Supporting Information

Rational synthesis, enrichment, and ^{13}C NMR spectra of endohedral C_{60} and C_{70} encapsulating a helium atom

Yuta Morinaka,[a] Fumiyuki Tanabe,[a] Michihisa Murata,[a] Yasujiro Murata,*[a] and Koichi Komatsu*[ab]

[a]*Institute for Chemical Research, Kyoto University, Uji, Kyoto 611-0011, Japan*
[b]*Department of Environmental and Biological Chemistry, Fukui University of Technology, Gakuen, Fukui 910-8505, Japan*

Contents

Complete Reference 20. Gaussian 03, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Wallingford CT, 2004.

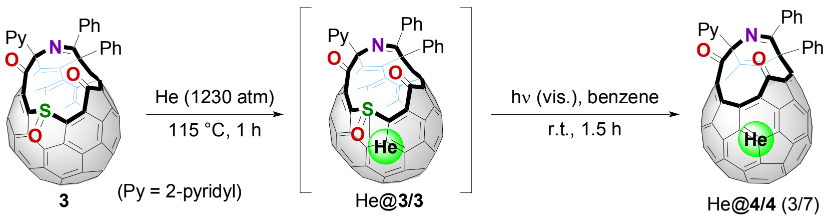
1. General

The ^{1}H and ^{13}C NMR measurements were carried out with a Varian Mercury 300 instrument and a JEOL AL-400 instrument. The NMR chemical shifts are reported in ppm with reference to residual protons and carbons of $CDCl_3$ (δ 7.26 ppm in ^{1}H NMR, δ 77.0 ppm in ^{13}C NMR), CD_2Cl_2 (δ 5.32 ppm in ^{1}H NMR, δ 53.5 ppm in ^{13}C NMR), acetone-d_6 (δ 2.04 ppm in ^{1}H NMR), benzene-d_6 (δ 7.20 ppm in ^{1}H NMR), and 1,2-dichlorobenzene-d_4 (ODCB-d_4) (δ 132.35 ppm in ^{13}C NMR). FAB mass spectra were recorded on a JEOL MStation JMS-700. APCI mass spectra were measured on a Finnigan-MAT TSQ 7000 spectrometer. The high-pressure liquid chromatography (HPLC) was performed with the use of a Cosmosil Buckyprep column (250 mm length, 4.6-mm inner diameter) for analytical purpose, and the same column (two directly connected columns; 250 mm length, 20 mm inner diameter) for preparative purpose. ODCB-d_4 was purchased from Aldrich Co. Zinc (sandy, 99.9%), titanium (IV) chloride, carbon disulfide (CS_2), benzene, and tetrahydrofuran (THF) were purchased from Wako Pure Chemical Industries, Ltd, and THF was distilled from sodium benzophenone ketyl under argon before use.

2. Computational Method

All calculations were conducted with Gaussian 03 packages. The structures were fully optimized with the MPWB1K functional and 6-31G** basis set without any symmetry assumptions.

3. Synthesis of C_{60} derivative He@4 with a 12-membered-ring opening



A powder of cage-opened C_{60} derivative **3** (600 mg, 0.553 mmol) wrapped in aluminum foil was heated at 115 °C in an autoclave under pressurized He gas (1230 atm) for 1 h. This high pressure (1230 atm) was generated by (i) introducing He gas (100 atm) into the autoclave, (ii) elevating the pressure up to 1050 atm by the use of a hydraulic compressor at room temperature, and (iii) heating the autoclave at 115 °C. After cooling to ambient temperature, the resulting powder was recovered from the autoclave and dissolved in benzene (1 L). The solution was irradiated with high-pressure mercury lamp for 1.5 h at room temperature through Pyrex glass. The solvent was removed *in vacuo* and the residual brown solid was subjected to flash column chromatography over silica gel. Elution with toluene-EtOAc (20:1) gave He@**4**/**4** (3/7) (158.8 mg, 0.153 mmol, 28%) as a brown solid, and following elution with toluene-EtOAc (5:1) gave unreacted **3** (307.4 mg, 0.284 mmol, 51%). The following NMR spectra were identical to the reported ones for empty compound.[1]

He@**4**/**4** (3/7): ^{1}H NMR (300 MHz, CS_2-acetone-d_6 (7:1)) δ 8.52 (m, 1H), 8.32 (m, 1H), 7.98-8.08 (m, 3H), 7.85 (m, 1H), 7.03-7.39 (m, 8H); ^{13}C NMR (75 MHz, CS_2-$CDCl_3$ (1:1)) δ 196.35, 189.11, 167.75, 161.87, 149.74, 148.48, 148.48, 148.43, 148.24, 147.63, 147.54, 147.52, 147.18, 147.14, 146.57, 146.24, 146.24, 146.06, 145.91, 145.75, 145.68, 145.57, 145.47, 145.42, 145.41, 145.18, 145.08, 145.03, 144.89, 144.56, 144.41, 144.03, 143.92, 143.72, 143.08, 142.59, 142.38, 142.15, 141.78, 141.64, 141.31, 140.98, 140.76, 140.45, 140.20, 140.11, 139.92, 139.79, 139.55, 139.45, 139.35, 139.35, 139.32, 138.47, 137.50, 137.11, 137.02, 137.02, 136.13, 135.57, 133.07, 132.60, 131.24, 130.85, 130.34, 129.93, 129.88, 129.65, 129.11, 128.89, 128.89, 128.57, 127.48, 127.48, 127.42, 126.94, 123.15, 122.65, 75.06, 52.44.

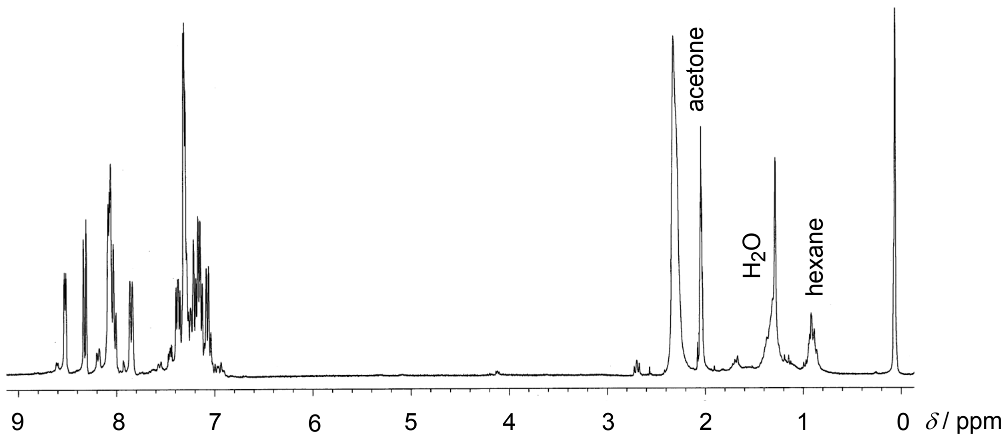


Fig. S1. [1]H NMR (300 MHz, CS_2-acetone-d_6 (7:1)) spectrum of He@**4**/**4** (3/7).

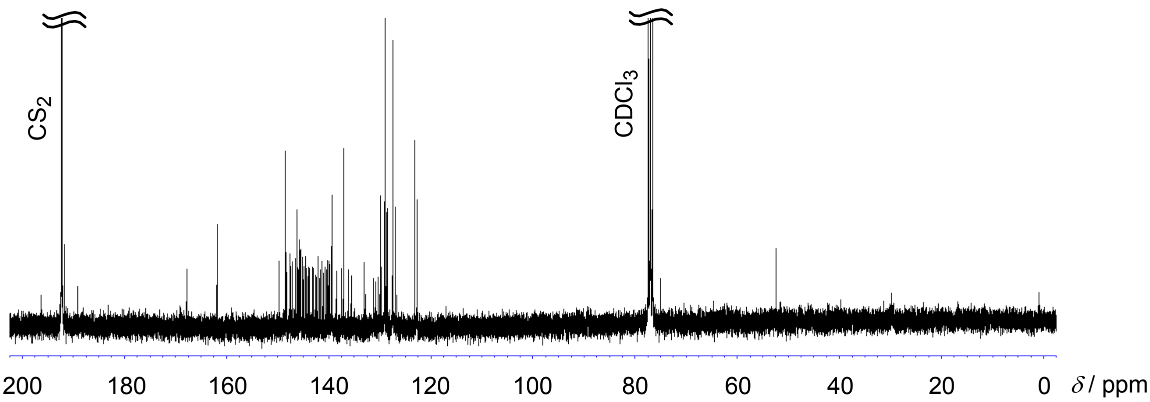


Fig. S2. [13]C NMR (75 MHz, CS_2-$CDCl_3$ (1:1)) spectrum of He@**4**/**4** (3/7).

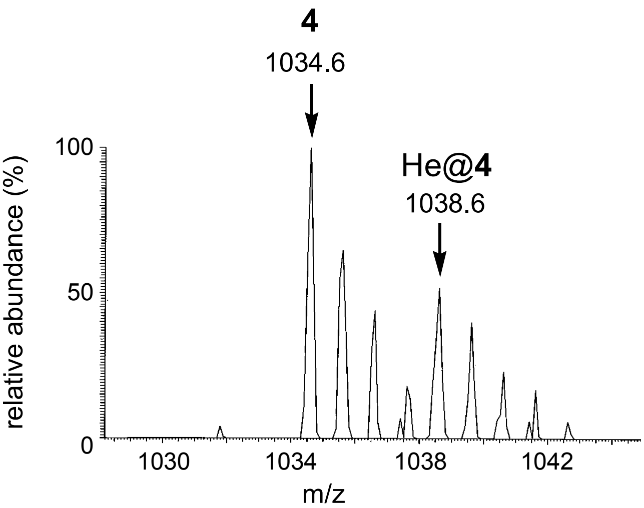
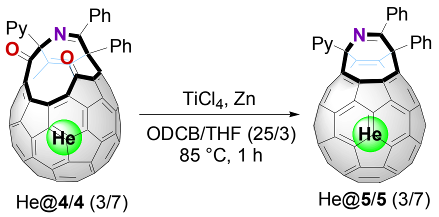


Fig. S3. APCI-MS spectrum (negative-ion mode) of He@**4**/**4** (3/7).

4. Synthesis of C_{60} derivative He@5 with an 8-membered-ring opening



To a stirred suspension of zinc powder (600 mg, 9.176 mmol) in dry THF (20 mL) was added titanium (IV) tetrachloride (500 μL, 4.560 mmol) drop by drop at 0 °C under argon atmosphere, and the mixture was refluxed for 2 h. A 3.0 mL portion of the resulting black slurry was added to a stirred solution of He@**4**/**4** (3/7) (143.0 mg, 0.138 mmol) in dry ODCB (25 mL) at room temperature under argon atmosphere. After heating at 85 °C for 1 h, the resulting brownish purple solution was cooled to room temperature. Then the solution was diluted with CS_2 (30 mL) and washed with aqueous solution of $NaHCO_3$ (saturated, 50 mL). The organic layer was dried over $MgSO_4$ and evaporated under reduced pressure to give a residual brown solid, which was then subjected to flash column chromatography over silica gel. Elution with toluene-EtOAc (20:1) gave He@**5**/**5** (3/7) (84.5 mg, 0.084 mmol, 61%) as a brown solid. The following NMR spectra were identical to the reported ones for empty compound.[1]

He@**5**/**5** (3/7): ^{1}H NMR (300 MHz, CS_2-acetone-d_6 (7:1)) δ 8.67 (m, 1H), 7.90-8.00 (m, 2H), 7.69-7.76 (m, 2H), 7.37-7.44 (m, 2H), 7.10-7.22 (m, 7H); ^{13}C NMR (75 MHz, CS_2-$CDCl_3$ (1:2)) δ 168.70, 165.32, 149.51, 148.62, 148.62, 148.30, 145.77, 145.60, 145.52, 145.45, 145.29, 144.74, 144.74, 144.59, 144.57, 144.33, 144.33, 144.19, 144.19, 144.04, 144.04, 143.92, 143.87, 143.78, 143.73, 143.59, 143.58, 143.40, 143.21, 141.69, 140.91, 140.91, 140.69, 140.68, 140.60, 140.34, 139.53, 139.14, 138.47, 138.32, 137.08, 137.03, 137.03, 136.71, 135.51, 135.38, 135.22, 134.89, 131.21, 131.01, 128.66, 128.58, 128.31, 128.31, 127.56, 127.42, 127.42, 127.36, 125.55, 122.90, 73.19, 56.56.

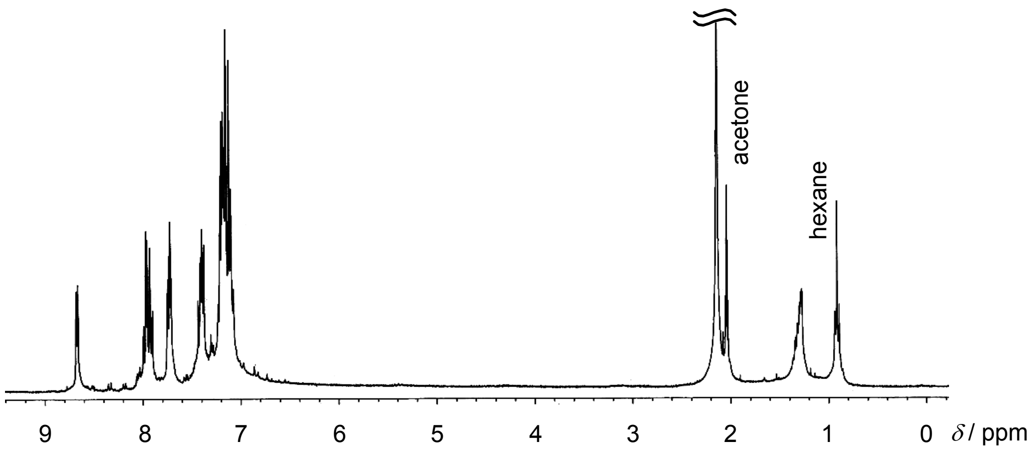


Fig. S4. [1]H NMR (300 MHz, CS_2-acetone-d_6 (7:1)) spectrum of He@**5**/**5** (3/7).

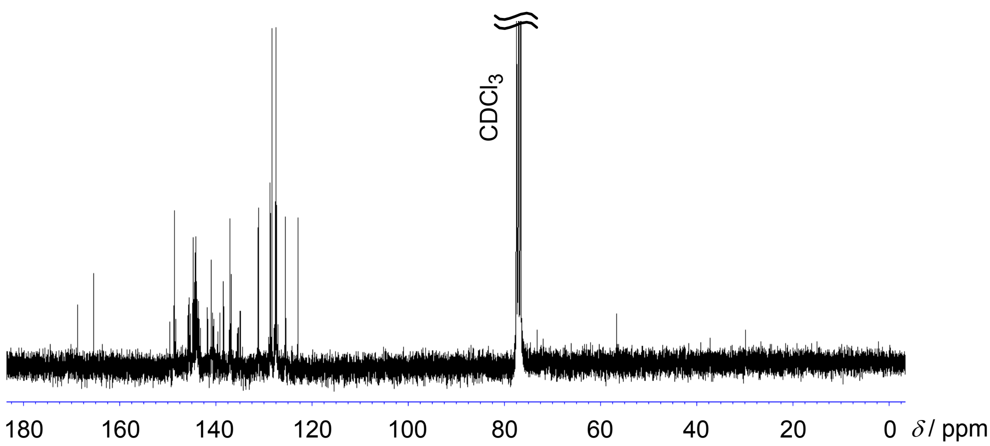
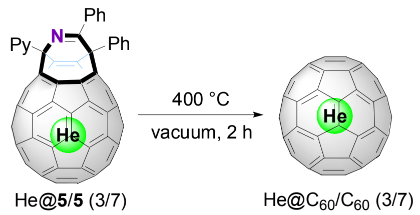


Fig. S5. [13]C NMR (75 MHz, CS_2-$CDCl_3$ (1:2)) spectrum of He@**5**/**5** (3/7).

.

5. Synthesis and enrichment of He@C_{60}

5-1. Synthesis of He@C_{60}



A powder of He@**5**/**5** (3/7) (70.0 mg, 0.070 mmol) lightly wrapped with a piece of aluminum foil was placed in a glass tube (inner diameter 20 mm), which was heated with an electric furnace at 400 °C for 2 h under vacuum (1 mmHg). The resulting black solid was dissolved in CS_2 (50 mL) and subjected to flash column chromatography over silica gel. Elution with CS_2 gave He@C_{60}/C_{60} (3/7) (38.3 mg, 0.053 mmol, 76%) as a brown solid.

He@C_{60}/C_{60} (3/7): ^{13}C NMR (75 MHz, ODCB-d_4) δ 142.80 (He@C_{60}), 142.78 (C_{60}); HRMS (+FAB), calcd for C_{60}He (M^+) 724.0026, found 724.0026.

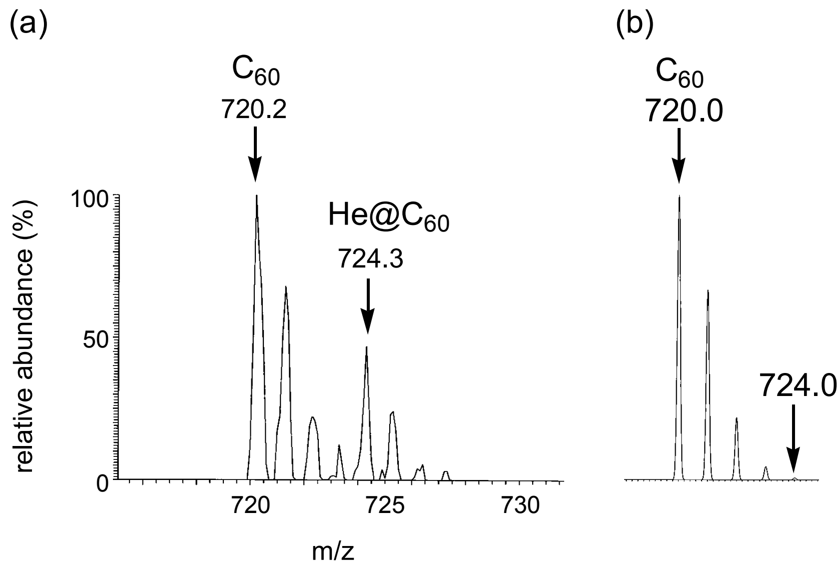


Fig. S6. (a) APCI-MS spectrum (negative-ion mode) of He@C_{60}/C_{60} (3/7) and (b) theoretical isotopic pattern for C_{60}.

5-2. Enrichment of He@C_{60}

The sample of He@C_{60}/C_{60} (3/7) was subjected to the recycle HPLC on Cosmosil Buckyprep column (two directly connected columns; 250 mm length, 20 mm inner diameter; mobile phase, toluene; 50 °C; flow rate was 9.9 mL/min).[2] After 10 recycling, the separated latter portion was evaporated and further subjected to the same HPLC. After 40 recycling, the latter potion was collected and was evaporated to give He@C_{60}/C_{60} (6/4). By repeating this procedure He@C_{60} at occupation level of 95% was obtained.

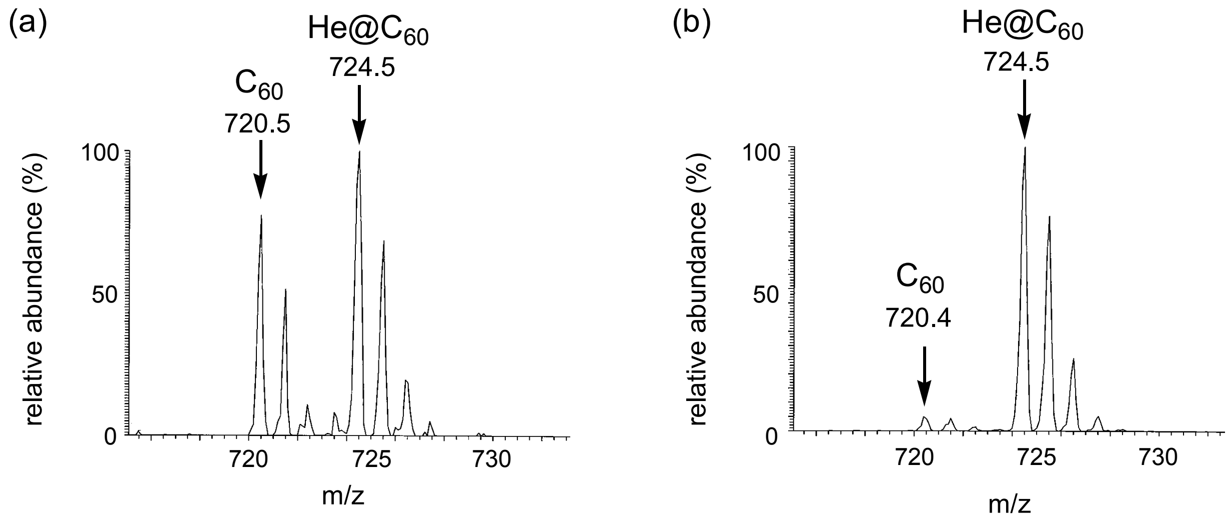
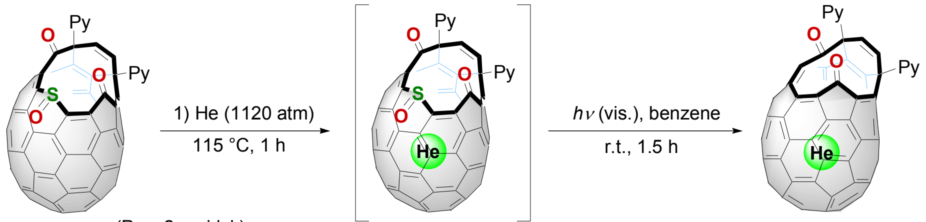


Fig. S7. APCI-MS spectrum (negative-ion mode) of a mixture of He@C_{60} and C_{60} after purification with the recycling HPLC. The occupation level of (a) 60% and (b) 95%.

6. Synthesis of C_{70} derivative He@7 with a 12-membered-ring opening



6 (Py = 2-pyridyl) He@**6**/**6** He@**7**/**7** (3/7)

A powder of cage-opened C_{70} derivative **6** (441.0 mg, 0.391 mmol) wrapped in aluminum foil was heated at 115 °C in an autoclave under pressurized He gas (1120 atm) for 1 h. This high pressure (1120 atm) was generated by (i) introducing He gas (110 atm) into the autoclave, (ii) elevating the pressure up to 1030 atm by the use of a hydraulic compressor at room temperature, and (iii) heating the autoclave at 115 °C. After cooling to ambient temperature, the resulting powder was recovered from the autoclave and dissolved in benzene (1 L). The solution was irradiated with high-pressure mercury lamp for 1.5 h at room temperature through Pyrex glass. The solvent was removed *in vacuo* and the residual brown solid was subjected to flash column chromatography over silica gel. Elution with toluene-EtOAc (10:1) gave He@**7**/**7** (3/7) (225.9 mg, 0.208 mmol, 53%) as a brown solid. The following NMR spectra were identical to the reported ones for empty compound.[3]

He@**7**/**7** (3/7): ^{1}H NMR (300 MHz, CS_2-CD_2Cl_2 (1:1)) δ 8.80 (m, 1H), 8.51 (m, 1H), 7.94 (m, 1H), 7.76 (m, 2H), 7.70 (m, 1H), 7.40 (m, 1H), 7.22 (m, 1H), 6.72 (d, J = 9.9 Hz, 1H), 6.59 (d, J = 9.9 Hz, 1H); ^{13}C NMR (75 MHz, ODCB-d_4) δ 198.37, 187.50, 165.81, 164.11, 151.17, 150.84, 150.71, 150.61, 150.45, 150.31, 149.91, 149.32, 149.19, 149.19, 148.87, 148.68, 148.37, 148.34, 148.13, 148.09, 148.05, 147.89, 147.89, 147.75, 147.69, 147.48, 146.93, 146.69, 146.58, 145.86, 145.60, 145.37, 145.29, 144.45, 144.21, 144.01, 143.70, 143.70, 143.32, 143.17, 142.92, 142.78, 142.17, 142.07, 141.60, 140.66, 139.79, 138.43, 138.15, 137.99, 137.91, 137.81, 137.09, 137.09, 136.73, 136.73, 135.12, 134.52, 133.63, 133.32, 132.85, 123.19, 122.79, 122.42, 122.03, 59.98, 52.92 (the signals at the range of δ 126.0 ~ 132.5 were overlapped with the signals of ODCB-d_4).

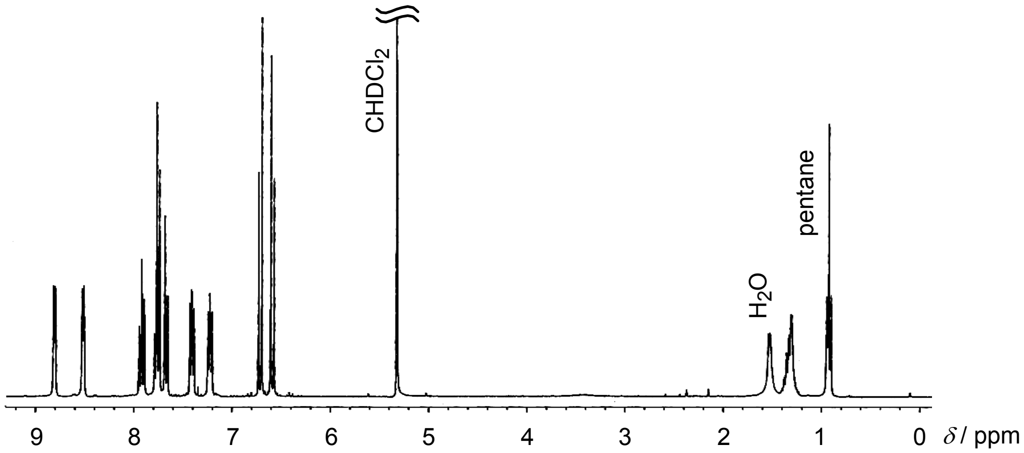


Fig. S8. [1]H NMR (300 MHz, CS_2-CD_2Cl_2 (1:1)) spectrum of He@**7**/**7** (3/7).

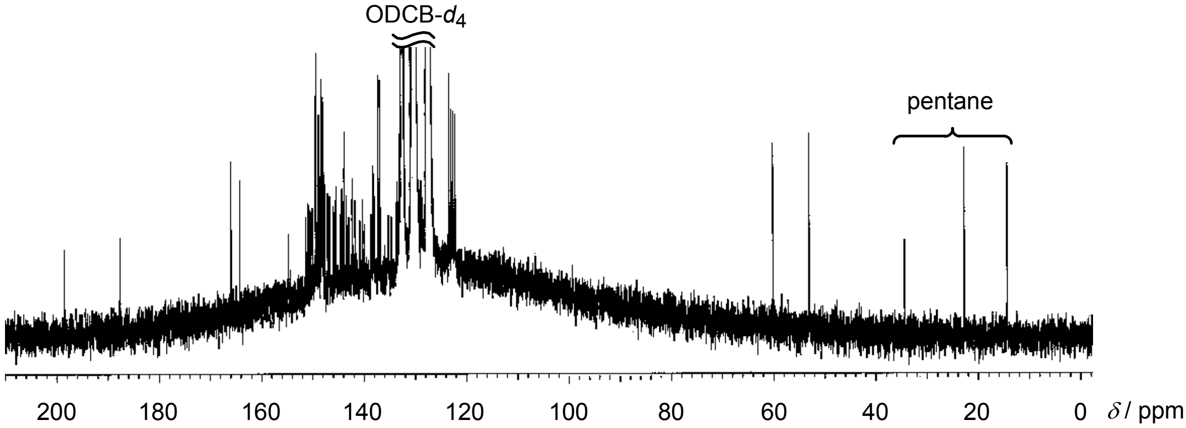


Fig. S9. [13]C NMR (75 MHz, ODCB-d_4) spectrum of He@**7**/**7** (3/7).

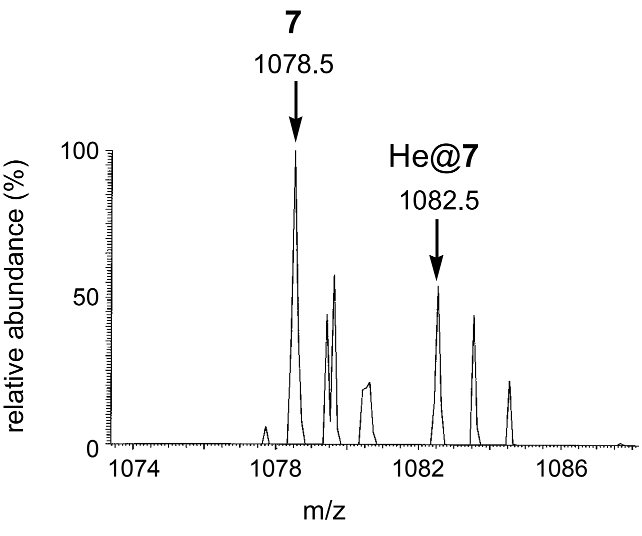
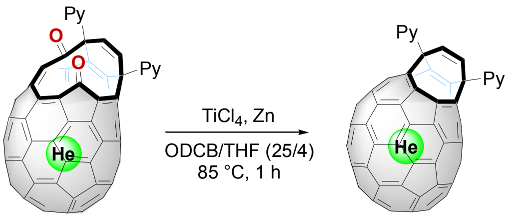


Fig. S10. APCI-MS spectrum (negative-ion mode) of He@**7**/**7** (3/7).

7. Synthesis of C_{70} derivative He@8 with an 8-membered-ring opening



He@**7**/**7** (3/7) (Py = 2-pyridyl) He@**8**/**8** (3/7)

To a stirred suspension of zinc powder (600 mg, 9.176 mmol) in dry THF (20 mL) was added titanium (IV) tetrachloride (500 μL, 4.560 mmol) drop by drop at 0 °C under argon atmosphere, and the mixture was refluxed for 2 h. A 4.1 mL portion of the resulting black slurry was added to a stirred solution of He@**7**/**7** (3/7) (200.0 mg, 0.185 mmol) in dry ODCB (25 mL) at room temperature under argon atmosphere. After heating at 85 °C for 1 h, the resulting brown solution was cooled to room temperature. Then the solution was diluted with CS_2 (30 mL) and washed with aqueous solution of $NaHCO_3$ (saturated, 50 mL). The organic layer was dried over $MgSO_4$ and evaporated under reduced pressure to give a residual brown solid, which was then subjected to flash column chromatography over silica gel. Elution with toluene-EtOAc (10:1) gave He@**8**/**8** (3/7) (157.6 mg, 0.150 mmol, 81%) as a brown solid. The following NMR spectra were identical to the reported ones for empty compound.[3]

He@**8**/**8** (3/7): ^{1}H NMR (300 MHz, CS_2-$CDCl_3$ (1:1)) δ 9.00 (m, 1H), 8.59 (m, 1H), 8.40 (m, 1H), 8.09 (m, 1H), 7.88 (m, 1H), 7.73 (m, 1H), 7.49 (m, 1H), 6.50 (d, J = 9.6 Hz, 1H), 6.30 (d, J = 9.3 Hz, 1H); ^{13}C NMR (75 MHz, CS_2-$CDCl_3$ (1:1)) δ 168.20, 165.41, 153.42, 150.79, 150.61, 150.40, 150.13, 150.00, 150.00, 149.82, 149.34, 149.34, 149.03, 148.46, 148.42, 148.27, 148.33, 148.02, 147.94, 147.89, 147.87, 147.82, 147.75, 147.44, 147.23, 147.20, 147.17, 147.11, 146.84, 146.18, 145.78, 145.72, 145.29, 145.22, 144.99, 144.86, 144.67, 144.27, 144.14, 143.91, 143.91, 143.82, 143.80, 143.12, 142.42, 142.03, 141.67, 141.43, 140.92, 140.43, 139.90, 139.55, 139.15, 138.16, 137.15, 137.08, 136.91, 136.30, 136.02, 135.36, 134.99, 133.29, 132.20, 132.02, 131.66, 131.03, 130.88, 130.49, 128.86, 127.58, 126.46, 124.93, 124.62, 124.41, 124.06, 123.37, 122.27, 122.05, 121.90, 117.49, 54.29, 52.87.

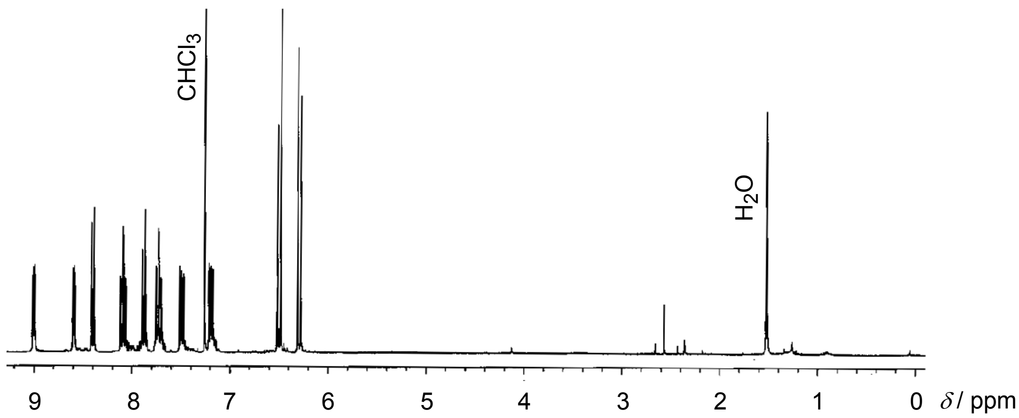


Fig. S11. ^{1}H NMR (300 MHz, CS_2-$CDCl_3$ (1:1)) spectrum of He@**8**/**8** (3/7).

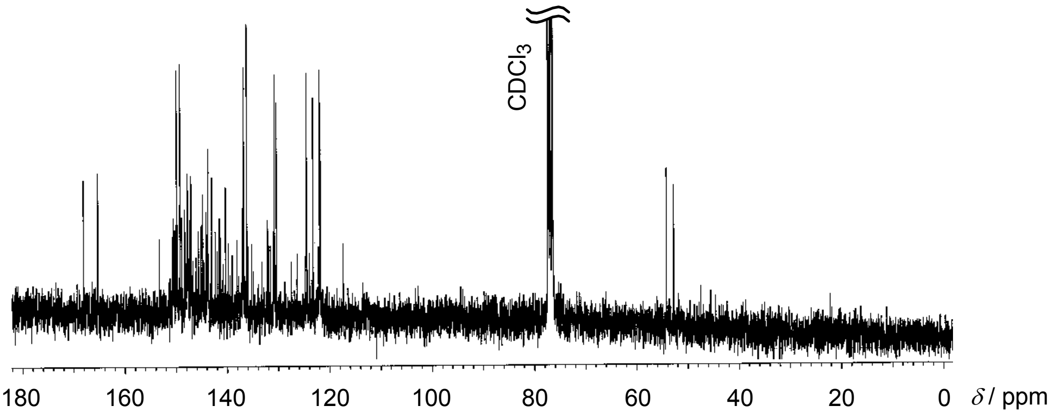
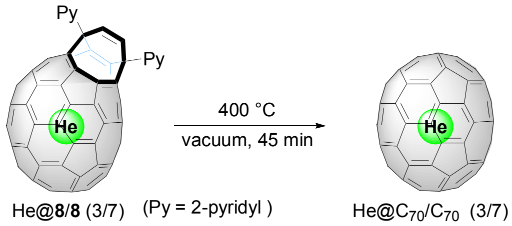


Fig. S12. ^{13}C NMR (75 MHz, CS_2-$CDCl_3$ (1:1)) spectrum of He@**8**/**8** (3/7).

8. Synthesis and enrichment of He@C_{70}

8-1. Synthesis of He@C_{70}



A powder of He@**8/8** (3/7) (137.1 mg, 0.130 mmol) lightly wrapped with a piece of aluminum foil was placed in a glass tube (inner diameter 20 mm), which was heated with an electric furnace at 400 °C for 45 min under vacuum (1 mmHg). The resulting black solid was dissolved in CS_2 (50 mL) and subjected to flash column chromatography over silica gel. Elution with CS_2 gave He@C_{70}/C_{70} (3/7) (29.9 mg, 0.041 mmol, 27%) as a brown solid.

He@C_{70}/C_{70} (3/7): ^{13}C NMR (100 MHz, CS_2-CD_2Cl_2 (1:1)) δ 150.91 (He@C_{70} & C_{70}), 148.36 (He@C_{70} & C_{70}), 147.67(He@C_{70} & C_{70}), 145.66 (He@C_{70}), 145.64 (C_{70}), 131.18 (He@C_{70}), 131.15 (C_{70}); HRMS (+FAB), calcd for C_{70}He (M^+) 844.0026, found 844.0031.

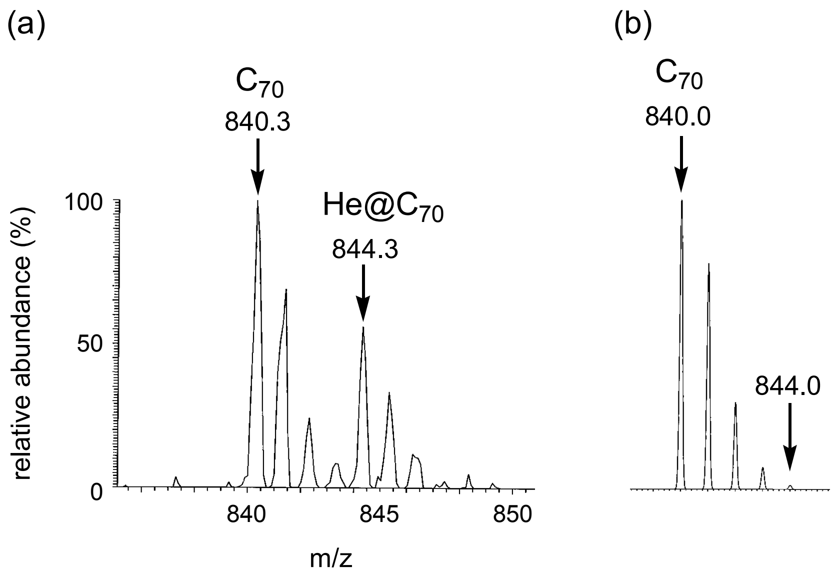


Fig. S13. (a) APCI-MS spectrum (negative-ion mode) of He@C_{70}/C_{70} (3/7) and (b) theoretical isotopic pattern for C_{70}.

8-2. Enrichment of He@C_{70}

The sample of He@C_{70}/C_{70} (3/7) was subjected to the recycle HPLC on Cosmosil Buckyprep column (two directly connected columns; 250 mm length, 20 mm inner diameter; mobile phase, toluene; 50 °C; flow rate was 6.0 mL/min).[4] After 25 recycling, the latter portion was separated and was evaporated to give He@C_{70}/C_{70} (6/4).

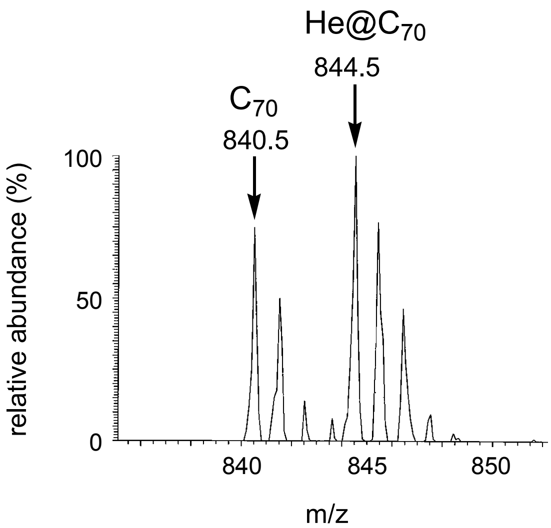
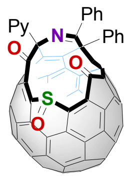


Fig. S14. APCI-MS spectrum (negative-ion mode) of He@C_{70} (He@C_{70}/C_{70} = 6/4) obtained after purification with the recycling HPLC.

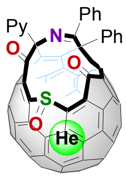
9. Optimized Geometries

9-1. Cage-opened C_{60} derivatives

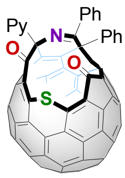
Total energies without and with BSSE correction (E and E_{CP} in hartrees, respectively), and Cartesian coordinates for compounds **3**, He@**3**, **1**, and H_2@**1** calculated at the MPWB1K/6-31G** level.



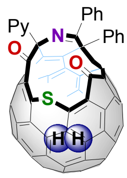
3
(Py = 2-pyridyl)



He@**3**



1



H_2@**1**

3

E = –3788.7685794

Charge = 0, Multiplicity = 1

C	-3.179447	-1.500712	-3.123782
C	-1.763397	-1.395183	-3.338682
C	-1.201177	-0.168465	-3.570352
C	-2.009880	1.018147	-3.557526
C	-3.358503	0.928287	-3.285260
C	-3.958916	-0.359938	-3.075161
C	-1.091454	-2.339535	-2.487794
C	0.068039	0.132414	-2.995130
C	-1.216304	2.054197	-2.968157
C	-3.958484	1.855817	-2.363123
C	-4.954678	-0.225751	-2.045099
C	-3.401946	-2.565359	-2.191198
C	-3.174973	2.816207	-1.757062
C	-1.786332	2.935202	-2.079880
C	-3.297661	3.052754	-0.346656
C	-1.066020	3.277598	-0.888383
C	0.114104	-2.031180	-1.854933
C	0.084605	1.529932	-2.684480
C	-1.999860	3.294475	0.195172
C	0.842822	1.980436	-1.631273
C	0.732913	-0.762496	-2.171005
C	-4.931039	1.138674	-1.587210
C	-5.171048	-1.252742	-1.149025
C	0.364332	-2.568995	-0.521776
C	-4.395282	-2.460648	-1.236518
C	-2.118863	-3.100466	-1.834169
C	-5.374803	-0.965368	0.246103
C	-4.163034	-2.943622	0.096320
C	-1.903358	-3.577027	-0.570786
C	0.236951	2.877003	-0.680256
C	-5.071781	1.406345	-0.238120
C	1.738830	-0.229072	-1.304023
C	-4.774452	-2.020583	1.013804
C	-2.950135	-3.523774	0.415165
C	-0.650864	-3.317986	0.068057
C	-0.910091	-3.204078	1.463893
C	1.354946	-1.915148	0.322346
C	1.850486	1.110318	-1.117762
C	2.156037	2.585228	0.883909
C	-2.331813	-3.263627	1.679526
C	-2.930299	-2.386759	2.565630
C	-2.117040	-1.435313	3.266733
C	-4.149761	-1.730708	2.209155
C	-4.206538	2.357282	0.400486
C	-5.299018	0.340611	0.690234
C	-4.579255	0.648525	1.894599
C	1.048947	-1.744026	1.660270
C	0.701430	2.840392	0.669305
C	-0.211457	2.819559	1.692493
C	-0.134009	-2.338931	2.180752
C	-0.759649	-1.459266	3.116193
C	-4.043584	-0.361870	2.645333
C	-2.769921	-0.161951	3.255621

C	0.007802	-0.287792	3.227707
C	-3.840033	1.867844	1.704433
C	-1.623616	2.863393	1.460909
C	-0.614326	0.925791	3.297334
C	-2.566622	2.063990	2.242272
C	-2.036559	1.015070	3.107314
C	2.481614	-1.213202	-0.432858
C	2.857710	1.692723	-0.188580
N	3.676077	0.750958	0.493569
C	3.503009	-0.501034	0.456573
C	3.751853	2.643823	-0.982801
C	4.419147	-1.313264	1.298869
C	3.282154	-2.116749	-1.383682
C	5.444732	-0.658598	1.976182
C	6.310049	-1.356616	2.789608
C	6.161106	-2.723716	2.956175
C	5.137063	-3.380986	2.303574
C	4.273934	-2.681843	1.479476
C	4.219589	-1.479137	-2.186394
C	4.984755	-2.192917	-3.086163
C	4.820208	-3.561560	-3.203069
C	3.888591	-4.203287	-2.411084
C	3.123643	-3.487057	-1.505964
N	3.135989	3.700136	-1.486274

C	3.845587	4.555893	-2.201337
C	5.196550	4.396373	-2.449614
C	5.831941	3.294596	-1.911773
C	5.101513	2.396718	-1.155894
O	2.770815	3.034960	1.803773
O	2.375431	-0.016015	2.864241
S	0.295038	2.473349	3.377226
C	1.360228	-0.595701	2.634092
O	-0.517322	3.356273	4.251323
H	5.529324	0.409464	1.865996
H	7.098712	-0.830938	3.305166
H	6.836273	-3.270185	3.596389
H	5.005367	-4.443894	2.432509
H	3.481939	-3.217743	0.987251
H	4.346151	-0.407949	-2.106060
H	5.707972	-1.678267	-3.699257
H	5.414680	-4.123078	-3.906457
H	3.752334	-5.270479	-2.491456
H	2.407588	-4.011130	-0.892480
H	3.310409	5.409399	-2.592608
H	5.730815	5.120550	-3.042571
H	6.887042	3.136246	-2.073361
H	5.555286	1.535525	-0.695380

He@**3**

E = –3791.6678036

E_{CP} = –3791.666761176306

Charge = 0, Multiplicity = 1

C	-3.174471	-1.517862	-3.115373
C	-1.758154	-1.413050	-3.329957
C	-1.195423	-0.187352	-3.567229
C	-2.002978	0.999894	-3.559898
C	-3.351007	0.912434	-3.286189
C	-3.950621	-0.374411	-3.068178
C	-1.085833	-2.354271	-2.475988
C	0.074281	0.116373	-2.994771
C	-1.208603	2.038339	-2.976160
C	-3.949874	1.845412	-2.368745

C	-4.944053	-0.232987	-2.037726
C	-3.397498	-2.578676	-2.177999
C	-3.165810	2.807933	-1.767824
C	-1.777460	2.923984	-2.092132
C	-3.288259	3.052887	-0.359012
C	-1.056308	3.272302	-0.903389
C	0.119265	-2.040968	-1.843909
C	0.092215	1.515452	-2.691218
C	-1.989698	3.295310	0.180134
C	0.851397	1.971291	-1.641021
C	0.738838	-0.774315	-2.166306
C	-4.921209	1.133557	-1.587550
C	-5.160775	-1.254709	-1.137079
C	0.370776	-2.570315	-0.507872

C	-4.388149	-2.464657	-1.220820
C	-2.113730	-3.112178	-1.818709
C	-5.364426	-0.958597	0.256021
C	-4.154517	-2.937574	0.114971
C	-1.897283	-3.576763	-0.550676
C	0.246500	2.872477	-0.694088
C	-5.063526	1.410224	-0.240373
C	1.746104	-0.236676	-1.303166
C	-4.765406	-2.010020	1.028509
C	-2.942383	-3.516296	0.436036
C	-0.644438	-3.314863	0.086499
C	-0.902453	-3.192241	1.481705
C	1.362686	-1.912495	0.331929
C	1.859066	1.103526	-1.123881
C	2.166383	2.588964	0.870255
C	-2.323506	-3.249487	1.698568
C	-2.920928	-2.367964	2.580365
C	-2.107026	-1.413613	3.275795
C	-4.140499	-1.713539	2.221758
C	-4.199091	2.365303	0.393222
C	-5.290775	0.349771	0.693969
C	-4.572156	0.664822	1.897398
C	1.057532	-1.732575	1.668893
C	0.711739	2.843544	0.655260
C	-0.200715	2.829414	1.678949
C	-0.125403	-2.323717	2.193204
C	-0.749911	-1.439004	3.124222
C	-4.034314	-0.342634	2.650956
C	-2.759832	-0.140403	3.258615
C	0.018062	-0.267433	3.229462
C	-3.832614	1.883277	1.700371
C	-1.613145	2.872346	1.448034
C	-0.603865	0.946492	3.293897
C	-2.557309	2.079682	2.234441
C	-2.026356	1.035364	3.104236
C	2.489454	-1.216243	-0.427723
C	2.867140	1.690255	-0.198099
N	3.685029	0.751628	0.488976
C	3.511133	-0.500400	0.458167
C	3.761540	2.637378	-0.996783
C	4.424947	-1.309315	1.306159
C	3.289204	-2.124140	-1.374976
C	5.446776	-0.651693	1.986356
C	6.309526	-1.346697	2.805048
C	6.161706	-2.713627	2.974103
C	5.141238	-3.373743	2.318811
C	4.280630	-2.677616	1.489560
C	4.228159	-1.490172	-2.178764
C	4.992734	-2.207547	-3.076155
C	4.825958	-3.576210	-3.189594
C	3.892713	-4.214296	-2.396603
C	3.128323	-3.494468	-1.493822
N	3.144519	3.688047	-1.510583
C	3.854340	4.540857	-2.228896
C	5.206876	4.383965	-2.470194
C	5.843481	3.288338	-1.921398
C	5.112769	2.393603	-1.162044
O	2.782109	3.043475	1.787132
O	2.385878	0.000427	2.864453
S	0.306153	2.493895	3.365523
C	1.370176	-0.579321	2.636932
O	-0.505812	3.382400	4.234332
H	5.530115	0.416271	1.874249
H	7.095191	-0.818784	3.322888
H	6.834881	-3.257710	3.618435
H	5.010342	-4.436510	2.449689
H	3.491375	-3.215808	0.995473
H	4.356424	-0.418993	-2.101100
H	5.717224	-1.695686	-3.690080
H	5.419966	-4.140569	-3.891097
H	3.754734	-5.281462	-2.474333
H	2.410945	-4.015657	-0.879409
H	3.318055	5.389730	-2.628637
H	5.741376	5.105530	-3.066111
H	6.899823	3.132364	-2.077083
H	5.567511	1.537550	-0.693083
He	-2.220955	-0.348278	-0.393701

1

E = –3713.6330266

Charge = 0, Multiplicity = 1

C	-3.228909	-0.581252	-3.302052
C	-1.812840	-0.432531	-3.489755
C	-1.241937	0.808533	-3.401293
C	-2.040725	1.958209	-3.079916
C	-3.389405	1.807963	-2.829322
C	-3.999050	0.512893	-2.953176
C	-1.142931	-1.568225	-2.916953
C	0.031555	0.945089	-2.775385
C	-1.235710	2.805763	-2.253740
C	-3.974355	2.465674	-1.691652
C	-4.986415	0.379785	-1.914495
C	-3.453097	-1.850711	-2.677960
C	-3.178631	3.231232	-0.864636
C	-1.793326	3.428967	-1.161977
C	-3.282411	3.087287	0.559169
C	-1.059847	3.458402	0.068529
C	0.066421	-1.440370	-2.231084
C	0.062791	2.217250	-2.118933
C	-1.976499	3.173184	1.127422
C	0.833690	2.383286	-0.993788
C	0.689670	-0.136436	-2.209968
C	-4.946934	1.577661	-1.117695
C	-5.204988	-0.844916	-1.316788
C	0.320647	-2.309773	-1.085155
C	-4.440014	-1.994162	-1.722054
C	-2.171847	-2.468831	-2.480577
C	-5.396729	-0.930609	0.105778
C	-4.204006	-2.810832	-0.564439
C	-1.952469	-3.259725	-1.387630
C	0.245369	3.023840	0.157475
C	-5.074138	1.483620	0.255408
C	1.703062	0.148878	-1.241103
C	-4.802011	-2.154831	0.566592
C	-2.994255	-3.462714	-0.415696
C	-0.695607	-3.184803	-0.709515
C	-0.949478	-3.444980	0.667618
C	1.318923	-1.907191	-0.103190
C	1.831364	1.397835	-0.724339
C	2.175535	2.342000	1.568711
C	-2.370314	-3.551263	0.867981
C	-2.954529	-2.930995	1.957585
C	-2.126271	-2.210154	2.879682
C	-4.168041	-2.190947	1.791312
C	-4.190823	2.227384	1.109636
C	-5.303565	0.214346	0.874226
C	-4.567124	0.192526	2.107465
C	1.022649	-2.108303	1.231552
C	0.726228	2.644439	1.444887
C	-0.169990	2.323912	2.440642
C	-0.160323	-2.813736	1.585669
C	-0.767620	-2.211411	2.731345
C	-4.038432	-0.983321	2.564113
C	-2.757761	-0.964781	3.190061
C	0.017939	-1.122888	3.149329
C	-3.814870	1.411109	2.231754
C	-1.586488	2.415631	2.226684
C	-0.584636	0.053558	3.517596
C	-2.528912	1.443726	2.778876
C	-2.006264	0.202059	3.337818
C	2.443087	-1.032255	-0.656380
C	2.855652	1.718552	0.308741
N	3.657907	0.623798	0.732821
C	3.476698	-0.575692	0.377348
C	3.766073	2.814109	-0.242247
C	4.415338	-1.573626	0.958320
C	3.231675	-1.673086	-1.808429
C	5.485980	-1.102530	1.712946
C	6.377766	-1.975909	2.296078
C	6.212453	-3.343099	2.149643
C	5.145652	-3.823099	1.416575
C	4.255857	-2.946034	0.822669
C	4.159009	-0.858902	-2.446644
C	4.918229	-1.335742	-3.496016

C	4.759260	-2.639744	-3.929963
C	3.837870	-3.455504	-3.303219
C	3.078331	-2.977022	-2.249311
N	3.169547	3.973968	-0.461720
C	3.892027	4.966639	-0.950601
C	5.237910	4.849041	-1.245481
C	5.852924	3.635585	-1.007653
C	5.108296	2.591915	-0.490096
O	2.805655	2.560457	2.559889
O	2.400719	-0.828132	2.848677
S	0.395321	1.469561	3.878536
C	1.362213	-1.281458	2.483464
H	5.585518	-0.038846	1.848893
H	7.201087	-1.589403	2.876554
H	6.907756	-4.028062	2.609915
H	4.999699	-4.885957	1.302669
H	3.430562	-3.351725	0.265854
H	4.281891	0.164062	-2.116727
H	5.633303	-0.686471	-3.976603
H	5.349712	-3.016631	-4.750221
H	3.705402	-4.474899	-3.630846
H	2.370099	-3.635812	-1.772240
H	3.372558	5.900557	-1.111857
H	5.784114	5.687782	-1.645082
H	6.902998	3.501613	-1.217254
H	5.545307	1.632920	-0.268228

H_2@**1**

E = –3714.8075252

E_{CP} = –3714.806570573809

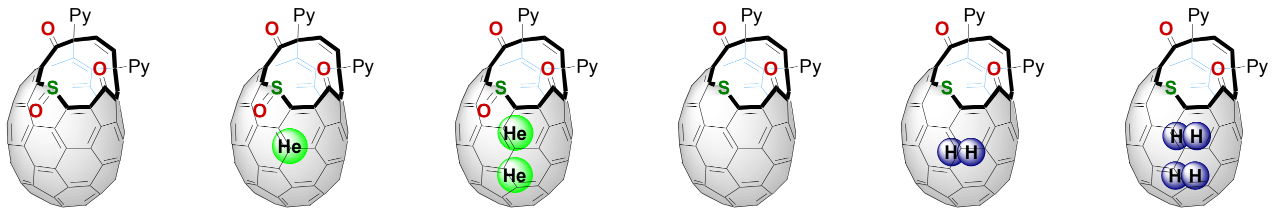
Charge = 0, Multiplicity = 1

C	-3.219799	-0.641507	-3.288934
C	-1.804205	-0.496055	-3.479532
C	-1.233978	0.746161	-3.412006
C	-2.032725	1.900594	-3.111016
C	-3.381687	1.755620	-2.860069
C	-3.990858	0.458348	-2.960516
C	-1.132790	-1.621305	-2.888921
C	0.039484	0.894619	-2.789604
C	-1.227763	2.762421	-2.300132
C	-3.965684	2.433044	-1.733775
C	-4.977348	0.343628	-1.919016
C	-3.443068	-1.900122	-2.643500
C	-3.169945	3.213244	-0.920451
C	-1.784763	3.405942	-1.220550
C	-3.273239	3.095423	0.505683
C	-1.050787	3.457927	0.008857
C	0.076944	-1.479932	-2.206314
C	0.070441	2.177067	-2.155130
C	-1.967459	3.192285	1.072455
C	0.842448	2.363872	-1.034150
C	0.699895	-0.175771	-2.207933
C	-4.937631	1.555533	-1.143815
C	-5.194384	-0.869941	-1.299328
C	0.331882	-2.326226	-1.044376
C	-4.429579	-2.026387	-1.684622
C	-2.161184	-2.513836	-2.435903
C	-5.385936	-0.929278	0.124479
C	-4.192690	-2.821935	-0.512900
C	-1.940433	-3.284429	-1.328939
C	0.254599	3.024919	0.105663
C	-5.063714	1.486578	0.230863
C	1.714902	0.127898	-1.246566
C	-4.790534	-2.144839	0.606115
C	-2.981851	-3.469928	-0.352998
C	-0.683211	-3.195315	-0.653004
C	-0.936122	-3.428061	0.728864
C	1.330086	-1.903351	-0.070783
C	1.842339	1.385180	-0.749921
C	2.183460	2.364263	1.529577
C	-2.356340	-3.531554	0.931290
C	-2.940361	-2.891532	2.009060
C	-2.112959	-2.153863	2.917814
C	-4.154381	-2.156128	1.829863
C	-4.181913	2.246493	1.072271

C	-5.292438	0.229228	0.872684
C	-4.557688	0.231405	2.106813
C	1.034753	-2.078749	1.267436
C	0.735294	2.669131	1.399907
C	-0.161205	2.369553	2.401937
C	-0.147474	-2.778391	1.634357
C	-0.754659	-2.155950	2.768805
C	-4.026550	-0.935636	2.581880
C	-2.746037	-0.904769	3.206849
C	0.030100	-1.060215	3.167744
C	-3.807414	1.453112	2.211291
C	-1.577776	2.456398	2.186213
C	-0.574295	0.120715	3.517531
C	-2.520899	1.496161	2.756964
C	-1.996001	0.264753	3.335371
C	2.455434	-1.042487	-0.642737
C	2.865339	1.723862	0.278466
N	3.671524	0.637432	0.717231
C	3.491801	-0.567728	0.380044
C	3.771496	2.817102	-0.283514
C	4.430111	-1.556281	0.976600
C	3.235018	-1.710099	-1.785539
C	5.504070	-1.074333	1.719560
C	6.395891	-1.939581	2.314688
C	6.227060	-3.308751	2.192534
C	5.156340	-3.799081	1.472084
C	4.266574	-2.930341	0.866198
C	4.152434	-0.911668	-2.457143
C	4.898279	-1.414808	-3.503928
C	4.735199	-2.729558	-3.902288
C	3.823280	-3.529798	-3.242554
C	3.077582	-3.024905	-2.191332
N	3.179461	3.984067	-0.475675
C	3.898405	4.976680	-0.969850
C	5.236219	4.852087	-1.296612
C	5.846455	3.630798	-1.088091
C	5.105301	2.586754	-0.566512
O	2.812517	2.592591	2.519176
O	2.414167	-0.775234	2.864963
S	0.403413	1.543295	3.856374
C	1.374932	-1.231404	2.505730
H	5.606501	-0.008596	1.836181
H	7.222123	-1.544985	2.885479
H	6.922630	-3.987184	2.661973
H	5.007329	-4.863403	1.377461
H	3.437846	-3.343247	0.319858
H	4.276973	0.120044	-2.157129
H	5.605492	-0.777126	-4.010944
H	5.314626	-3.126427	-4.720979
H	3.687113	-4.557144	-3.542605
H	2.375297	-3.671434	-1.689350
H	3.382856	5.916418	-1.108186
H	5.780300	5.691689	-1.697265
H	6.890536	3.491289	-1.322531
H	5.540168	1.622373	-0.364660
H	-2.269248	-0.504955	-0.013317
H	-2.238098	0.222828	-0.178376

9-2. Cage-opened C_{70} derivatives

Total energies without and with BSSE correction (E and E_{CP} in hartrees, respectively), and Cartesian coordinates for compounds **6**, He@**6**, He_2@**6**, **2**, H_2@**2**, and $(H_2)_2$@**2** calculated at the MPWB1K/6-31G** level.



6 He@**6** He_2@**6** **2** H_2@**2** $(H_2)_2$@**2**

(Py = 2-pyridyl)

6

E = –3938.795066

Charge = 0, Multiplicity = 1

C	3.161062	-0.071466	0.713681
C	2.510260	-0.834049	1.727970
C	2.099241	-2.162966	1.364360
C	2.385029	-2.621546	0.046451
C	3.672530	-2.174990	-0.550822
C	1.834726	-0.279315	-3.215476
C	0.578545	-1.121579	-3.252990
C	0.314387	-2.345603	-2.735429
C	1.391059	-3.226628	-0.684218
C	0.073207	-3.430809	-0.163742
C	-0.028596	-3.339028	1.209926
C	0.981795	-2.695501	1.979233
C	0.317672	-2.035608	3.054612
C	0.698827	-0.765740	3.385689
C	1.757018	-0.149922	2.655375
C	1.346790	1.186943	2.389528
C	1.640537	1.765365	1.173721
C	2.693213	1.172189	0.410040
C	1.653559	1.833655	-1.599215
C	1.294328	1.045518	-2.656256
C	-0.062544	1.074670	-3.094567
C	-0.482668	-0.212850	-3.441867
C	-1.815563	-0.599292	-3.397075
C	-2.095659	-1.860633	-2.755386
C	-1.014746	-2.625042	-2.230645
C	-1.142335	-3.261579	-0.961421
C	-2.407416	-3.207664	-0.288032
C	-2.474467	-3.154827	1.165078
C	-1.279337	-3.165049	1.877810
C	-1.075923	-2.361358	3.018299
C	-2.063917	-1.467872	3.459364
C	-1.657396	-0.115269	3.805788
C	-0.299302	0.215464	3.686322
C	0.105306	1.411946	3.056269
C	-0.813695	2.334001	2.561573
C	-0.538726	2.951503	1.274071
C	0.636511	2.596418	0.532864
C	0.591569	2.557696	-0.893948
C	-0.641333	2.820508	-1.552426
C	-0.984958	2.040410	-2.712603
C	-2.329387	1.759882	-3.010611
C	-2.744078	0.447965	-3.350032
C	-4.058096	0.246683	-2.824116
C	-4.364323	-0.970536	-2.269510
C	-3.361932	-2.003982	-2.190162
C	-3.518186	-2.689819	-0.973432
C	-4.654634	-2.111916	-0.294829
C	-4.667031	-2.009522	1.068161
C	-3.552382	-2.517495	1.808670
C	-3.343787	-1.666020	2.921578
C	-4.300889	-0.593747	2.841409
C	-3.915418	0.684775	3.163875
C	-2.561716	0.934012	3.584084

C	-2.142076	2.149701	2.989675
C	-3.243997	2.682631	2.246691
C	-2.996435	3.338606	1.072170
C	-1.646453	3.447825	0.573863
C	-1.701342	3.372753	-0.828727
C	-3.076848	3.190210	-1.221360
C	-3.391854	2.380492	-2.282692
C	-4.487311	1.457996	-2.187443
C	-5.246629	1.402656	-1.038626
C	-4.953563	2.290422	0.053872
C	-3.881976	3.162465	-0.039849
C	-5.186309	1.577530	1.277521
C	-4.356701	1.786948	2.361078
C	-5.594067	0.240383	0.943285
C	-5.146170	-0.819530	1.707285
C	-5.617466	0.126735	-0.486944
C	-5.168217	-1.036392	-1.089880
C	4.063165	1.109219	-1.665610
C	4.197761	-0.796051	-0.084196
C	3.001919	1.832278	-0.901307
C	4.607957	-0.034053	-1.297087
C	3.510268	3.253302	-0.683953
C	5.379624	-1.049477	0.843422
C	6.374907	-0.099800	0.995728
C	7.398332	-0.366843	1.882820
C	7.385985	-1.558790	2.581700
C	6.334904	-2.430902	2.368630
N	5.348311	-2.185315	1.520868
N	4.303138	3.415130	0.363628
C	4.827959	4.612023	0.568547
C	4.600000	5.698073	-0.256830
C	3.783575	5.518350	-1.355832
C	3.226649	4.274108	-1.576999
O	4.273595	-2.806334	-1.372628
O	2.922680	-0.593398	-3.583985
S	1.596918	-3.554341	-2.429853
O	0.987746	-4.880301	-2.697276
H	4.369412	1.570892	-2.592488
H	5.344052	-0.515569	-1.921651
H	6.328132	0.825104	0.443422
H	8.193461	0.347846	2.028751
H	8.166758	-1.808532	3.281410
H	6.281096	-3.369327	2.901774
H	5.464582	4.708788	1.436891
H	5.052974	6.652037	-0.041766
H	3.580290	6.334727	-2.031417
H	2.582329	4.095572	-2.423277

He@**6**

$E = -3941.6960299$

$E_{CP} = -3941.695194858822$

Charge = 0, Multiplicity = 1

C	3.165649	-0.072363	0.710334
C	2.513240	-0.830284	1.726606
C	2.100804	-2.160415	1.369144
C	2.386072	-2.626556	0.053942
C	3.673478	-2.182674	-0.546105
C	1.843449	-0.296214	-3.208935
C	0.586556	-1.138171	-3.239056
C	0.318261	-2.361582	-2.722297
C	1.391790	-3.237154	-0.671957
C	0.073396	-3.438057	-0.150373
C	-0.027947	-3.337647	1.222196
C	0.983464	-2.689724	1.987035
C	0.320265	-2.023033	3.058146
C	0.703097	-0.752133	3.383323
C	1.762084	-0.140808	2.651474
C	1.355097	1.196525	2.381848
C	1.650798	1.771571	1.165469
C	2.702488	1.172620	0.404397
C	1.665852	1.828793	-1.605016
C	1.305491	1.032396	-2.654883
C	-0.051691	1.060087	-3.090457
C	-0.473174	-0.228606	-3.429091
C	-1.806467	-0.613184	-3.384833
C	-2.092260	-1.874056	-2.744931

C	-1.012430	-2.637906	-2.217884	C	-3.867732	3.174743	-0.054344
C	-1.143034	-3.272024	-0.948224	C	-5.167038	1.588126	1.266809
C	-2.410423	-3.216988	-0.276924	C	-4.341914	1.804940	2.350730
C	-2.476384	-3.155726	1.177096	C	-5.576079	0.249999	0.938330
C	-1.279126	-3.158688	1.888346	C	-5.136449	-0.808970	1.706390
C	-1.073460	-2.347611	3.022809	C	-5.600154	0.129426	-0.489624
C	-2.059475	-1.449728	3.457869	C	-5.162732	-1.040054	-1.088438
C	-1.650889	-0.096055	3.798306	C	4.074009	1.100342	-1.669818
C	-0.292652	0.232322	3.679401	C	4.200841	-0.802337	-0.084529
C	0.113810	1.426589	3.046958	C	3.014451	1.828593	-0.907881
C	-0.802636	2.352032	2.551893	C	4.614063	-0.044597	-1.299069
C	-0.526321	2.966795	1.262412	C	3.524991	3.249097	-0.694235
C	0.648518	2.603950	0.522533	C	5.381318	-1.054875	0.845348
C	0.604401	2.559190	-0.903847	C	6.376149	-0.104825	0.998615
C	-0.628036	2.822363	-1.563703	C	7.397632	-0.370560	1.888316
C	-0.972117	2.031349	-2.716743	C	7.383939	-1.561600	2.588763
C	-2.315505	1.750749	-3.015684	C	6.333478	-2.434148	2.374520
C	-2.731710	0.435739	-3.346765	N	5.348694	-2.189786	1.524249
C	-4.045940	0.236688	-2.823789	N	4.312170	3.414569	0.357026
C	-4.358773	-0.980215	-2.268793	C	4.838161	4.611520	0.558945
C	-3.361746	-2.018917	-2.186097	C	4.616918	5.693849	-0.273094
C	-3.521734	-2.702904	-0.966746	C	3.806300	5.510252	-1.375812
C	-4.656818	-2.117916	-0.289187	C	3.248313	4.265990	-1.593931
C	-4.667313	-2.008015	1.074374	O	4.273608	-2.817096	-1.366241
C	-3.553914	-2.514956	1.818834	O	2.929540	-0.611296	-3.581954
C	-3.339702	-1.652237	2.924088	S	1.595455	-3.575371	-2.415621
C	-4.291435	-0.576979	2.838831	O	0.979426	-4.899585	-2.675428
C	-3.903431	0.703364	3.155116	H	4.382799	1.559203	-2.597282
C	-2.551764	0.955048	3.575774	H	5.348707	-0.529979	-1.922380
C	-2.130990	2.172655	2.982635	H	6.330425	0.819477	0.445189
C	-3.231710	2.705234	2.236524	H	8.192299	0.344471	2.035143
C	-2.983559	3.358473	1.058959	H	8.163165	-1.810251	3.290597
C	-1.632644	3.465382	0.559629	H	6.278563	-3.371876	2.908794
C	-1.687059	3.384448	-0.844390	H	5.470086	4.711379	1.430374
C	-3.062791	3.197787	-1.237083	H	5.070461	6.648040	-0.060192
C	-3.376443	2.378056	-2.292650	H	3.608338	6.323729	-2.056469
C	-4.469030	1.452563	-2.192258	H	2.608169	4.084299	-2.442749
C	-5.225975	1.402332	-1.044019	He	-2.072414	0.155278	0.143761
C	-4.935035	2.297385	0.042343				

He_2@**6**

$E = -3944.5939699$

$E_{CP} = -3944.591474854503$

Charge = 0, Multiplicity = 1

C	3.165505	-0.069506	0.709634
C	2.513586	-0.830330	1.724020
C	2.104341	-2.160796	1.365086
C	2.390622	-2.623737	0.049038
C	3.677856	-2.176590	-0.549492
C	1.849687	-0.285631	-3.207656
C	0.594082	-1.129408	-3.238964
C	0.327840	-2.354313	-2.724306
C	1.399123	-3.238849	-0.676676
C	0.081470	-3.443938	-0.155128
C	-0.021775	-3.341279	1.217467
C	0.987770	-2.691940	1.982623
C	0.324013	-2.029591	3.056689
C	0.704839	-0.758893	3.384034
C	1.761814	-0.144812	2.651006
C	1.354198	1.192473	2.385300
C	1.652259	1.772849	1.171641
C	2.703733	1.177017	0.408111
C	1.668766	1.836993	-1.601799
C	1.310295	1.042731	-2.654503
C	-0.047768	1.067361	-3.088544
C	-0.467211	-0.221310	-3.429000
C	-1.800165	-0.606385	-3.387729
C	-2.081827	-1.866154	-2.746172
C	-1.002434	-2.631649	-2.220681
C	-1.133424	-3.269935	-0.952951
C	-2.398834	-3.209994	-0.280752
C	-2.467202	-3.153958	1.171889
C	-1.272528	-3.164012	1.885052
C	-1.069235	-2.356229	3.022830
C	-2.056814	-1.460691	3.461049
C	-1.650271	-0.107268	3.803855
C	-0.292299	0.223084	3.683845
C	0.113056	1.418469	3.052040
C	-0.805764	2.338775	2.554906
C	-0.529830	2.954323	1.267453
C	0.647446	2.601069	0.528572
C	0.604723	2.560526	-0.898141
C	-0.629219	2.818518	-1.556281
C	-0.971416	2.034432	-2.713062
C	-2.315284	1.752838	-3.010811
C	-2.728651	0.440622	-3.345993
C	-4.043755	0.242249	-2.822260
C	-4.350636	-0.972901	-2.265847
C	-3.349272	-2.007017	-2.183944
C	-3.507916	-2.690365	-0.967316
C	-4.644093	-2.108172	-0.292122
C	-4.657430	-2.003585	1.069742
C	-3.544557	-2.512362	1.812220
C	-3.336491	-1.658746	2.922731
C	-4.293320	-0.586234	2.838965
C	-3.907714	0.692221	3.157817
C	-2.554354	0.941496	3.578667
C	-2.134308	2.155181	2.982042
C	-3.235686	2.685628	2.236682
C	-2.988715	3.339351	1.061718
C	-1.638042	3.447130	0.565752
C	-1.691393	3.370396	-0.835611
C	-3.067019	3.187827	-1.228455
C	-3.379905	2.374788	-2.286859
C	-4.477261	1.455069	-2.191841
C	-5.243744	1.405157	-1.046608
C	-4.951442	2.296485	0.044408
C	-3.875830	3.164980	-0.049351
C	-5.180825	1.583383	1.269320
C	-4.348663	1.791597	2.351507
C	-5.588379	0.245456	0.938139
C	-5.137173	-0.812275	1.704289
C	-5.613649	0.129283	-0.492027
C	-5.158580	-1.035026	-1.089486
C	4.077638	1.111427	-1.664648
C	4.202588	-0.796418	-0.085383
C	3.016312	1.836893	-0.902395

C	4.616916	-0.034937	-1.297201
C	3.524048	3.257829	-0.685283
C	5.382403	-1.048403	0.845702
C	6.374916	-0.096394	1.002054
C	7.396060	-0.361723	1.892206
C	7.384368	-1.554334	2.590051
C	6.336133	-2.428755	2.372861
N	5.351625	-2.184779	1.522115
N	4.309678	3.422977	0.367189
C	4.833004	4.620610	0.571824
C	4.610500	5.704025	-0.258482
C	3.801578	5.520800	-1.362474
C	3.246383	4.275795	-1.583451
O	4.279971	-2.809229	-1.369482
O	2.936435	-0.600008	-3.579548
S	1.604322	-3.569774	-2.421471
O	0.987465	-4.892235	-2.688154
H	4.387977	1.573505	-2.589988
H	5.352648	-0.517974	-1.921023
H	6.327770	0.828959	0.450552
H	8.188932	0.354799	2.041388
H	8.163472	-1.802703	3.292102
H	6.282724	-3.367706	2.905099
H	5.463647	4.720265	1.444190
H	5.061811	6.658739	-0.043257
H	3.602695	6.335061	-2.041906
H	2.607575	4.094360	-2.433311
He	-2.575897	0.339418	0.050822
He	0.098352	-0.444541	-0.240272

2

$E = -3863.6591055$

Charge = 0, Multiplicity = 1

C	-3.181875	-0.298517	-0.620296
C	-2.540830	-1.235641	-1.482757
C	-2.124547	-2.476752	-0.883350
C	-2.406160	-2.679464	0.497736
C	-3.689298	-2.138932	1.002319
C	-1.806270	0.280949	3.316289
C	-0.547679	-0.526628	3.514318
C	-0.295513	-1.826253	3.209543
C	-1.401354	-3.096313	1.345247
C	-0.079203	-3.369810	0.858104
C	0.017809	-3.555532	-0.508383
C	-1.000619	-3.098761	-1.391036
C	-0.342227	-2.647600	-2.573212
C	-0.732305	-1.465248	-3.136083
C	-1.787913	-0.729949	-2.519639
C	-1.378494	0.632992	-2.504515
C	-1.662433	1.421926	-1.410569
C	-2.704562	0.976554	-0.542511
C	-1.651251	2.019551	1.304291
C	-1.277881	1.468772	2.498101
C	0.081461	1.595353	2.913019
C	0.511845	0.404564	3.508816
C	1.845270	0.018900	3.505134
C	2.114237	-1.337290	3.092635
C	1.025521	-2.182182	2.726897
C	1.141702	-3.046075	1.599156
C	2.405504	-3.127739	0.920181
C	2.464394	-3.359055	-0.514213
C	1.265519	-3.510960	-1.202969
C	1.054129	-2.949349	-2.478569
C	2.036269	-2.153340	-3.088535
C	1.619803	-0.893762	-3.683413
C	0.260343	-0.552813	-3.617848
C	-0.144502	0.737405	-3.213470
C	0.771629	1.739741	-2.907650
C	0.503503	2.584820	-1.753744
C	-0.660312	2.364457	-0.945578
C	-0.602091	2.599444	0.461301
C	0.633850	2.998073	1.043783
C	0.994495	2.466661	2.332399
C	2.344556	2.259922	2.663598
C	2.769292	1.038091	3.241657
C	4.075268	0.740067	2.744356

C	4.376652	-0.560869	2.428552
C	3.373842	-1.589381	2.552323
C	3.522019	-2.492684	1.485485
C	4.654496	-2.054850	0.702660
C	4.654936	-2.215432	-0.654725
C	3.537420	-2.857928	-1.276233
C	3.320490	-2.238771	-2.530731
C	4.274343	-1.168498	-2.663965
C	3.877891	0.023816	-3.219235
C	2.519184	0.182999	-3.668062
C	2.097149	1.485636	-3.307858
C	3.201818	2.154267	-2.689713
C	2.959393	3.019289	-1.658464
C	1.613376	3.212937	-1.174425
C	1.681821	3.408924	0.215265
C	3.063350	3.317124	0.619987
C	3.394668	2.728946	1.813629
C	4.493876	1.808008	1.883506
C	5.241093	1.535951	0.757891
C	4.934594	2.198318	-0.480879
C	3.856342	3.065495	-0.543588
C	5.159551	1.264991	-1.547598
C	4.319781	1.259741	-2.643620
C	5.576763	0.017346	-0.968248
C	5.127493	-1.169944	-1.512917
C	5.611408	0.178959	0.457147
C	5.170690	-0.847642	1.275842
C	-4.056625	1.291066	1.521170
C	-4.215864	-0.861928	0.299673
C	-3.004926	1.865926	0.628797
C	-4.609158	0.103187	1.363248
C	-3.528651	3.216738	0.150109
C	-5.407674	-1.273466	-0.554914
C	-6.411745	-0.369677	-0.859023
C	-7.447404	-0.795965	-1.666430
C	-7.438364	-2.095028	-2.138536
C	-6.378017	-2.910071	-1.789339
N	-5.380006	-2.512197	-1.017438
N	-4.318935	3.170634	-0.910735
C	-4.851026	4.302392	-1.341683
C	-4.634033	5.527158	-0.737839
C	-3.820875	5.566000	0.377849
C	-3.256151	4.391028	0.833555
O	-4.286770	-2.609789	1.928518
O	-2.894200	0.043299	3.737410
S	-1.614537	-2.978372	3.091651
H	-4.348877	1.906762	2.358752
H	-5.338426	-0.258490	2.071160
H	-6.359417	0.638720	-0.480319
H	-8.249631	-0.122225	-1.925150
H	-8.229463	-2.469880	-2.767248
H	-6.327134	-3.929188	-2.145419
H	-5.484320	4.227093	-2.214641
H	-5.091416	6.419708	-1.132445
H	-3.625198	6.497883	0.885427
H	-2.611198	4.380134	1.698044

H_2@**2**

$E = –3864.8314698$

$E_{CP} = –3864.830618707344$

Charge = 0, Multiplicity = 1

C	-3.175076	-0.306471	-0.611313
C	-2.533150	-1.215045	-1.502240
C	-2.112456	-2.472562	-0.942014
C	-2.391815	-2.716972	0.433148
C	-3.675839	-2.194915	0.956035
C	-1.802111	0.180442	3.329988
C	-0.539017	-0.627254	3.497906
C	-0.279776	-1.917019	3.159252
C	-1.381354	-3.147538	1.267182
C	-0.057778	-3.398415	0.770231
C	0.038220	-3.546875	-0.600832
C	-0.984295	-3.071509	-1.468709
C	-0.331110	-2.582615	-2.638070
C	-0.729901	-1.387355	-3.166975
C	-1.787639	-0.676057	-2.527813
C	-1.386955	0.688633	-2.478643

C	-1.673665	1.446880	-1.364196
C	-2.708906	0.970231	-0.503281
C	-1.663061	1.976446	1.362573
C	-1.283235	1.392329	2.538773
C	0.076355	1.513408	2.952382
C	0.514876	0.309749	3.515153
C	1.850211	-0.068016	3.500824
C	2.126539	-1.411079	3.052056
C	1.042705	-2.252727	2.665783
C	1.163213	-3.089045	1.517877
C	2.427054	-3.147308	0.835735
C	2.483706	-3.336556	-0.605499
C	1.284484	-3.476179	-1.296043
C	1.066912	-2.879600	-2.555022
C	2.041778	-2.060376	-3.145265
C	1.616371	-0.787259	-3.704577
C	0.255632	-0.455941	-3.626300
C	-0.156218	0.821352	-3.188958
C	0.753073	1.823625	-2.861691
C	0.480672	2.639395	-1.686727
C	-0.678988	2.388233	-0.880648
C	-0.618646	2.583578	0.532326
C	0.616958	2.971661	1.122271
C	0.983027	2.404975	2.393805
C	2.334110	2.196697	2.717491
C	2.767259	0.963552	3.263659
C	4.074415	0.686609	2.757738
C	4.382650	-0.603717	2.407051
C	3.386806	-1.642177	2.504602
C	3.539874	-2.518107	1.415123
C	4.666076	-2.048713	0.641382
C	4.664354	-2.171682	-0.719864
C	3.550070	-2.804745	-1.356091
C	3.327219	-2.152696	-2.592912
C	4.273939	-1.073354	-2.699178
C	3.869483	0.130651	-3.222604
C	2.508572	0.294364	-3.663665
C	2.079590	1.585413	-3.270069
C	3.182010	2.242763	-2.636126
C	2.935649	3.078689	-1.582182
C	1.589261	3.255698	-1.091942
C	1.660114	3.411570	0.303161
C	3.042210	3.313858	0.703262
C	3.379353	2.694536	1.879330
C	4.484151	1.778955	1.923576
C	5.231220	1.542614	0.790569
C	4.916833	2.235939	-0.429225
C	3.833738	3.098568	-0.467645
C	5.147019	1.333503	-1.520647
C	4.304938	1.352986	-2.614688
C	5.573746	0.073654	-0.975469
C	5.129752	-1.101061	-1.550536
C	5.610217	0.196580	0.453758
C	5.176265	-0.854094	1.245729
C	-4.056654	1.217558	1.573121
C	-4.205464	-0.901228	0.292117
C	-3.016935	1.827260	0.689956
C	-4.599787	0.029963	1.385702
C	-3.574050	3.173843	0.238033
C	-5.402951	-1.260658	-0.579123
C	-6.261188	-0.263318	-1.015692
C	-7.316411	-0.626805	-1.827079
C	-7.468442	-1.957124	-2.174400
C	-6.539081	-2.865442	-1.705962
N	-5.521996	-2.529625	-0.927013
N	-4.472096	3.099639	-0.733546
C	-5.041425	4.219610	-1.144916
C	-4.758086	5.462458	-0.608314
C	-3.835410	5.531258	0.416173
C	-3.230382	4.367320	0.850712
O	-4.263340	-2.689514	1.875893
O	-2.884227	-0.071100	3.757066
S	-1.591760	-3.073759	3.016321
H	-4.350119	1.808257	2.428012
H	-5.323819	-0.357067	2.085119
H	-6.075947	0.764219	-0.738925
H	-8.009490	0.117944	-2.187032
H	-8.281340	-2.284598	-2.801880
H	-6.611562	-3.911421	-1.967957
H	-5.762837	4.120655	-1.943963

H	-5.250803	6.344631	-0.983062
H	-3.586167	6.477263	0.871361
H	-2.502850	4.382530	1.646157

$(H_2)_2$@**2**

E = – 3866.0036747

E_{CP} = –3866.001340132286

Charge = 0, Multiplicity = 1

C	-3.188006	-0.289270	-0.621839
C	-2.546572	-1.217468	-1.492984
C	-2.130052	-2.465931	-0.907710
C	-2.410830	-2.684324	0.470962
C	-3.693202	-2.147044	0.982439
C	-1.820735	0.239011	3.309400
C	-0.561731	-0.570645	3.497977
C	-0.306521	-1.868227	3.185458
C	-1.408074	-3.119671	1.312270
C	-0.086468	-3.393289	0.823043
C	0.010847	-3.556246	-0.545998
C	-1.006820	-3.083866	-1.422244
C	-0.347762	-2.615773	-2.597124
C	-0.738368	-1.427537	-3.146823
C	-1.796068	-0.699702	-2.525746
C	-1.389245	0.664519	-2.499602
C	-1.676972	1.444875	-1.400784
C	-2.717519	0.988199	-0.536511
C	-1.665730	2.007683	1.319856
C	-1.293032	1.437685	2.505171
C	0.066420	1.557968	2.920194
C	0.496726	0.361103	3.501644
C	1.830419	-0.022214	3.496764
C	2.102043	-1.373050	3.072201
C	1.015595	-2.218123	2.700797
C	1.134486	-3.073153	1.567064
C	2.398887	-3.139575	0.887437
C	2.458265	-3.351225	-0.548846
C	1.259344	-3.496888	-1.238453
C	1.048243	-2.917760	-2.505764
C	2.030139	-2.114568	-3.106038

H	1.261058	-0.118393	-0.288896
H	1.988690	-0.095857	-0.134228

C	1.613634	-0.849457	-3.686518
C	0.254215	-0.510199	-3.617917
C	-0.152237	0.775437	-3.202809
C	0.764431	1.773651	-2.885524
C	0.494448	2.606374	-1.724535
C	-0.672968	2.380043	-0.923460
C	-0.615415	2.597475	0.485459
C	0.621488	2.985978	1.072750
C	0.980359	2.436818	2.353117
C	2.329881	2.228904	2.685077
C	2.754094	1.000698	3.248440
C	4.061972	0.710523	2.752512
C	4.365566	-0.586463	2.423991
C	3.364020	-1.617848	2.534821
C	3.514776	-2.508935	1.458954
C	4.647532	-2.059995	0.682902
C	4.649274	-2.204663	-0.675915
C	3.531128	-2.839349	-1.304017
C	3.314663	-2.205668	-2.550667
C	4.269608	-1.135095	-2.672953
C	3.872497	0.063103	-3.215014
C	2.513150	0.226527	-3.660992
C	2.090365	1.524747	-3.287629
C	3.194870	2.187082	-2.662727
C	2.950824	3.040284	-1.622504
C	1.604120	3.228783	-1.138637
C	1.671052	3.409073	0.252662
C	3.052365	3.313442	0.658340
C	3.382347	2.711156	1.845283
C	4.481859	1.789358	1.905831
C	5.231999	1.531310	0.778852
C	4.926357	2.207934	-0.452657
C	3.847066	3.075109	-0.506795
C	5.153207	1.286411	-1.529289
C	4.313577	1.292867	-2.625871

C	5.571135	0.032435	-0.963668
C	5.123257	-1.149505	-1.522012
C	5.603764	0.177761	0.463717
C	5.162212	-0.858835	1.269994
C	-4.070240	1.280806	1.530296
C	-4.220806	-0.863440	0.292926
C	-3.019353	1.865350	0.643179
C	-4.617382	0.091502	1.364193
C	-3.540789	3.221670	0.178690
C	-5.412741	-1.267159	-0.565836
C	-6.405429	-0.353690	-0.878336
C	-7.442487	-0.772107	-1.688012
C	-7.445610	-2.073156	-2.154753
C	-6.395044	-2.897817	-1.798575
N	-5.395988	-2.507605	-1.024069
N	-4.335060	3.186765	-0.879645
C	-4.864453	4.323736	-1.300016
C	-4.640418	5.543030	-0.687828
C	-3.823146	5.570296	0.425164
C	-3.261386	4.389715	0.870026
O	-4.291360	-2.628131	1.902817
O	-2.907231	-0.002738	3.731717
S	-1.622719	-3.021861	3.059882
H	-4.365348	1.889606	2.371951
H	-5.345787	-0.278086	2.068888
H	-6.344312	0.655546	-0.503179
H	-8.236495	-0.090839	-1.952313
H	-8.238315	-2.442171	-2.784893
H	-6.353468	-3.918725	-2.150707
H	-5.501192	4.257523	-2.171195
H	-5.095588	6.440348	-1.074089
H	-3.621831	6.497584	0.938918
H	-2.612981	4.369979	1.731742
H	0.086009	-0.586701	-0.211620
H	-0.154519	-0.518659	0.487438
H	2.606849	0.077521	-0.428462
H	2.377043	0.400687	0.201591

10. References

1 Y. Murata, M. Murata, K. Komatsu, *Chem*. *Eur*. *J*., 2003, **9**, 1600.

2 M. Murata, Y. Murata, K. Komatsu, *J*. *Am*. *Chem*. *Soc*., 2006, **128**, 8024.

3 Y. Murata, S. Maeda, M. Murata, K. Komatsu, *J*. *Am*. *Chem*. *Soc*., 2008, **130**, 6702.

4 M. Murata, S. Maeda, Y. Morinaka, Y. Murata, K. Komatsu, *J*. *Am*. *Chem*. *Soc*., 2008, **130**, 15800.