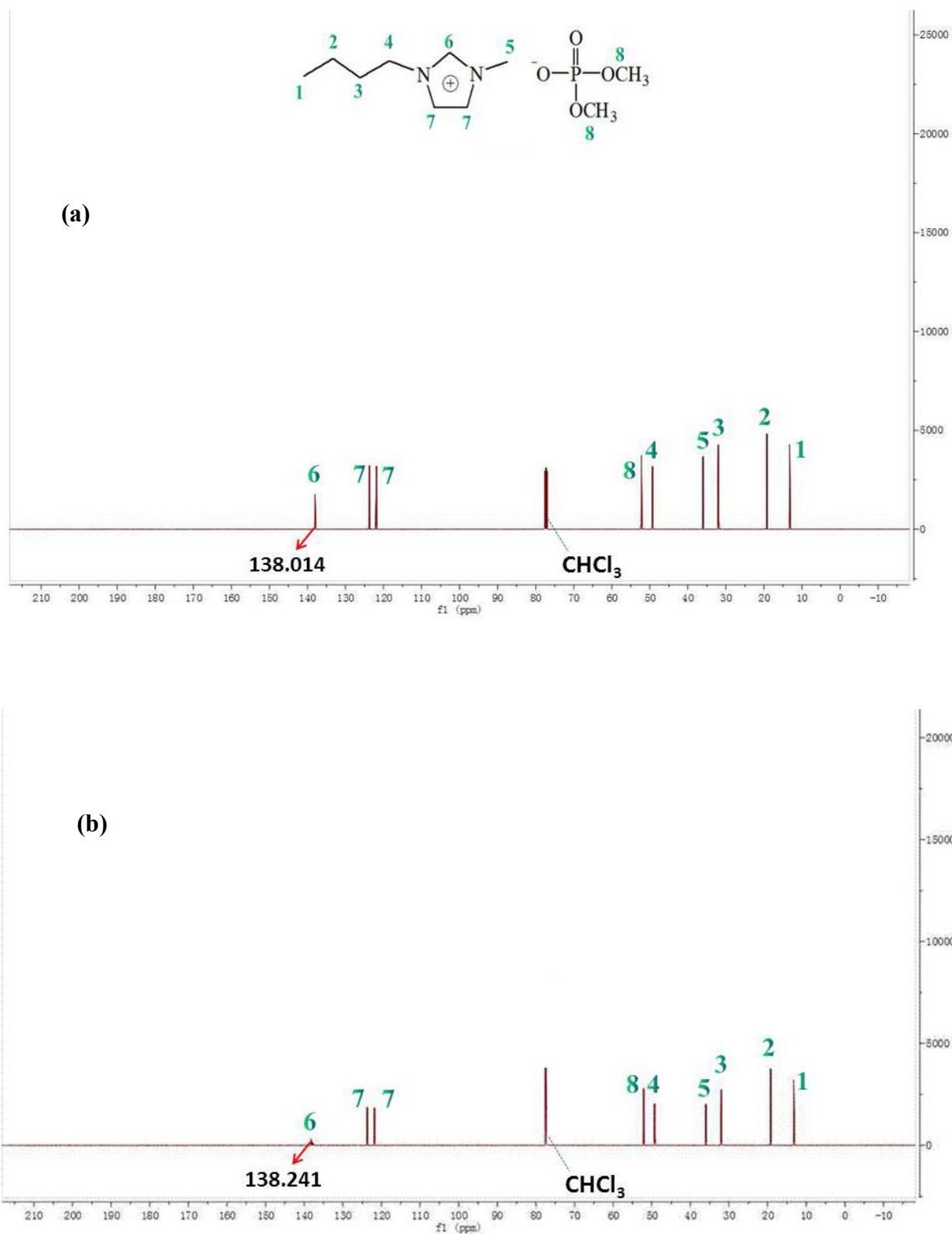


Figure S17 ^{13}C NMR spectra for $[\text{C}_4\text{C}_1\text{im}][\text{DMP}]$ (1-butyl-3-methylimidazolium dimethylphosphate) in CDCl_3 with tetramethylsilane (TMS) as the internal standard: (a) fresh ionic liquid; (b) ionic liquid+ NH_3 .

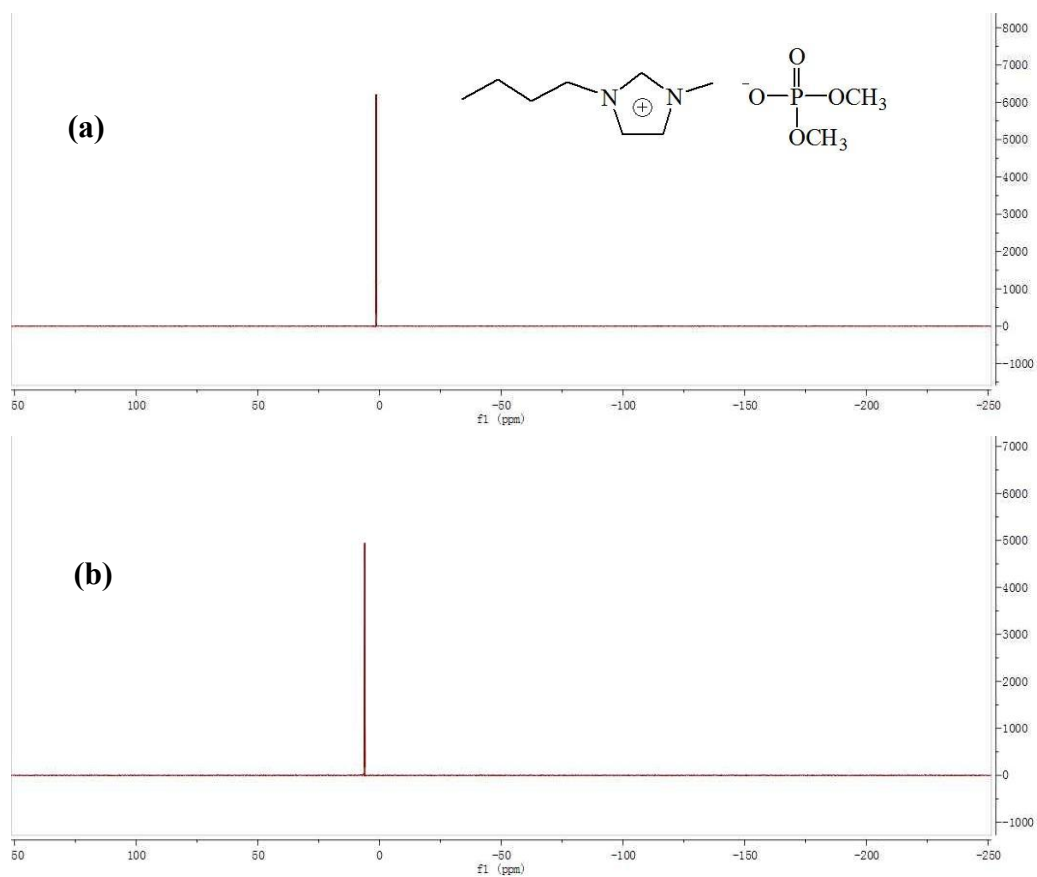


Figure S18 ^{31}P NMR spectra for [C₄C₁im][DMP] (1-butyl-3-methylimidazolium dimethylphosphate): (a) fresh ionic liquid; (b) ionic liquid+NH₃.

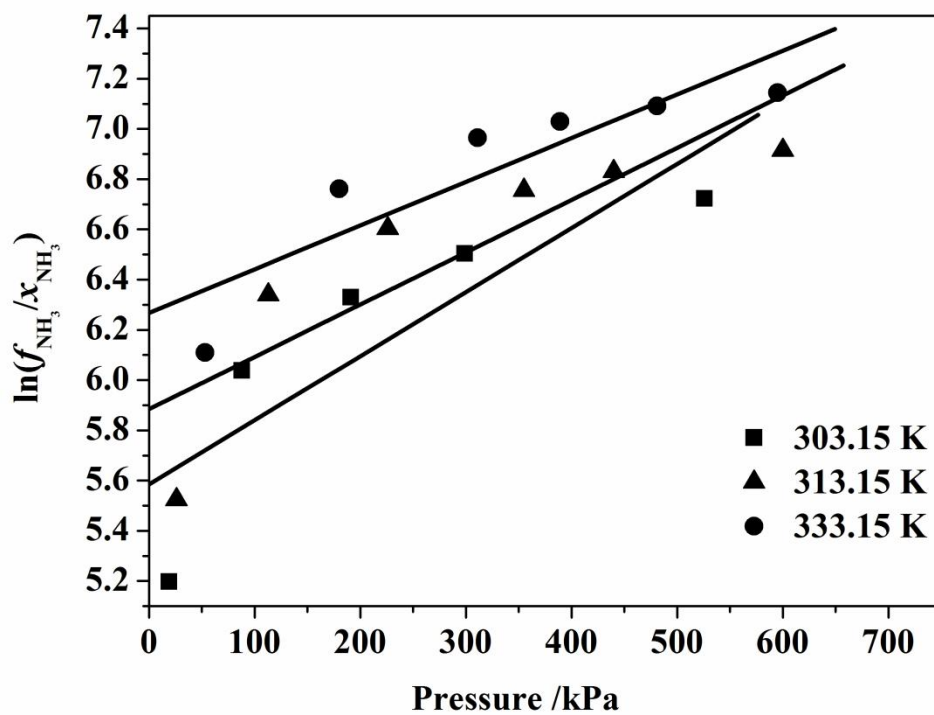


Figure S19 K-K equation analysis of the solubilities of NH_3 in $[\text{C}_4\text{C}_{1\text{im}}][\text{DMP}]$

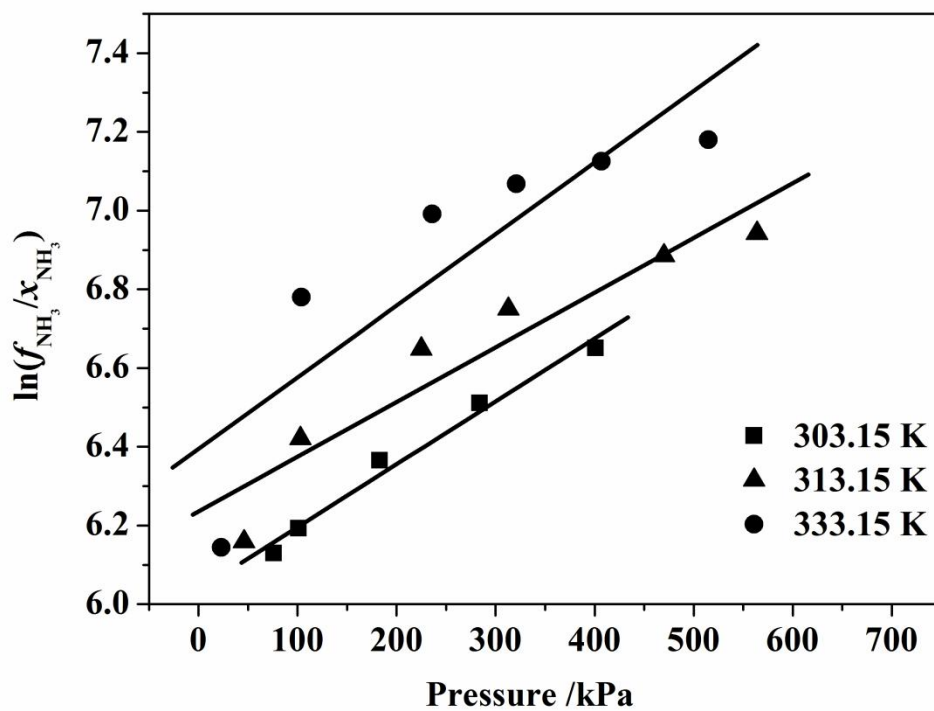


Figure S20 K-K equation analysis of the solubilities of NH_3 in $[\text{C}_2\text{C}_{1\text{im}}][\text{DEP}]$

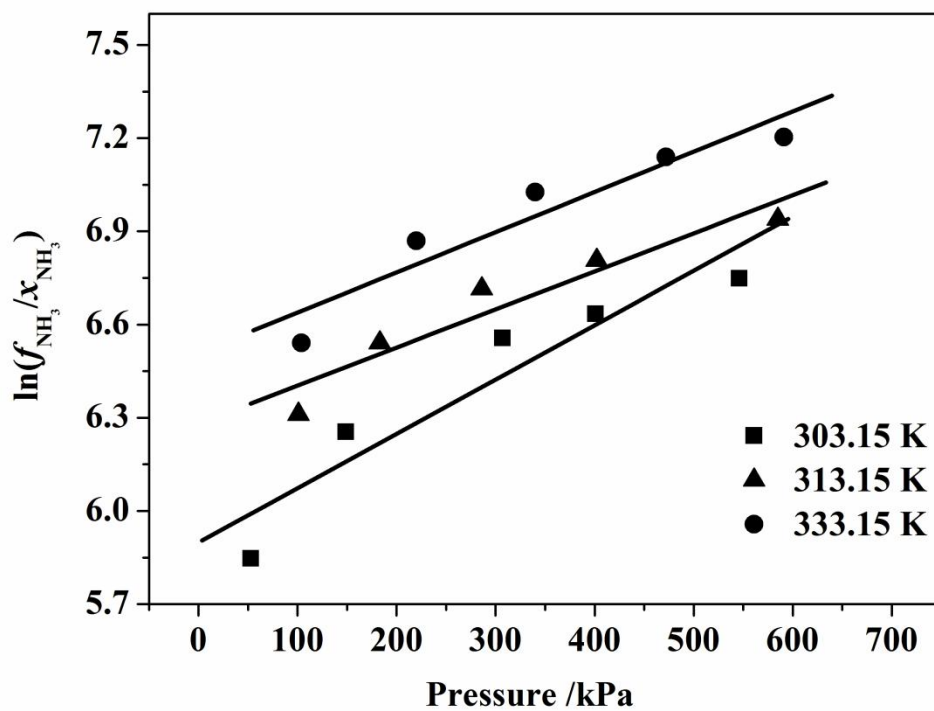


Figure S21 K-K equation analysis of the solubilities of NH_3 in $[\text{C}_2\text{C}_{1\text{im}}][\text{DMP}]$

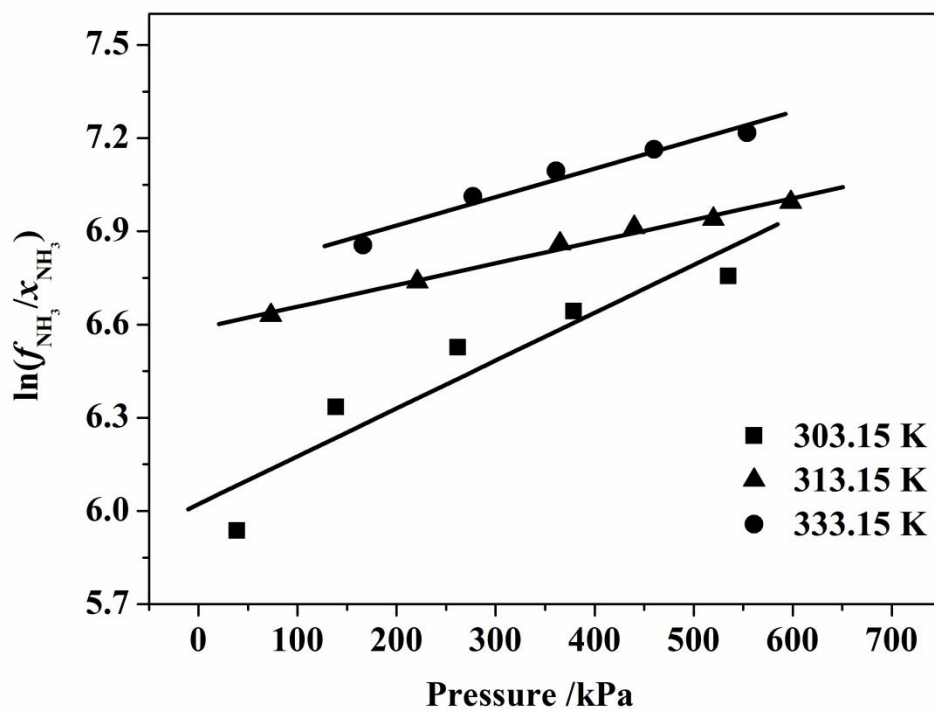


Figure S22 K-K equation analysis of the solubilities of NH_3 in $[\text{C}_1\text{C}_1\text{im}][\text{DMP}]$

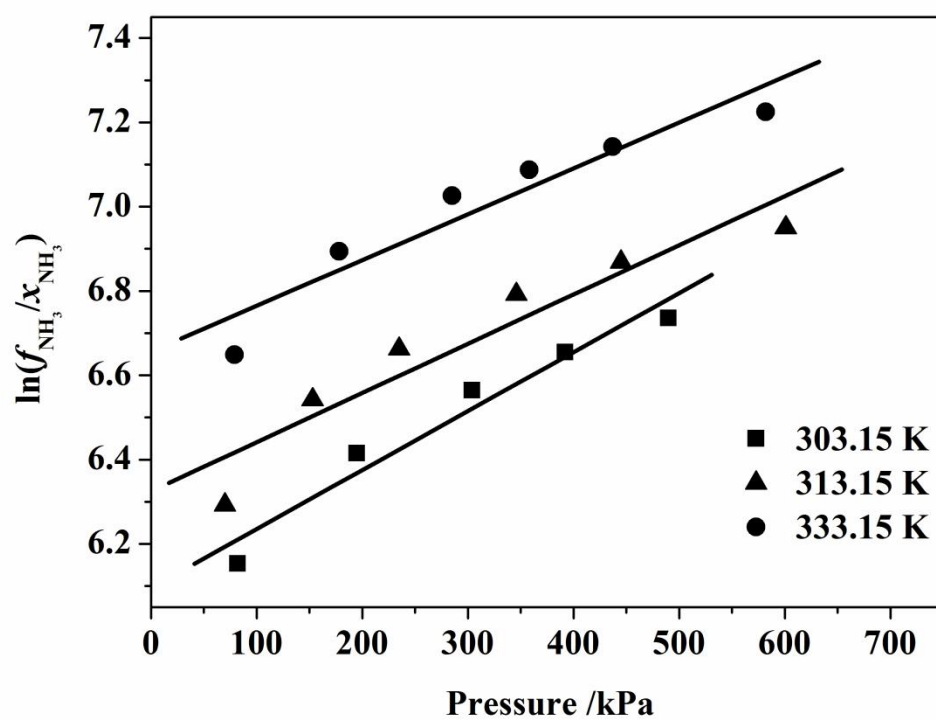


Figure S23 K-K equation analysis of the solubilities of NH_3 in $[\text{C}_4\text{C}_{1\text{im}}][\text{DBP}]$

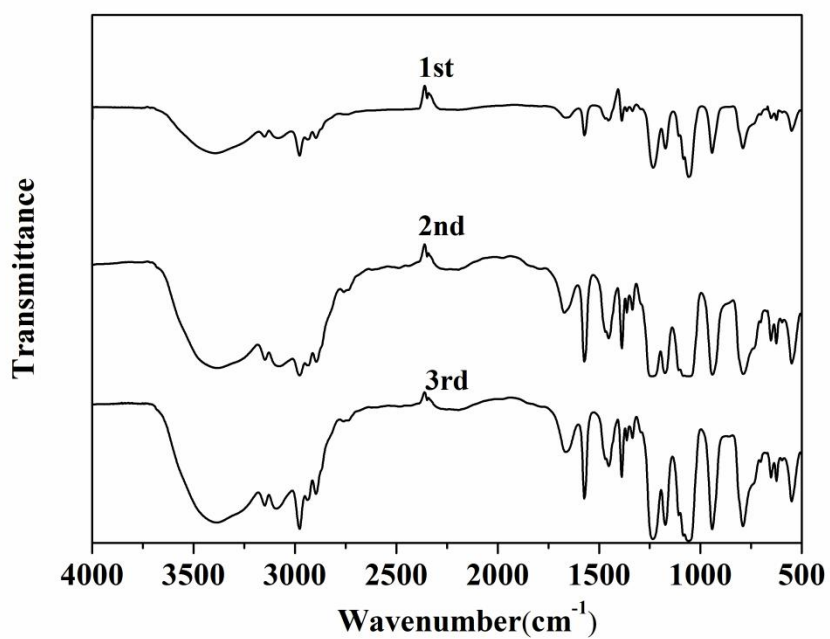


Figure S24 FT-IR spectra of three consecutive cycles of NH_3 absorption and desorption in $[\text{C}_2\text{C}_1\text{im}][\text{DEP}]$

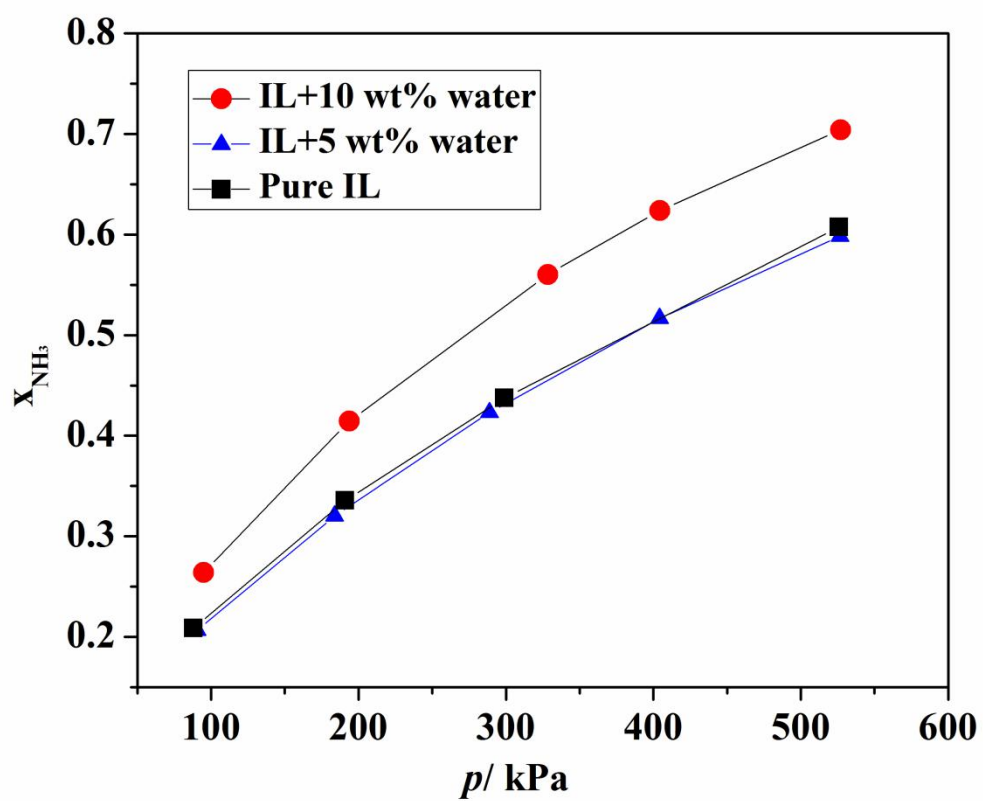


Figure S25 The effect of water on NH_3 absorption in $[\text{C}_4\text{C}_{1\text{im}}][\text{DMP}]$ at 303.15 K