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Supporting Information

Synthetic Route for an Ionic Liquid Precursor

Xintong Liu*

Department of Chemistry, Renmin University of China, Beijing 100872, China

Contents

1 Materials

Pyrrole, 1-methylimidazole, sodium hydride and ammonium hexafluorophosphate were purchased from Shanghai Aladdin Biochemical Technologies Co., Ltd.. 1,8-Dibromooctane, sodium sulphate, chloroform-d, dimethyl sulfoxide-d_6 (DMSO-d_6) and methanol were purchased from Beijing Tongguang Fine Chemicals Co., Ltd.. N,N-Dimethylformamide (DMF), dichloromethane (DCE), acetonitrile, petroleum ether (PE) and silica gel were purchased from Meryer Shanghai Chemical Technology Co., Ltd.. All commercially available chemicals were used without further purification unless otherwise noted.

2 Instruments

1H-NMR and 13C-NMR spectra spectra were recorded on a Bruker Avance DMX 400 MHz Spectrometer in $CDCl_3$ or DMSO-d_6. Chemical shifts (δ) are given in ppm and they were referenced to the internal solvent signals. Rotary evaporation was performed with an EYELA SB-2000 rotary evaporator and SHB-III circulating water vacuum pump. All the reactions were carried out on a ETS-D5 magnetic heating stirrer. Silica gel column chromatography and thin layer chromatography were used to isolate and purify the reaction mixture.

3 Experimental details

(**a**) Synthesis of Py-C8-Br:

Pyrrole (15 mmol) dissolved in 20 mL DMF was added dropwise to a mixture of 1,8-dibromooctane (50 mmol), NaH (1.8 g, 60% w/w) and dry DMF (40 mL) at 0°C. The reaction mixture was stirred overnight and quenched with H2O (60 mL). The resulting mixture was extracted with DCM (4×30 mL). The combined organic layers were dried by anhydrous Na_2SO_4 and evaporated under reduced pressure to afford a clear, brownish liquid. The crude product was purified by column chromatography on silica gel using petroleum ether as eluent to obtain pure product as a colorless and transparent liquid in 50-70% yield.

(**b**) Synthesis of (Py-C8-MIm)Br:

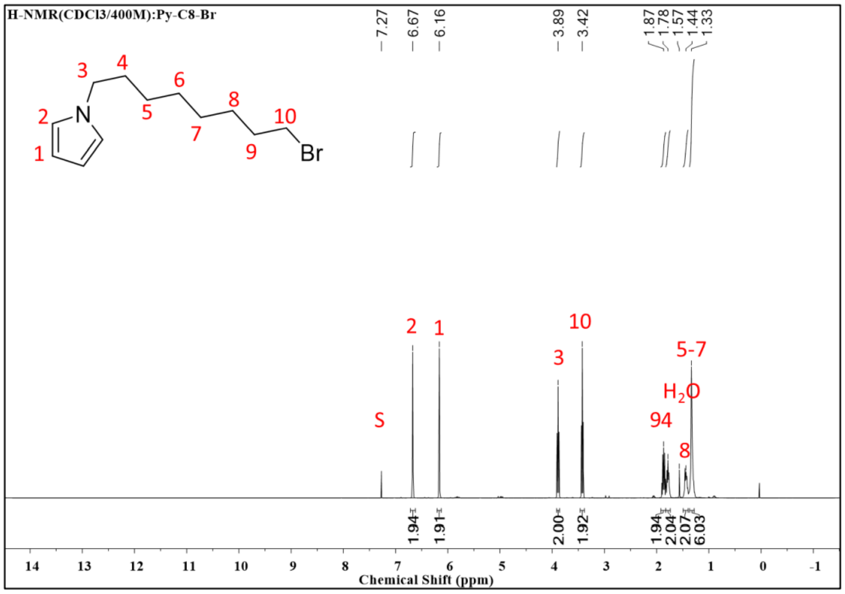
To a solution of 1-methylimidazole (18 mmol) in CH_3CN (25 mL) was added a mixture of Py-C8-Br (12 mmol) and CH_3CN (5 mL) dropwise. The mixture was stirred at 60°C for 48 hours under nitrogen atmosphere. The crude product was purified by column chromatography on silica gel using CH_2Cl_2/CH_3OH (10：1) as eluent to afford the pure product as a brownish liquid in 70-80% yield.

(**c**) Synthesis of (Py-C8-MIm)PF_6:

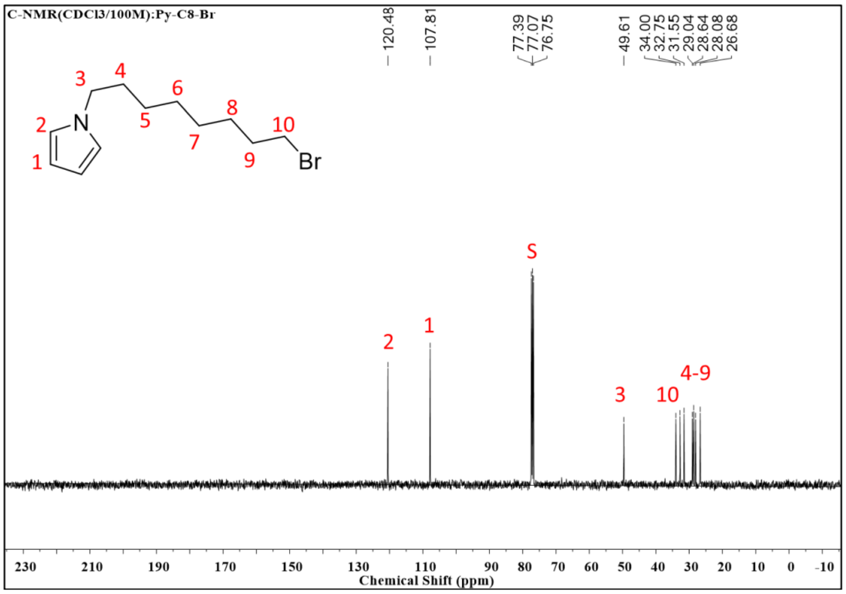
(Py-C8-MIm)Br (9 mmol) was added dropwise to a solution of ammonium hexafluophosphate (24 mmol) in 100 mL mixture of deionized water and DCM (1：1). The mixture was stirred vigorously overnight at room temperature under nitrogen atmosphere. After separated and washed with deionized water, the organic phase was dried over anhydrous Na_2SO_4, then filtered and evaporated under reduced pressure to afford a clear, brownish liquid in 80-90% yield.

4 Spectroscopic data

Py-C8-Br:

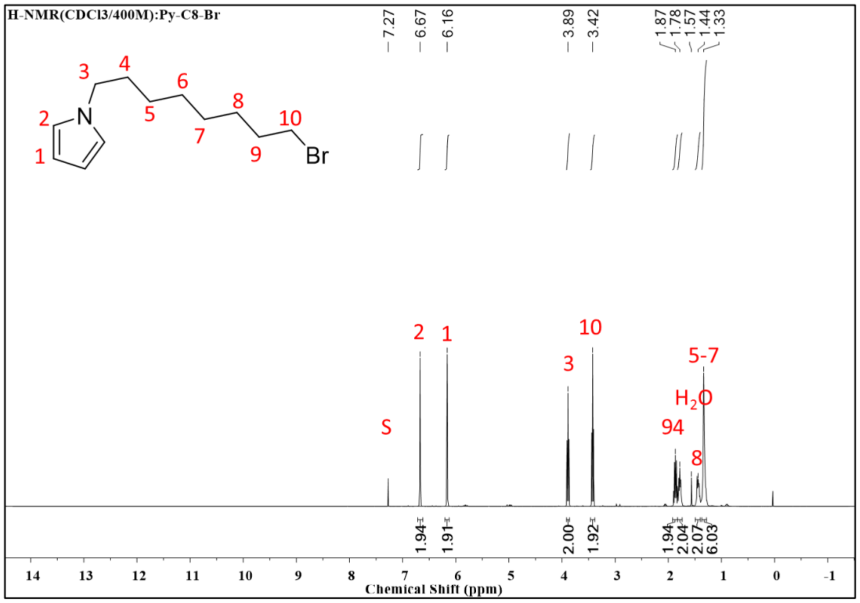


^{1}H NMR (400 MHz, CDCl3) δ 6.67 (t, J = 2.1 Hz, 2H), 6.16 (t, J = 2.1 Hz, 2H), 3.89 (t, J = 7.2 Hz, 2H), 3.42 (t, J = 6.8 Hz, 2H), 1.92-1.83 (m, 2H), 1.82-1.74 (m, 2H), 1.49-1.40 (m, 2H), 1.37-1.28 (m, 6H).

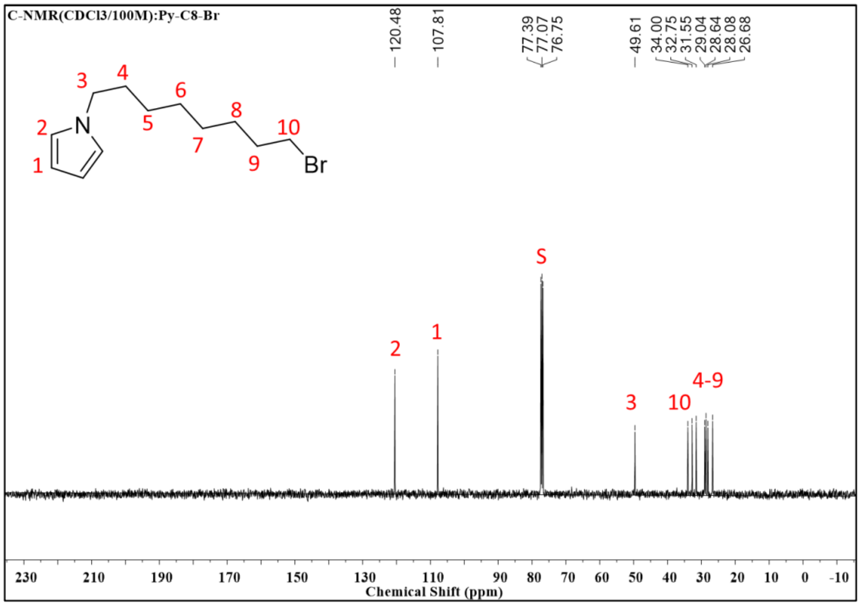


^{13}C NMR (101 MHz, CDCl3) δ 120.48, 107.81, 49.61, 34.00, 32.75, 31.55, 29.04, 28.64, 28.08, 26.68.

(Py-C8-MIm)Br:



^{1}H NMR (400 MHz, CDCl3) δ 6.67 (t, J = 2.1 Hz, 2H), 6.16 (t, J = 2.1 Hz, 2H), 3.89 (t, J = 7.2 Hz, 2H), 3.42 (t, J = 6.8 Hz, 2H), 1.92-1.83 (m, 2H), 1.82-1.74 (m, 2H), 1.49-1.40 (m, 2H), 1.37-1.28 (m, 6H).



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