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Supporting Information

for

Controlling the reactivity of La@C_{82} by reduction: reaction of the La@C_{82} anion with alkyl halide with high regioselectivity

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Additional experimental data

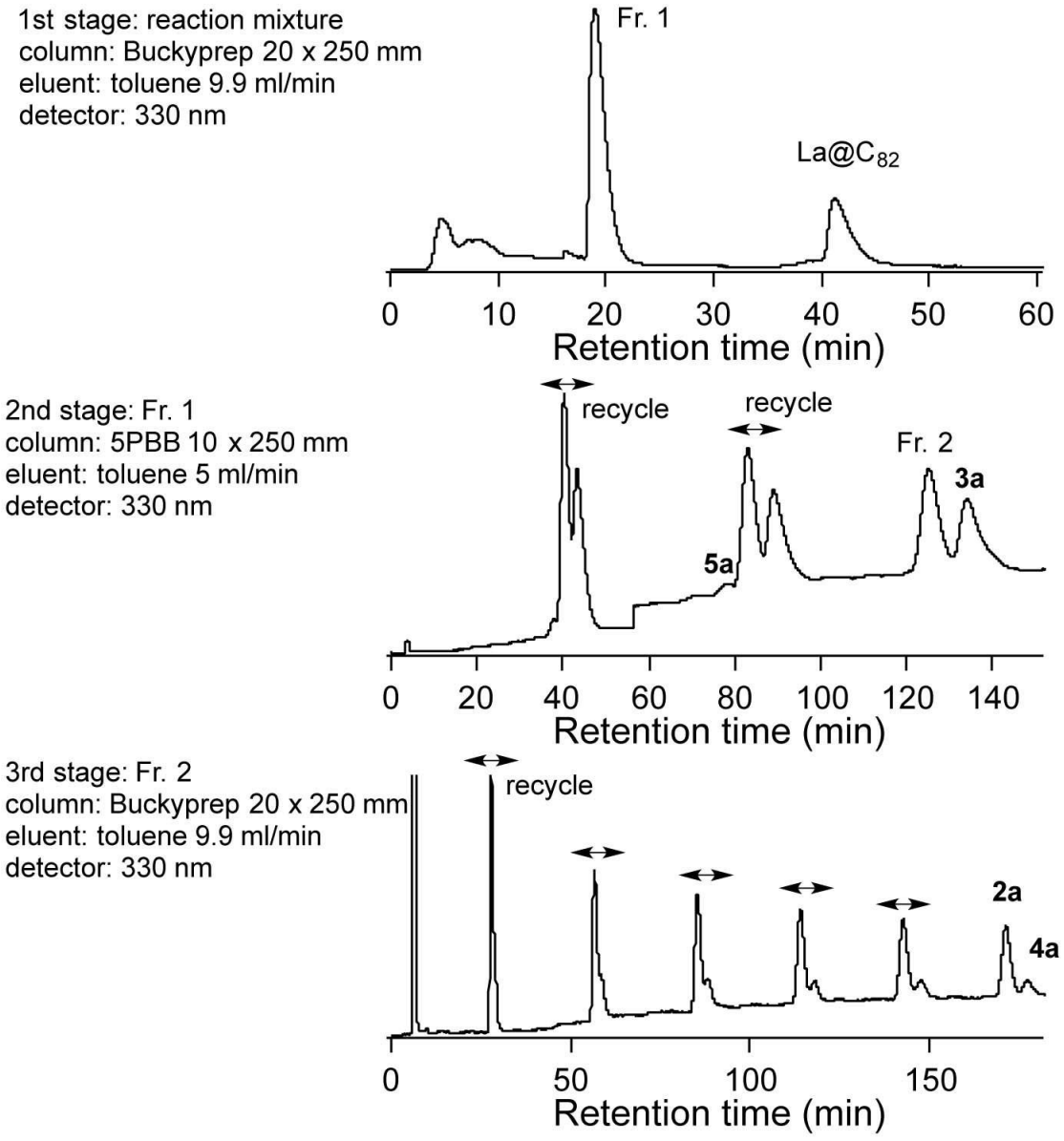

Figure S1: HPLC separation/isolation schemes for **2a**, **3a**, **4a**, and **5a**.

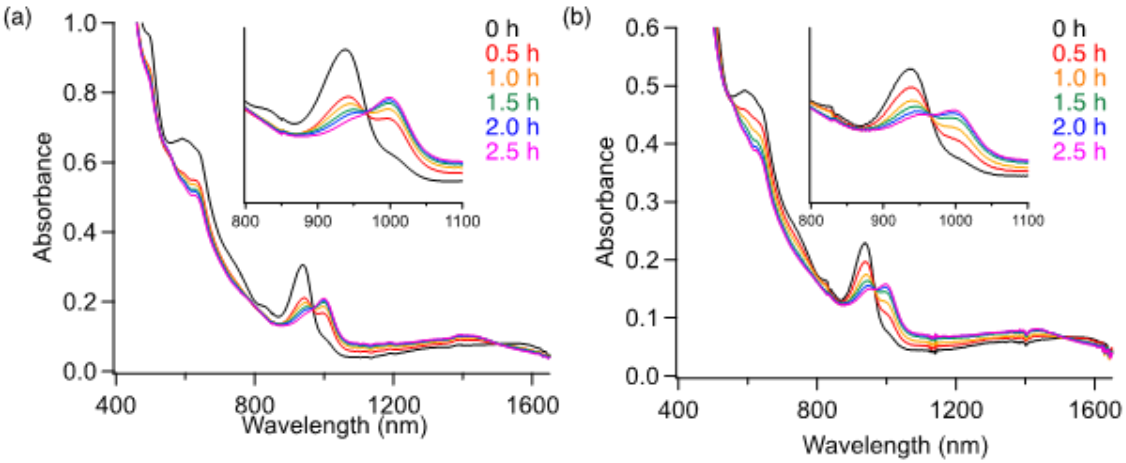

Figure S2: Changes in absorption spectra during the reaction of La@C_{2v}-C_{82} with (a) **1b** and (b) **1c**.

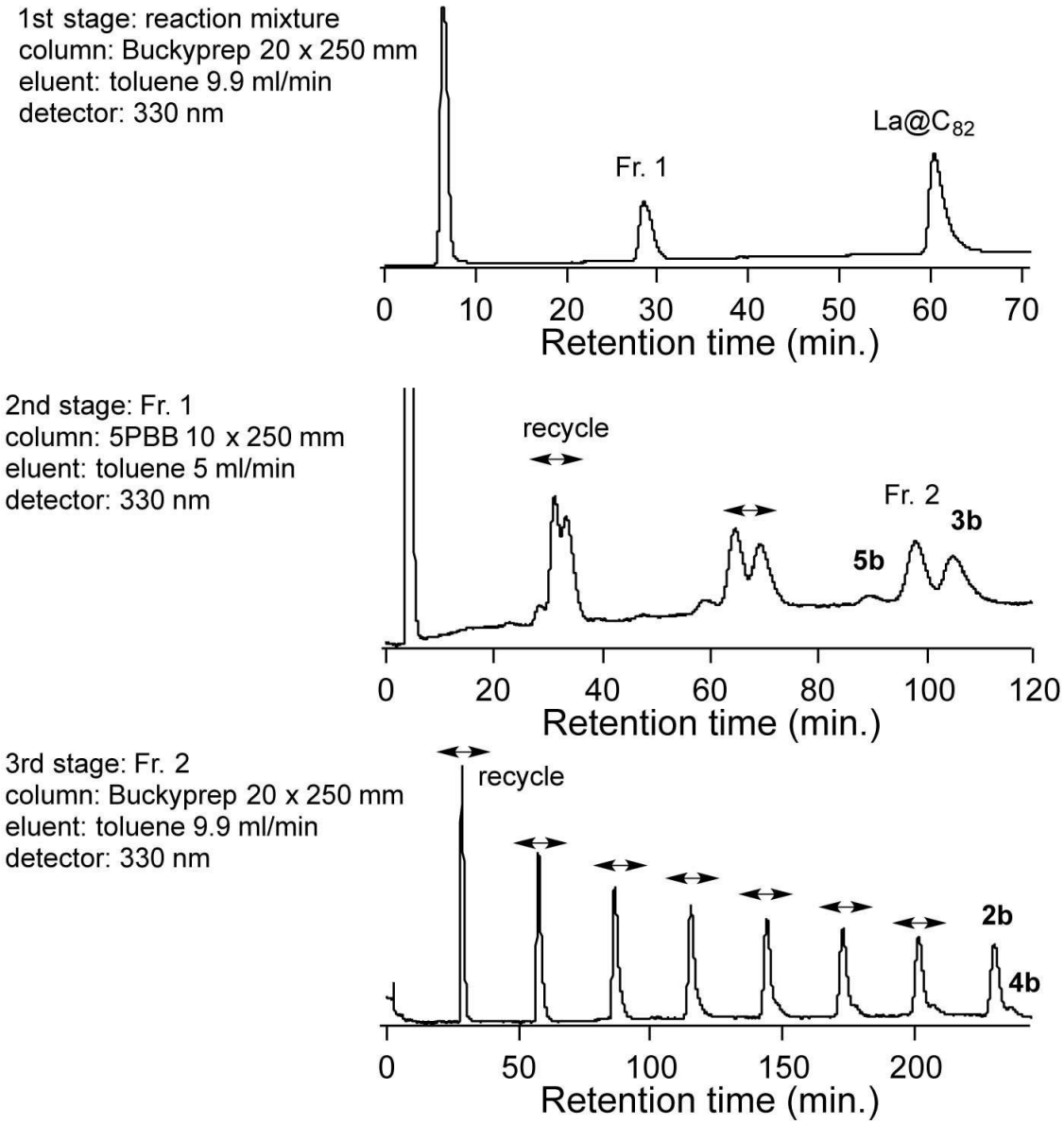

Figure S3: HPLC separation/isolation schemes for **2b**, **3b**, **4b**, and **5b**.

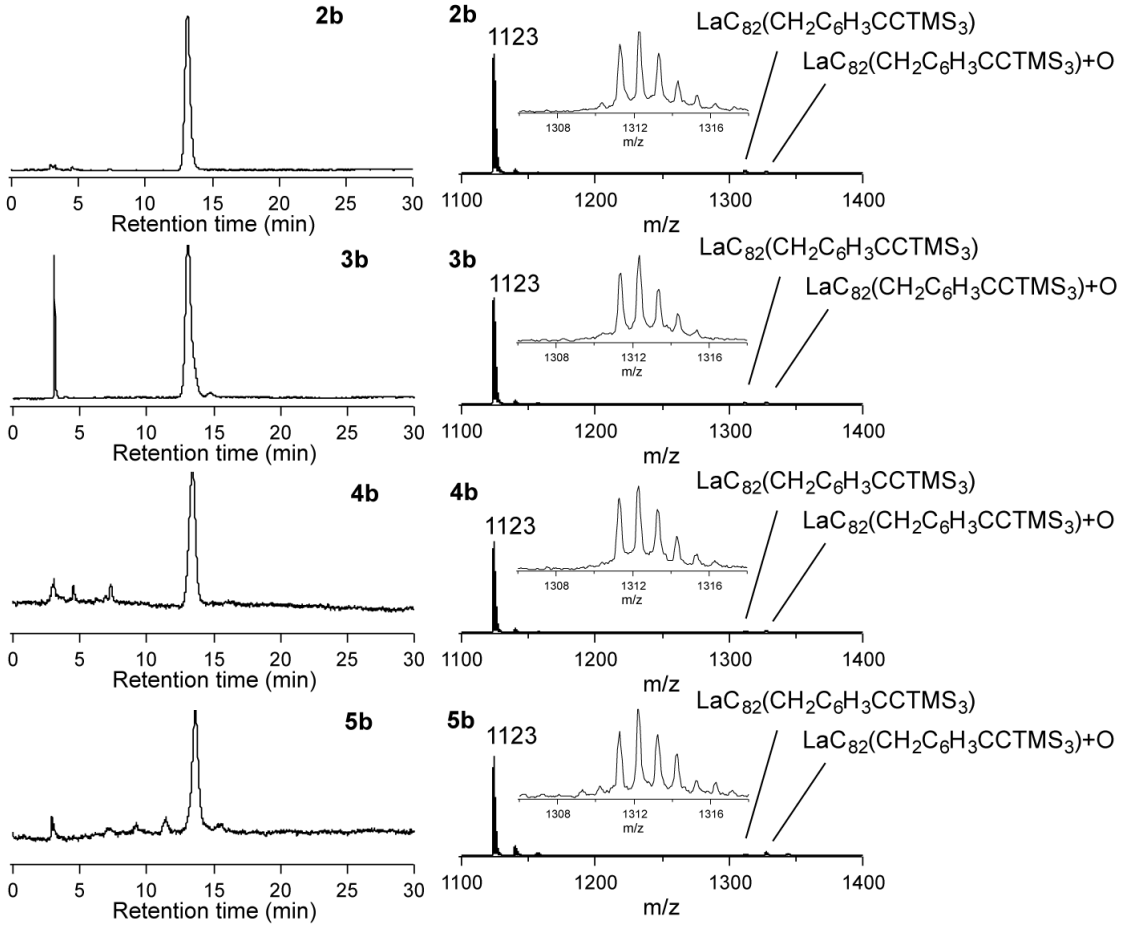

Figure S4: HPLC profiles and MALDI–TOF mass (positive mode) spectra of **2b**, **3b**, **4b**, and **5b**. HPLC conditions: column, Buckyprep (4.6 mm × 250 mm); eluent, toluene; flow rate, 1.0 mL/min; detector, UV detector, 330 nm.

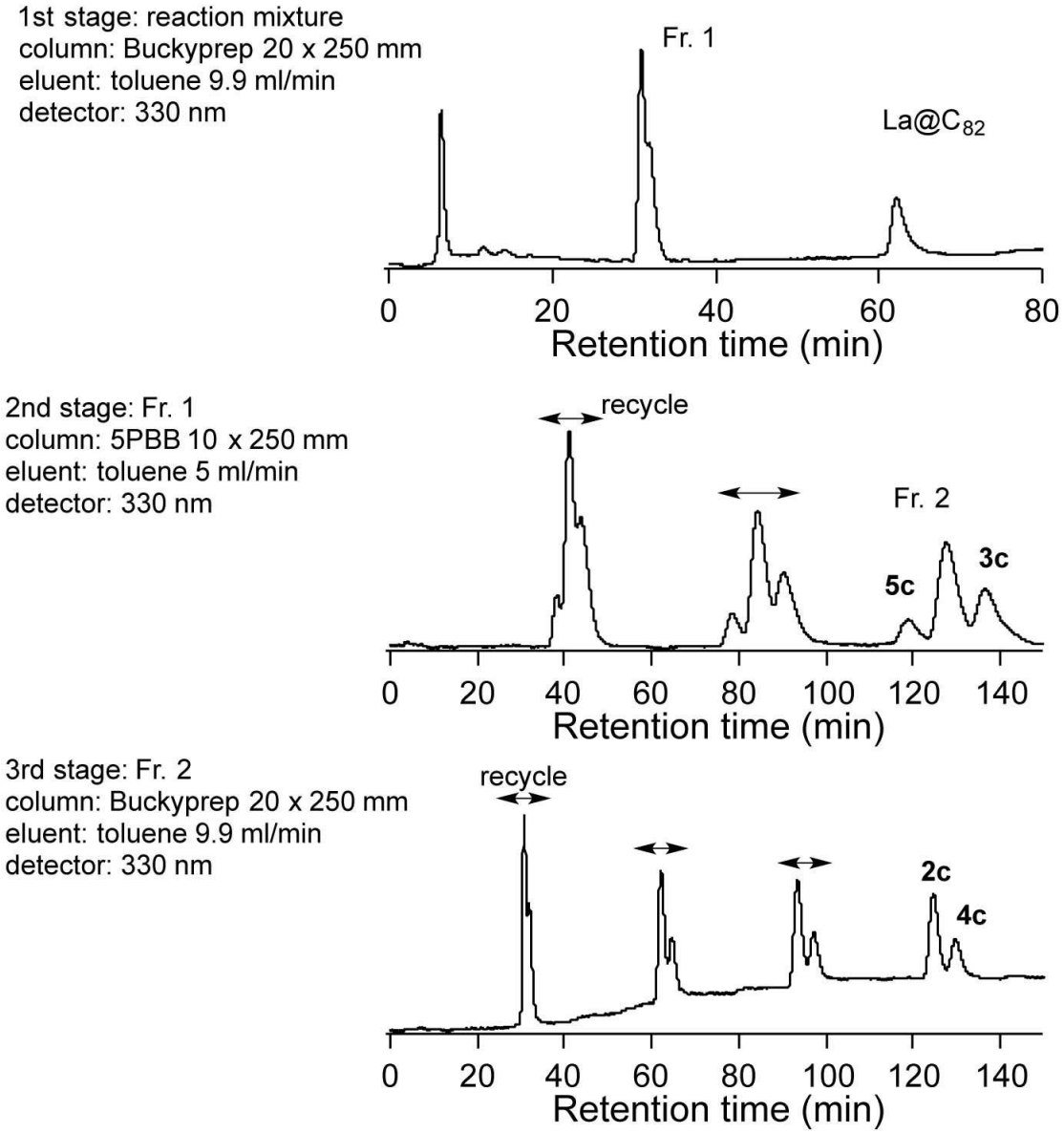

Figure S5: HPLC separation/isolation schemes for **2c**, **3c**, **4c**, and **5c**.

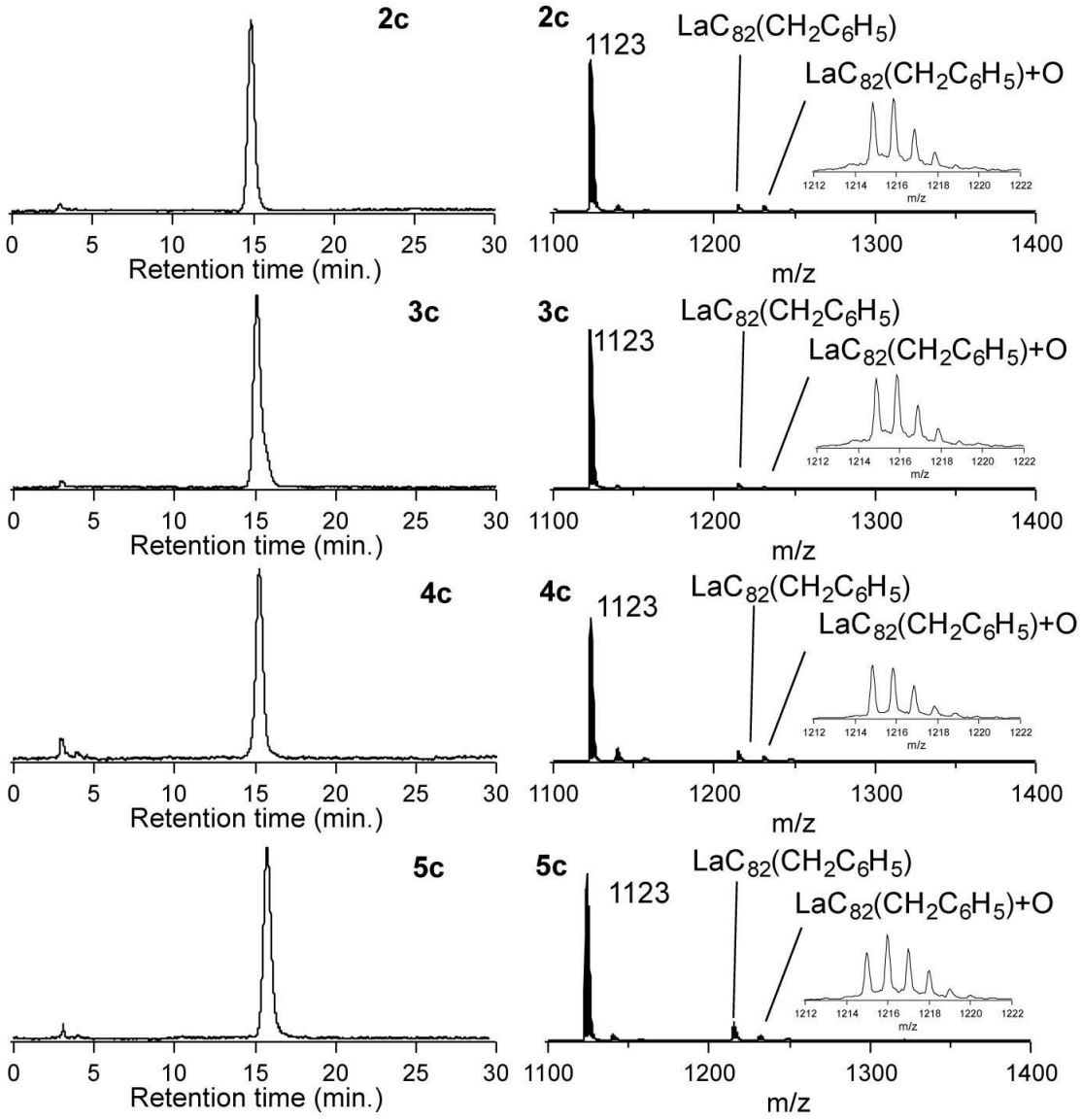

Figure S6: HPLC profiles and MALDI–TOF mass (positive mode) spectra of **2c**, **3c**, **4c**, and **5c**. HPLC conditions: column, Buckyprep (4.6 mm × 250 mm); eluent, toluene; flow rate, 1.0 mL/min; detector, UV detector, 330 nm.

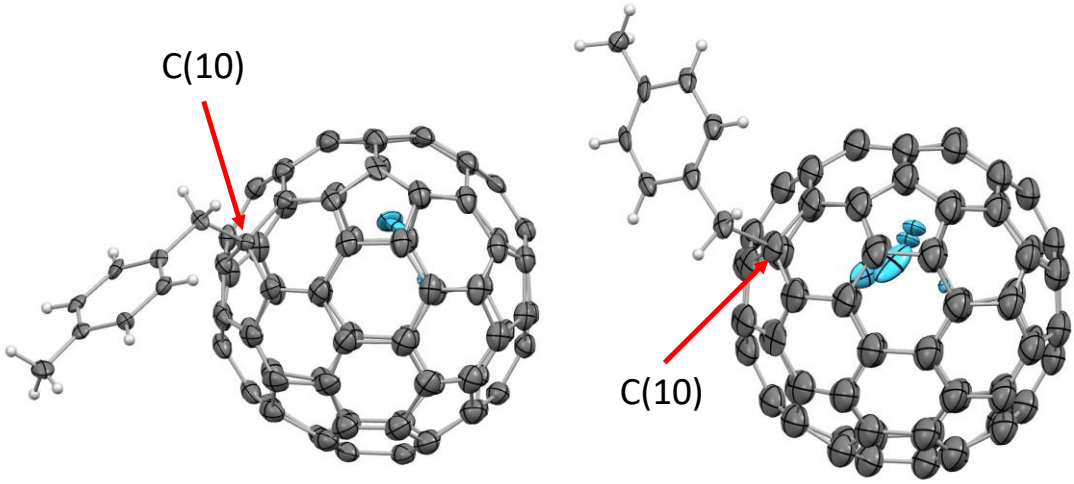

Figure S7: ORTEP drawings of an independent unit of **3a**.

Table S1: Crystal data of 2(**3a**)•3CS_2 (CCDC No. 2299232).

formula	$C_{183}H_{18}La_2S_6$
formula weight	2686.16
color, habit	black, block
crystal system	monoclinic
space group	$P2_1$ (No. 4)
T (K)	90
a (Å)	16.4784(8)
b (Å)	14.5513(8)
c (Å)	19.6146(9)
α (º)	90
β (º)	90
γ (º)	90
V (Å^3)	4703.2(4)
Z	2
ρ_{calc}	1.897
μ (mm^{-1})	1.110
crystal size (mm)	0.690 x 0.240 x 0.180
radiation (λ/Å)	fine-focus sealed tube (0.71073)
reflection collected	70164
independent reflections	36557
data ($I > 2\sigma(I)$)/parameter/restraints	33932/1771/4430
R_{int}	0.0486
R_1/wR_2/GOF (all data)	0.2235/0.5384/2.461
R_1/wR_2/GOF ($I > 2\sigma(I)$)	0.2180/0.5297/2.554

The reason for the large R value is that the quality of the crystal is poor. This crystal data suggested an orthorhombic space group, but an initial structure could not be obtained. Therefore, the initial structure was shown in the monoclinic space group when the symmetry was lowered. This crystal data was analyzed based on this initial structure.