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°C, found 28-30°C. IR(cm⁻¹): 1032 vs (SO).

$^1$H NMR (CDCl₃, 400Hz, r.t. ppm): 2.60 (3H, s, Me), 7.39 (5H, m, Ph), 7.53 (2H, m, Ph). $^{13}$C NMR (CDCl₃, 100Hz, r.t. ppm): $\delta = 43.75, 123.29, 129.17, 130.81, 145.62.$

**Ethyl phenyl sulfoxide:** yellow oil. B.p.: 284°C, found 285-287°C. IR(cm⁻¹): 1018 vs (SO).

$^1$H NMR (CDCl₃, 400Hz, r.t. ppm): $\delta = 1.05$ (3H, t, Me), 2.73 (2H, m, CH₂), 7.37 (3H, m, Ph), 7.48 (2H, m, Ph). $^{13}$C NMR (CDCl₃, 100Hz, r.t. ppm): $\delta = 6.06, 50.49, 124.38, 129.33, 131.08, 143.78.$

**Diphenyl sulfoxide:** white crystal. M.p.: 70°C, found 70-72°C. IR(cm⁻¹): 1034 vs (SO).

$^1$H NMR (CDCl₃, 400Hz, r.t. ppm): $\delta = 7.38$ (6H, m, Ph), 7.57 (4H, m, Ph). $^{13}$C NMR (CDCl₃, 100Hz, r.t. ppm): $\delta = 123.80, 128.31, 130.02, 144.69.$

**Dibutyl sulfoxide:** white solid. M.p.: 31°C, found 31-33°C. IR(cm⁻¹): 1023 vs (SO).

$^1$H NMR (CDCl₃, 400Hz, r.t. ppm): $\delta = 0.99$ (6H, t, Me), 1.49 (4H, m, CH₂), 1.85 (4H, m, CH₂), 2.97 (4H, m, CH₂). $^{13}$C NMR (CDCl₃, 100Hz, r.t. ppm): $\delta = 13.53, 21.78, 23.95, 52.50.$

**Dimethyl sulfoxide:** colorless liquid. B.p.: 189°C, found 190-192°C. IR(cm⁻¹): 1015 vs (SO).

$^1$H NMR (CDCl₃, 400Hz, r.t. ppm): $\delta = 2.47$ (6H, s, Me). $^{13}$C NMR (CDCl₃, 100Hz, r.t. ppm): $\delta = 41.30.$

**2-(Phenylsulfinyl)ethanol:** pale yellow oil. B.p.: 362°C, found 360-363°C. IR(cm⁻¹): 3343s (OH), 1018 vs (SO).

$^1$H NMR (DMSO, 100Hz, r.t. ppm): $\delta = 2.97$ (1H, m, CH₂OH), 3.67 (1H, m, CH₂SO), 3.84 (1H, m, CH₂SO), 5.10 (1H, t, OH), 7.54 (3H, m, Ph), 7.62 (2H, m, Ph). $^{13}$C NMR (DMSO, 100Hz, r.t. ppm): $\delta = 54.32, 59.92, 123.78, 129.20, 130.65, 144.66.$
**Methyl 2-(pheylsulfinyl) acetate:** pale yellow oil. B.p.: 341 °C, found 342-344 °C. IR (cm⁻¹): 1043 vs (SO). ¹H NMR (CDCl₃, 400Hz, r.t. ppm): δ = 3.54 (3H, s, Me), 3.69 (1H, m, CH₂), 7.39 (3H, m, Ph), 7.54-7.56 (2H, m, Ph). ¹³C NMR (CDCl₃, 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 °C, found 297-300 °C. IR (cm⁻¹): 1037 vs (SO). ¹H NMR (CDCl₃, 400Hz, r.t. ppm): δ = 3.45 (2H, m, CH₂), 5.11 (1H, d, CH=CH₂), 5.24 (1H, d, SOCH₂), 5.56 (1H, m, SOCH₂), 7.43 (3H, m, Ph), 7.52 (2H, m, Ph). ¹³C NMR (CDCl₃, 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 °C, found 295-298 °C. IR (cm⁻¹): 1015. ¹H NMR (CDCl₃, 400Hz, r.t. ppm): δ = 3.68 (3H, s, OMe), 4.53 (2H, s, SOCH₂), 7.60 (2H, m, Ph), 7.66 (1H, m, Ph), 7.95 (2H, m, Ph). ¹³C NMR (CDCl₃, 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 °C, found 292-294 °C. IR (cm⁻¹): 1020 vs (SO). ¹H NMR (CDCl₃, 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). ¹³C NMR (CDCl₃, 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 °C, found 123-125 °C. IR (cm⁻¹): 1027 vs (SO). ¹H NMR (CDCl₃, 400Hz, r.t. ppm): δ = 4.10 (2H, m, SOCH₂), 7.02 (2H, m, Ph), 7.35 (3H, m, Ph), 7.46 (5H, m, Ph). ¹³C NMR (CDCl₃, 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°C, \(^{11}\) found 135-137°C. IR(cm\(^{-1}\)): 1028vs (SO). \(^1\)H NMR (CDCl\(_3\), 400Hz, r.t. ppm): \(\delta = 3.94\) (4H, m, CH\(_2\)SOCH\(_2\)), 7.31-7.38 (4H, m, Ph), 7.43 (6H, m, Ph). \(^{13}\)C NMR (CDCl\(_3\), 100Hz, r.t. ppm): \(\delta = 57.18, 128.42, 128.99, 130.16, 130.86\).

**Dibenzothiophene oxide**: off-white to pale yellow solid. M.p.:194-196°C, \(^{12}\) found 195-197°C. IR(cm\(^{-1}\)): 1018vs (SO). \(^1\)H NMR (CDCl\(_3\), 400Hz, r.t. ppm): \(\delta = 7.56\) (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): \(\delta = 120.89, 126.55, 128.55, 131.55, 136.10, 144.12\).

**E2. Spectroscopic data**

**E2.1 NMR spectra comparison**

\(^{11}\)B NMR of [Bmim] BF\(_4\) (1) and [Bmim] BF\(_4\) + H\(_2\)O\(_2\) (35%) (2) system.
$^{19}$F NMR of [Bmim] BF$_4$ (1) and [Bmim] BF$_4$ + H$_2$O$_2$ (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 H₂O₂ concentration in ionic liquid.

The line is the spectra for 3.8 mol/L H₂O₂ 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\(_2\)O\(_2\) concentrations.

**E2.3 Raman spectra comparison**

Pure [Bmim]BF\(_4\) ionic liquid
Pure H₂O₂ (35%)

The line is the spectra for 3.4 mol/L H₂O₂ concentration in ionic liquid.
The line is the spectra for 4.1 mol/L H₂O₂ concentration in ionic liquid.

E3. References


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