

Supplementary Information

“A Reversible Zwitterionic SO₂-Binding Organic Liquid”

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I. Experimental Section

General. All reactions were run under an atmosphere of argon, unless otherwise indicated. Solvents were transferred by plastic syringe. Flasks were oven-dried and cooled under a stream of argon. Ethanol was purchased from Fisher and used without further purification. SO₂ was purchased from Aldrich chemical company and used without purification. High-resolution mass spectra (HRMS) were obtained on a LTQ Orbitrap™ Mass Spectrometer from Thermo Scientific Company as m/e (relative intensity). Accurate masses are reported for the molecular ion (M+1) or a suitable fragment ion. IR measurements were performed on NaCl disks using a Nicolet Magna-750 spectrometer running on OMNIC software. Proton nuclear magnetic resonance (¹H NMR) spectra were recorded with a Varian (300 MHz) spectrometer. Chemical Shifts are reported in delta (δ) units, parts per million (ppm) downfield from trimethylsilane. Coupling constants are reported in Hertz (Hz). Carbon-13 nuclear magnetic resonance (¹³C NMR) spectra were recorded with a Varian 300 (75.5MHz) spectrometer. Chemical shifts are reported in delta (δ) units, parts per million (ppm) relative to the singlet of the terminal CH₃ on the butyl groups of dibutylamine at 14.2 ppm.

1-(*N,N*-Di-*n*-butylamino)-1-undecanol (DBUA)

11-(*N,N*-Di-*n*-butylamino)-1-undecanol was prepared according to a modified literature procedure.¹ Dibutylamine (9.4 mL, 55.70 mmol) and 11-bromo-1-undecanol (4.0g, 15.92 mmol) were charged into a clean dry 250 mL flask. Ethanol (100 mL) was added, the resulting solution was heat to reflux under an argon atmosphere for 18h. At which point the reaction mixture was allowed to cool to room temperature and then the solvent was removed in *vacuo* to afford a white solid. This crude product was dissolved in water (100 mL, and the pH was adjusted to 9.0 using solid Na₂CO₃. This solution was extracted with CHCl₃ (3 X 30 mL), the organic layers were combined, dried over MgSO₄, filtered, and then concentrated to provide a pale yellow oil. Excess dibutylamine was distilled off under vacuum at 90 °C. The final product was recovered as a pale yellow oil (4.2g, 88% yield.) ¹H NMR (300 MHz, CDCl₃) δ 3.65 (t, *J* = 6.44 Hz, 2H), 2.40 (br s, 6H), 1.55 (t, *J* = 6.7 Hz, 2H), 1.44-1.27 (m, 24H), 0.90 (t, *J* = 6.7 Hz, 6H) ¹³C NMR (75.5 MHz, neat) δ 61.6, 54.3, 53.9, 33.1, 30.0, 29.5, 27.8, 27.4, 26.3, 20.8, 14.2. FTIR (NaCl, film): 3332, 2927, 2855, 1464, 1375, 1060, 732 cm⁻¹ HRMS calculated [M+1] for C₁₉H₄₁NO 300.3266 found 300.3255.

DBUA-SO₂

DBUA was syringed into oven-dried round bottom flask fitted with a rubber septa and massed. The septa was punctured with a needle connected to a N₂ bubbler and a polyetheretherketone (PEEK) 1/16" tube connected to a lecture bottle of SO₂. The flask was placed in an ice water bath and then DBUA was then sparged with SO₂ to form the zwitterion. Once uptake had finished, the flask was quickly vacuumed and refilled with N₂ three times to remove any gaseous SO₂ in the flask. The flask was then massed to record the SO₂ gravimetric uptake. ¹H NMR (300 MHz, CDCl₃) δ 10.2 (br s, 1H) 3.70 (t, *J* = 6.70 Hz, 2H), 2.95 (br s, 6H), 1.69 (m, 6H), 1.59 (t, *J* = 6.44 Hz, 2H), 1.39-1.28 (m, 18 H), 0.90 (t, *J* = 7.37 Hz, 6H). ¹³C NMR (75.5 MHz, neat) δ 61.0, 52.5, 31.4, 30.1, 27.3, 26.9, 25.8, 23.9, 20.6, 14.2. FTIR (NaCl, film): 3384, 2928, 2856, 2646, 2548, 1468, 1381, 1322, 1144, 1076, 678 cm⁻¹.

Stripping of SO₂ was performed by placing DBUA-SO₂ and a 1" stir bar in a flask fitted with a jacketed condenser. The flask was then placed under vacuum and then placed in an oil bath set to 70 °C. The flask as heated under vacuum for 40 minutes while stirring. The flask was then cooled and massed.

¹ Qi, W.; Li, H.; Wu, L. *Adv. Mater.* **2007**, *17*, 198

II. Spectral data for DBUA and DBUA-SO₂

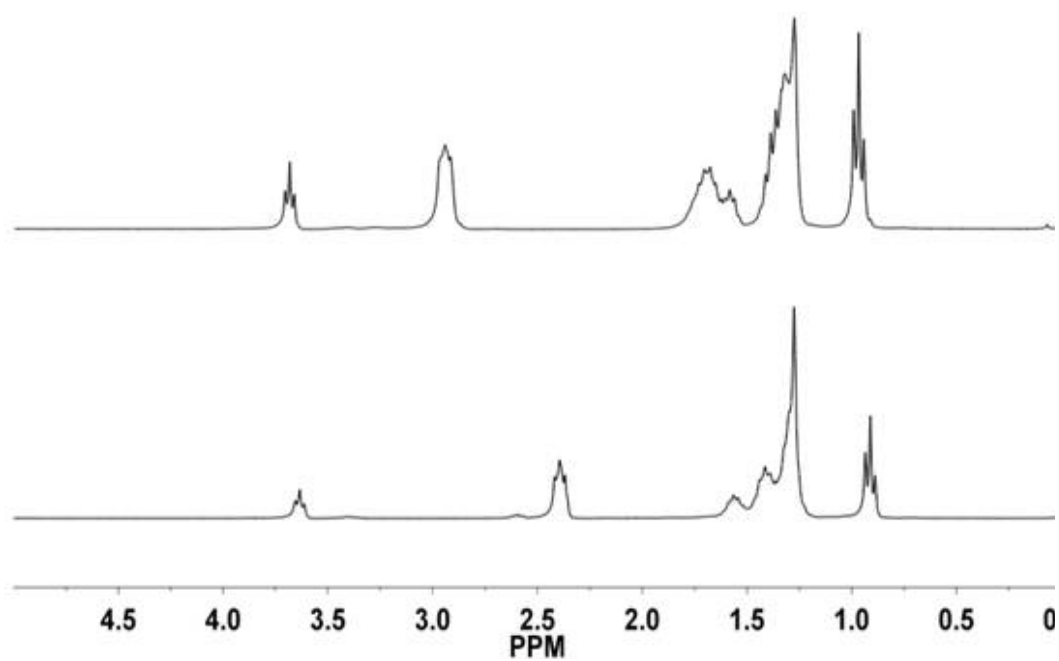


Figure 1S. ¹H NMR of DBUA (bottom) and DBUA with SO₂ (top)

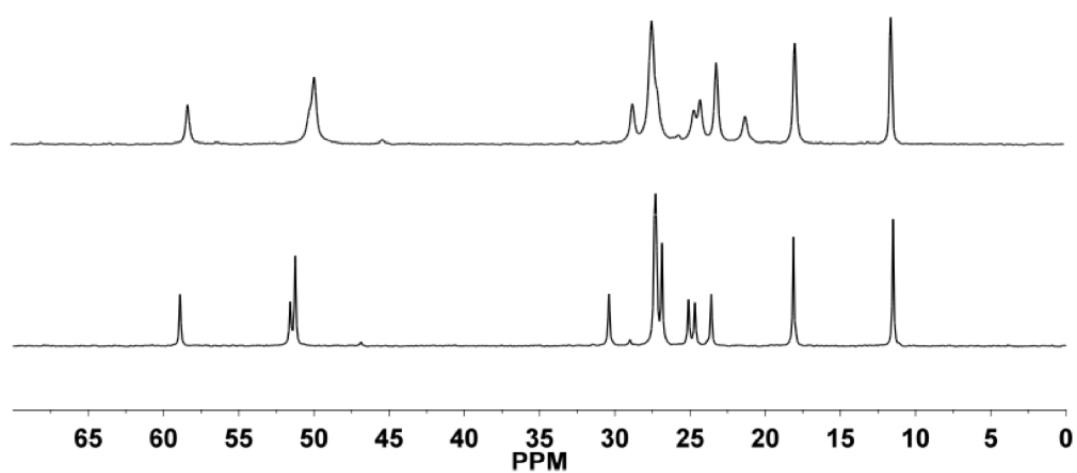


Figure 2S. ¹³C NMR of DBUA (bottom) and with SO₂ (top)

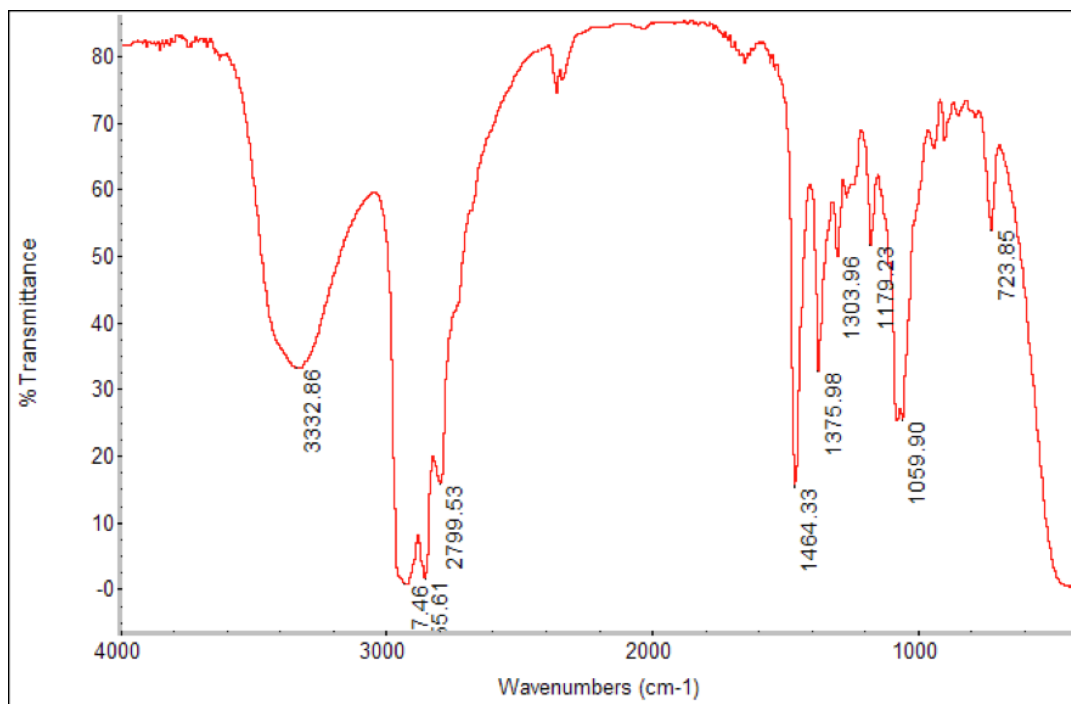


Figure 3S. IR of DBUA

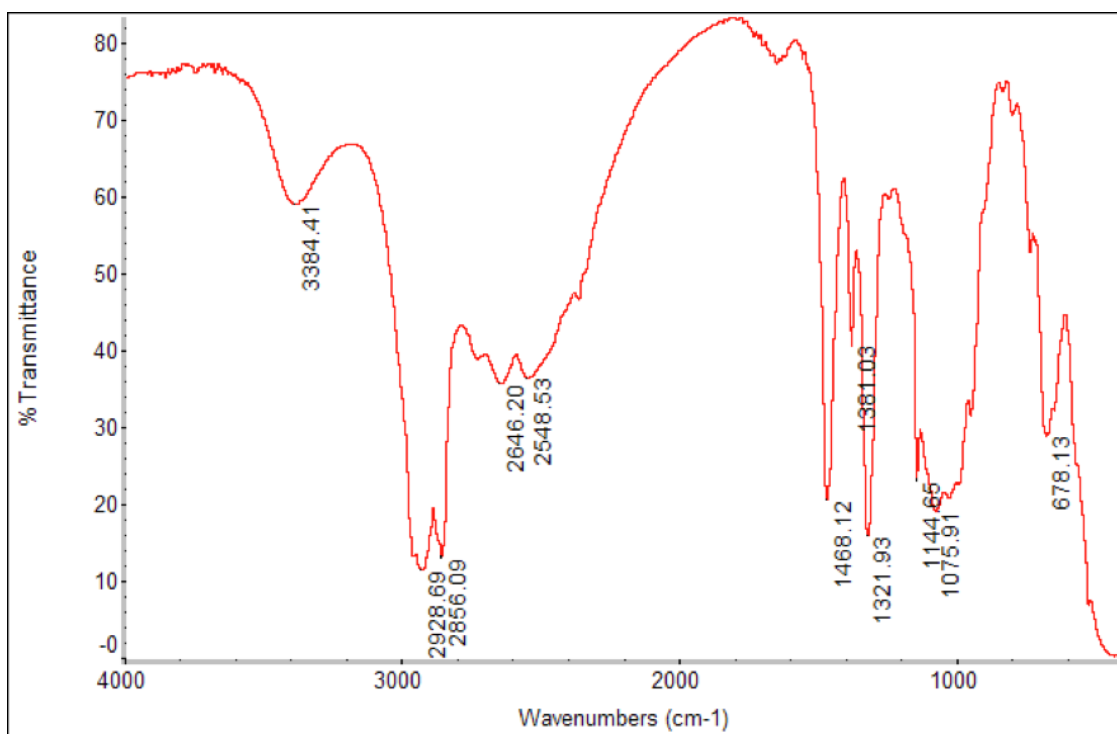


Figure 4S. IR of DBUA+SO₂

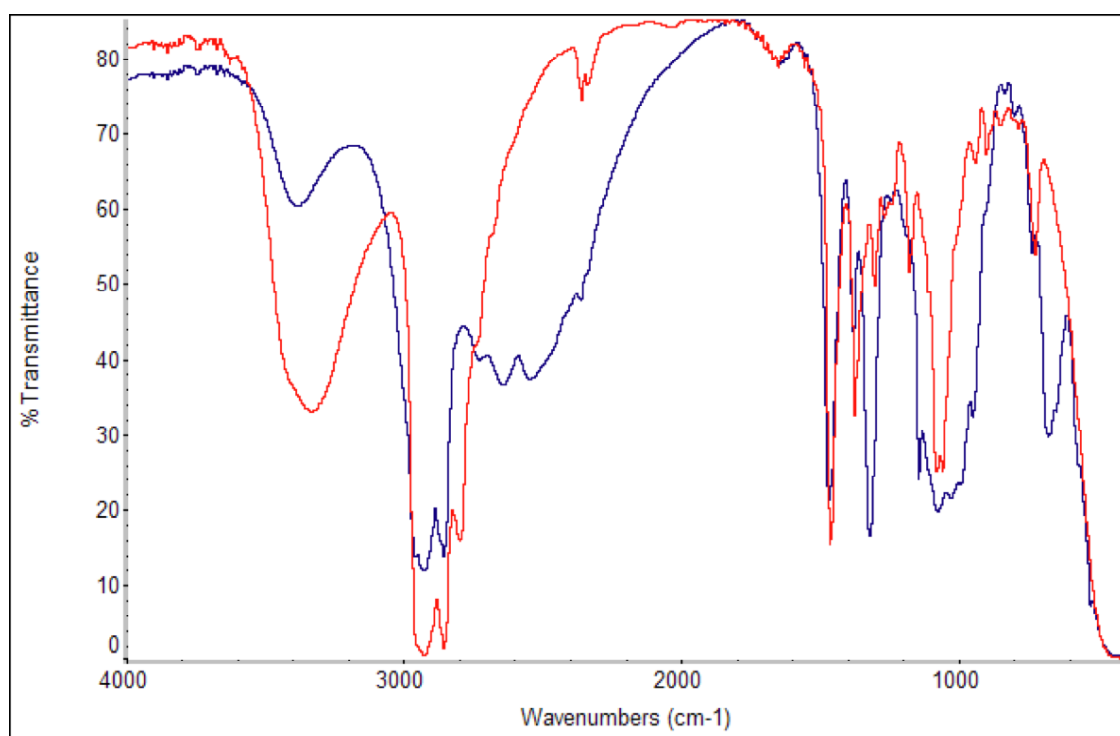


Figure 5S. IRs of DBUA with and without SO₂