Supplementary Material (ESI) for Chemical Communications

Supporting information for

Structural Similarities in C_s(16)-C_{86} and C_2(17)-C_{86}†

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Experimental and computation section

Synthesis of C_{86}. The 8 × 150 mm graphite rods were core-drilled (6.0 mm diameter), and were packed with a mixture of Sm_2O_3 and graphite powder with atomic ratio of 1:40. The packed rods were preheated at about 800°C under a dinitrogen atmosphere for 12 hours. The rods were then vaporized in a Krätschmer-Huffman arc-discharge generator with pressure of 200 torr.[1] The discharging electric current and voltage were 80 A and 30 V, respectively. The raw soot was collected and extracted repeatedly with *o*-dichlorobenzene with ultrasonication until the extract was colorless, without special nitrogen protection. After removing the solvent with a rotary evaporator, chlorobenzene was added to redissolve the dry powder.

HPLC separation of C_{86}. The extract was subjected to a four-stage HPLC isolation process that did not involve recycling.The first-stage of chromatography was carried out on a Buckyprep-M column with chlorobenzene eluent, and the eluent from 9.0 to 10.5 minutes was collected as F1 (dashed portion). F1 was subjected to the second-stage separation utilizing a Buckyprep column with toluene eluent, and F2 was collected. The third-stage isolation for F2 was performed on a 5PBB column with toluene eluent, the dashed part located between two main peaks was collected as F3, which was condensed and re-injected into the same column in order to get rid of both the front and the rear impurities. All the columns used were 10 × 250 mm (Nacalai Tesque).

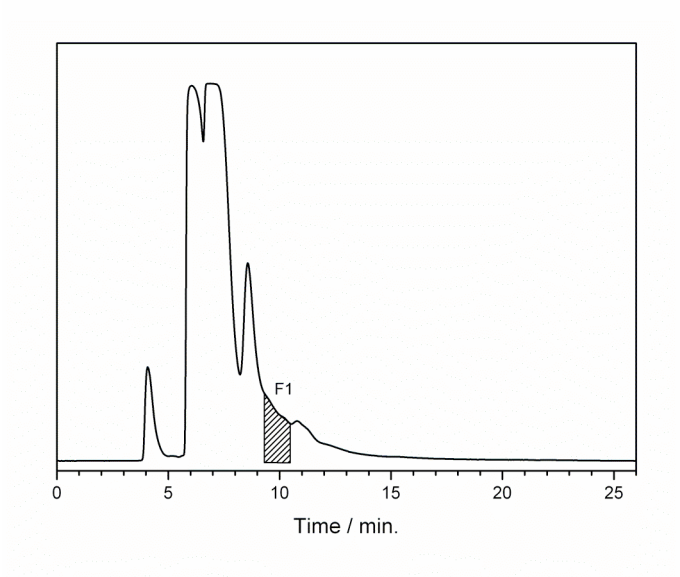


Fig S-1 The first-stage HPLC separation of raw extract on Buckyprep-M column with chlorobenzene as eluent at flow rate 4.5 mL/min and detecting wavelength 450 nm. Dashed area was collected as F1.

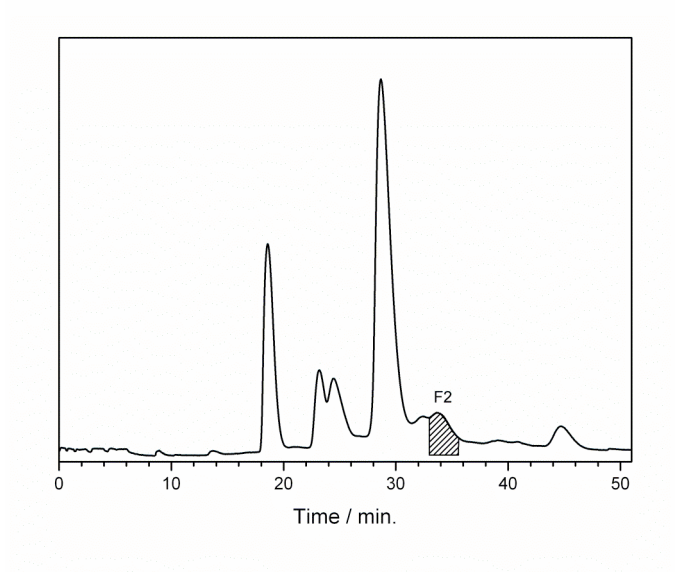


Fig. S-2 The second-stage HPLC profile of F1 on Buckyprep column with toluene as eluent at flow rate 4.5 mL/min and detecting wavelength 450 nm. Dashed area was collected as F2.

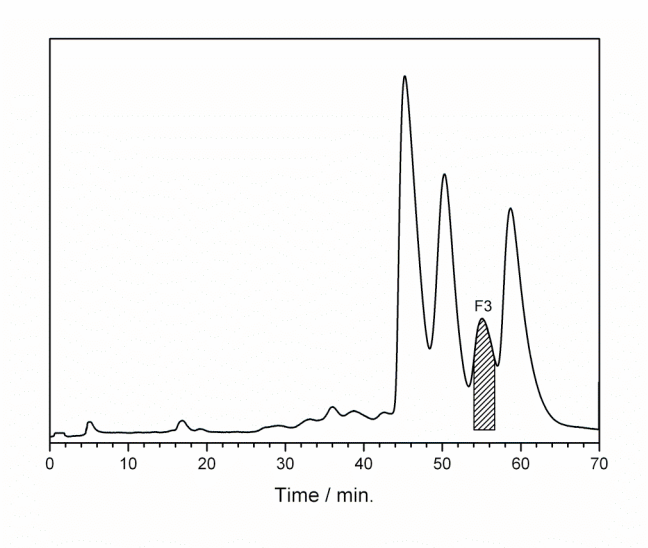


Fig. S-3 The third-stage HPLC profile of F1-1 on 5PBB column with toluene as eluent at flow rate 4.5 mL/min and detecting wavelength 450 nm. Dashed area was collected as F3, which contains the C_{86}.

Computational Details. All computations were at density function theory (DFT) level. Geometries of C86(16)-Cs were fully optimized by the PBEPBE function [2] with split-valence *d*-polarized 3-21G(d) basis set. All calculations were carried out with the GAUSSIAN 03 program.[3]

References

1 Sun, D.-Y.; Liu, Z.-Y. ; Guo, X.-H. ; Xu, W.-G.; Liu, S.-Y. *J. Phys. Chem. B* 1997, **101**, 3927-3930.

2 a) Becke, A. D. *Phys. Rev. A*, 1988, **38**, 3098-3100; b) Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B*, 1988, **37**, 785-789.

3 Gaussian 03, Revision C.02. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; and Pople, J. A.; Gaussian, Inc., Wallingford CT, 2004

Figures

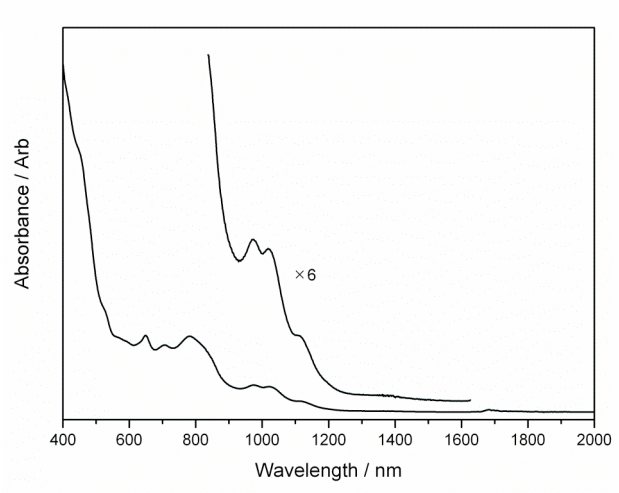


Fig. S-4 UV-Vis-NIR absorption spectrum of the isolated C_{86} in carbon disulfide

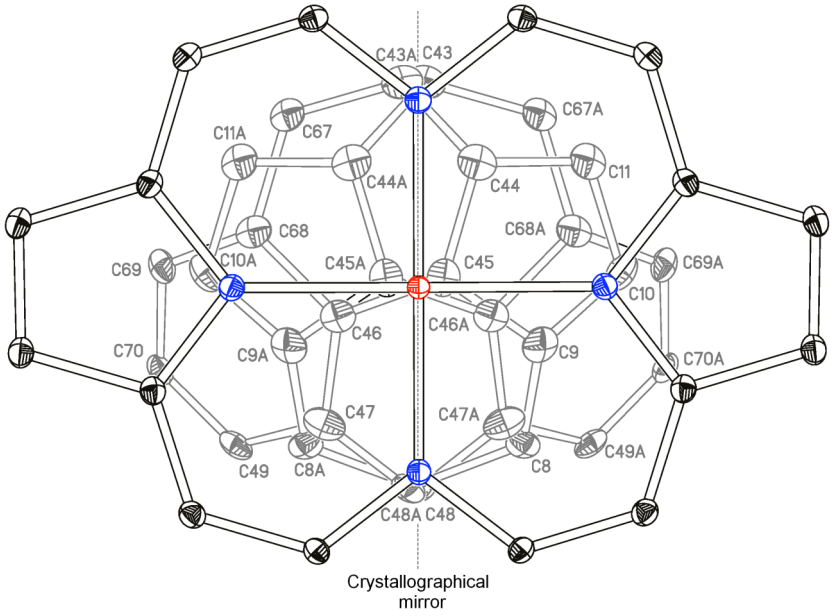


Fig. S-5 Orientation of two positions of C_{86} with respect to porphyrin plane in C_{86} + Ni^{II}(OEP) system. For clarity, only partial atoms of the fullerene are shown. The crystallographical mirror is perpendicular to the paper.

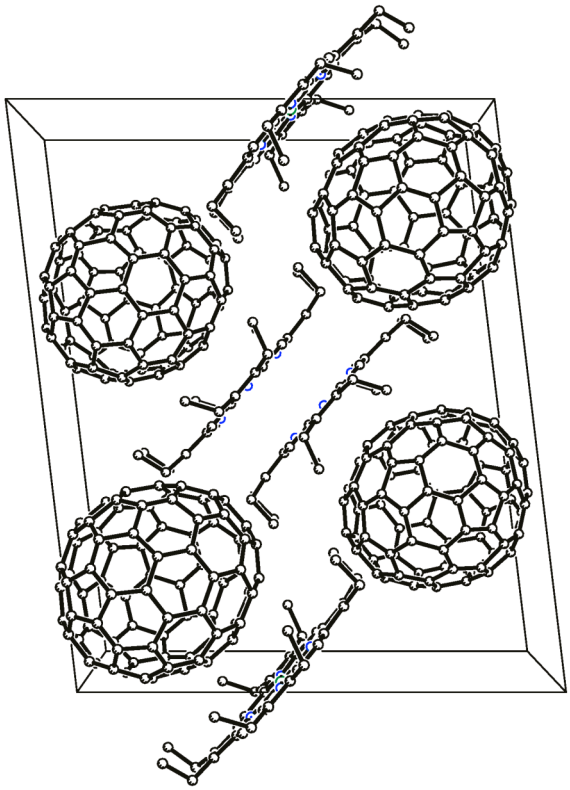


Fig S-6 A perspective view of the packing in $[C_{86}\bullet Ni^{II}(OEP)\bullet 2C_6H_5CH_3]$ with atoms denoted by uniform circles of arbitrary size. For clarity, the hydrogen atoms and toluene solvents are not shown.

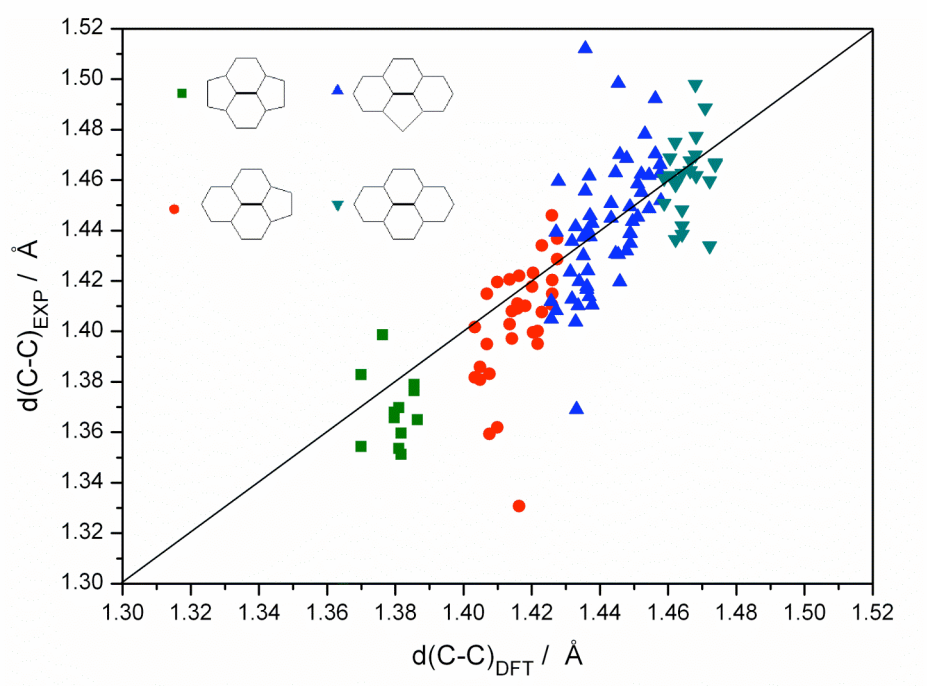
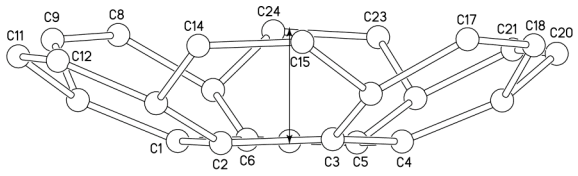
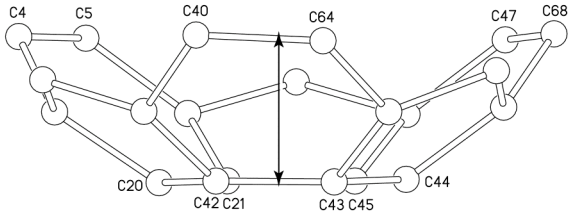


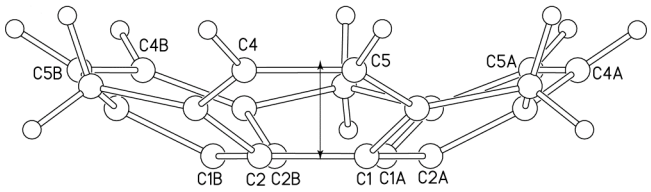
Fig. S-7 Correlation between the experimentally obtained and the DFT calculated C─C bond distances in $C_s(16)$-C_{86}. Correlation between the C─C bond length and the type of fragment in which the corresponding bonds are involved (the bonds under consideration are shown in bold)



Cornonene motif, 1.25 Å depth



Sumanene motif, 1.66 Å average depth



Sumanane, 1.11 Å depth

Fig. S-8. A comparison of the bowl depth of the coronene and sumanene motifs in the structure of $C_s(16)C_{86}$. A comparison is made to the structure of sumanene, $C_{21}H_{12}$.