Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information

A temperature-responsive C_2 wagging vibration in $Sc_2C_2@C_s$-C_{82}

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Contents

Experimental Section:

1. The synthesis and purification of $Sc_2C_2@C_s$-C_{82} and $Sc_2C_2@D_{2d}$-C_{84}

Graphite rods were core-drilled and subsequently packed with a mixture of Sc/Ni_2 alloy and graphite powder in a weight ratio of 2:1. These rods were then vaporized in a Krätschmer-Huffman generator at 200 Torr He. The resulting soot was Soxlet-extracted with toluene for 12 h. $Sc_2C_2@C_s$-C_{82} and $Sc_2C_2@D_{2d}$-C_{84} were isolated from various empty fullerenes and other scandium metallofullerenes by HPLC.

2. HPLC data of purified $Sc_2C_2@C_s$-C_{82} and $Sc_2C_2@D_{2d}$-C_{84}

Several separations stage were repeated several times to obtain purified $Sc_2C_2@C_s$-C_{82} and $Sc_2C_2@D_{2d}$-C_{84}. Figure S2 and Figure S3 are showing the HPLC data of purified $Sc_2C_2@C_s$-C_{82} and $Sc_2C_2@D_{2d}$-C_{84} with Buckyprep-M columns.

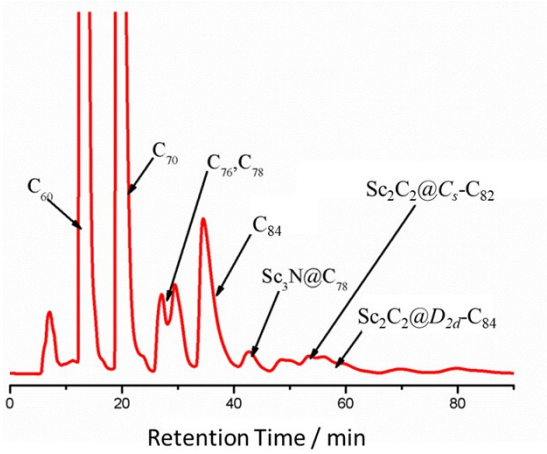

Figure S1. The first stage HPLC profile of toluene extract of the soot containing scandium endohedral metallofullerenes (20 × 250 mm Buckyprep column; flow rate 12 mL/min; toluene as eluent).

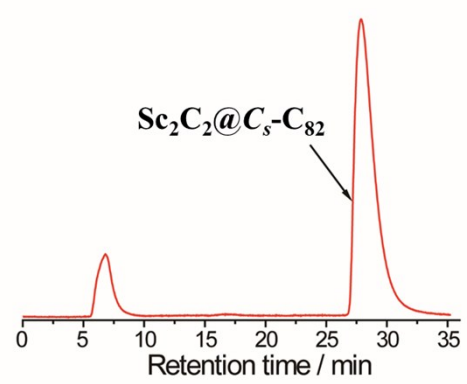

Figure S2. Chromatogram of the isolated $Sc_2C_2@C_s$-C_{82} (20×250 mm Buckyprep-M column; flow rate 12 mL/min; toluene as eluent).

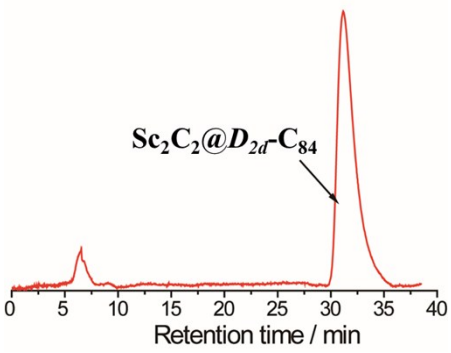

Figure S3. Chromatogram of the isolated $Sc_2C_2@D_{2d}$-C_{84} (20×250 mm Buckyprep-M column; flow rate 12 mL/min; toluene as eluent).

3. UV/Vis-NIR spectra of purified $Sc_2C_2@C_s$-C_{82} and $Sc_2C_2@D_{2d}$-C_{84}

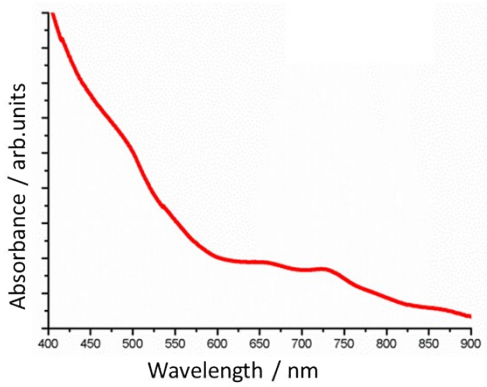

Figure S4. UV/Vis-NIR spectrum of purified $Sc_2C_2@C_s$-C_{82} in toluene.

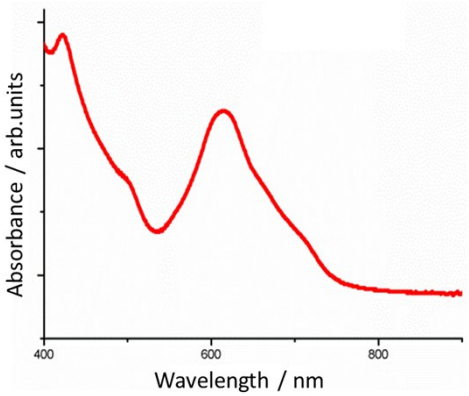

Figure S5. UV/Vis-NIR spectrum of purified $Sc_2C_2@D_{2d}$-C_{84} in toluene.

4. MALDI-TOF mass spectra of purified $Sc_2C_2@C_s$-C_{82} and $Sc_2C_2@D_{2d}$-C_{84}

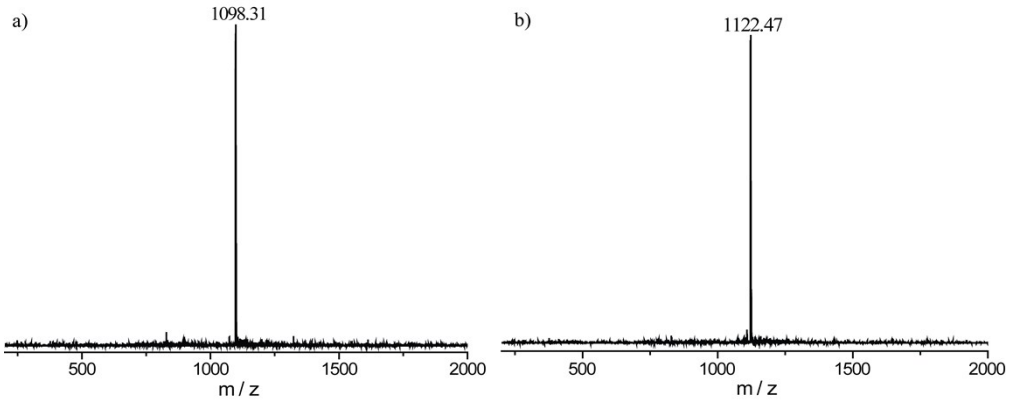

Figure S6. MALDI-TOF mass spectra of the (a) $Sc_2C_2@C_s$-C_{82} and (b) $Sc_2C_2@D_{2d}$-C_{84}.

5. The temperature-dependent Raman spectra of $Sc_2C_2@D_{2d}$-C_{84}

Raman spectra were studied with 633 nm excitation from laser. About 15 μg $Sc_2C_2@D_{2d}$-C_{84} were dissolved in carbon disulfide (CS_2, 99.999%, Sigma-Aldrich). The signals were detected on an N_2-cooled camera through a single pass monochromator. The instrument model is Renishaw invia plus, and a resolution of 1 cm^{-1} is used for all Raman measurements and 30 min accumulation time. Measurements were performed at selected temperatures from 80 K to 393 K.

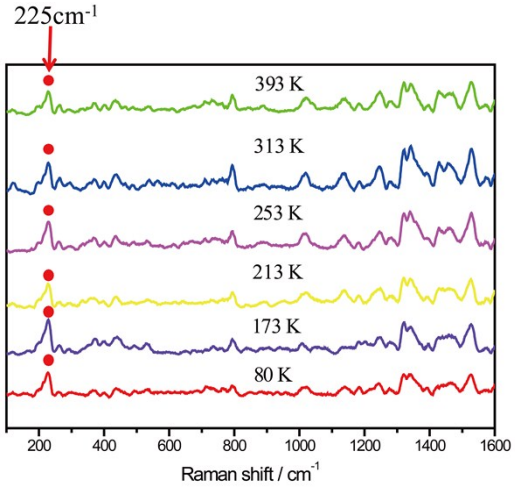

Figure S7. The experimental Raman spectra of $Sc_2C_2@D_{2d}$-C_{84} from 80 K to 393 K.

6. The temperature-dependent Raman spectra of $Sc_2C_2@C_s$-C_{82} from 80 K to 293 K

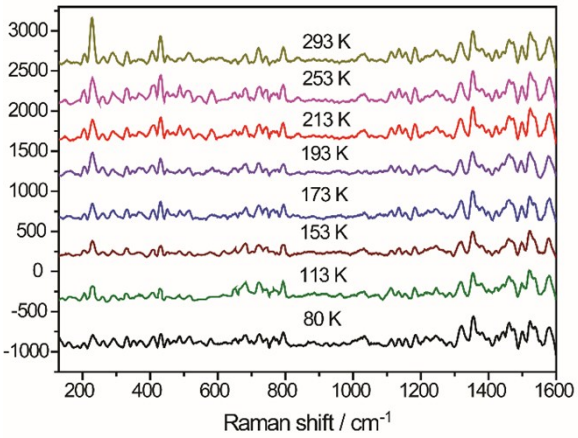

Figure S8. The experimental Raman spectra of $Sc_2C_2@C_s$-C_{82} from 80 K to 293 K.

7. The calculated and experimental Raman spectrum of $Sc_2C_2@D_{2d}$-C_{84} at B3LYP/DZP level

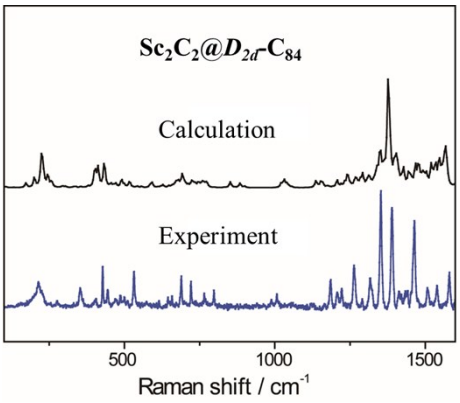

Figure S9. The calculated and experimental Raman spectrum of $Sc_2C_2@D_{2d}$-C_{84} at B3LYP/DZP level.

8. The calculated Raman spectrum of C_{82}-C_s(6) and $Sc_2C_2@C_s$-C_{82} at B3LYP/DZP level

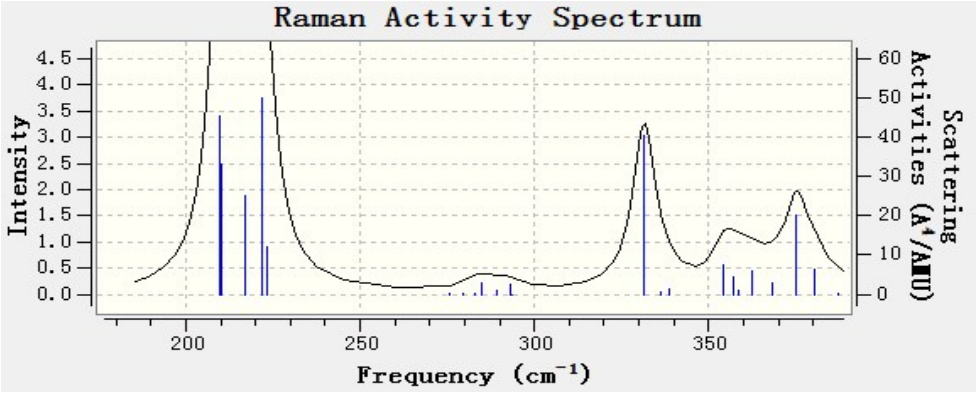

Figure S10. The calculated Raman spectrum of C_{82}-C_s(6) at B3LYP/DZP level.

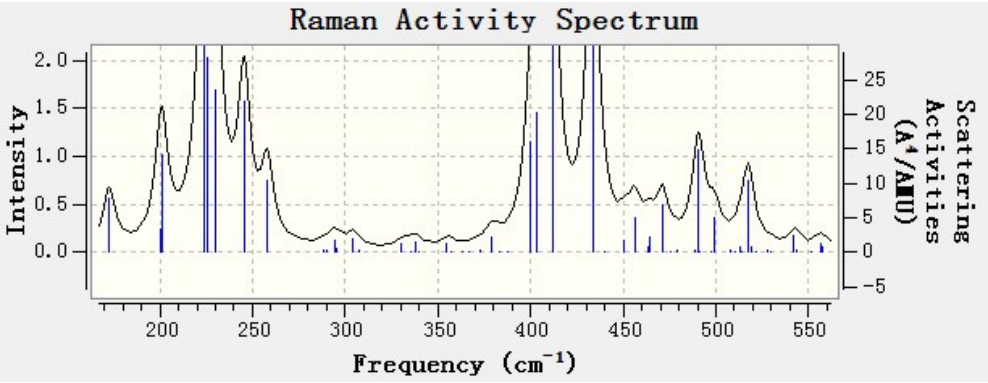

Figure S11. The calculated Raman spectrum of $Sc_2C_2@C_s$-C_{82} at B3LYP/DZP level.