Supporting Information of

X-Ray Structures of $Sc_2C_2@C_{2n}$ (n = 40, 41, 42): In-Depth Understanding of the Core-Shell Interplay in Carbide Cluster Metallofullerenes

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Experimental section.

Preparation of $Sc_2C_2@C_{2n}$

The soot containing scandium metallofullerenes was prepared according to the reported procedure.[13] The Sc/C composite rod (4.7 × 10 × 150 mm, 2.0 atom%) was arc-vaporized at 150 A and 40 V under helium at 50 Torr. The raw soot was collected and extracted with CS_2. The samples under study were separated and isolated from various empty fullerenes and other scandium metallofullerenes by a multi-stage HPLC method. The purity of all samples is estimated to be higher than 99% with both HPLC analysis and LD-TOF mass spectrometry. The visible-NIR spectra of the isolated $Sc_2C_2@C_{2n}$ are shown in Fig. S1.

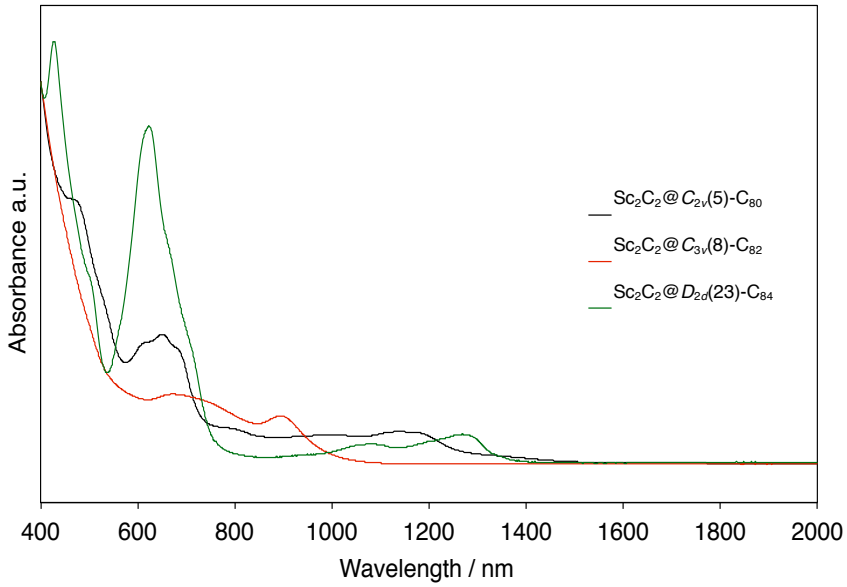

Figure S1. Vis-NIR spectra of $Sc_2C_2@C_{2n}$ (n = 40, 41, 42) under study.

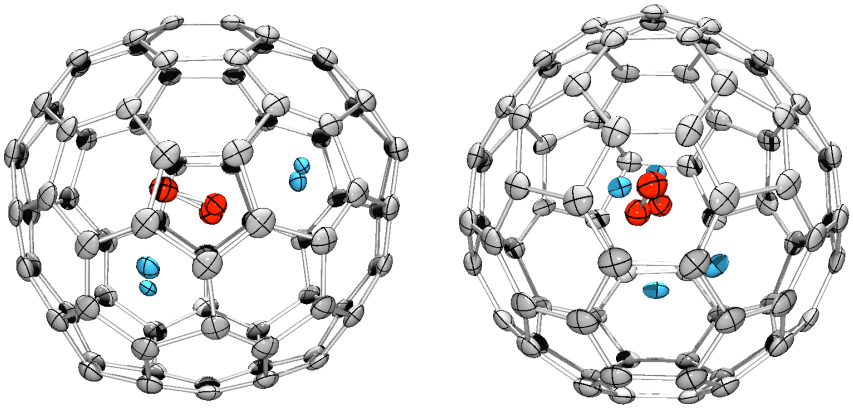

Figure S2. X-ray structures of $Sc_2C_2@C_{80}$ showing.

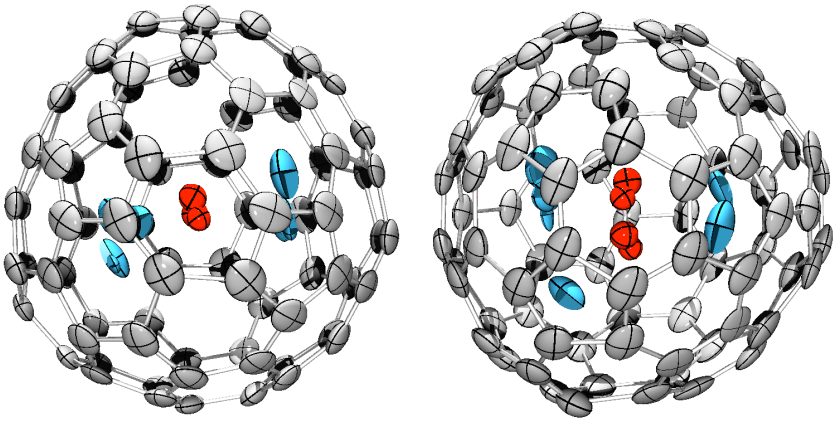

Figure S3. X-ray structures of $Sc_2C_2@C_{82}$ showing cluster disorder.

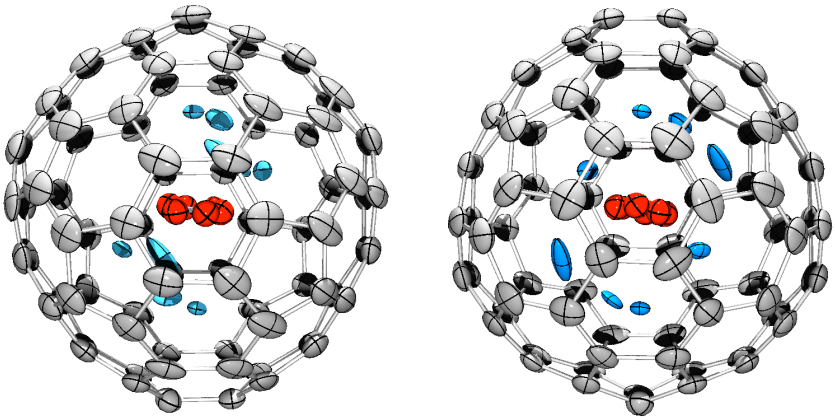

Figure S4. X-ray structures of $Sc_2C_2@C_{84}$ showing cluster disorder.