

Supplementary Information

Preparation of endohedral fullerene containing lithium (Li@C₆₀) and
isolation as pure hexafluorophosphate salt ([Li⁺@C₆₀][PF₆⁻])

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Fig. S1. LDI-TOF mass spectra of Li@C₆₀-enriched brown solid (**B**) in the range of m/z 680 to 800.

(a) Linear positive mode and (b) reflectron negative mode.

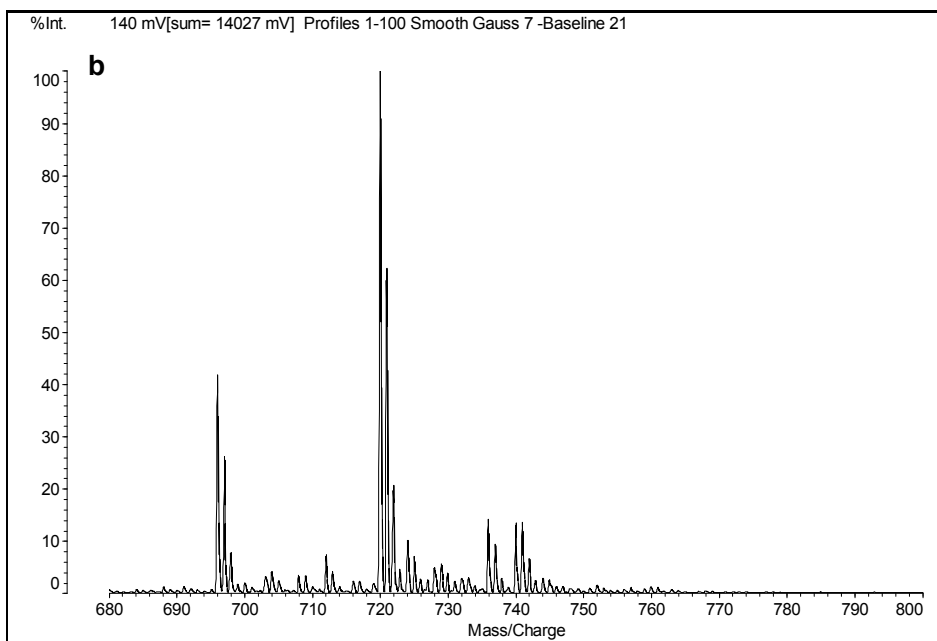
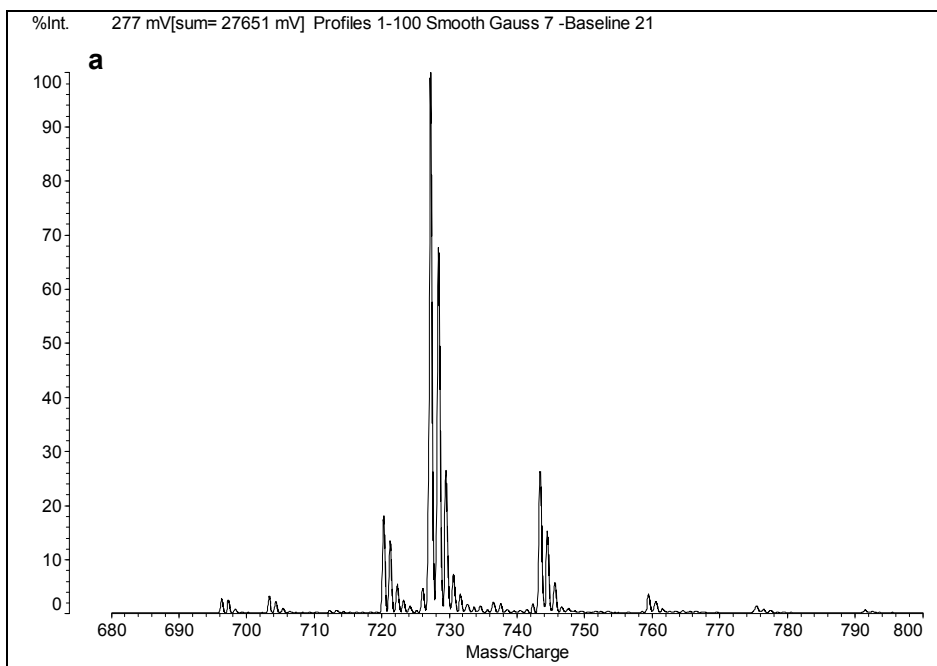


Fig. S2. Dynamic light scattering of 1-chloronaphthalene solutions of (a) Li@C₆₀-enriched brown solid (**B**) and (b) C₆₀.

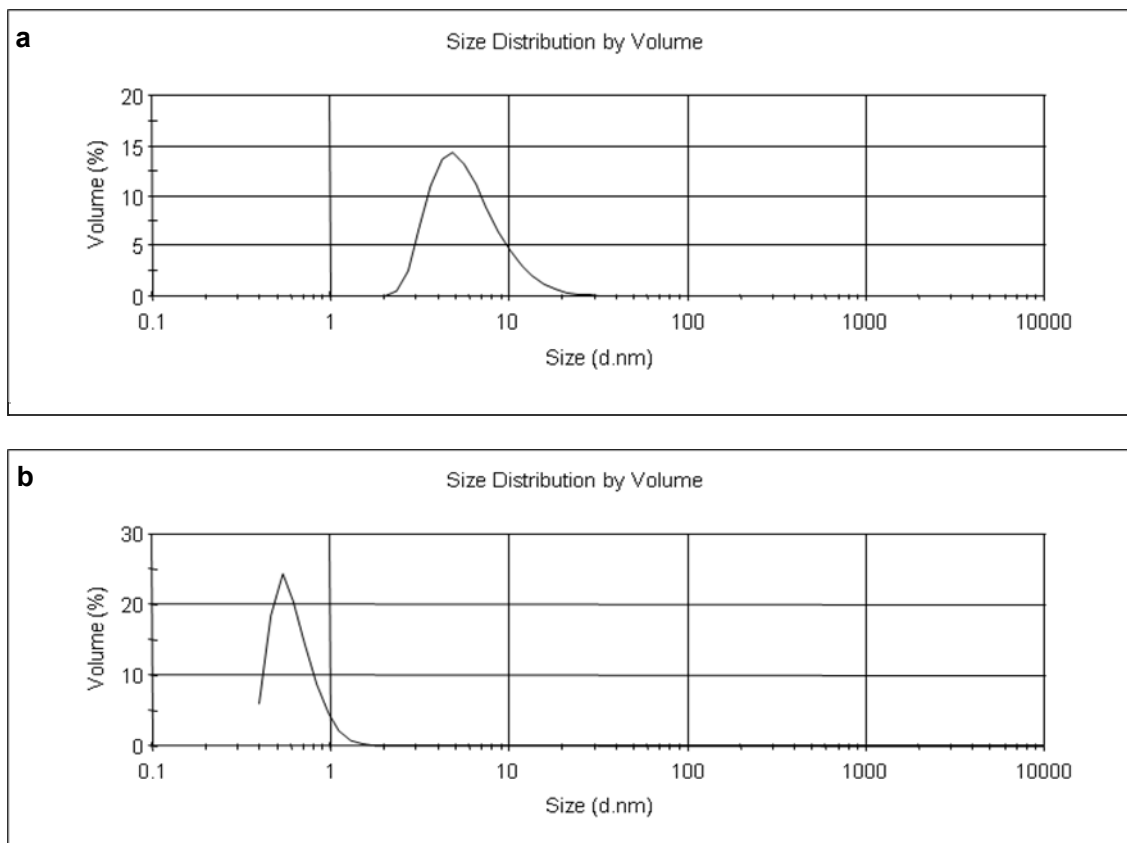


Fig. S3. LDI-TOF mass spectra of $[\text{Li}^+@C_{60}][\text{PF}_6^-]$. (a) Reflectron positive mode and (b) reflectron negative mode. The spectra in the range of m/z 700 to 800 are shown in the inset.

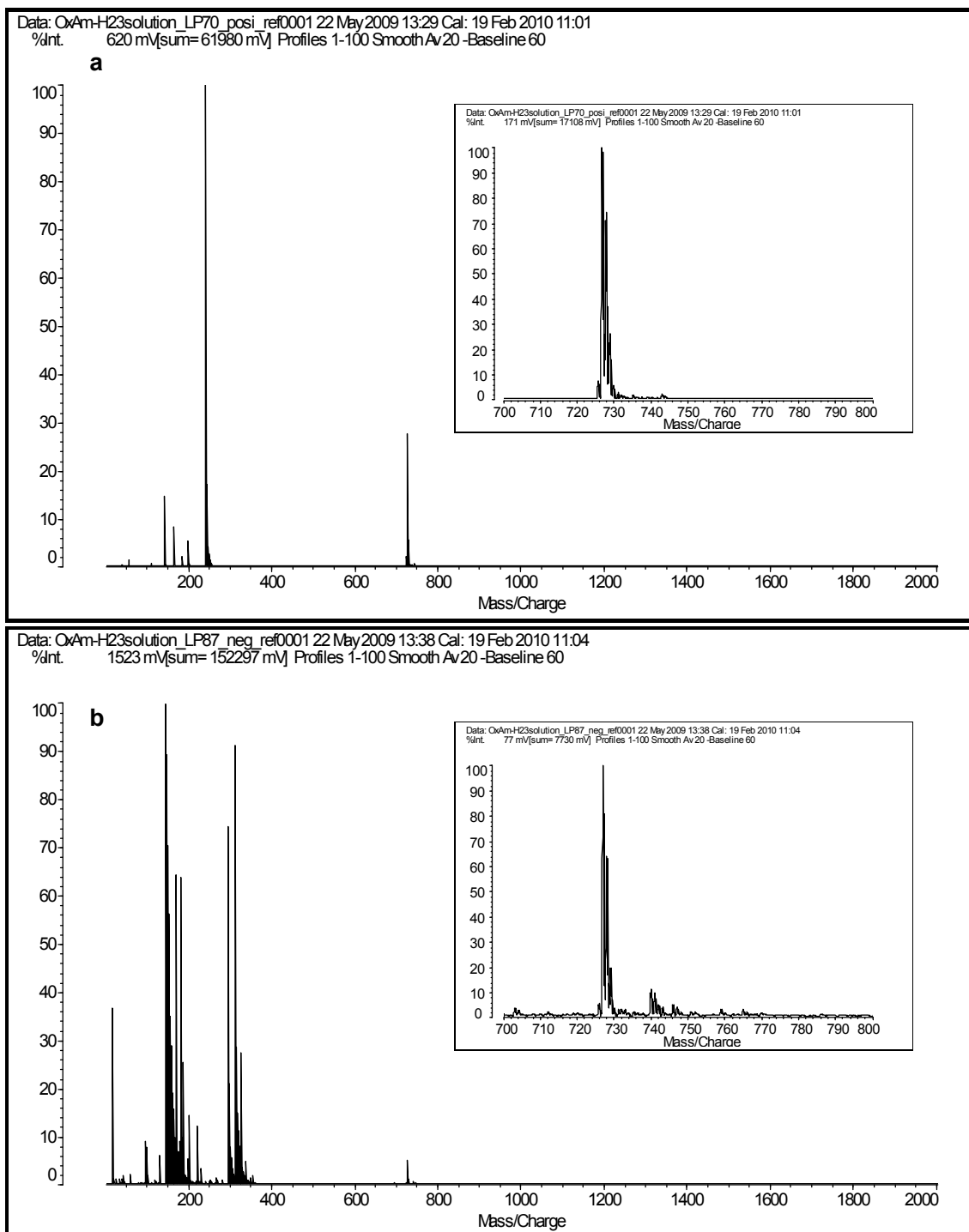


Fig. S4. A ^7Li NMR spectrum of $[\text{Li}^+\text{@C}_{60}][\text{PF}_6^-]$
(117 MHz, *o*-dichlorobenzene- d_4 /acetonitrile- $d_3 = 1/1$).

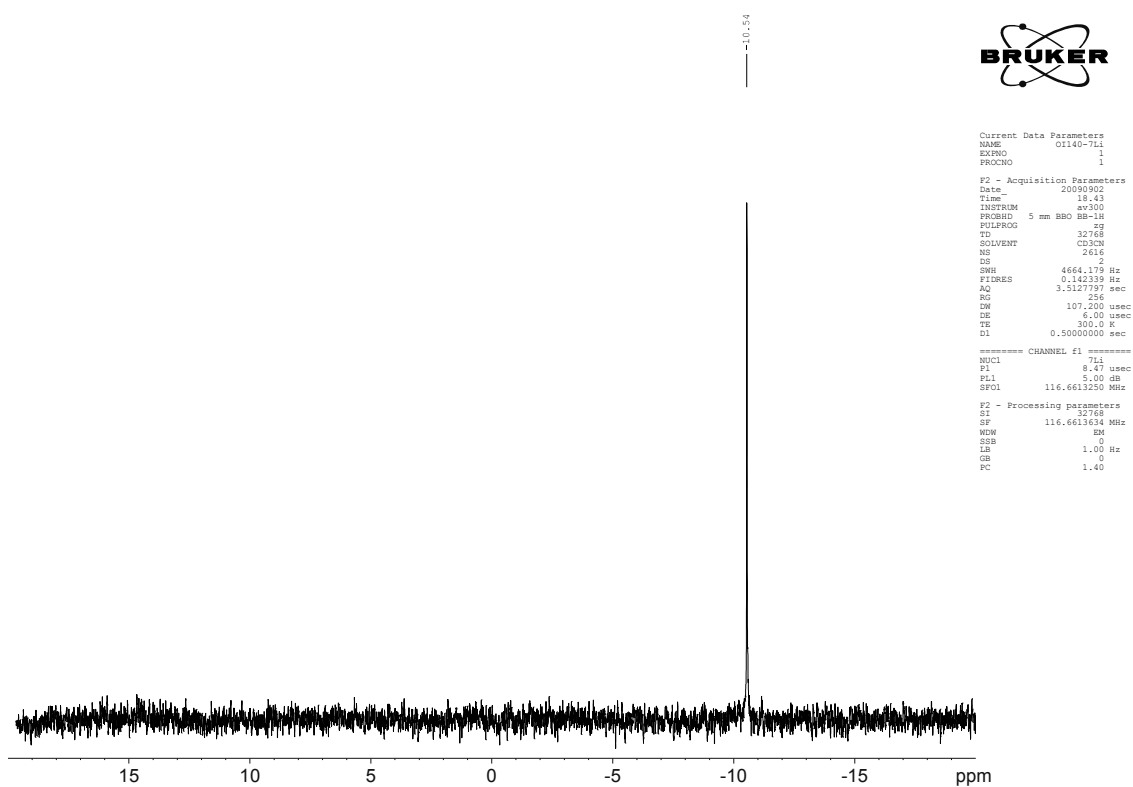
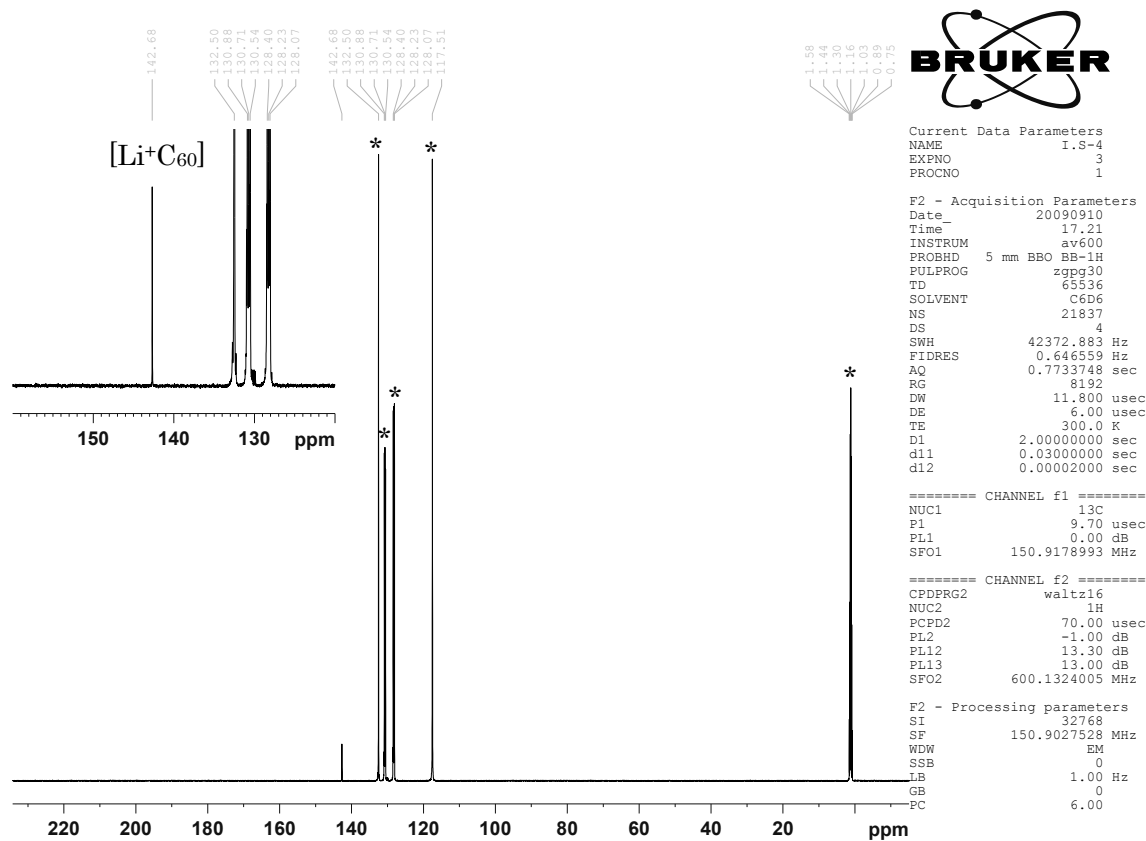


Fig. S5. A $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of $[\text{Li}^+\text{C}_{60}][\text{PF}_6^-]$ (151 MHz, *o*-dichlorobenzene- d_4 /acetonitrile- $d_3 = 1/1$). The spectrum in the range of 120 to 160 ppm is shown in the inset.



*: solvents