Supplementary Information

Two-Dimensional Hopping Motion of Encapsulated La Atoms in Silylated $La_2@C_{80}$

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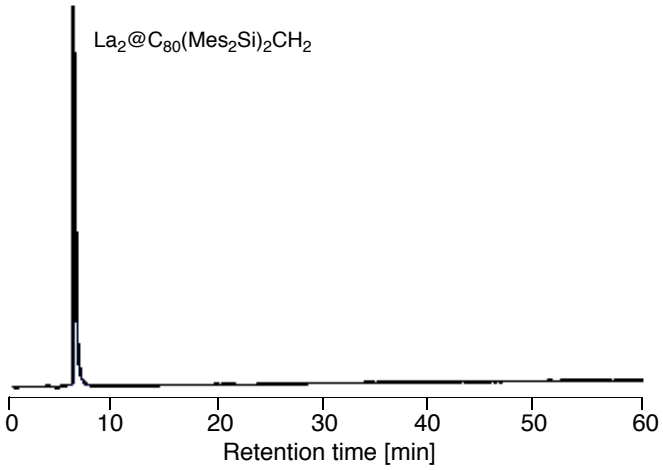
(a)



(b)

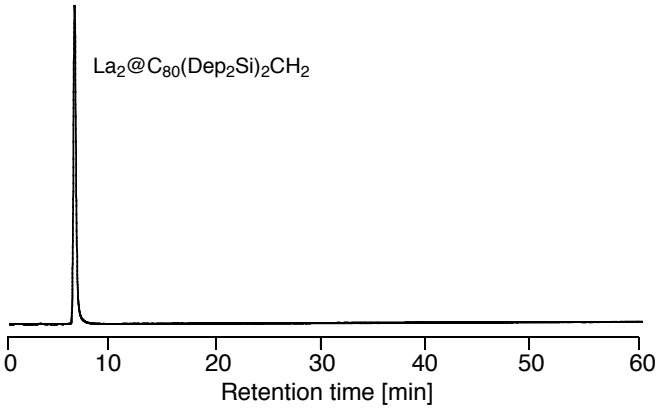
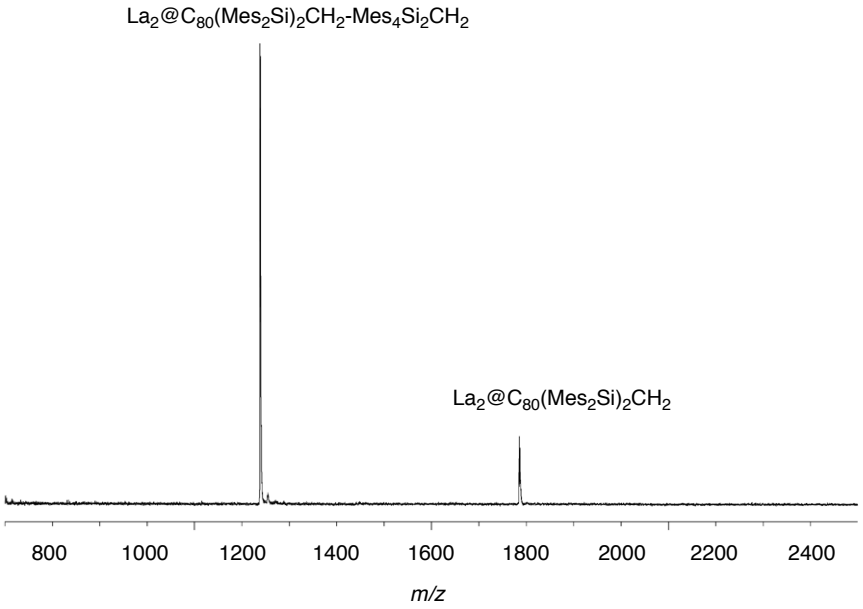


Figure S1. HPLC profiles of isolated (a) **3a** and (b) **3b**; column, Buckyprep ϕ4.6 mm × 250 mm; eluent, toluene 1.0 mL/min. 330 nm UV detection was used.

(a)



(b)

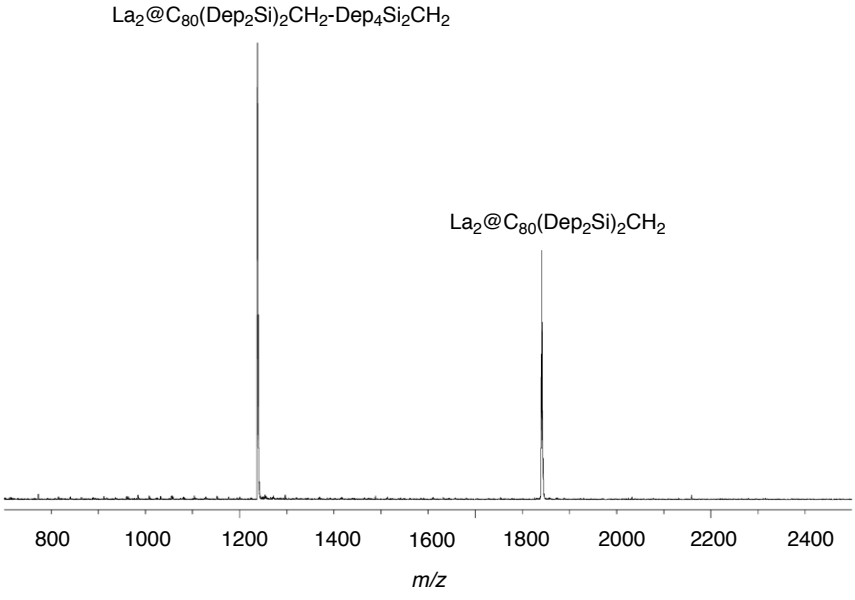


Figure S2. MALDI-TOF Mass spectra of isolated (a) **3a** and (b) **3b**. The spectra were recorded in negative mode with 9-nitroanthracene as matrix.

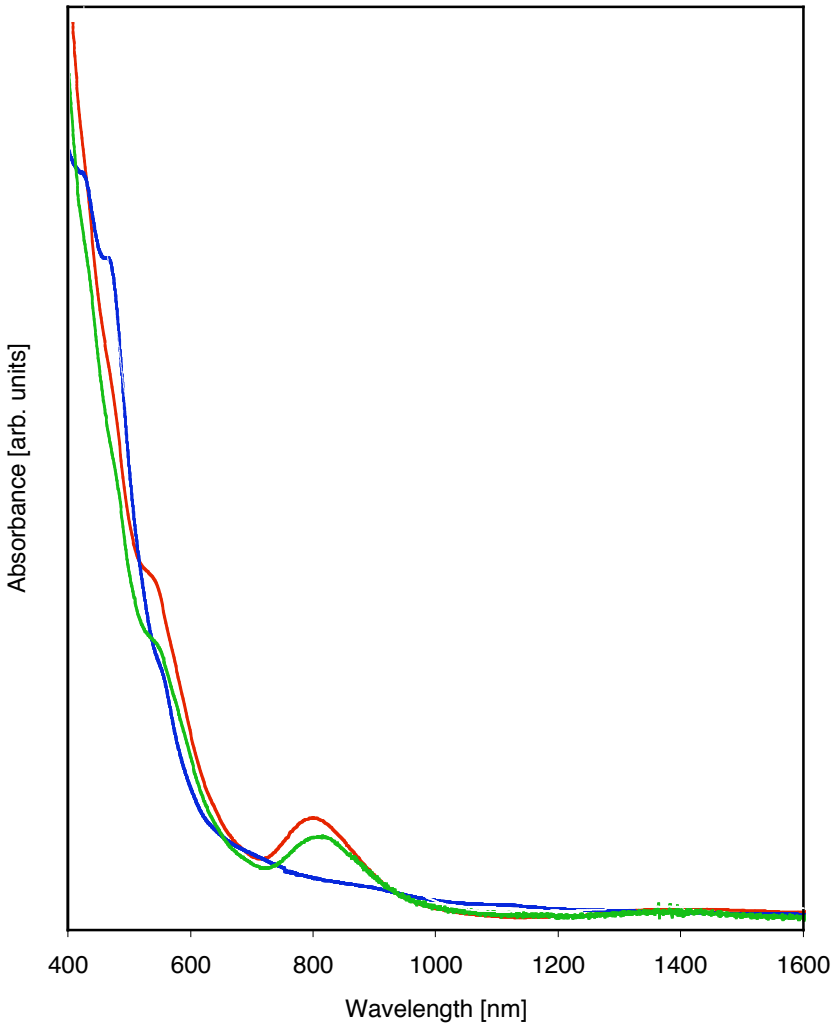
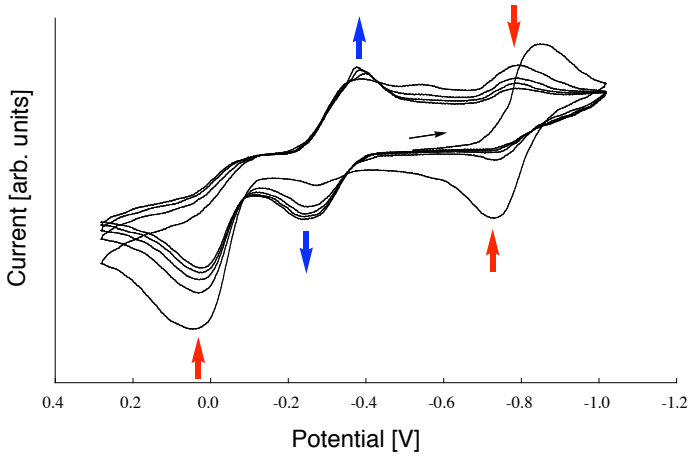


Figure S3. Vis-near-IR spectra of isolated **3a** (green line), **3b** (red line), and $La_2@C_{80}$ (blue line).

(a)



(b)

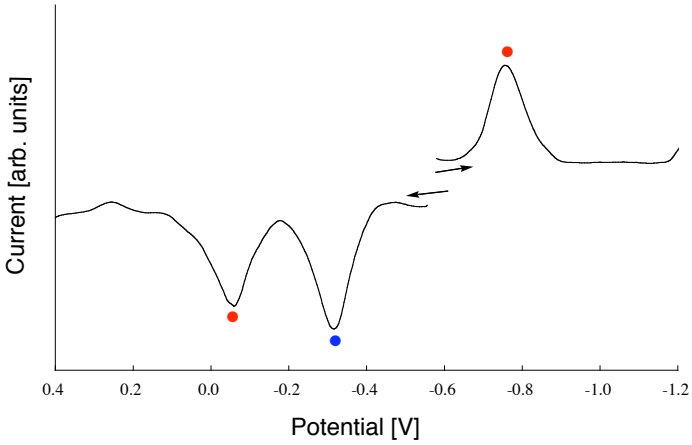
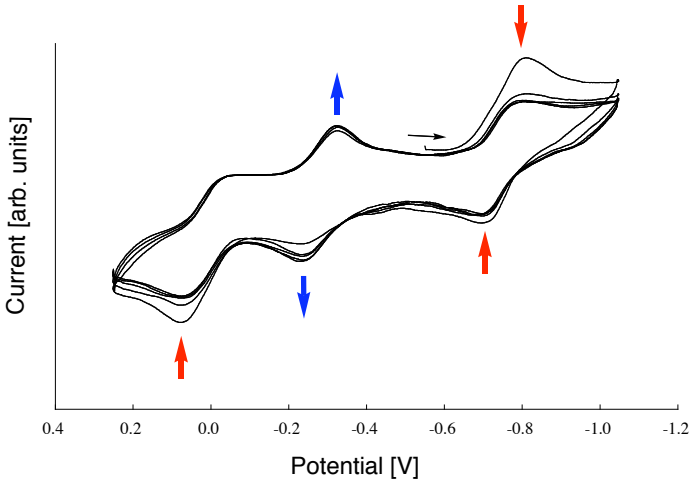


Figure S4. (a) Cyclic and (b) differential pulse voltammograms of **3a**. The peaks of **3a** and the peaks of $La_2@C_{80}$ formed by retro-cycloaddition are marked as red and blue arrows (circles), respectively.

(a)



(b)

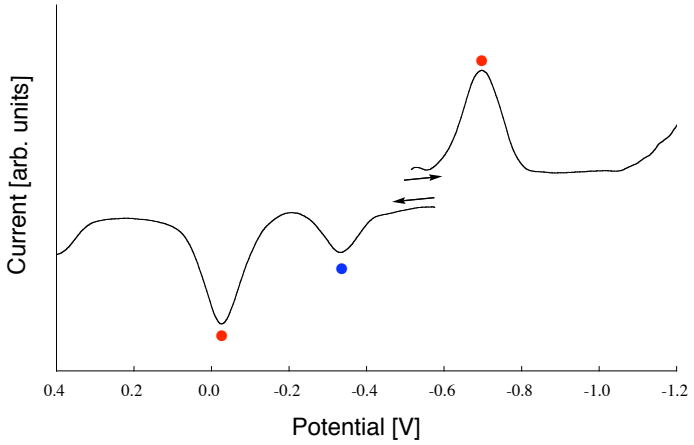


Figure S5. (a) Cyclic and (b) differential pulse voltammograms of **3b**. The peaks of **3b** and the peaks of $La_2@C_{80}$ formed by retro-cycloaddition are marked as red and blue arrows (circles), respectively.

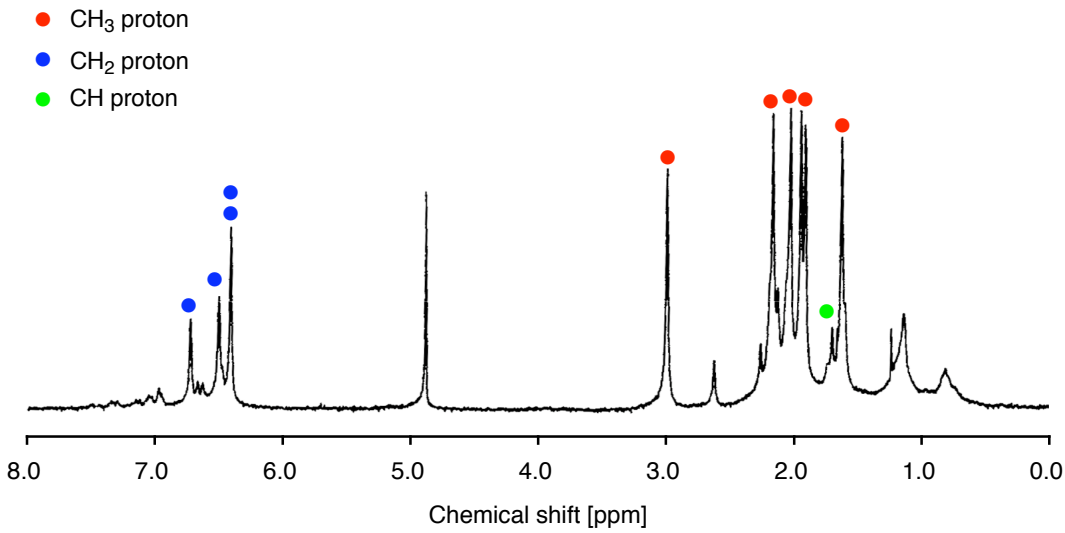


Figure S6. ^{1}H NMR spectrum (300 MHz) of **3a** in CS_2/CD_2Cl_2 (3/1) at 213 K.

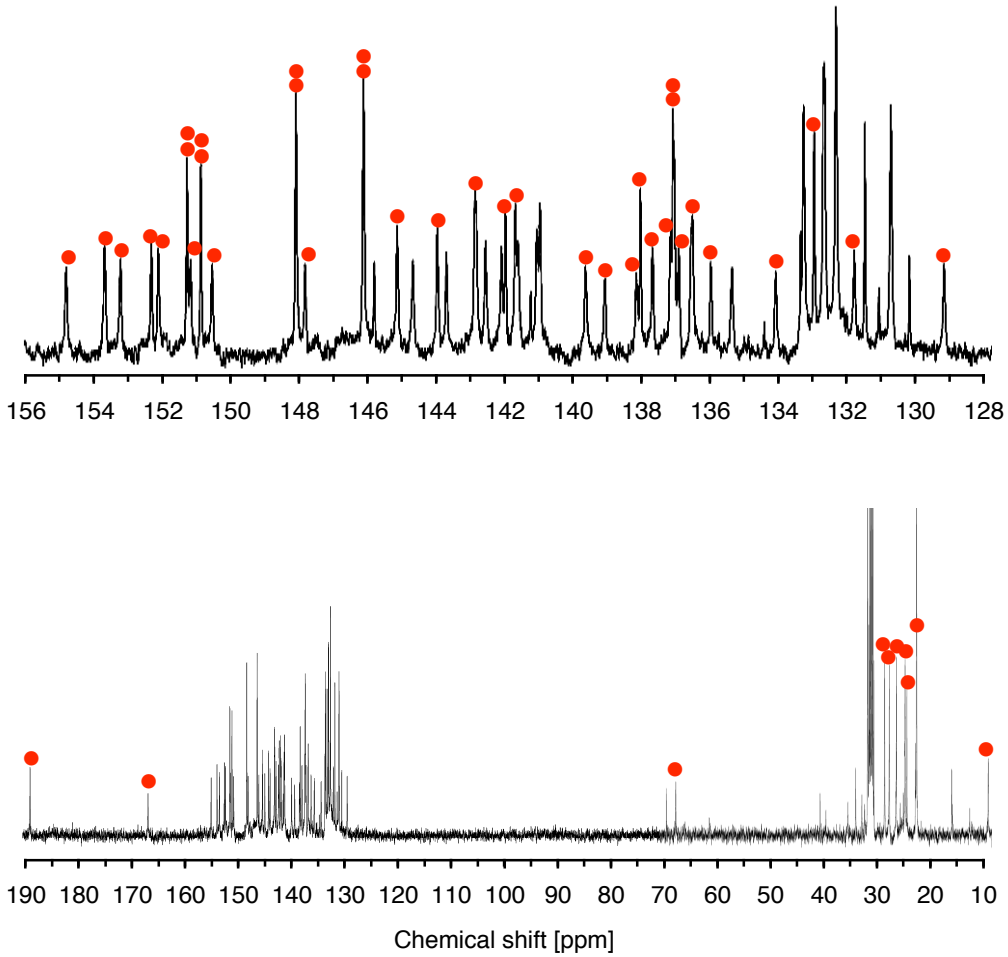


Figure S7. ^{13}C NMR spectrum (125 MHz) of **3a** in CS_2/CD_2Cl_2 (3/1) at 213 K.

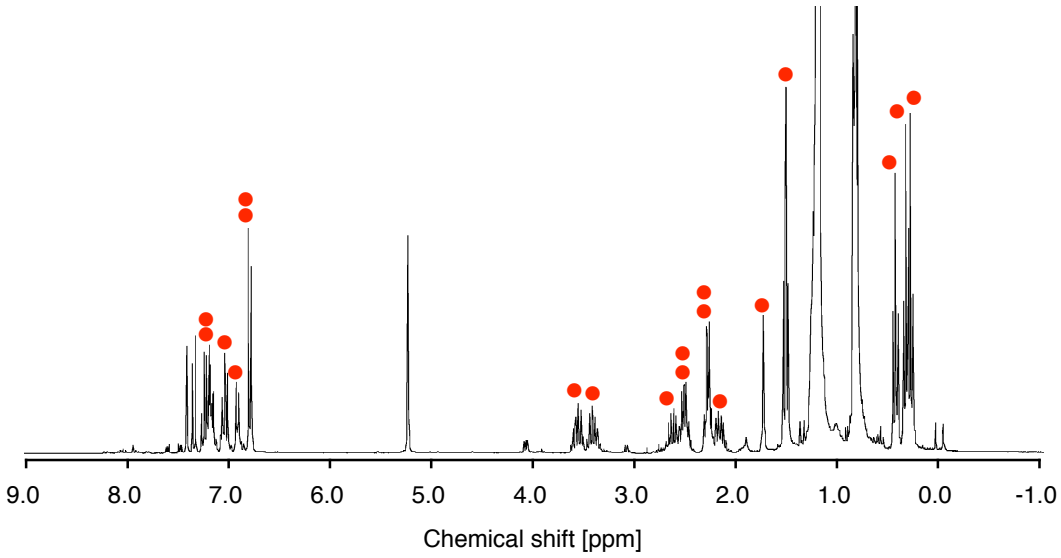


Figure S8. ^{1}H NMR spectrum (500 MHz) of **3b** in CS_2/CD_2Cl_2 (3/1) at 288 K.

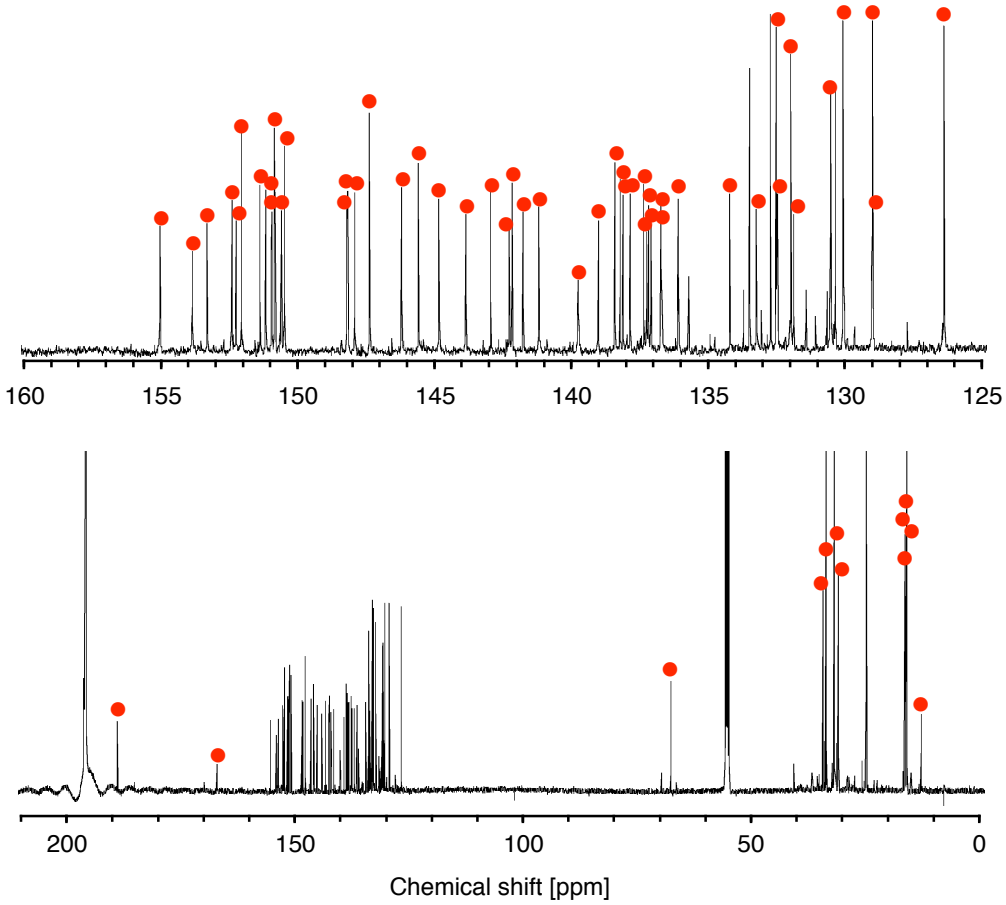


Figure S9. ^{13}C NMR spectrum (500 MHz) of **3b** in CS_2/CD_2Cl_2 (3/1) at 288 K.

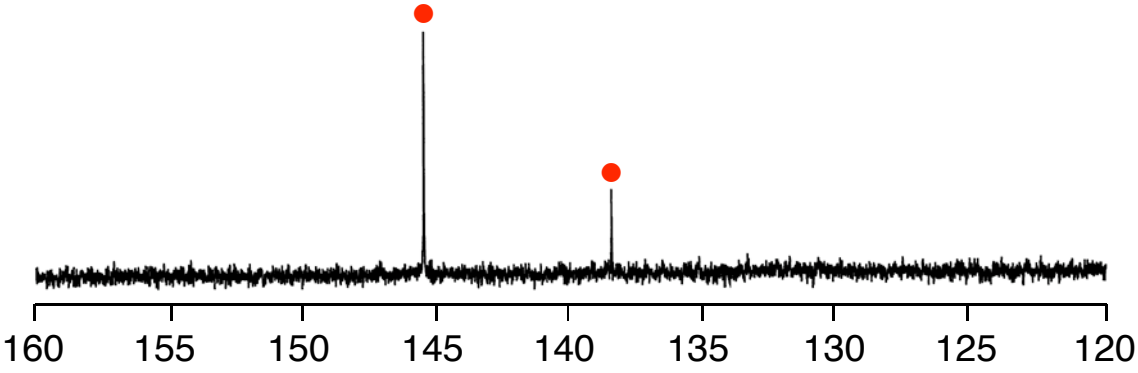


Figure S10. ^{13}C NMR spectrum (150 MHz) of $La_2@C_{80}$ in CS_2 (acetone-d_6 in capillary as lock solvent) at 298 K.

Table S1. Redox Potentials[a] of **3a**, **3b** and $La_2@C_{80}$

Compound	E_{ox}	E_{red}
3a	-0.06[b]	-0.76
3b	-0.03[b]	-0.70
$La_2@C_{80}$	0.56[c]	-0.31[c]

[a]Values are obtained by differencial pulse voltammetry in Volts relative to ferrocene/ferrocenium couple. Conditions: 0.1 M $(n\text{-Bu})_4NPF_6$ in 1,2-dichlorobenzene; working electrode, Pt disk; counter electrode, Pt wire; reference electrode, SCE. [b]Irreversible. [c]T. Suzuki, Y. Maruyama, T. Kato, K. Kikuchi, Y. Nakao, Y. Achiba, K. Kobayashi and S. Nagase, *Angew. Chem., Int. Ed. Engl.,* 1995, **34**, 1094.