Electronic Supplementary Information for Energy & Environmental Science

A green Li-organic battery working as a fuel cell in case of emergency

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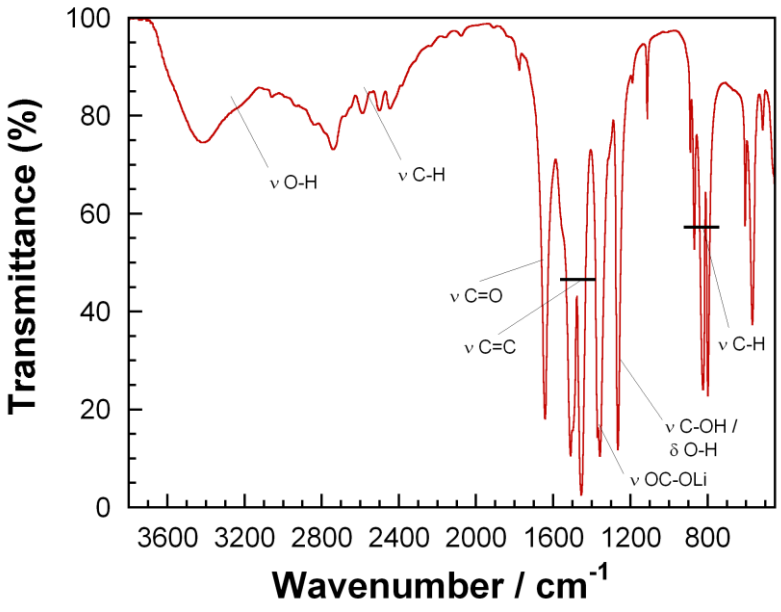
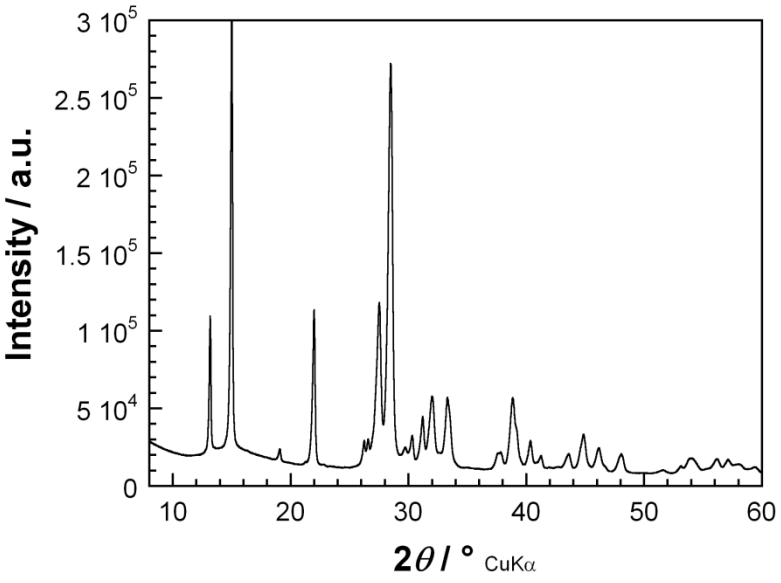
1. Characterizations of dilithium 2,5-dihydroxyterephthalate (Li_2-*p*-DHT)

(I)



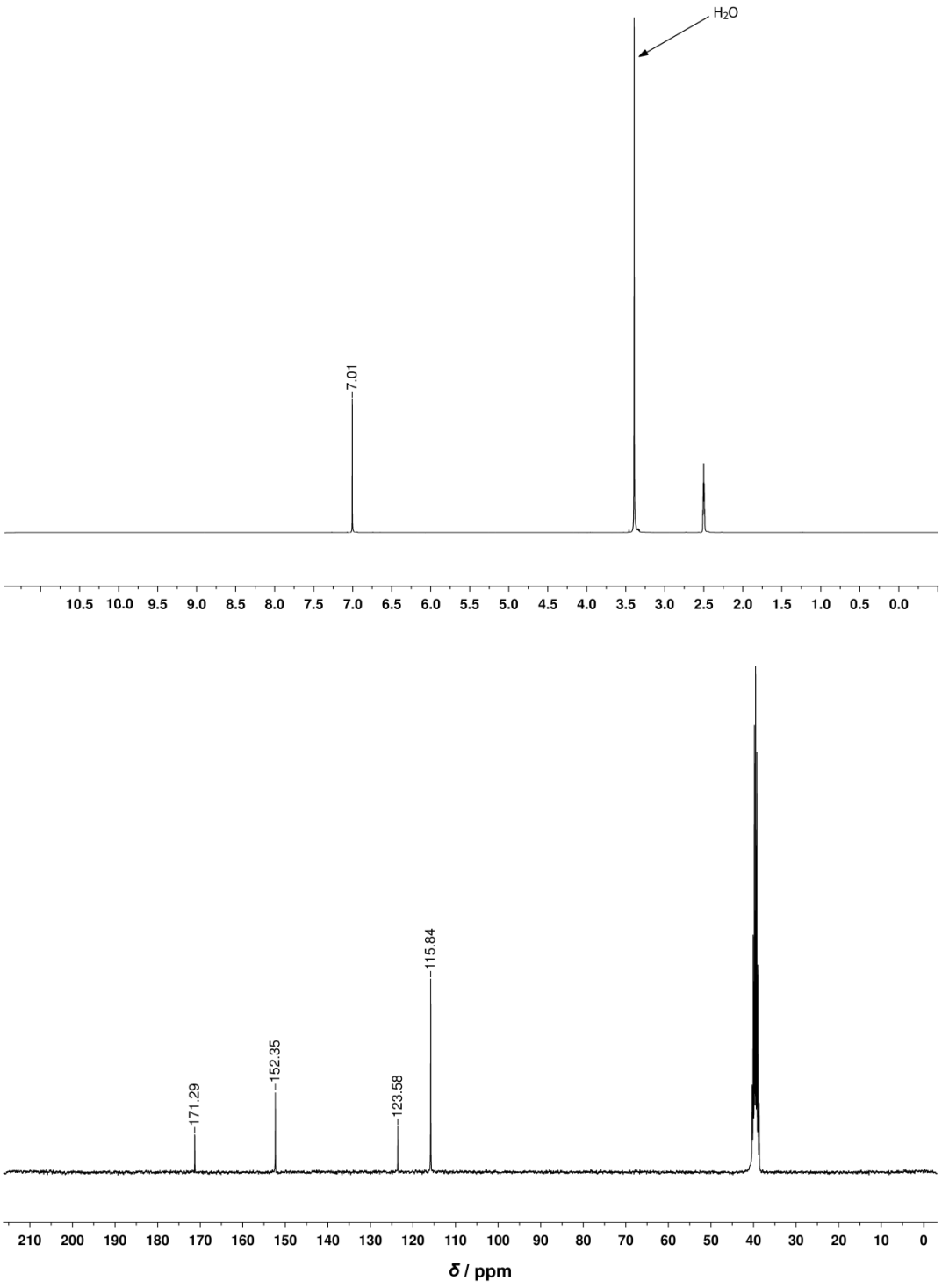
(II)



(III)

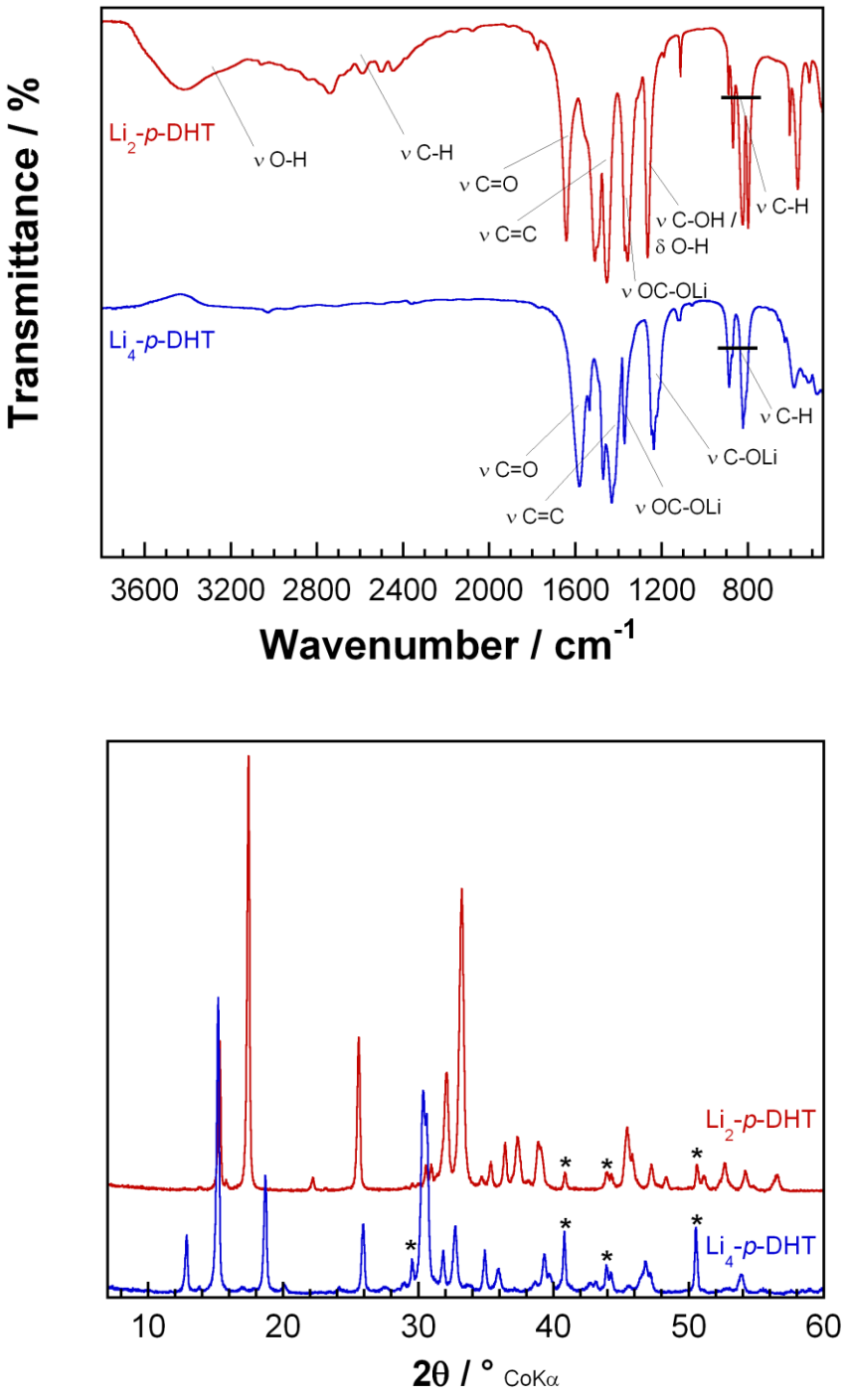
d[Å]	Intensity [%]	*d*[Å]	Intensity [%]
6.72	34	1.89	6
5.91	100	1.77	3
4.65	7	1.72	4
4.04	35	1.70	6
3.39	9	1.66	3
3.35	9	1.64	5
3.24	37	1.61	5
3.13	84	1.59	4
3.00	8	1.55	4
2.95	10	1.52	3
2.86	14	1.50	3
2.79	18	1.47	3
2.69	18	1.43	3
2.39	7	1.42	3
2.38	7	1.37	3
2.32	18	1.36	3
2.30	12	1.33	3
2.23	9	1.32	2
2.19	6	1.28	3
2.15	4	1.24	2
2.12	4	1.22	3
2.07	6	1.89	6
2.03	8	1.77	3
2.02	10	1.72	4
1.97	8	1.70	6
1.94	4	1.66	4

Supplementary Figure S1a. Typical FTIR spectrum (I) and X-ray powder diffraction pattern (II) of Li_2-*p*-DHT. (III) List of corresponding *d* spacing and relative intensities as deduced from XRPD data.

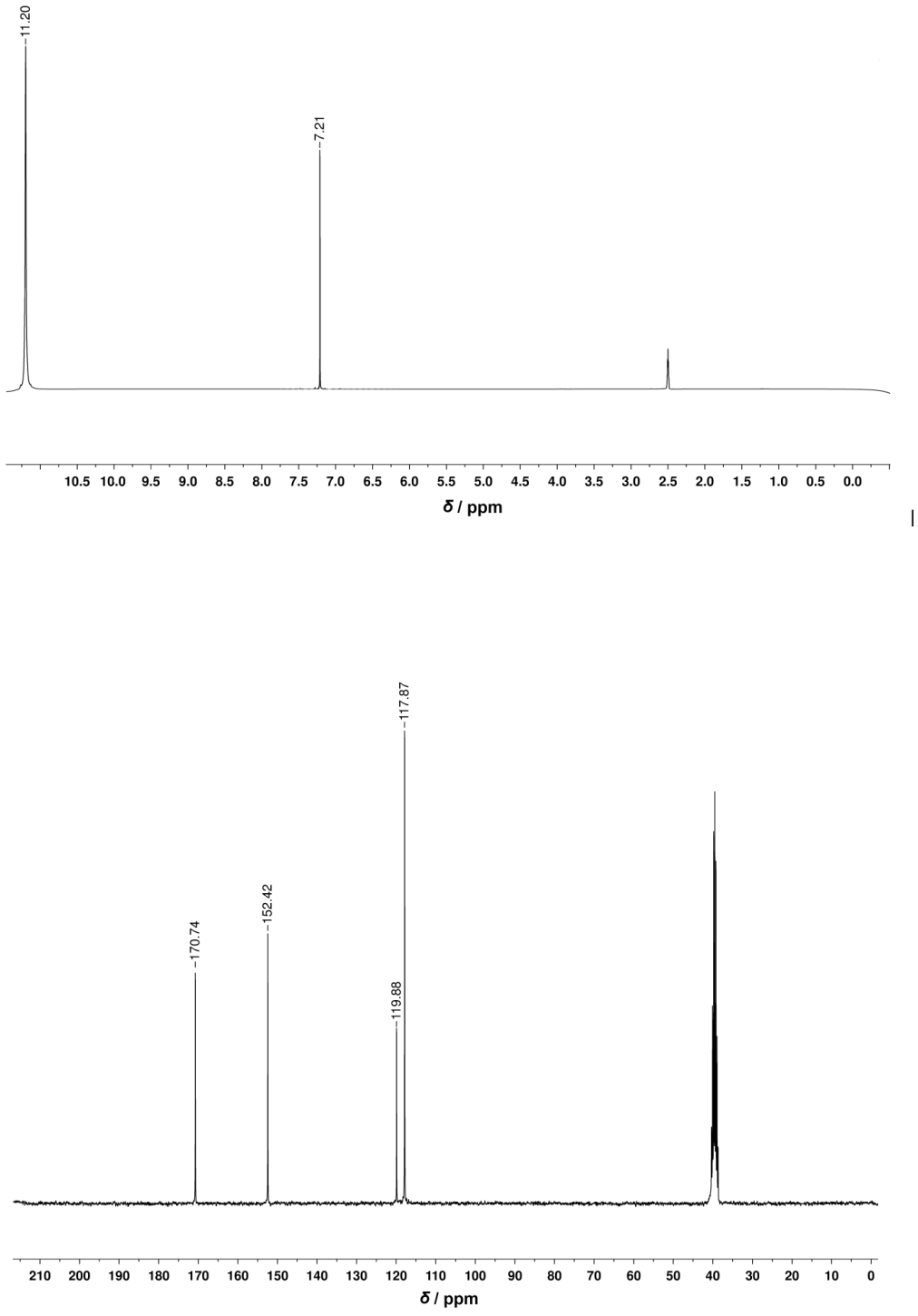


Supplementary Figure S1b. ^{1}H NMR (top) and ^{13}C NMR (bottom) spectra of Li_2-*p*-DHT measured in DMSO-d_6.

2. Characterizations of dilithium (2,5-dilithium-oxy)-terephthalate (Li_4-*p*-DHT)

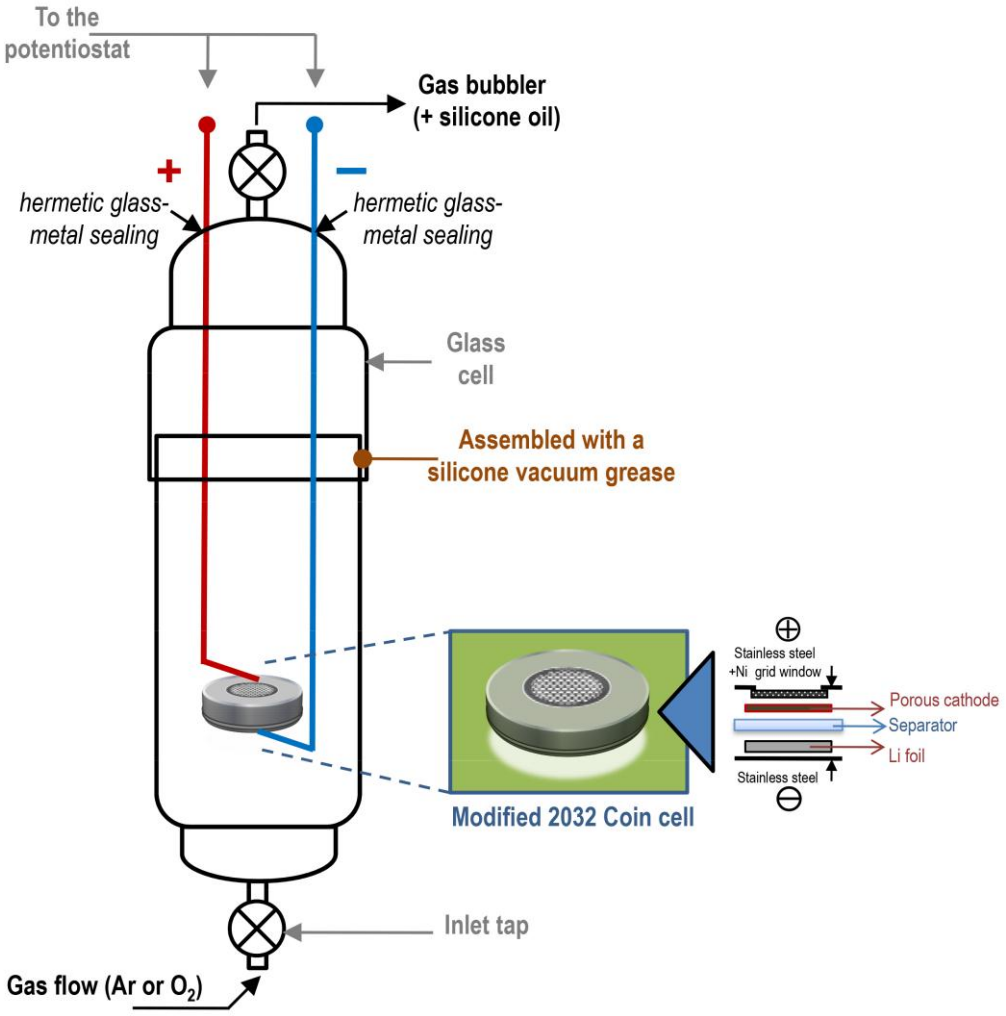


Supplementary Figure S2a. Comparison of both FTIR spectra and XRPD patterns for Li_2-*p*-DHT (red line) and Li_4-*p*-DHT (blue line). Note that (*i*) the KBr pellet containing Li_4-*p*-DHT was prepared in glove box and (*ii*) XRPD patterns were extracted from the TRXRPD experiment performed under N_2 shown in Fig. 3 (*: peaks from sample holder).



Supplementary Figure S2b. Typical ^{1}H NMR (top) and ^{13}C NMR (bottom) spectra of Li_4-*p*-DHT measured in H_2SO_4/DMSO-d_6 (50/50 in volume). This acidic medium makes a derivatization reaction of Li_4-*p*-DHT by full reprotonation possible, which leads to NMR data related to 2,5-dihydroxyterephthalic acid (H_4-*p*-DHT).

3. Experimental set-up



Supplementary Figure S3. Schematic of the homemade glass container used for the electrochemical assessments of Li_4-*p*-DHT/Li half-cells under different controlled atmospheres (e.g., Ar, O_2 or ambient air). A modified 2032 coin cell including a nickel grid window that exposes the porous cathode to the inner atmosphere could be then electrically connected to a potentiostat. In a practical application, a sealed cell integrating a specific lid like a soda can should be shaped (air contact by peeling away this lid).