

Supplementary Information

Improving SO₂ Capture by Tuning Functional Groups on the Cation of Pyridinium-based Ionic Liquids

Shaojuan Zeng,^{a,b} Hongyan He,^a Hongshuai Gao,^a Xiangping Zhang,^{*,a} Jian Wang,^{a,b} Ying

Huang,^{a,b} Suojiang Zhang^{*,a}

^aBeijing Key Laboratory of Ionic Liquids Clean Process, Key Laboratory of Green Process and Engineering, State Key Laboratory of Multiphase Complex Systems, Institute of Process Engineering, Chinese Academy of Sciences, Beijing, 100190, China

^bCollege of Chemical and Engineering, University of Chinese Academy of Sciences, Beijing 100049, China

*Email: sjzhang@home.ipe.ac.cn; xpzhang@home.ipe.ac.cn

1. NMR data of the pyridinium-based ILs

[NEt₂C₂Py][SCN]: ¹H NMR(d₆-DMSO) : 0.73 (t, 3H), 2.44 (m, 2H), 2.86 (m, 2H), 4.65 (t, 2H), 8.15 (t, 2H), 8.61 (t, 1H), 9.00 (d, 2H); ¹³C NMR(d₆-DMSO) : 145.86, 145.60, 130.31, 127.76, 59.52, 53.01, 46.70, 12.12.

After the absorption of SO₂: ¹H NMR(d₆-DMSO) : 0.83(t, 3H), 2.58(m, 2H), 2.99(m, 2H), 4.70(t, 2H), 8.17(t, 2H), 8.61(t, 1H), 9.01(d, 2H); ¹³C NMR(d₆-DMSO) : 146.02, 145.69, 129.27, 127.92, 58.72, 52.53, 46.67, 11.56.

[C₄OPy][SCN]: ¹H NMR(CDCl₃) : 1.12 (t, 3H), 3.52 (m, 2H), 4.00 (m, 2H), 5.04 (t, 2H), 8.20 (t, 2H), 8.67 (t, 1H), 9.16 (d, 2H); ¹³C NMR(CDCl₃) : 145.92, 145.28, 131.67, 128.27, 77.39, 68.26, 66.88, 14.92.

After the absorption of SO₂: ¹H NMR(CDCl₃) : 1.12 (t, 3H), 3.51 (m, 2H), 3.98 (m, 2H), 4.96 (t, 2H), 8.17 (t, 2H), 8.63 (t, 1H), 9.04 (d, 2H); ¹³C NMR(CDCl₃) : 145.92, 145.16, 129.26, 128.30, 77.34, 68.19, 66.86, 14.88.

[C₄CNPy][SCN]: ¹H NMR(d₆-DMSO) : 1.66 (t, 3H), 2.09 (m, 2H), 2.63 (m, 2H), 4.73 (t, 2H), 8.23 (t, 2H), 8.67 (t, 1H), 9.16 (d, 2H); ¹³C NMR(d₆-DMSO) : 145.55, 144.69, 129.76, 128.17, 120.28, 59.96, 29.76, 21.54, 15.83.

After the absorption of SO₂: ¹H NMR(d₆-DMSO) : 1.65 (t, 3H), 2.08 (m, 2H), 2.58 (m, 2H), 4.71 (t, 2H), 8.21 (t, 2H), 8.66 (t, 1H), 9.13 (d, 2H); ¹³C NMR(d₆-DMSO) : 145.55, 144.68, 129.67, 128.17, 120.28, 59.84, 29.75, 21.52, 15.81.

2. Densities and viscosities of the ILs at different temperatures

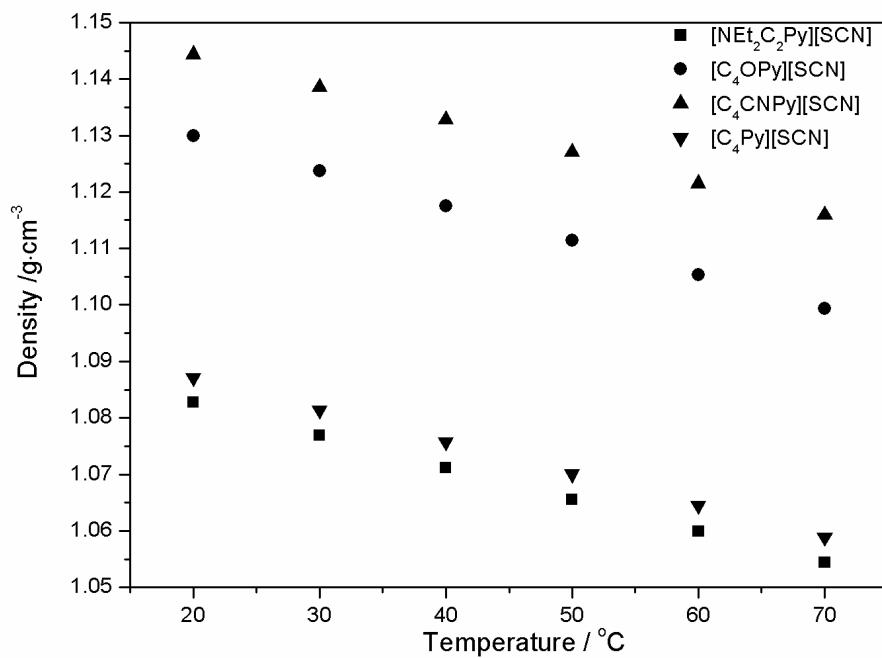


Fig.S1 Variation in the densities of pyridinium-based ILs with temperature

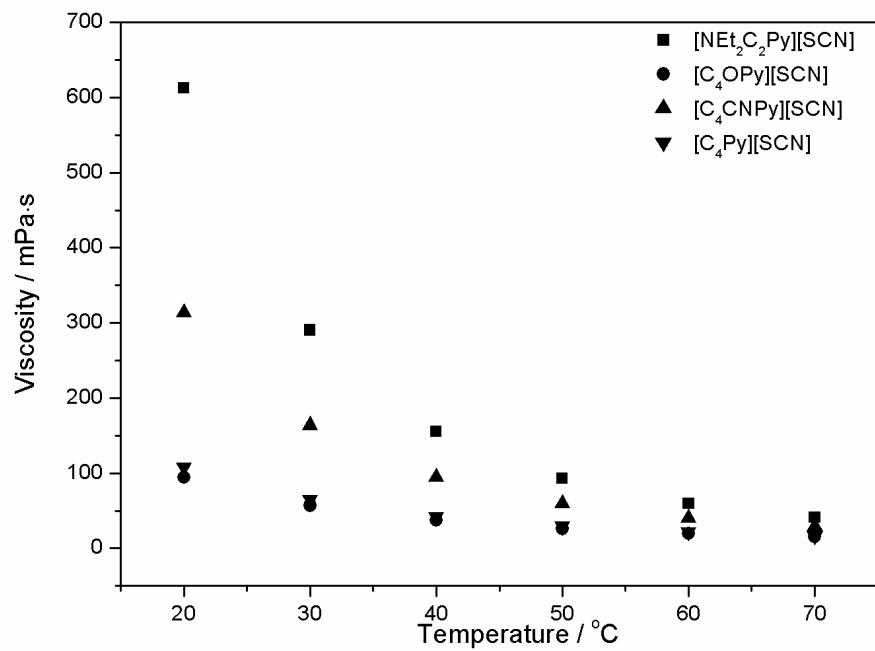


Fig.S2 Variation in the viscosities of pyridinium-based ILs with temperature

3. TGA results for the pyridinium-based ILs

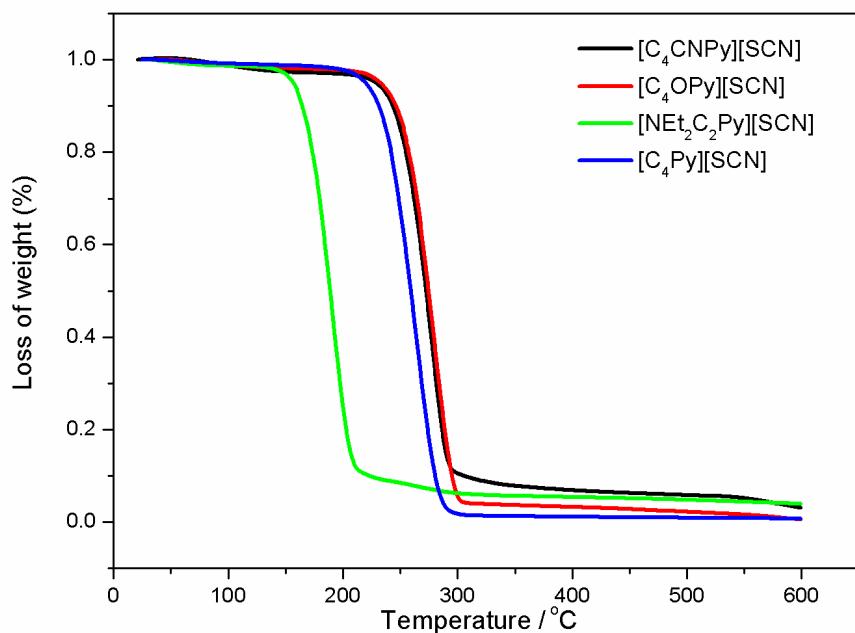


Fig.S3 TGA results for the pyridinium-based ILs with a $10^{\circ}\text{C min}^{-1}$ temperature heating rate to 600°C under N_2 atmosphere

4. Effect of water on SO_2 absorption for $[\text{C}_4\text{OPy}][\text{SCN}]$

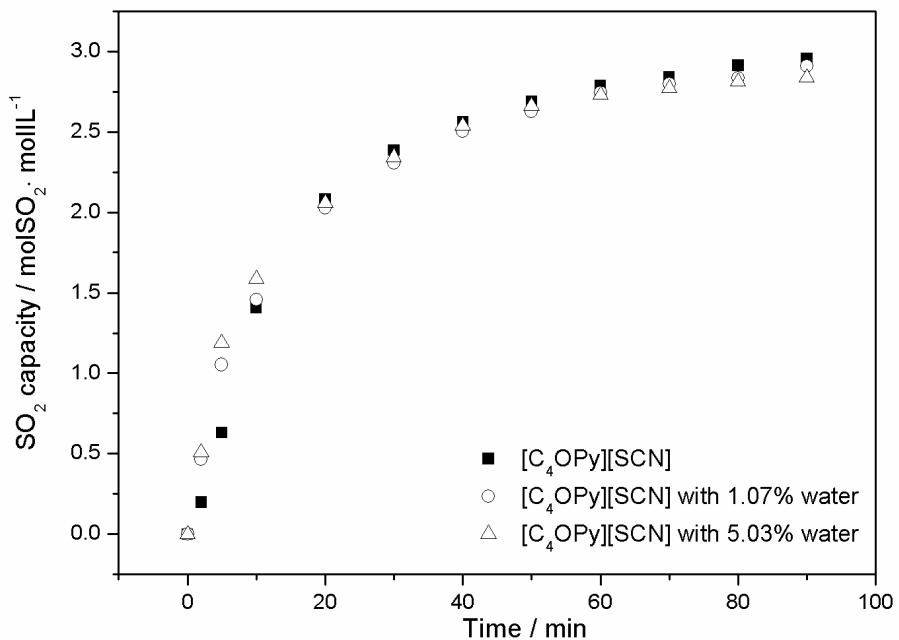


Fig.S4 Effect of water on the SO₂ absorption capacity by [C₄OPy][SCN] at 20°C and 0.1 MPa

5. FTIR and NMR spectra of the pyridinium-based ILs

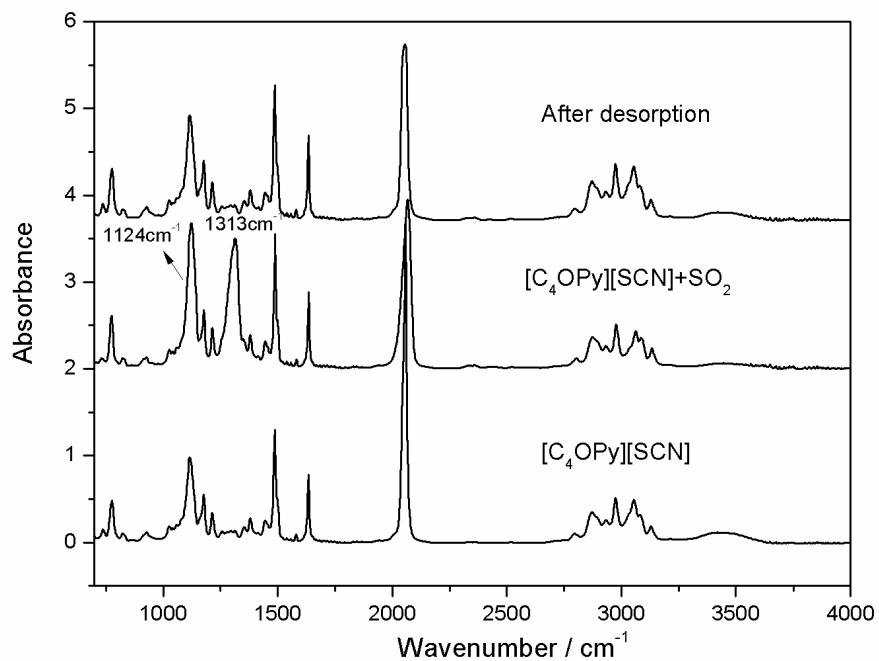


Fig.S5 FT-IR spectra of [C₄OPy][SCN] before and after SO₂ absorption and after SO₂ desorption

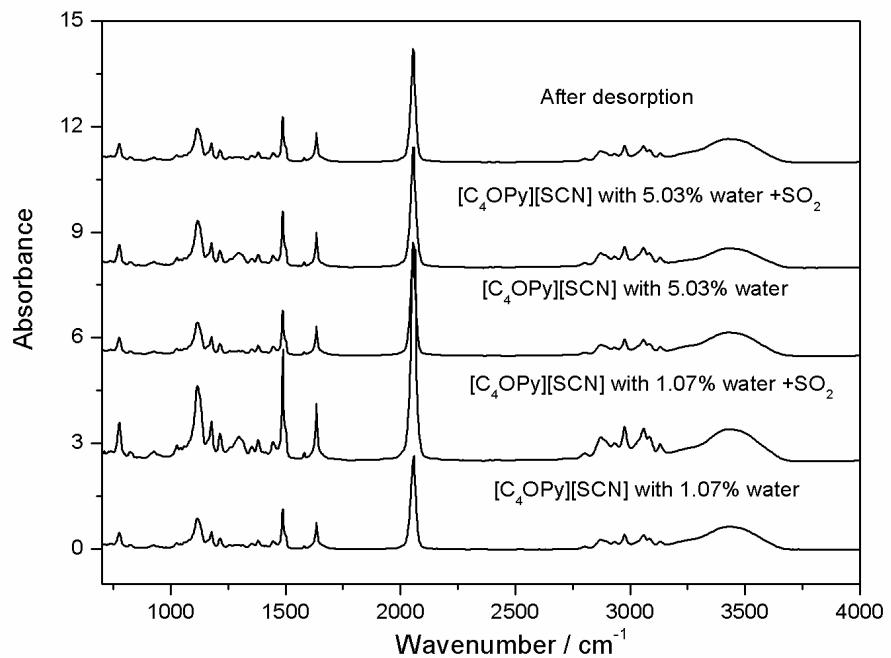
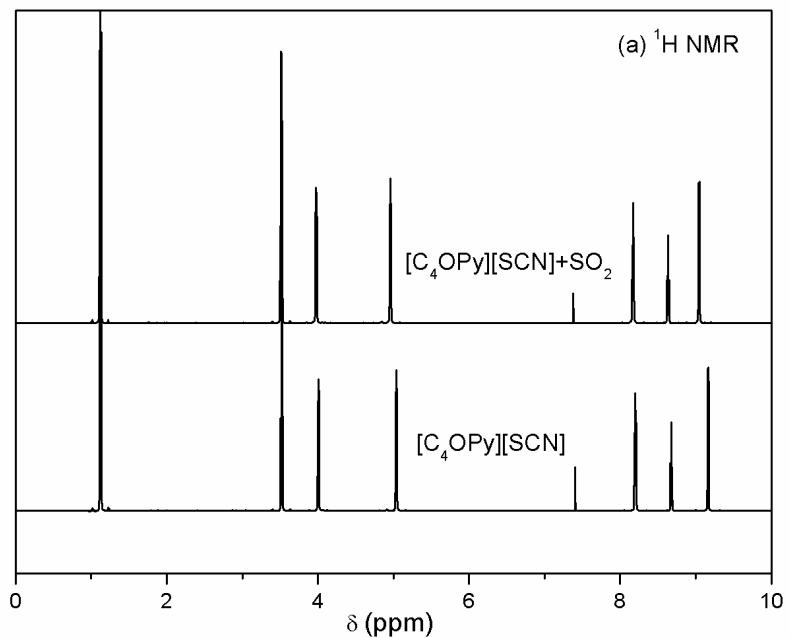


Fig.S6 FT-IR spectra of [C₄OPy][SCN] with water before and after absorption of SO₂ and after desorption



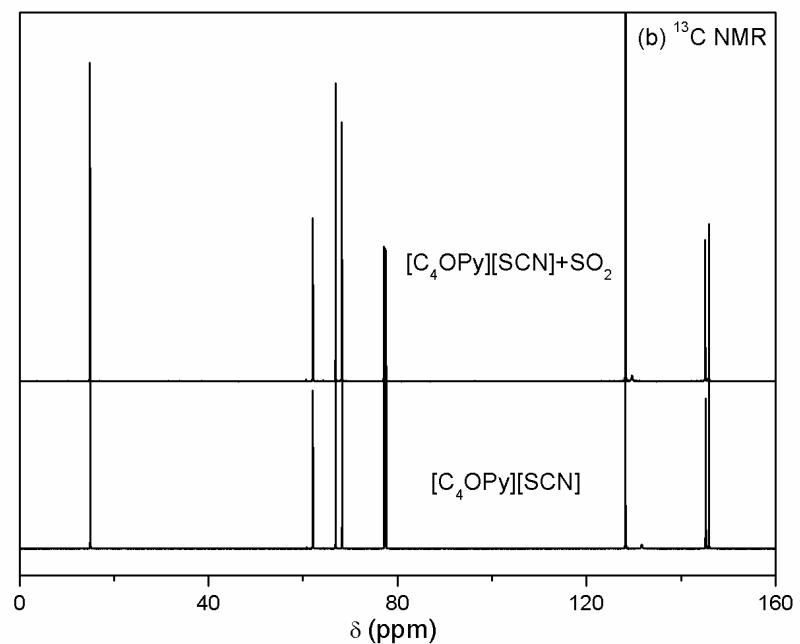


Fig.S7 ^1H NMR (a) and ^{13}C NMR (b) spectra of $[\text{C}_4\text{OPy}][\text{SCN}]$ before and after SO_2 absorption