

Electronic Supplementary Information

Improving the electrochemical performance of organic Li-ion battery electrodes

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Notes: no significant peaks are seen in the 4000-1700 cm⁻¹ region.

1. Experimental details

General Methods

Solvents and reagents were purchased from Aldrich or Alfa Aesar and were used as received. ^1H and ^{13}C NMR spectra were recorded at 400 MHz and 100 MHz on a JEOL ECP-400 spectrometer, at room temperature, respectively. Chemical shifts (δ) were expressed in part per million (ppm) relative to residual D_2O or an internal standard. Infrared spectra were performed with a PerkinElmer Spectrum One FT-IR spectrometer in the $650\text{--}4000\text{ cm}^{-1}$ frequency range equipped with an attenuated total reflectance probe (ATR). The positive electrode was prepared without binder by mixing organic compounds with 33% carbon SP (in total mass) in the solid state (Method A) or in the liquid state (Method B). Mechanical mixing was carried out on a Restch during 1 hour. The powder and 2 balls (diameter 20 mm) were stowed in a milling container (55mL). Electrochemical performances were tested vs. lithium in Swagelok[®]-type cells using Li metal disc as negative electrode and a fibreglass separator soaked with a molar LiTFSI solution in DMC as the electrolyte. Cells were cycled in galvanostatic mode using an Arbin BT-2043 system. The morphology of the samples was observed using a high resolution scanning electron microscopy (HRSEM LEO 1550).

Synthesis of dilithium benzenediacylate (1): Method A

221.7 mg of lithium carbonate (3 mmol) and 654.6 mg of benzenediacylic acid **4** (3 mmol) were stirred in 20 mL of a $\text{H}_2\text{O}/\text{EtOH}$ solution (1:1 v/v) at 50°C for 48 hours. Solvents were eliminated by drying in a ventilated oven at 100°C for 15 hours. The white crystalline powder was then transferred into a glovebox and dried under vacuum at 100°C for 12 hours and 676 mg of dilithium *trans,trans* benzenediacylate **1** was obtained (yield = 98%).

$\nu_{\text{max}}/\text{cm}^{-1}$ 1638, 1574, 1510, 1422, 1396, 1259, 1105, 971, 890, 843, 826, 708, 668; ^1H NMR (400 MHz, D_2O) δ (ppm): 6.53 (d, 15.7 Hz, 2H, CH-CO_2); 7.37 (d, 16.1 Hz, 2H, CH=CH-CO_2); 7.58 (s, 4H, C_6H_4); ^{13}C NMR (100 MHz, D_2O) δ (ppm): 124.9 (CH-CO_2); 128.3 (CH phenylene); 136.4 (C-CH=CH-CO_2); 140.3 (CH=CH-CO_2); 175.8 (CO_2).

Method B

221.7 mg of lithium carbonate (3 mmol), 345.1 mg of carbon SP and 654.6 mg of benzenediacylic acid **4** (3 mmol) were stirred in 20 mL of a $\text{H}_2\text{O}/\text{EtOH}$ solution (1:1 v/v) at 50°C for 48 hours. Solvents were eliminated by drying in a ventilated oven at 100°C for 15 hours. The powder was then transferred into a glovebox and dried under vacuum at 100°C for 12 hours. 1.012 g of the mixture dilithium *trans,trans* benzenediacylate **1**/carbon SP was obtained (yield = 98%).