Electronic Supplementary Information

Exohedrally stabilized C_{70} isomer with adjacent pentagons characterized by crystallography

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1. Multi-stage separation of $^{\#8064}C_{70}Cl_{10}$ by HPLC.

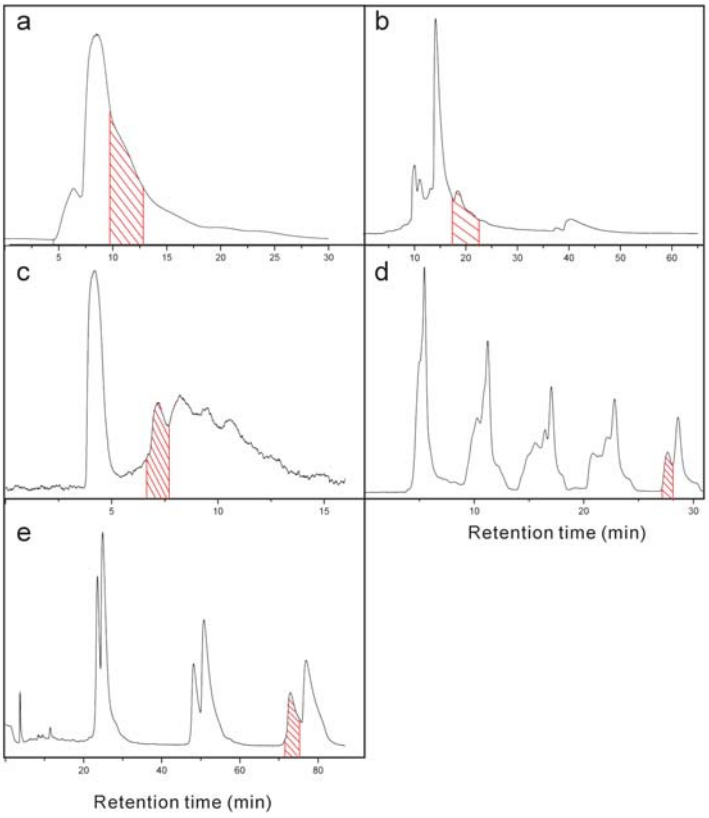

Figure S1. Multi-stage HPLC chromatograms for the separation of $^{\#8064}C_{70}Cl_{10}$. The collected components were highlighted by red shadow.

The procedure for the purification of $^{\#8064}C_{70}Cl_{10}$ includes five stages of HPLC runs, of which the last two runs were performed in a recyclic mode. All the separations were carried out at room temperature using toluene as the eluant. The crude toluene extraction of carbon soot was first separated using a pyrenebutyric acid bonded silica column (I.D. 20 × 250 mm) at a flow rate of 10 ml/min, and the component with the retention time ranging from 9.0 to 13.0 min was collected for the subsequent HPLC stage (Fig. S1a). Then a buckyprep column (I.D. 10 × 250 mm) was used to separate the collected sample at a flow rate of 4 ml/min, and the component with retention time from 17.5 to 22.5 min was collected (Fig. S1b). The third stage of the isolation was performed using a buckyprep-M column (I.D. 10 × 250 mm) at a flow rate of 4 ml/min, and collecting the component ranging from 6.1 to 7.5 min (Fig. S1c). The following two steps of the isolation were performed using recyclic HPLC. The sample was isolated by a 5PBB column at a flow rate of 4 ml/min, and then the peak containing $C_{70}Cl_{10}$ was collected after fifth cycles (Fig. S1d). The obtained sample was further purified by a

buckyprep column (I.D. 4.6 × 250 mm) at a flow rate of 1 ml/min (Fig. S1e). The component highlighted by the red shadow in Fig. S1e was corresponded to the purified $^{\#8064}C_{70}Cl_{10}$.

2. Crystallographic identification for $^{\#8064}C_{70}Cl_{10}$.

By evaporation of its chloroform solution, single crystals of $^{\#8064}C_{70}Cl_{10}$ were obtained. X-ray diffraction data were collected on a Bruker CCD diffractometer (MoKα radiation (0.71073 Å), graphite monochromator). The structure was solved and refined using SHELTXL.[1] CCDC 809403 contains the crystallographic data of $^{\#8064}C_{70}Cl_{10}$ can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

3. Computational details.

The geometrical optimization and electronic structure of pristine $^{\#8064}C_{70}$ was calculated at the GGA/DNP level, in which the generalized gradient approximation (GGA) in the Perdew, Burke, and Ernzerhof (PBE)[2] form as well as a double numerical polarized (DNP) basis set were employed. The nucleus independent chemical shifts (NICS)[3,4] at the center of the rings in the remainder carbon framework were calculated at B3LYP/6-31G*[5,6] level of theory. All of the computation works were performed using the DMol[3] code[7,8] and Gaussion03 program[9]. Fig. S2 shows the HOMO and LUMO of $^{\#8064}C_{70}$. The amounts of Kekulé structures for the three $C_{30}H_{12}$ isomers are indicated in Fig. S3, and the NICS values for the ring centers of the C_{30} fragments shown in Fig. S4 are listed in Table S1.

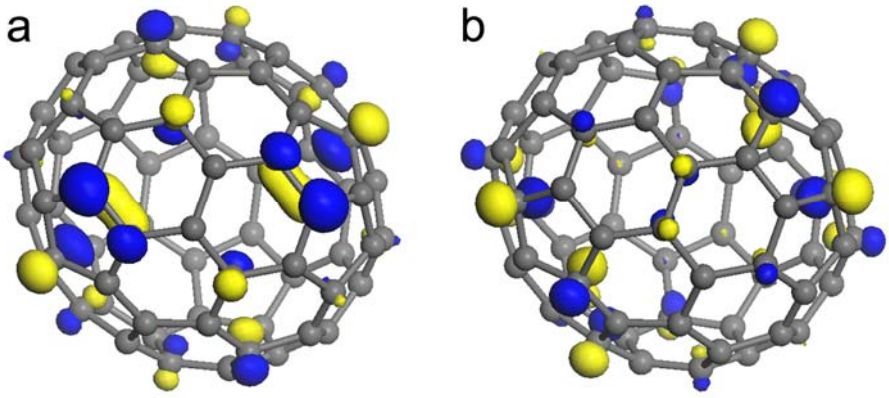

Figure S2. The HOMO (a) and LUMO (b) of $^{\#8064}C_{70}$.

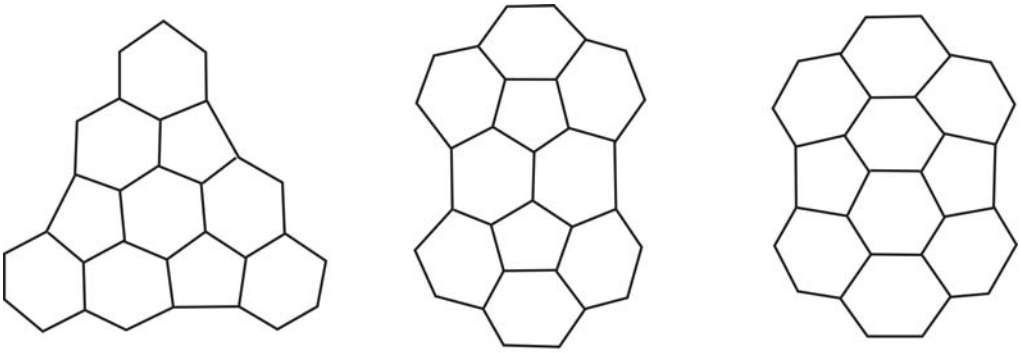

Figure S3. The frameworks of the three $C_{30}H_{12}$ isomers. The amounts of Kekulé structures are written below the frameworks.

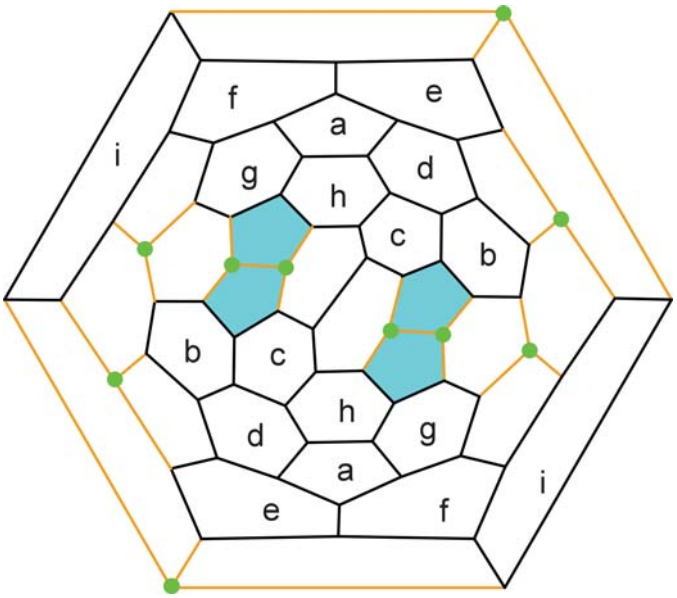

Figure S4. The numeration of the rings in the C_{30} fragments.

Table S1. B3LYP/6-31G* calculated NICS values of the ring centers

Ring	NICS
a	- 1.7
b	-12.8
c	-5.3
d	-7.2
e	-10.4
f	-8.8
g	-10.4
h	-13.5
i	-12.1

4. Coordinates of the optimized pristine $^{\#8064}C_{70}$.

carbon	x	y	z	carbon	x	y	z
1	3.82383	-0.57193	-0.19827	36	0.31944	-2.6612	-2.43882
2	2.55449	-2.58413	0.34354	37	2.28138	1.46717	-2.78965
3	-3.2893	1.79635	-0.59276	38	-2.54786	0.83419	-2.71909
4	-0.59404	0.44143	3.35208	39	1.10877	0.86169	-3.39719
5	1.54521	-2.85366	-1.73646	40	-3.63197	-1.37441	1.05425
6	-0.95764	-2.32409	3.18801	41	-2.28245	2.08673	1.66314
7	2.0691	1.47612	2.93062	42	0.27957	-3.588	1.66494
8	-1.28216	0.56025	-3.37951	43	2.90723	2.14305	1.94547
9	-1.55434	3.336	-0.38391	44	2.92028	2.81059	-0.82681
10	-2.55449	2.58413	0.34354	45	3.60051	-0.06745	1.13925
11	-2.73189	0.74534	2.03991	46	2.73189	-0.74534	2.03991
12	-1.54521	2.85366	-1.73646	47	-2.18794	-3.32229	1.47079
13	-0.37946	3.81054	0.25261	48	-3.60051	0.06745	1.13925
14	3.2893	-1.79635	-0.59276	49	-0.84673	-3.22665	-1.8397
15	0.35833	-1.82612	3.22258	50	0.59404	-0.44143	3.35208
16	3.83393	0.54317	-1.12315	51	3.63197	1.37441	1.05425
17	-2.11144	-3.57837	0.0928	52	2.15352	2.6341	-2.04115
18	-2.0691	-1.47612	2.93062	53	-1.89433	-0.06571	2.93211
19	-0.35833	1.82612	3.22258	54	-1.00063	-3.41625	2.24567
20	1.89433	0.06571	2.93211	55	-0.82276	-3.82292	-0.5274
21	-2.92028	-2.81059	-0.82681	56	-1.10877	-0.86169	-3.39719
22	-3.82383	0.57193	-0.19827	57	-3.17109	-0.4178	-2.35767
23	-1.16293	2.63846	2.31548	58	2.65215	-1.93919	-1.8861
24	-3.71051	-1.75325	-0.35436	59	-2.15352	-2.6341	-2.04115
25	-3.83393	-0.54317	-1.12315	60	-2.28138	-1.46717	-2.78965
26	-0.31944	2.6612	-2.43882	61	-2.90723	-2.14305	1.94547
27	2.11144	3.57837	0.0928	62	3.71051	1.75325	-0.35436
28	2.18794	3.32229	1.47079	63	2.54786	-0.83419	-2.71909
29	1.55434	-3.336	-0.38391	64	0.37946	-3.81054	0.25261
30	-0.17869	1.4526	-3.26123	65	0.95764	2.32409	3.18801
31	1.16293	-2.63846	2.31548	66	-2.65215	1.93919	-1.8861
32	1.00063	3.41625	2.24567	67	0.17869	-1.4526	-3.26123
33	0.82276	3.82292	-0.5274	68	3.17109	0.4178	-2.35767
34	0.84673	3.22665	-1.8397	69	2.28245	-2.08673	1.66314
35	-0.27957	3.588	1.66494	70	1.28216	-0.56025	-3.37951

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