Supporting Information

1,4-Bis(trimethylsilyl)-2,5-Dimethoxybenzene As a Novel Redox Shuttle Additive for Overcharge Protection in LithiumIon Batteries

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Supplementary Figures and Tables

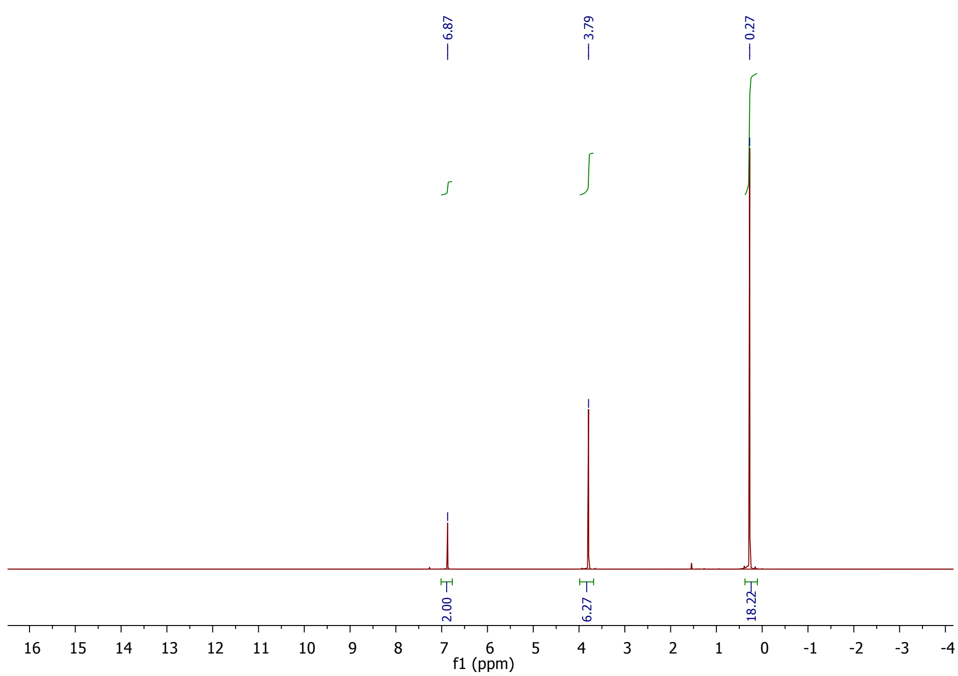

Figure S1. ^{1}H NMR of BTMSDB

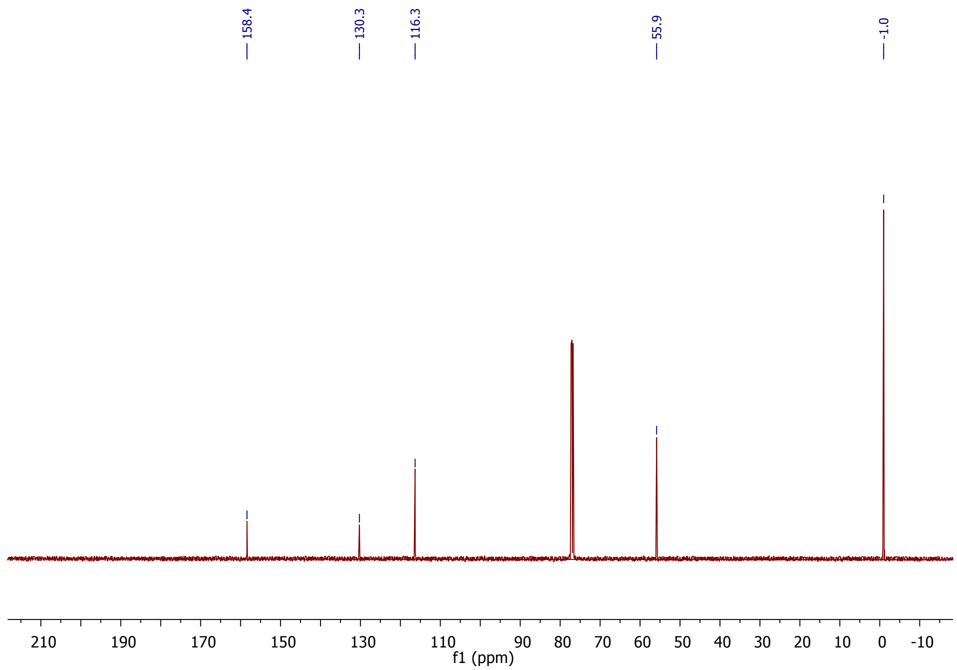

Figure S2. ^{13}C NMR of BTMSDB

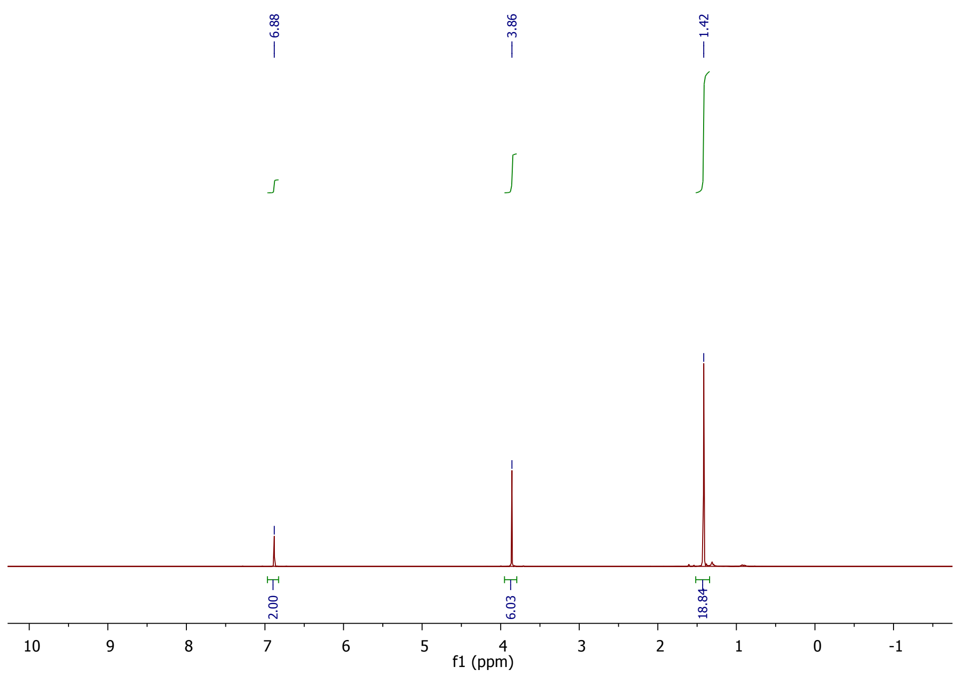

Figure S3. ^{1}H NMR of DDB

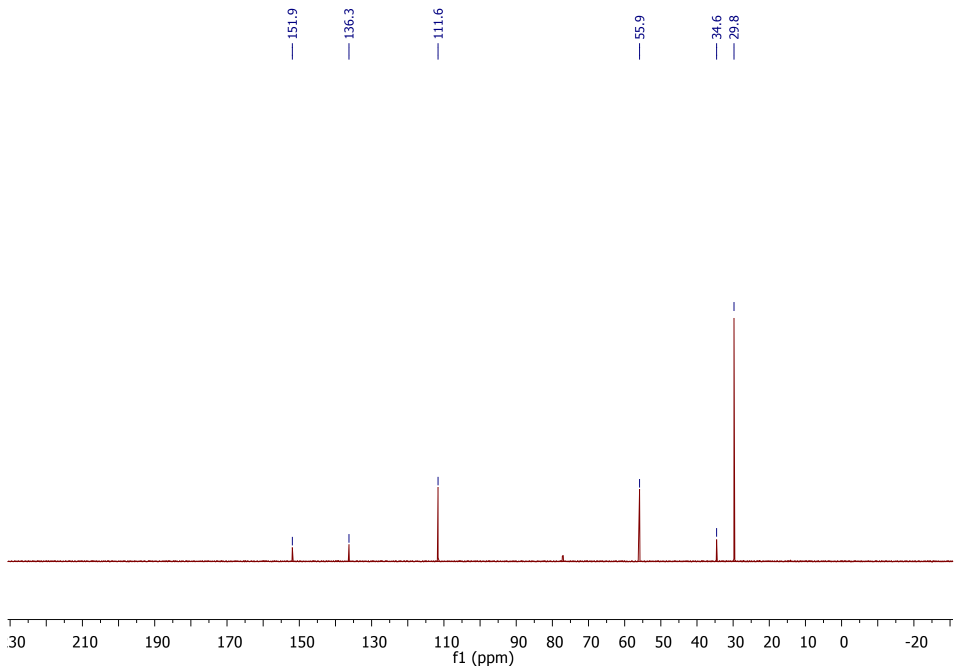

Figure S4. ^{13}C NMR of DDB

Table S1. Ratio of the anodic/cathodic peak currents *vs*. the scan rate

scan rate mV/s	**current ratio**
5	1.04
10	1.01
20	1.00
25	1.00
50	1.03
100	1.01

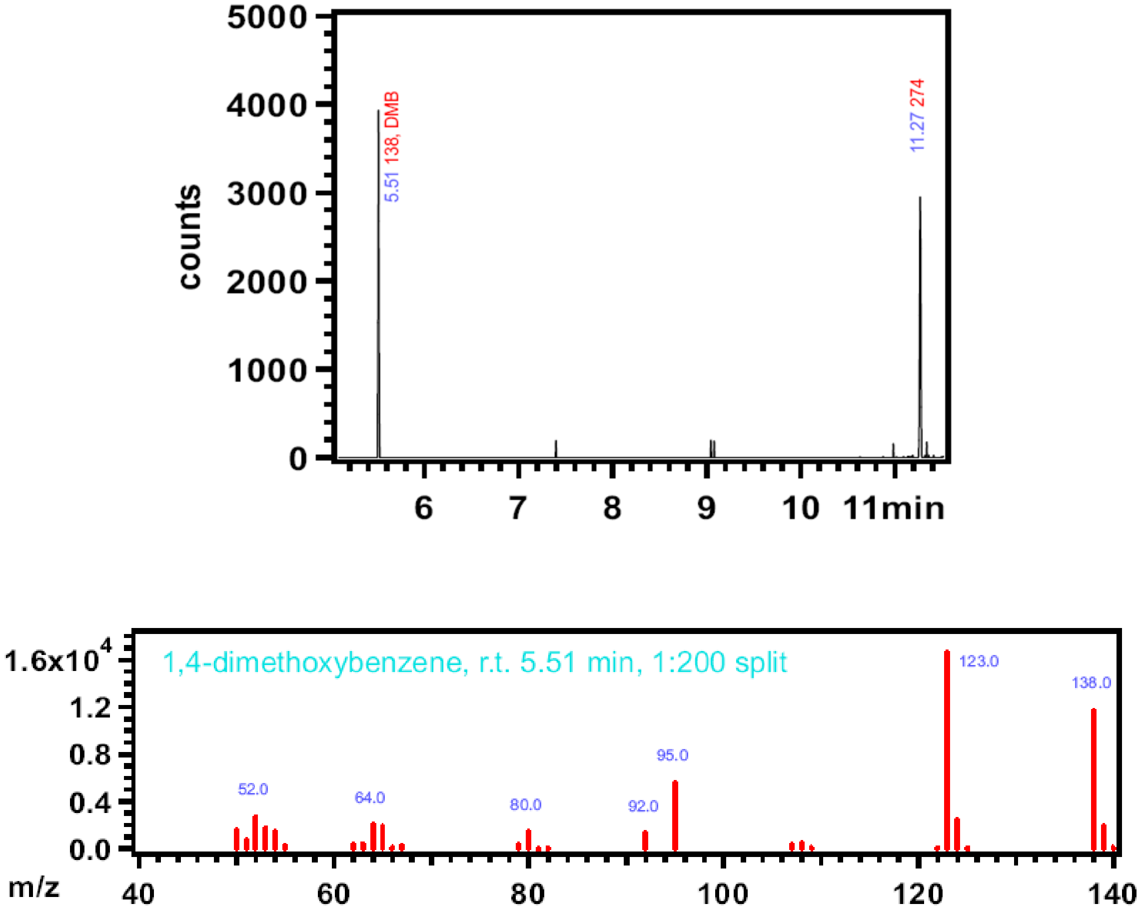

Figure S5. GCMS of the harvested electrolyte

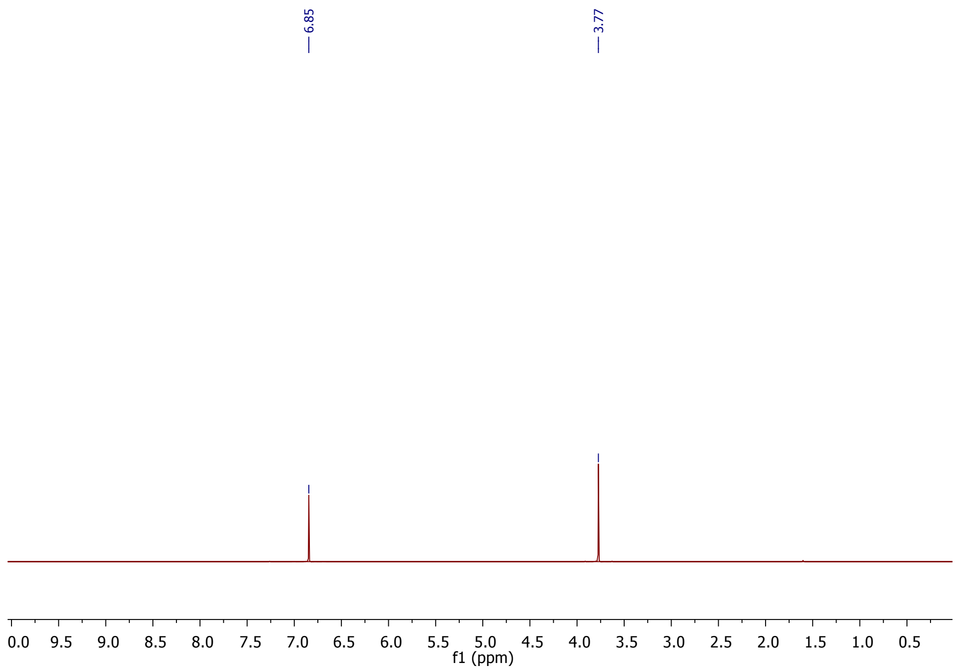

Figure S6. ^{1}H NMR of 1,4-dimethoxybenzene

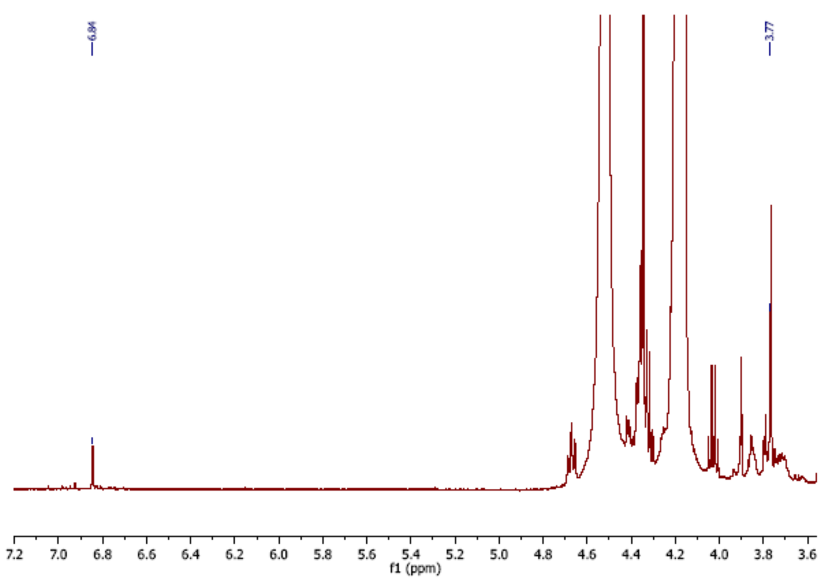

Figure S7. ^{1}H NMR of the harvested electrolyte

Table S2. Summary of *g*-factors and ^{1}H and ^{29}Si hyperfine coupling constants (hfcc, Gauss) [1] for radical cations of DDB and BTMDSB

Progenitor	(g-2)x10^4	hfcc calculated [a]	hfcc, chemical [b]	hfcc, electrochemical [c]
DDB	48.8 [b], 42.9 [c]	6H (MeO) 3.69, 2H 0.11, 18H (*t*Bu) 0.16	4H 3.22, 2H 1.02	4H 3.21, 2H 1.01, 18H 0.10
BTMSDB	49.1 [b], 48.4 [c]	6H (MeO) 3.82, 2H 0.80, 2 ^{29}Si 1.57	6H 3.34, 2H 1.76, 2 ^{29}Si 1.58	6H 3.32, 2H 1.77, 2 ^{29}Si 1.58

a) DFT calculation for the gas-phase radical cation

b) chemical oxidation by [bis(trifluoroacetoxy)iodo]benzene

c) electrochemical oxidation by constant potential bulk electrolysis.

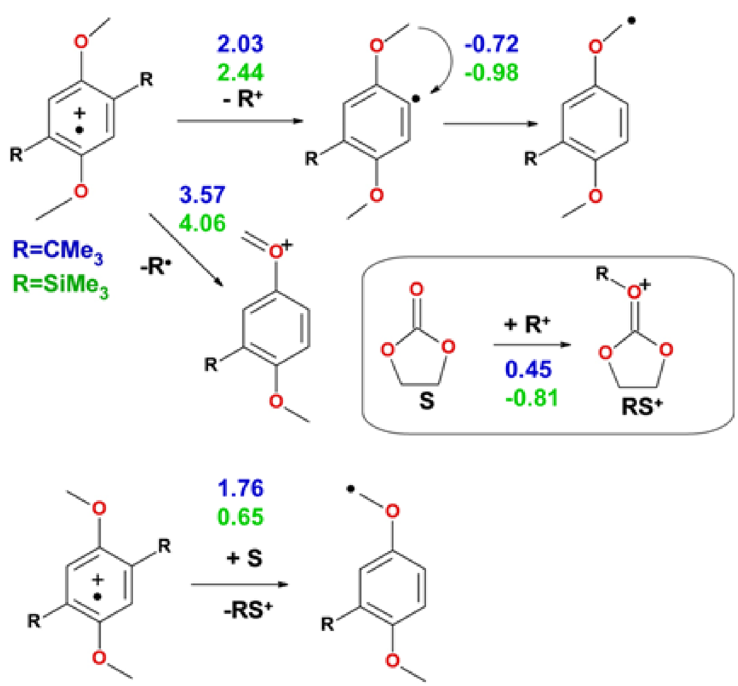

Figure S8. Decomposition reactions of radical cations

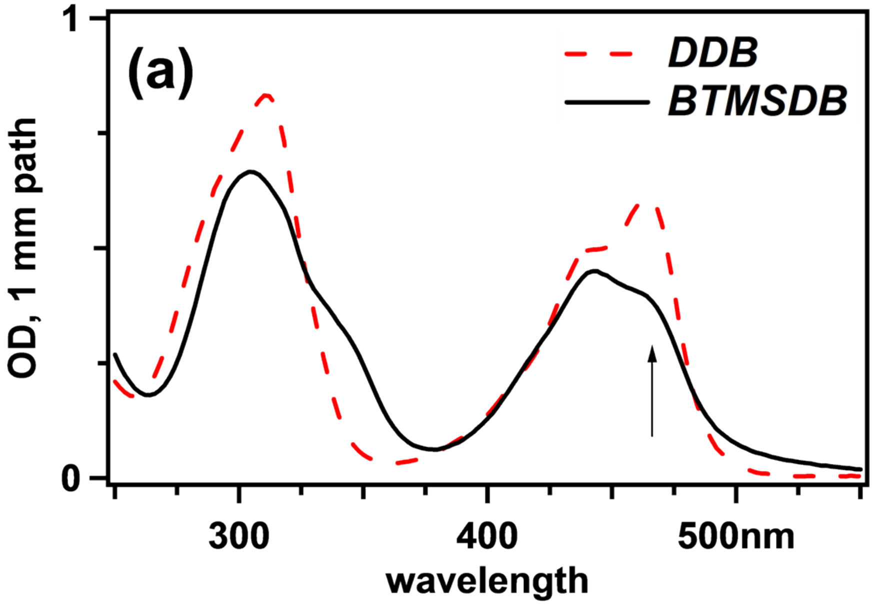

Figure S9. UV spectra of BTMSDB and DDB