Electronic Supplementary Information

Oxidation of Sulfides to Sulfoxides Mediated by Ionic Liquids

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E1. Characterization data of sulfoxides

Methyl phenyl sulfoxide: pale yellow oil. M.p.: 30℃, [1] found 28-30℃. IR(cm^{-1}): 1032vs (SO). ^{1}H NMR ($CDCl_3$, 400Hz, r.t. ppm): 2.60 (3H, s, Me), 7.39 (5H, m, Ph), 7.53 (2H, m, Ph). ^{13}C NMR ($CDCl_3$, 100Hz, r.t. ppm): δ = 43.75, 123.29, 129.17, 130.81, 145.62.

Ethyl phenyl sulfoxide: yellow oil. B.p.: 284℃,[2] found 285-287℃. IR(cm^{-1}): 1018vs (SO) . ^{1}H NMR ($CDCl_3$, 400Hz, r.t. ppm): δ = 1.05 (3H, t, Me), 2.73 (2H, m, CH_2), 7.37 (3H, m, Ph), 7.48 (2H, m, Ph). ^{13}C NMR ($CDCl_3$, 100Hz, r.t. ppm): δ = 6.06, 50.49, 124.38, 129.33, 131.08, 143.78.

Diphenyl sulfoxide: white crystal. M.p.:70℃,[3] found 70-72℃. IR(cm^{-1}): 1034vs (SO). ^{1}H NMR ($CDCl_3$, 400Hz, r.t. ppm): δ = 7.38 (6H, m, Ph), 7.57 (4H, m, Ph). ^{13}C NMR($CDCl_3$, 100Hz, r.t. ppm): δ = 123.80, 128.31, 130.02, 144.69.

Dibutyl sulfoxide: white solid. M.p.:31℃,[3] found 31-33℃.IR(cm^{-1}): 1023vs (SO). ^{1}H NMR ($CDCl_3$, 400Hz, r.t. ppm): δ = 0.99 (6H, t, Me), 1.49 (4H, m, CH_2), 1.85 (4H, m, CH_2), 2.97 (4H, m, CH_2). ^{13}C NMR ($CDCl_3$, 100Hz, r.t. ppm): δ = 13.53, 21.78, 23.95, 52.50.

Dimethyl sulfoxide: colorless liquid. B.p.: 189℃,[4] found 190-192℃. IR(cm^{-1}): 1015vs (SO). ^{1}H NMR ($CDCl_3$, 400Hz, r.t. ppm): δ = 2.47 (6H, s, Me). ^{13}C NMR ($CDCl_3$, 100Hz, r.t. ppm): δ = 41.30.

2-(Phenylsulfinyl)ethanol: pale yellow oil. B.p.: 362℃,[5] found 360-363℃. IR(cm^{-1}): 3343s (OH), 1018vs (SO). ^{1}H NMR (DMSO, 100Hz, r.t. ppm): δ = 2.97 (1H, m, CH_2OH), 3.67 (1H, m, CH_2SO), 3.84 (1H, m, CH_2SO), 5.10 (1H, t, OH), 7.54 (3H, m, Ph), 7.62 (2H, m, Ph). ^{13}C NMR (DMSO, 100Hz, r.t. ppm): δ = 54.32, 59.92, 123.78, 129.20, 130.65, 144.66.

Methyl 2-(pheylsulfinyl) acetate: pale yellow oil. B.p.: 341℃, [6] found 342-344℃. IR(cm^{-1}): 1043vs (SO). ^{1}H NMR ($CDCl_3$, 400Hz, r.t. ppm): δ = 3.54 (3H, s, Me), 3.69 (1H, m, CH_2), 7.39 (3H, m, Ph), 7.54-7.56 (2H, m, Ph). ^{13}C NMR ($CDCl_3$, 100Hz, r.t. ppm): δ = 52.63, 61.34, 124.03, 129.37, 131.73, 142.92, 165.17.

Phenyl allyl sulfoxide: yellow oil. B.p.: 297℃,[7] found 297-300℃. IR(cm^{-1}): 1037vs (SO). ^{1}H NMR ($CDCl_3$, 400Hz, r.t. ppm): δ = 3.45 (2H, m, CH_2), 5.11 (1H, d, $CH=CH_2$), 5.24 (1H, d, $SOCH_2$), 5.56 (1H, m, $SOCH_2$), 7.43 (3H, m, Ph), 7.52 (2H, m, Ph). ^{13}C NMR($CDCl_3$, 100Hz, r.t. ppm): δ = 59.76, 122.85, 123.27, 124.19, 128.01, 130.06, 141.85

Methoxymethyl phenyl sulfoxide: yellow oil. B.p.: 296 ℃,[8] found 295-298℃. IR(cm^{-1}):1015. ^{1}H NMR ($CDCl_3$, 400Hz, r.t. ppm): δ = 3.68 (3H, s, OMe), 4.53 (2H, s, $SOCH_2$), 7.60 (2H, m, Ph), 7.66 (1H, m, Ph), 7.95 (2H, m, Ph). ^{13}C NMR($CDCl_3$, 100Hz, r.t. ppm): δ = 61.19, 87.78, 128.74, 129.23, 134.07, 137.39

Phenyl isopropyl sulfoxide: yellow oil. B.p.: 290℃,[9] found 292-294℃. IR(cm^{-1}): 1020vs (SO). ^{1}H NMR ($CDCl_3$, 400Hz, r.t. ppm): δ = 1.05 (3H, d, Me), 1.14 (3H, d, Me), 2.75 (1H, m, SOCH), 7.41-7.44 (3H, m, Ph), 7.51 (2H, m, Ph). ^{13}C NMR ($CDCl_3$, 100Hz, r.t. ppm): δ = 13.82, 15.84, 54.45, 124.91, 128.83, 130.93, 141.68.

Benzyl phenyl sulfoxide: white solid. M.p.:124-126℃,[10] found 123-125℃. IR(cm^{-1}): 1027vs (SO). ^{1}H NMR($CDCl_3$, 400Hz, r.t. ppm): δ = 4.10 (2H, m, $SOCH_2$), 7.02 (2H, m, Ph), 7.35 (3H, m, Ph), 7.46 (5H, m, Ph). ^{13}C NMR ($CDCl_3$, 400Hz, r.t. ppm): δ = 63.57, 124.47, 128.26, 128.46, 128.86, 129.13, 130.37, 131.19, 142.72.

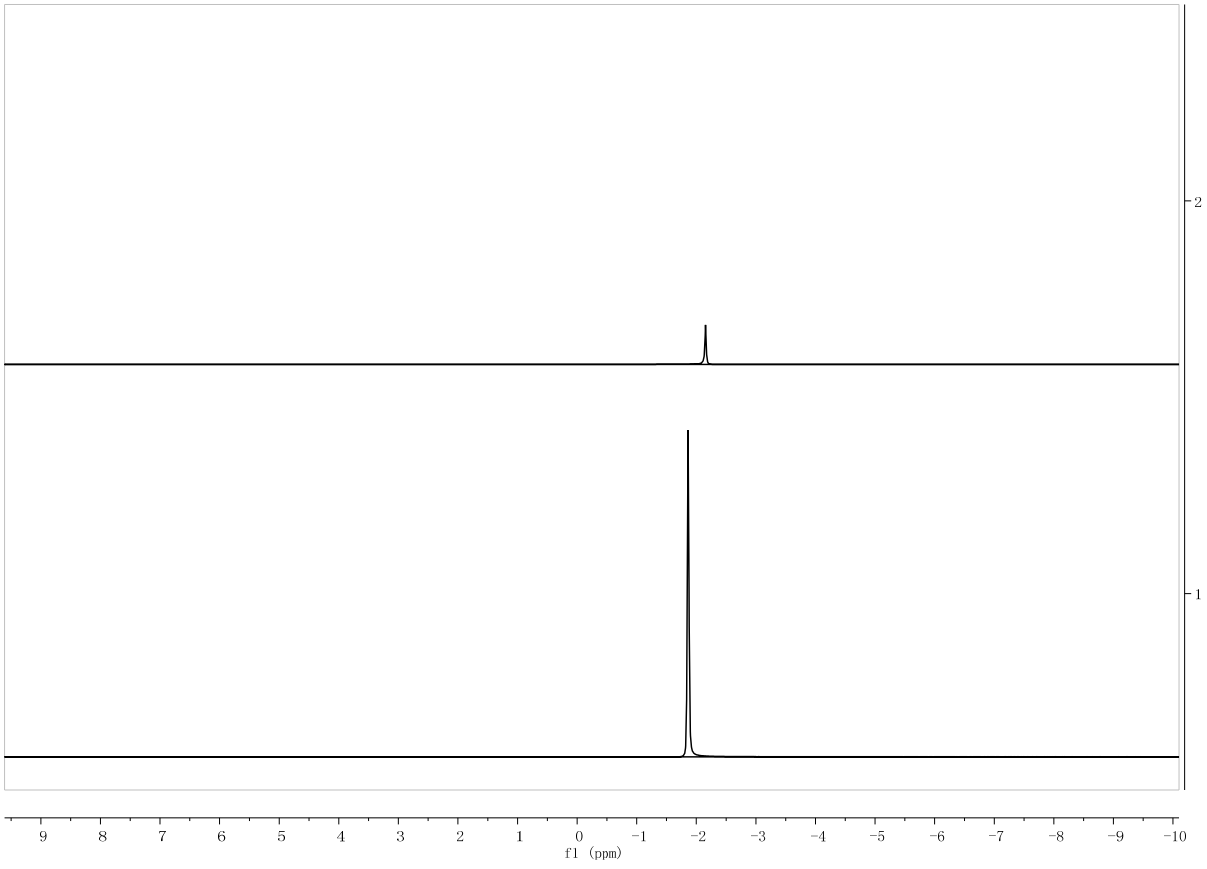
Dibenzyl sulfoxide: white crystalline powder. M.p.:135℃,[11] found 135-137℃.IR(cm^{-1}): 1028vs (SO). ^{1}H NMR ($CDCl_3$, 400Hz, r.t. ppm): δ = 3.94 (4H, m, CH_2SOCH_2), 7.31-7.38 (4H, m, Ph), 7.43 (6H, m, Ph). ^{13}C NMR ($CDCl_3$, 100Hz, r.t. ppm): δ = 57.18, 128.42, 128.99, 130.16, 130.86.

Dibenzothiophene oxide: off-white to pale yellow solid. M.p.:194-196℃,[12] found 195-197℃. IR(cm^{-1}): 1018vs (SO). ^{1}H NMR ($CDCl_3$, 400Hz, r.t. ppm): δ = 7.56 (m, 2H, Ph), 7.65 (2H, m, Ph), 7.87 (2H, m, Ph), 8.03-8.05 (2H, m, Ph). ^{13}C NMR ($CDCl_3$, 100Hz, r.t. ppm): δ = 120.89, 126.55, 128.55, 131.55, 136.10, 144.12.

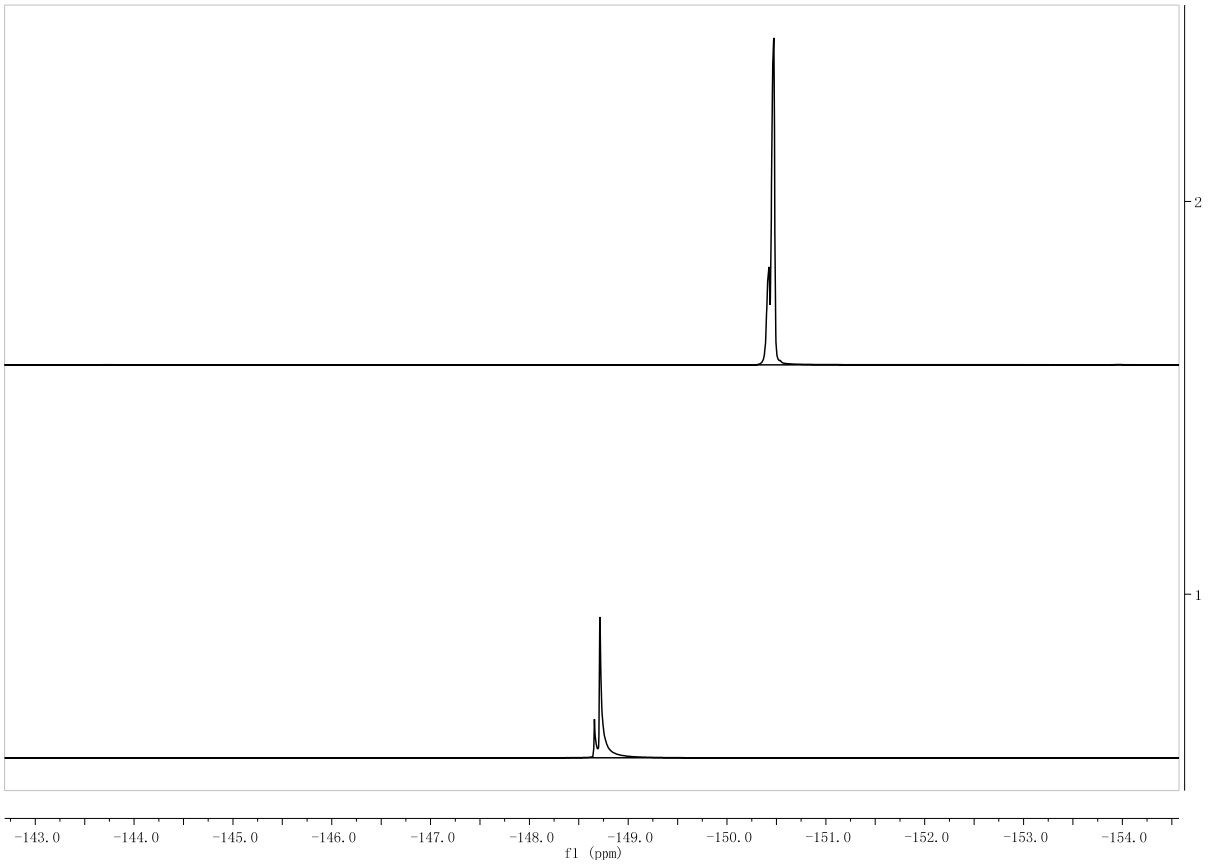
E2. Spectroscopic data

E2.1 NMR spectra comparison

^{11}B NMR of [Bmim] BF_4 (1) and [Bmim] BF_4 + H_2O_2 (35%)(2) system.

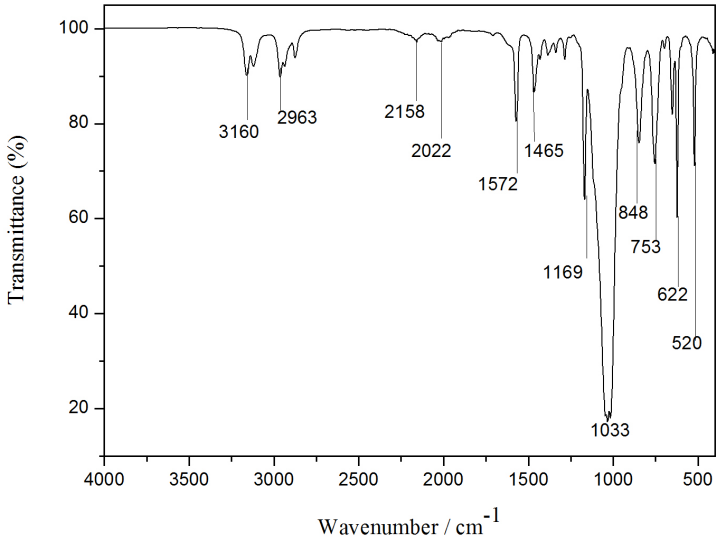


^{19}F NMR of [Bmim] BF_4 (1) and [Bmim] BF_4 + H_2O_2 (35%) (2) system.

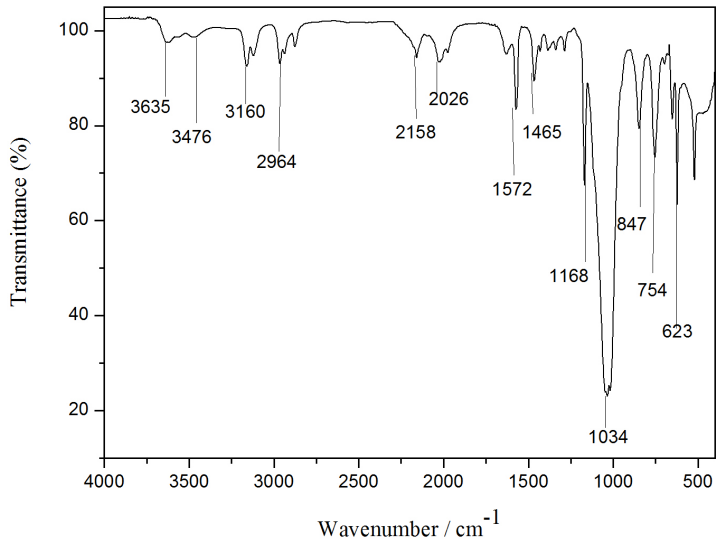


E2.2 IR spectra comparison

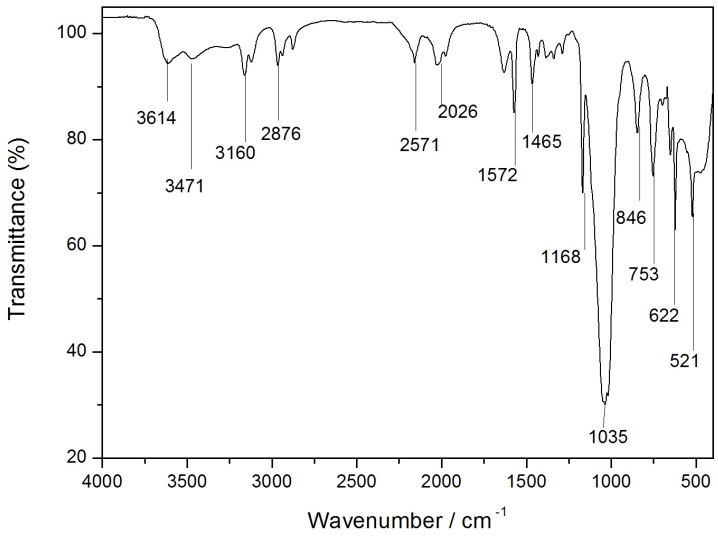
Pure [Bmim]BF_4 ionic liquid



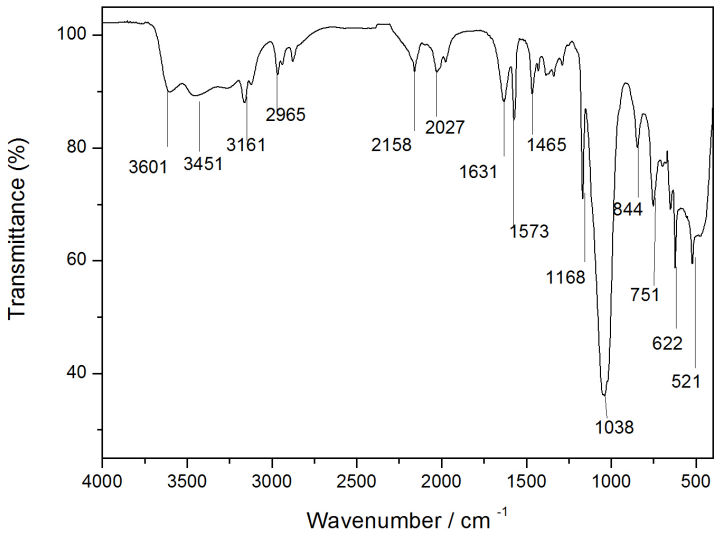
The line is the spectra for 0.23 mol/L H_2O_2 concentration in ionic liquid.



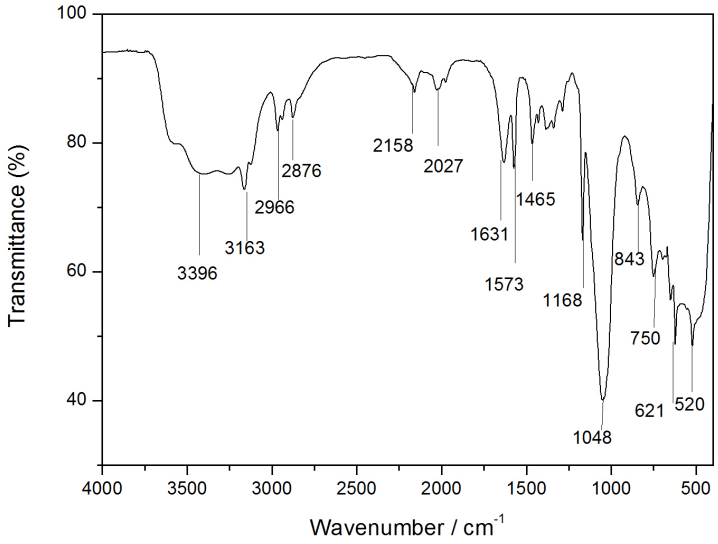
The line is the spectra for 0.53 mol/L H_2O_2 concentration in ionic liquid.



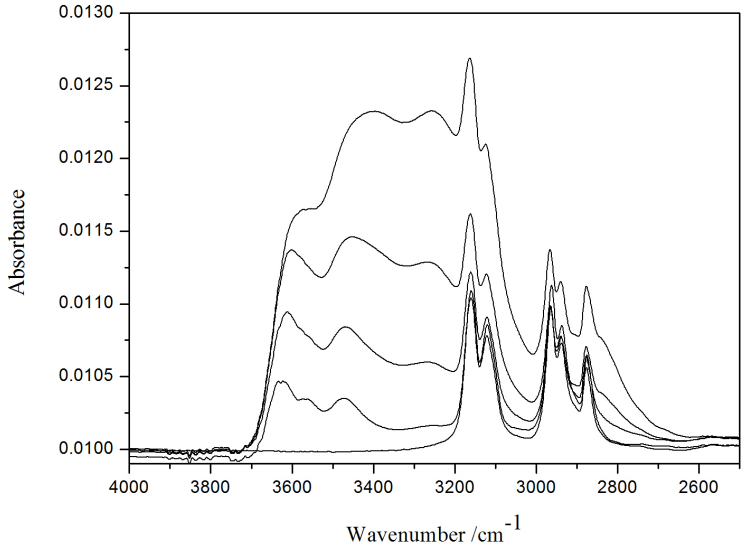
The line is the spectra for 1.5 mol/L H_2O_2 concentration in ionic liquid.



The line is the spectra for 3.8 mol/L H_2O_2 concentration in ionic liquid.

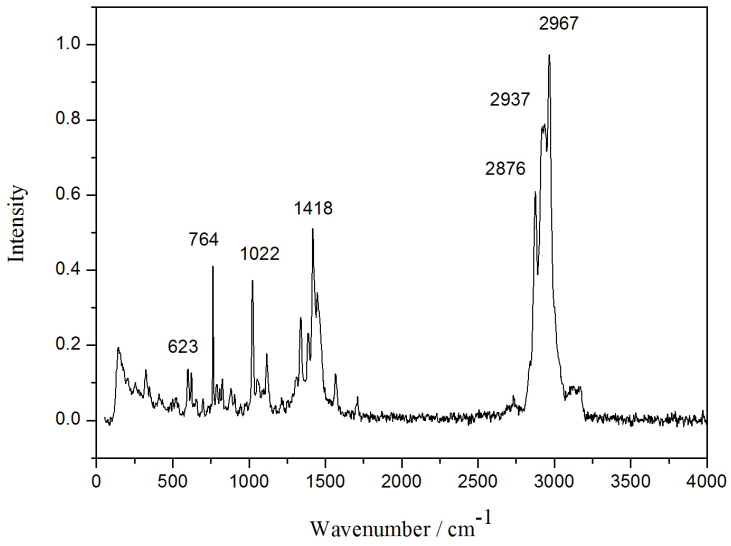


The IR spectra in the range of 3000 to 3500 cm^{-1} for the treatment of [Bmim]BF_4 with different H_2O_2 concentrations.

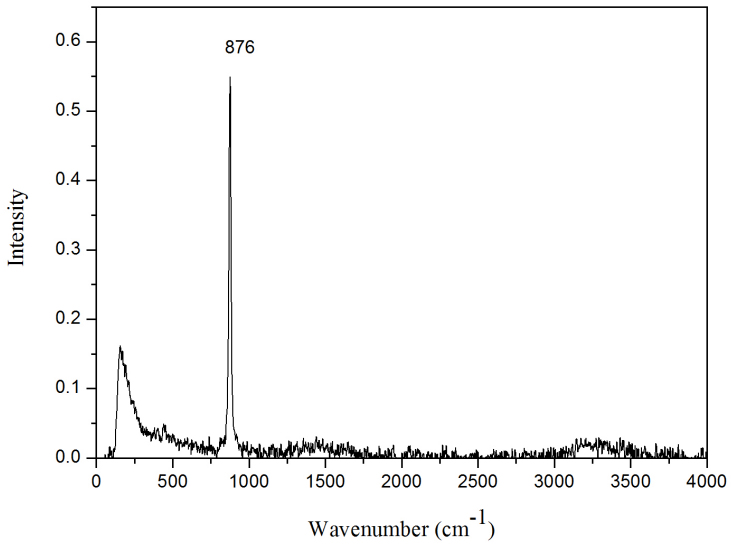


E2.3 Raman spectra comparison

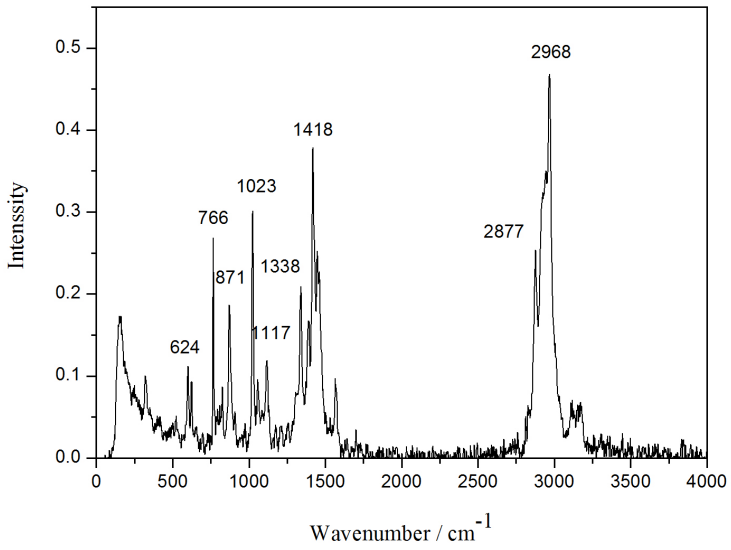
Pure [Bmim]BF_4 ionic liquid



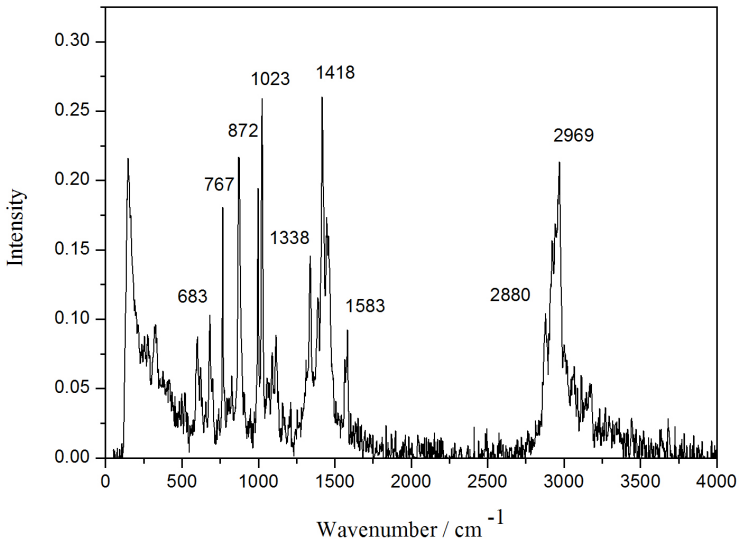
Pure H_2O_2 (35%)



The line is the spectra for 3.4 mol/L H_2O_2 concentration in ionic liquid.



The line is the spectra for 4.1 mol/L H_2O_2 concentration in ionic liquid.



E3. References

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