



Supporting Information

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Experimental and Theoretical Studies of the Scandium Carbide Endohedral
Metallofullerene $\text{Sc}_2\text{C}_2@C_{82}$ and Its Carbene Derivative

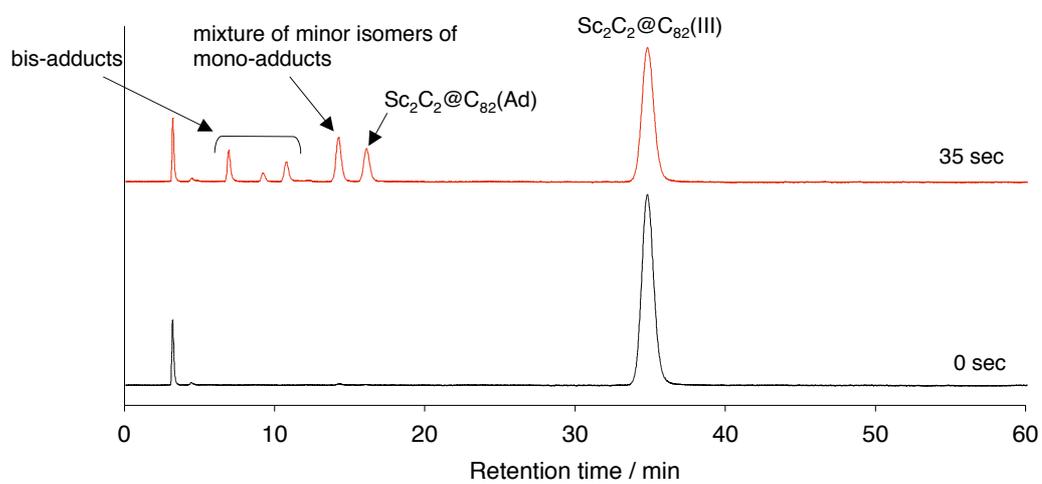
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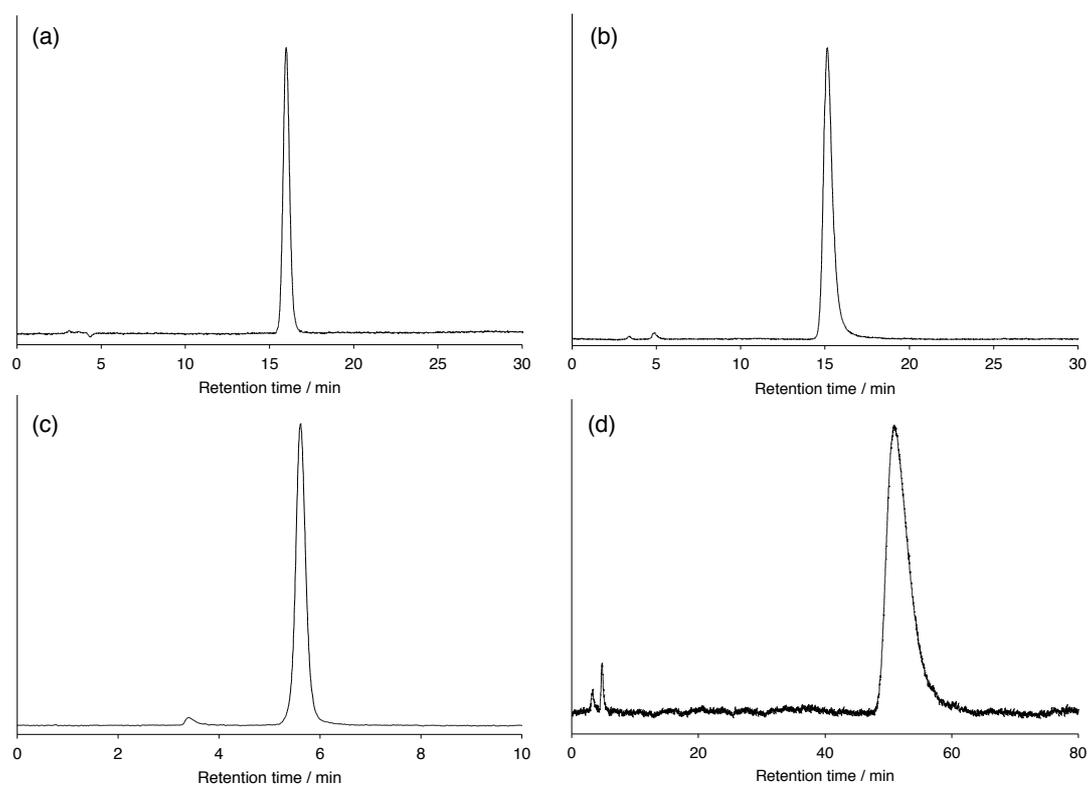
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Figure S1



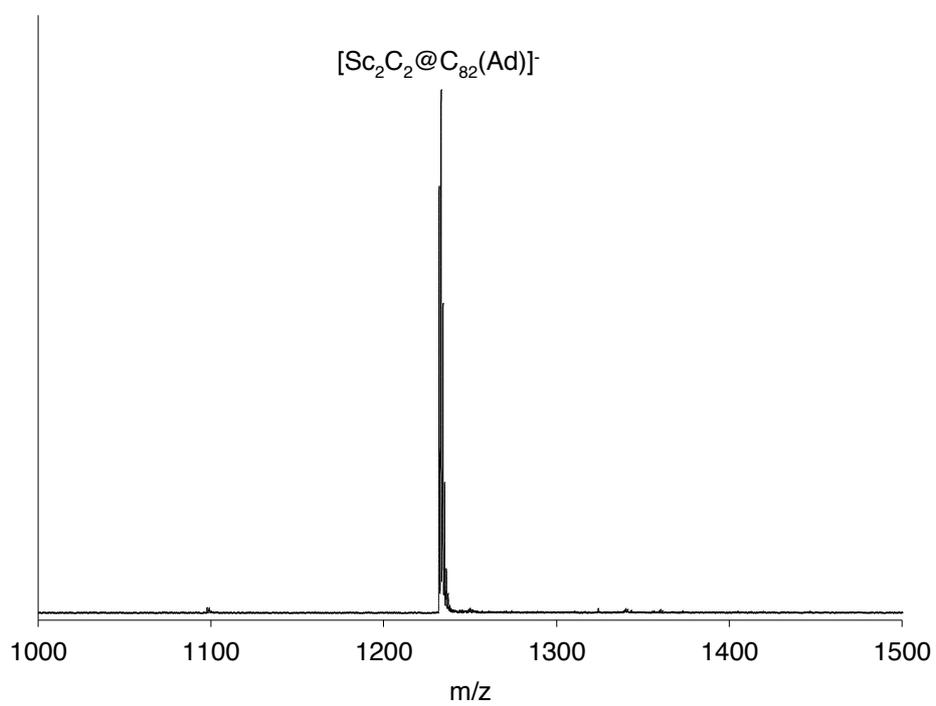
Conditions: column; Buckyprep $\phi 4.6 \times 20$ mm, eluent; toluene, flow rate; 1.0 mL/min. 330 UV detection was used.

Figure S2



Conditions: column; (a) Buckyprep $\phi 4.6 \times 20$ mm, (b) BuckyprepM $\phi 4.6 \times 20$ mm, (c) Buckyclutcher $\phi 4.6 \times 20$ mm, (d) 5PBB $\phi 4.6 \times 20$ mm, eluent; toluene, flow rate; 1.0 mL/min. 330 UV detection was used.

Figure S3



The spectrum was recorded in positive mode with 1,1,4,4-tetraphenyl-1,3-butadiene as matrix.

Figure S4

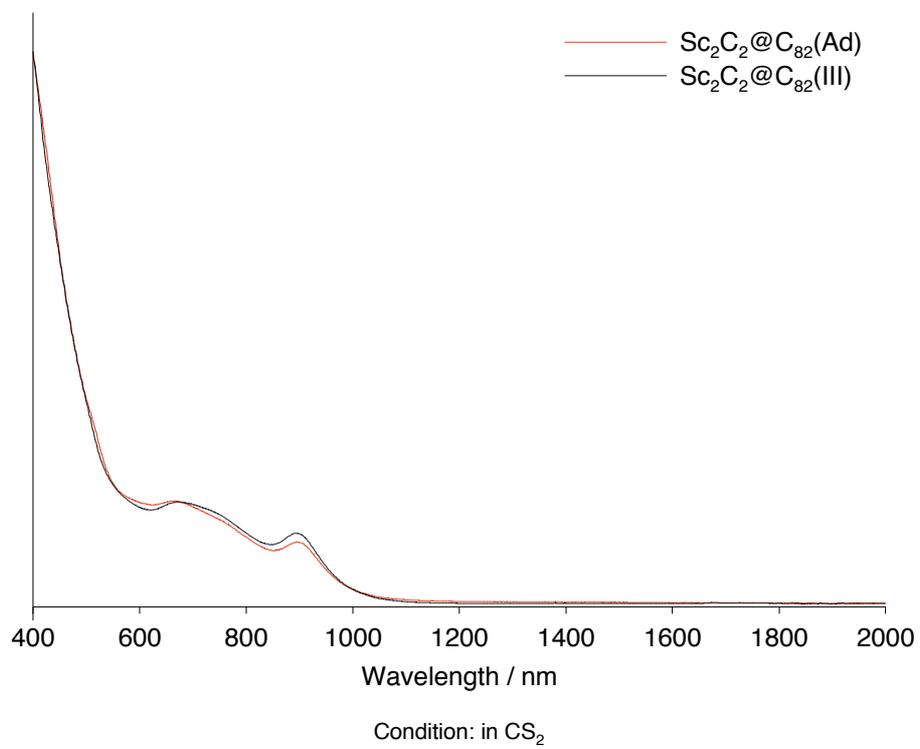
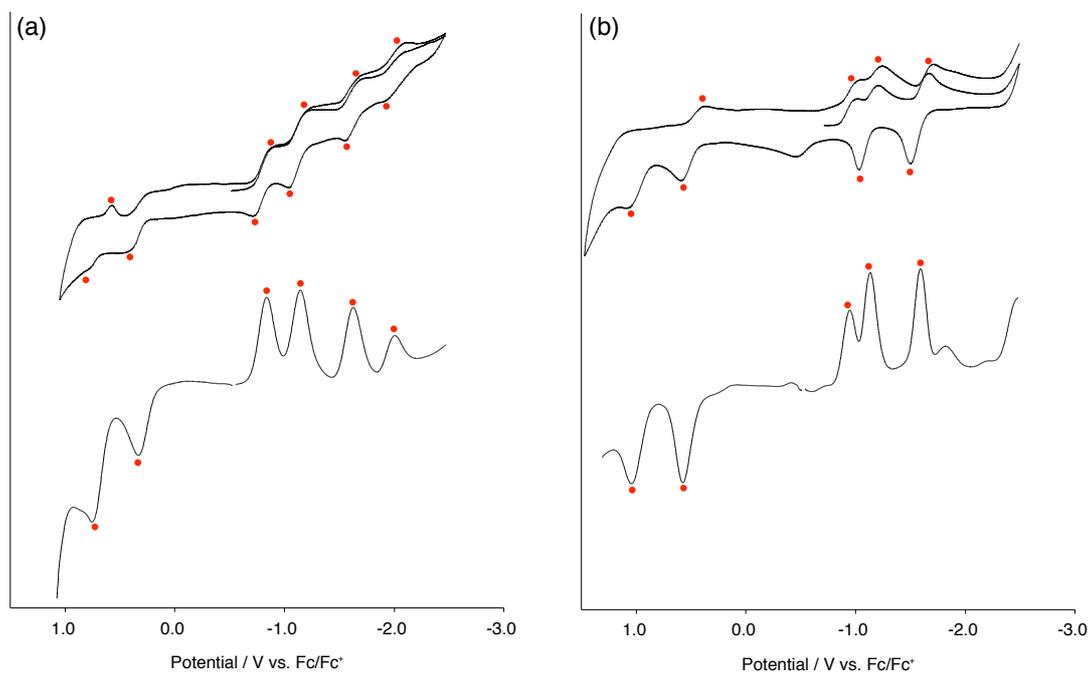
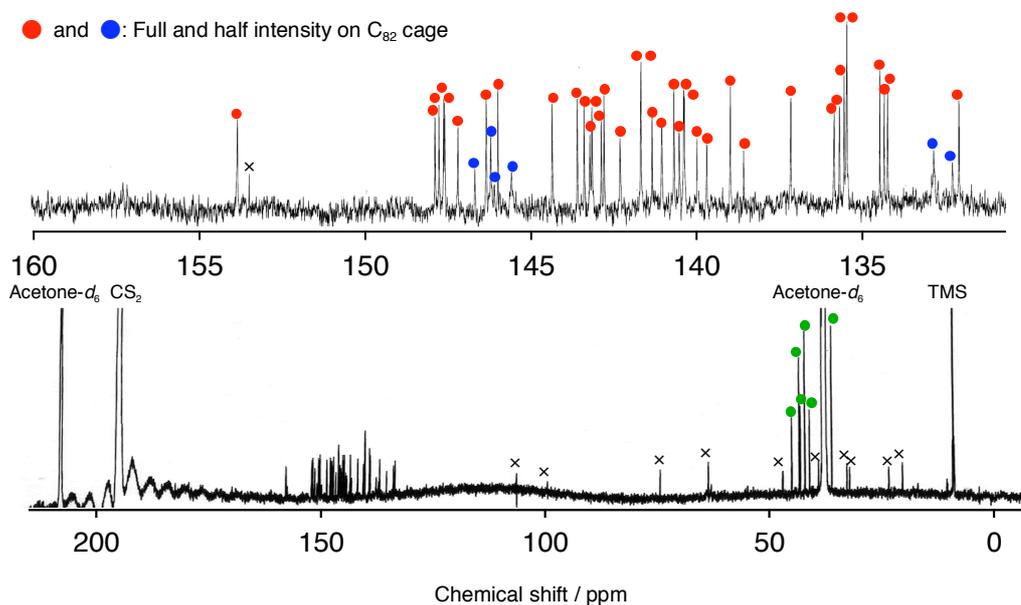


Figure S5



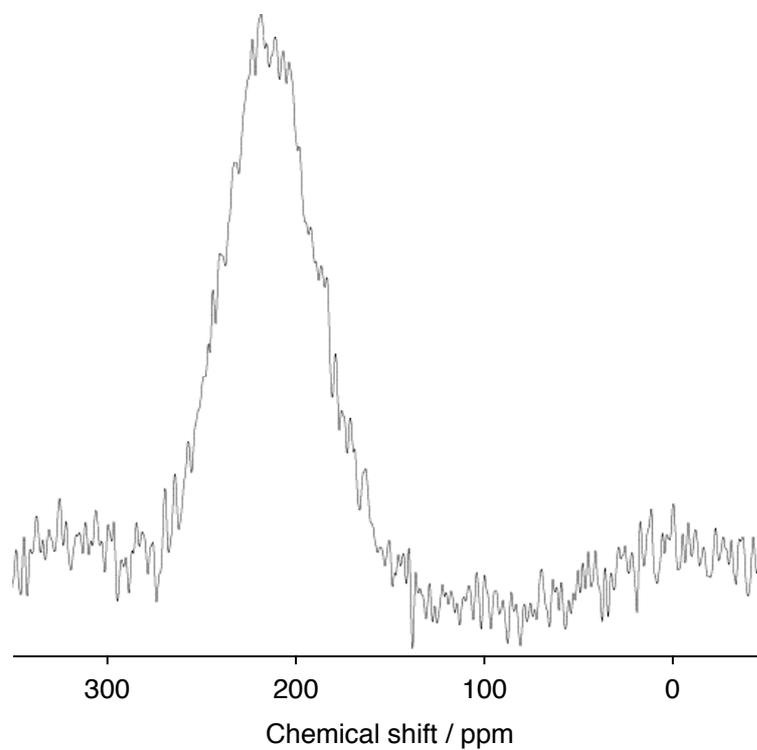
Conditions: working electrode and counter electrode, Pt wire; reference electrode, saturated calomel reference electrode (SCE); supporting electrolyte, 0.1 M *n*-Bu₄NPF₆ in *o*-dichlorobenzene. CV: scan rate, 20 mV/s. DPV pulse amplitude, 50 mV; pulse width, 50 ms; pulse period, 200 ms; scan rate, 20 mV/s.

Figure S6



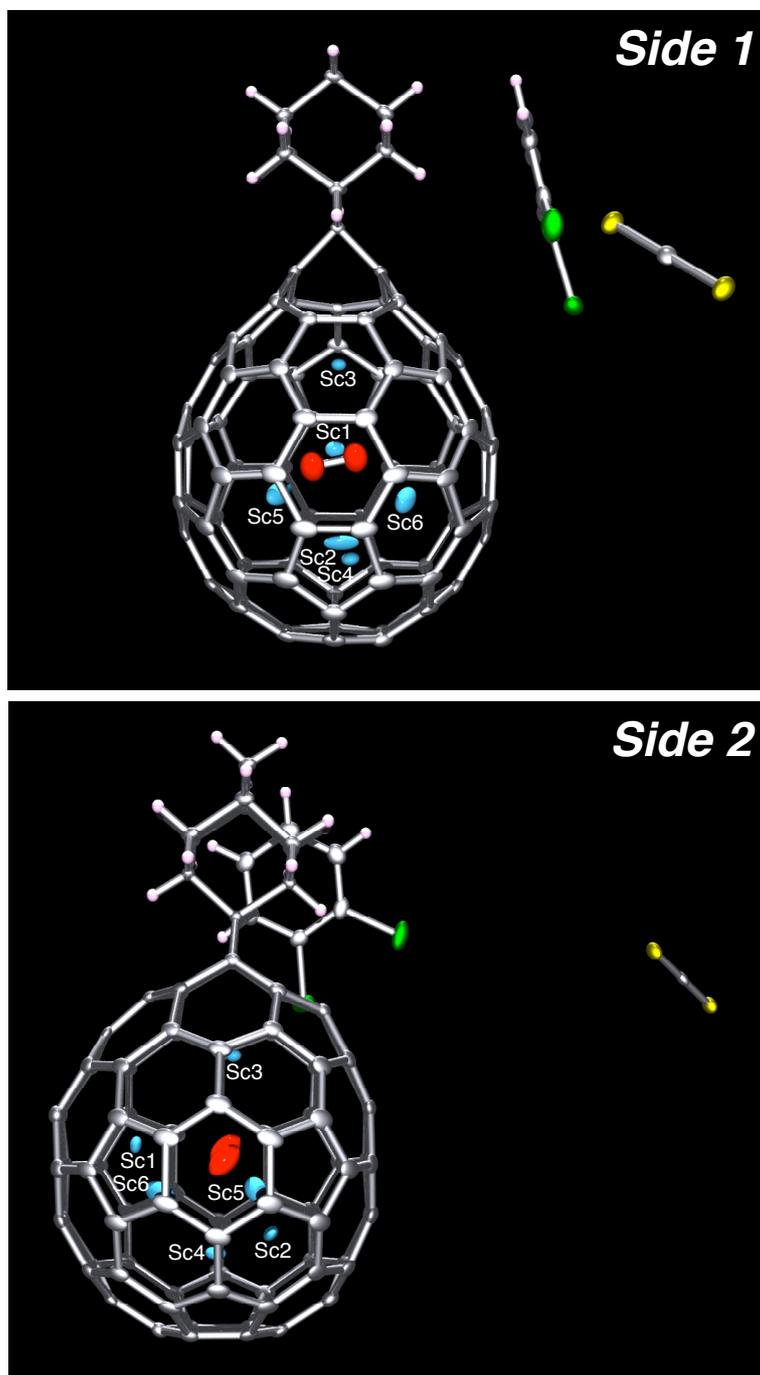
(125 MHz, CS₂, 293 K) δ 153.8(2C), 147.8(2C), 147.7(2C), 147.6(2C), 147.6(2C), 147.2(2C), 146.7(1C), 146.3(2C), 146.2(1C), 146.1(1C), 146.6(2C), 145.6(1C), 144.3(2C), 143.6(2C), 143.4(2C), 143.2(2C), 143.2(2C), 142.9(2C), 142.8(2C), 142.3(2C), 141.7(2C), 141.7(2C), 141.4(2C), 141.4(2C), 140.7(2C), 140.5(2C), 140.4(2C), 140.4(2C), 140.0(2C), 139.7(2C), 139.0(2C), 138.6(2C), 137.2(2C), 135.9(2C), 135.7(2C), 135.6(2C), 135.5(2C), 135.5(2C), 134.5(2C), 134.4(2C), 134.3(2C), 132.9(1C), 132.4(1C), 132.2(2C), 37.3(1C), 35.6(2C), 35.4(1C), 34.3(2C), 33.2(1C), 28.1(2C). The signals of carbon atom encapsulated in C₈₂ and quaternary carbon atom on the adamantyl part were not observed. It was used capillary containing acetone-d₆ as an internal lock. The signals marked with an cross come from some impurities.

Figure S7



(145.8 MHz, $\text{CS}_2/o\text{-dichlorobenzene-}d_4$, 293 K) δ 220. The chemical shift scale was calibrated using Sc_2O_3 in $\text{HCl}/\text{D}_2\text{O}$ as external reference (0 ppm).

Figure S8



At the 50% probability level.
Occupancies of Sc1–6 are 0.51, 0.51, 0.40, 0.40, 0.09 and 0.09, respectively.

Table S1

Compd.	oxE₂	oxE₁	redE₁	redE₂	redE₃	redE₄
Sc₂C₂@C₈₂(Ad)	+0.72	+0.38 ^a	-0.79	-1.12	-1.63	-2.00
Sc₂C₂@C₈₂(III)	+0.93 ^a	+0.47	-0.94 ^a	-1.15	-1.60	
Sc₂C₂@C₈₂(III)^b		+0.53	-0.97 ^a			

Half-cell potentials unless otherwise stated. Values are relative to ferrocene/ferrocenium couple.
^aIrreversible. Values are obtained by differential pulse voltammetry. ^bRef. 18