Supporting Information

Synthesis and Characterization of a Novel Non-IPR Isomer of Th@C_{76} : Th@C_1(17418)-C_{76}

Yunpeng Xia,[1,#] Yi Shen,[1,#] Qingyu Meng,[1] Yang-Rong Yao,[2] and Ning Chen[1,*]

[1]College of Chemistry, Chemical Engineering and Materials Science, and State Key Laboratory of Radiation Medicine and Protection, Soochow University, Suzhou, Jiangsu 215123, P. R. China

[2]Department of Materials Science and Engineering, CAS Key Laboratory of Materials for Energy Conversion, Anhui Laboratory of Advanced Photon Science and Technology, University of Science and Technology of China, Hefei, Anhui, 230026 China

Table of Contents

High-performance liquid chromatography (HPLC) isolation of Th@C_1(17418)-C_{76}

Th@C_1(17418)-C_{76} was purified by a four-stage HPLC process, as shown in Figure S1. The first stage was performed on a Buckyprep-M column (25 mm × 250 mm, Cosmosil Nacalai Tesque) with a 10 mL / min flow rate. After that, the fraction from 26 to 27.5 min (marked in blue) was collected and re-injected into a Buckyprep column (10 mm × 250 mm, Cosmosil Nacalai Tesque) for the second stage separation using toluene as the eluent with a 4 mL / min flow rate, the fraction from 46 to 49.5 min (marked in red) containing Th@C_1(17418)-C_{76} was collected. The third separation stage was conducted on a 5PBB column (10 mm × 250 mm, Cosmosil Nacalai Tesque) with a 4 mL/min flow rate. The fraction marker in orange from 65 to 73 min containing Th@C_1(17418)-C_{76} was collected. The final stage was performed on a Buckyprep column (10 mm × 250 mm, Cosmosil Nacalai Tesque) with a 4 mL / min flow rate. Finally, pure C_1(17418)-C_{76} was attained. The MALDI-TOF mass spectrometry in a positively charged mode pure was used to confirm the purity of the extracted Th@C_1(17418)-C_{76} (Figure 1).

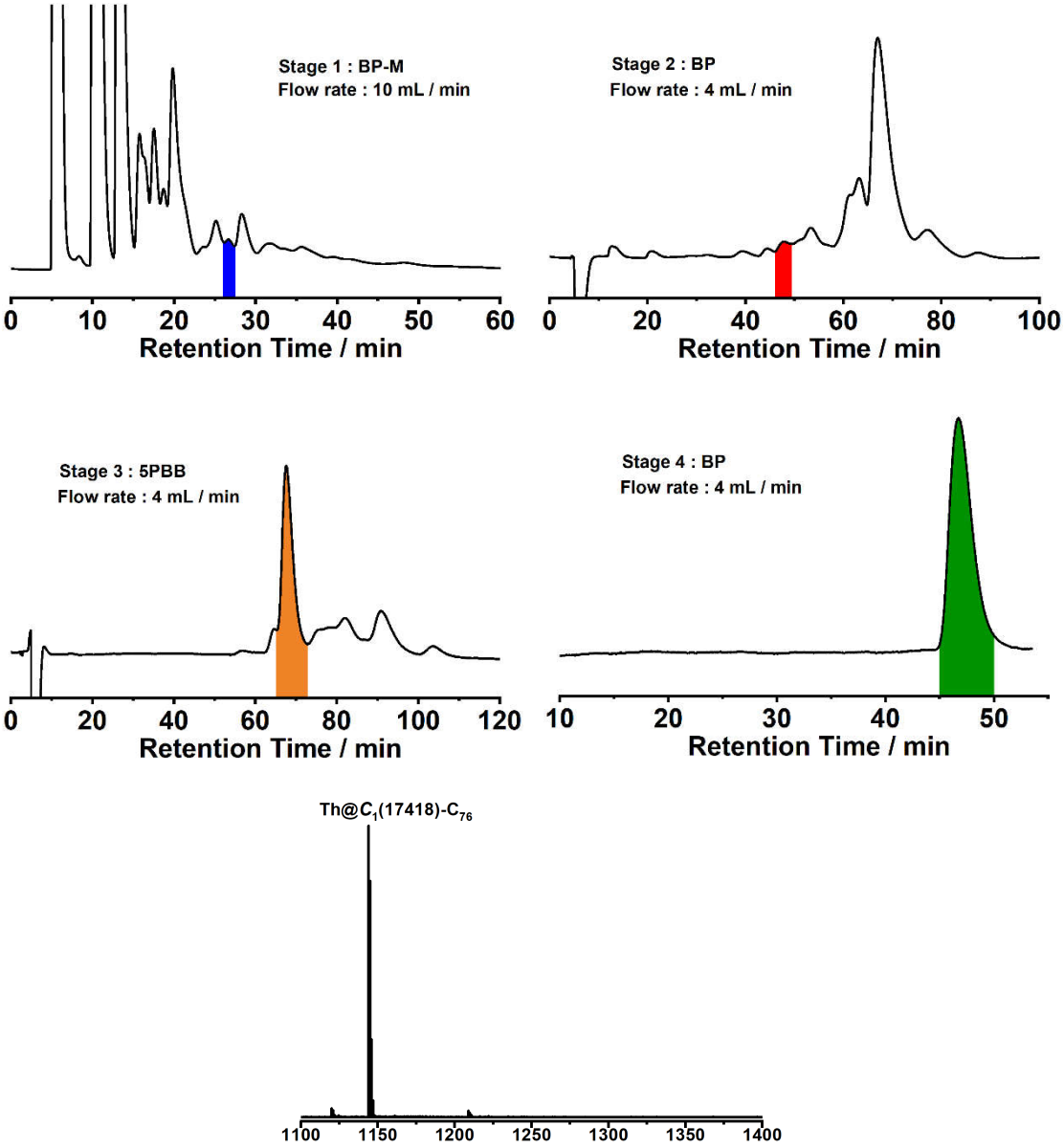

Figure S1. HPLC isolation procedures of Th@C_1(17418)-C_{76} and the pure sample's MALDI-TOF mass spectrum.

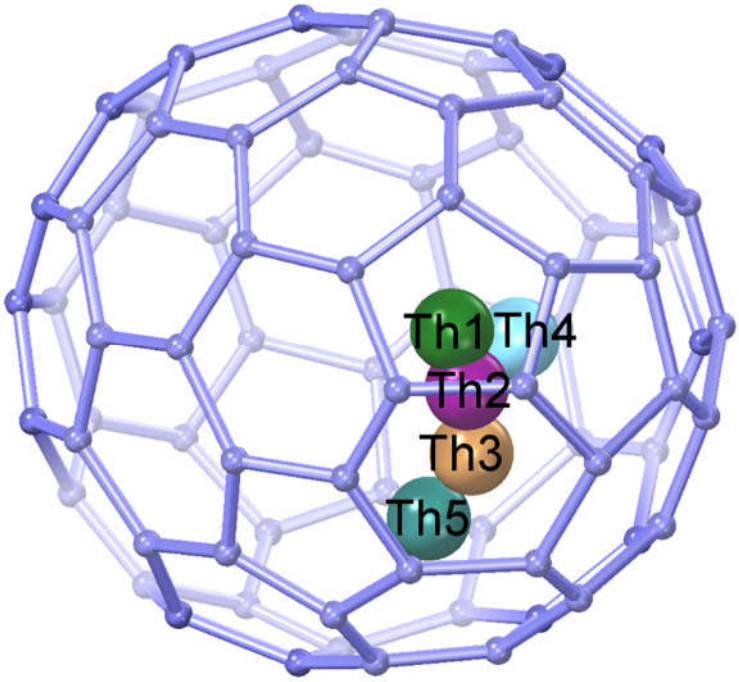

Figure S2. Ball and stick representation of disordered Th sites inside Th@C_1(17418)-C_{76}, five positions (Th1, Th2, Th3, Th4, and Th5) are observed.

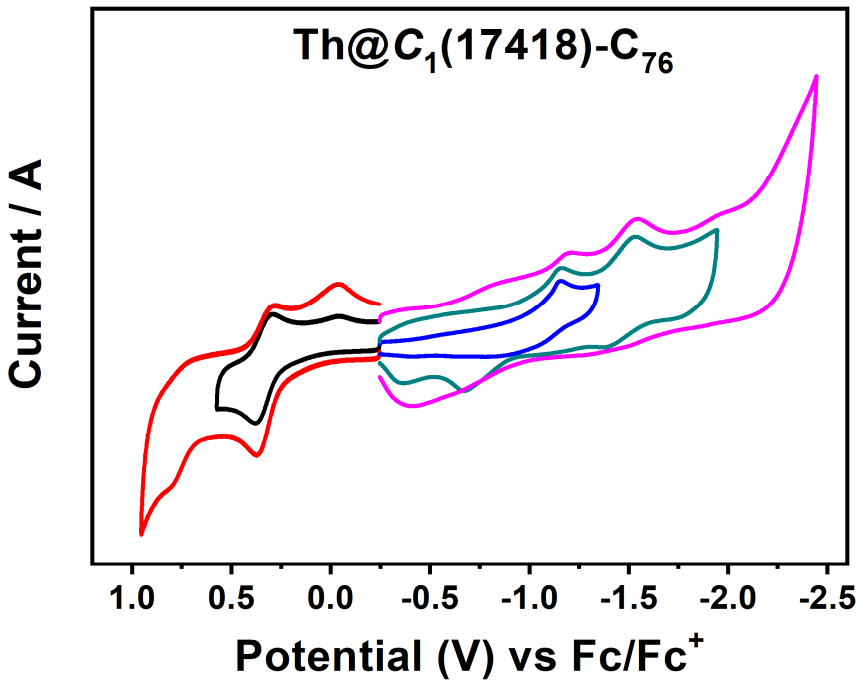

Figure S3. Cyclic voltammograms of Th@C_1(17418)-C_{76} in o-dichlorobenzene (0.05 M (n-Bu)4NPF6 as the supporting electrolyte; scan rate 100 mV/s).

Table S1. Occupancies of disordered thorium sites in Th@C_1(17418)-C_{76}.

Compounds	**Th@*C*$_1$(17418)-C$_{76}$**				
Labeling	**Th1**	**Th2**	**Th3**	**Th4**	**Th5**
Occupancy	0.504(3)	0.304(3)	0.1352(19)	0.0319(3)	0.0252(2)

Table S2. Closest Th-Cage distances (Å) in Th@C_1(17418)-C_{76}.

Compounds	**Th@*C*$_1$(17418)-C$_{76}$**				
Labeling	**Th1-C1**	**Th1-C2**	**Th1-C3**	**Th1-C4**	**Th1-C5**
Length / Å	2.449(10)	2.433(12)	2.376(12)	2.359(13)	2.382(12)

Table S3. Crystallographic information of Th@C_1(17418)-C_{76}

Crystal	Th@C_1(17418)-C_{76}·[Ni^{II}(OEP)]·$2C_6H_6$
Formula	C_{124} H_{56} N_4 Ni Th
Formula weight	1892.47
Crystal size, mm^3	0.1×0.08×0.06
Crystal system	Monoclinic
Space group	*C*2/*c*(No. 15)
a, Å	44.778(2)
b, Å	14.9844(11)
c, Å	25.431(2)
α, deg	90
β, deg	121.405(3)
γ, deg	90
Volume, Å3	14564(2)
Z	8
ρ, g cm^{-3}	1.726
F(000)	7568
θ, deg	2.756-58.099
T, K	120.0
Radiation (λ, mm^{-1})	μ(Ga Kα) = 6.129 mm^{-1}
R_1 / wR_2 (all data)	0.1339 / 0.2547
R_1 / wR_2 (I > 2.0σ(I))	0.0901 / 0.2256
obs reflects	10155
total reflects	15333
R_{int}	0.0881
Goodness-of-fit indicator	1.074
Parameters	1220
density, e $Å^{-3}$	-1.286 / 1.429