Prof. Dr. Hiroyuki Isobe

K. Nguyen

Education

1994: B.Sc. In Chemistry (Tokyo Institute of Technology, Prof. E. Nakamura)
1996: M. S. in Chemistry (Tokyo Institute of Technology; Prof. E. Nakamura)
1999: Ph. D. in Chemistry (The University of Tokyo; Prof. E. Nakamura)

Academia

1998–2004: Assistant Professor, The University of Tokyo
2004–2007: Associate Professor, The University of Tokyo
2007–2016: Professor, Tohoku University
2013–2017: Principal Investigator, Advanced Institute for Materials Research, Tohoku University
2013–2019: Research Director, Isobe Degenerate π-Integration, ERATO, JST
2016–present: Professor, Department of Chemistry, The University of Tokyo

Awards/Honors

2000: The 1st IUPAC Prize for Young Chemists
2004: The 53th Chemical Society of Japan Award for Young Chemists
2005: The 1st Osawa Award of Fullerene Nanotube Research Society
2008: The Young Scientists' Prize
2009: Nozoe Memorial Award for Young Organic Chemists
2017: Inoue Prize for Science
2018: Fujifilm Prize for Functional Materials

- Over 140 peer-reviewed publications
- *h*-index: 39 (May 2020)

Prof. Dr. Hiroyuki Isobe

K. Nguyen

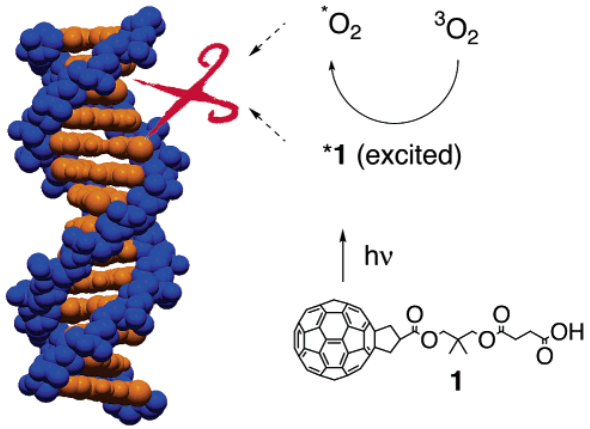
Supervisor throughout his studies: Prof. Dr. Eiichi Nakamura

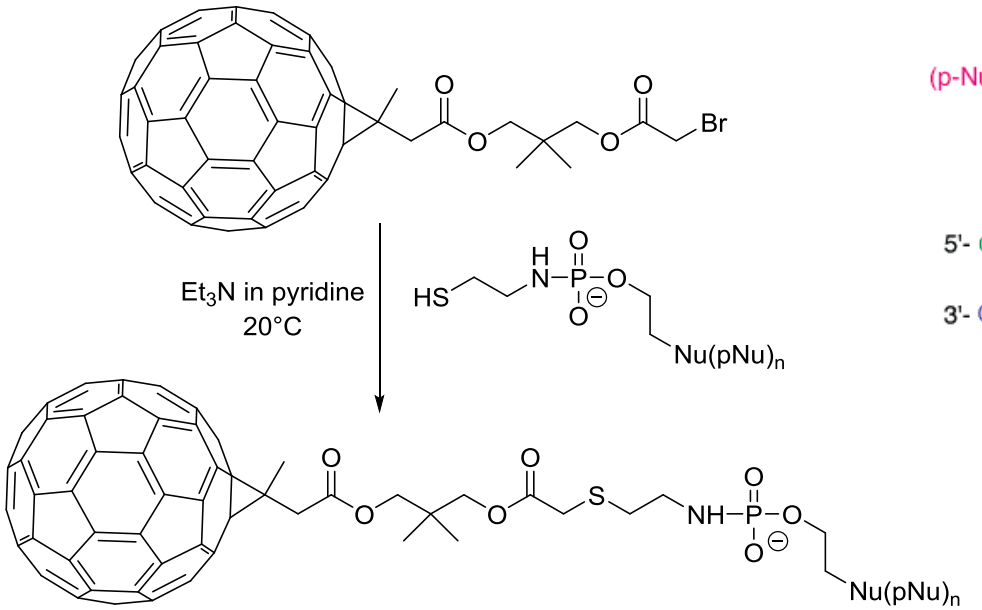
Fullerene chemistry

Organometallics (Catalysis, Mechanism)
Material Science (OPV, OLED, Perovskite)

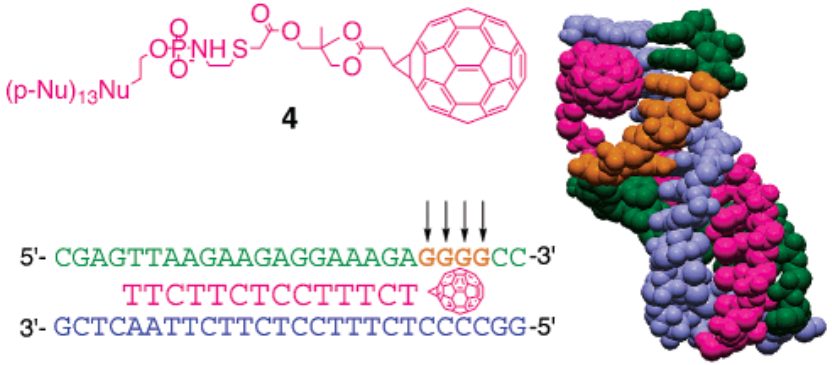
First publication: Fullerene - Oligonucleotide Conjugates

Biological activitiy towards DNA
→photoinduced DNA cleavage by singlet-oxygen



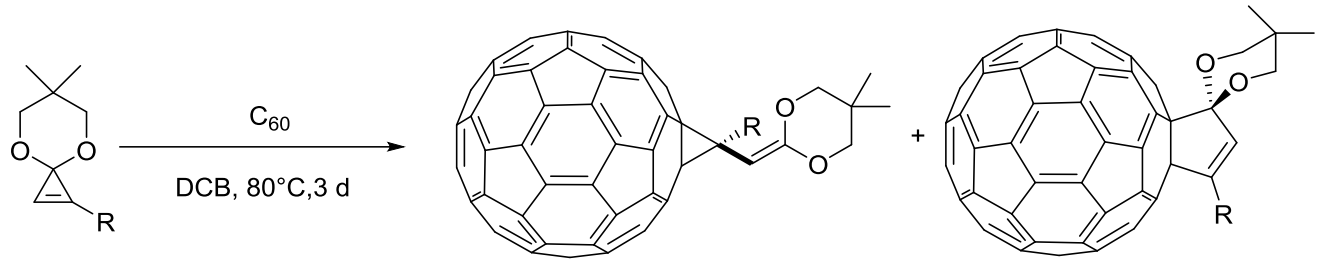


Binding of fullerene-DNA conjugate
to target DNA



Boutorine, A. S.; Tokuyama, H.; Takasugi, M.; Isobe, H.; Nakamura, E.; Hélène, *Angew. Chem., Int. Ed. Engl.* **1994**, *33*, 2462-2465.

[1+2] and [3+2] cyloaddition on [60]fullerene



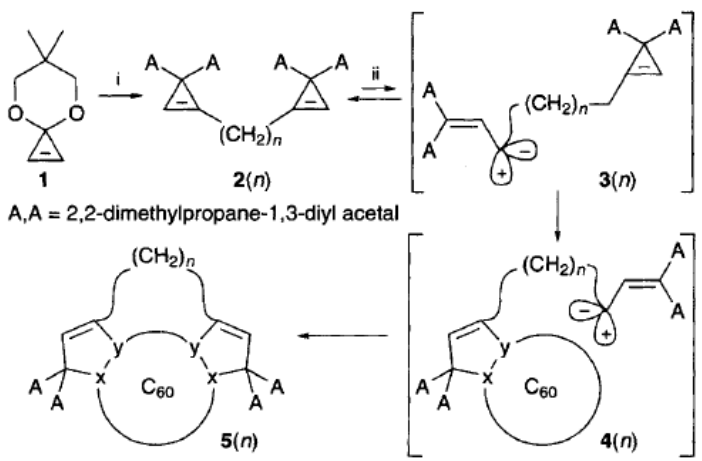
cyclopropenoneacetal methanofullerene propanofullerene

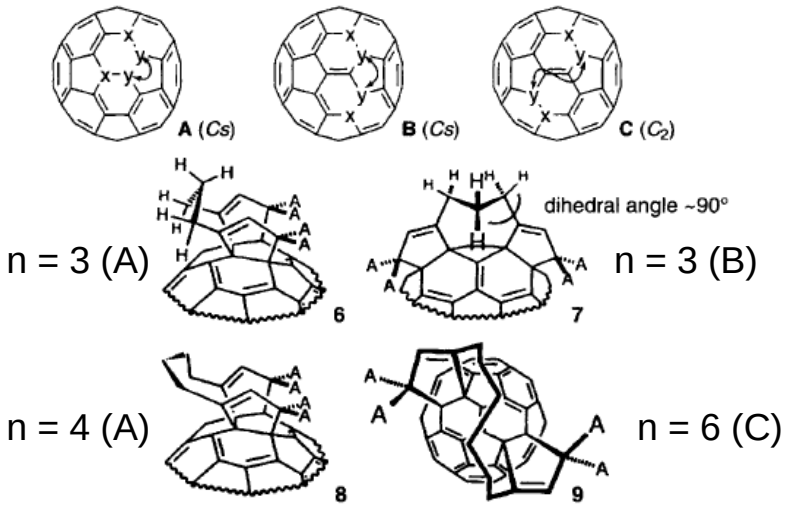
Temperature-dependence of cycloaddition

Temperature (°C)	[1+2] : [3+2]
80	9 : 1
100	67 : 33
140	7 : 93

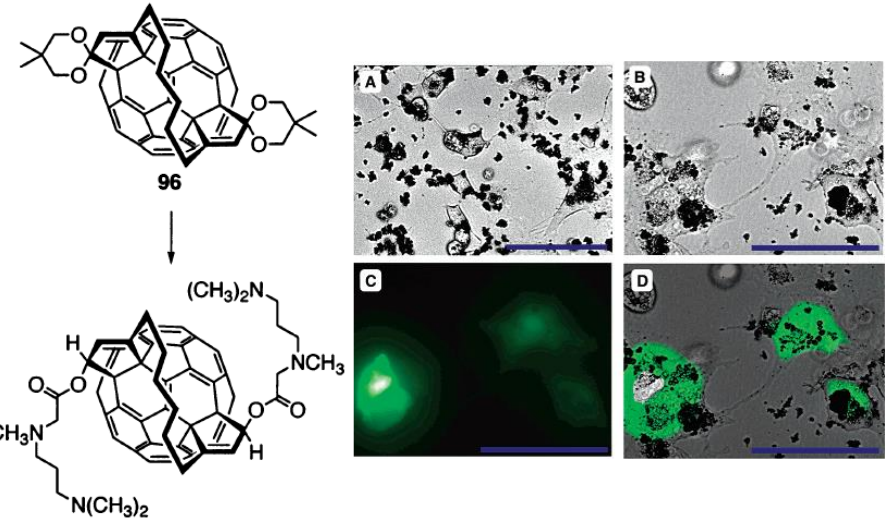
Tokuyama, H.; Isobe, H.; Nakamura, E. *Bull. Chem. Soc. Jpn.* **1995**, *68*, 935-941

Double [3+2] cycloddition on [60] fullerene





Application in gene delivery

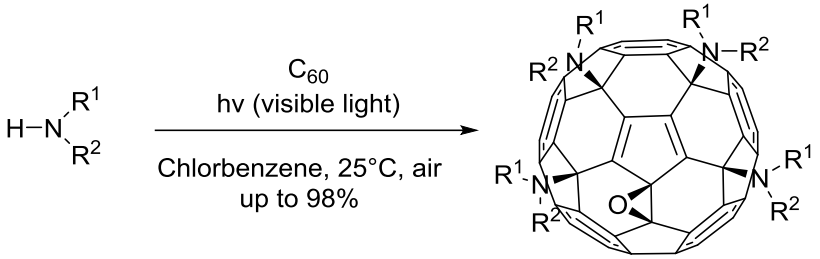


Nakamura, E.; Isobe, H.; Tokuyama, H.; Sawamura, M. *Chem. Commun.* **1996**, *15*, 1747-1748.

Nakamura, E.; Isobe, H.; Tomita, N.; Sawamura, M.; Jinno, S.; Okayama, H. *Angew. Chem. Int. Ed.* **2000**, *39*, 4254-4257

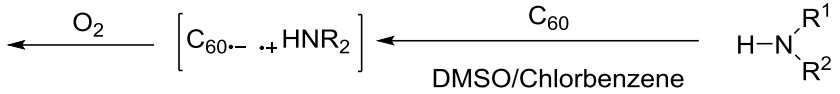
Functionalization on [60] fullerenes

Amination



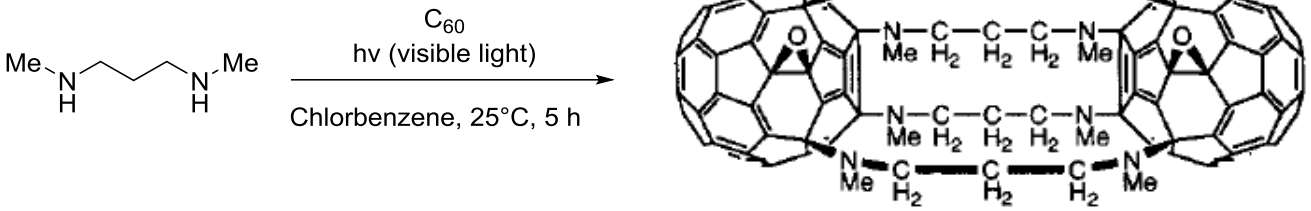
Isobe, H.; Tomita, N.; Nakamura, E. *Org. Lett.* **2000**, *2* (23), 3663-3665.

Contact-ion pair via SET



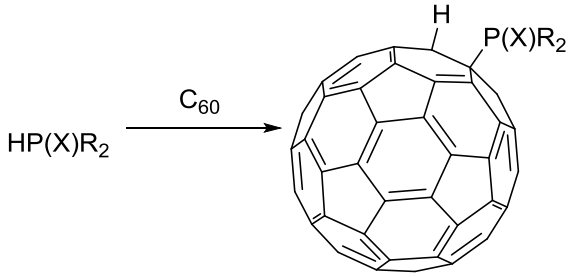
Isobe, H.; Tanaka, T.; Nakanishi, W.; Lemiègre, L.; Nakamura, E. *J. Org. Chem.* **2005**, *70* (12), 4826-4832.

Cage structure bearing two fullerene end caps



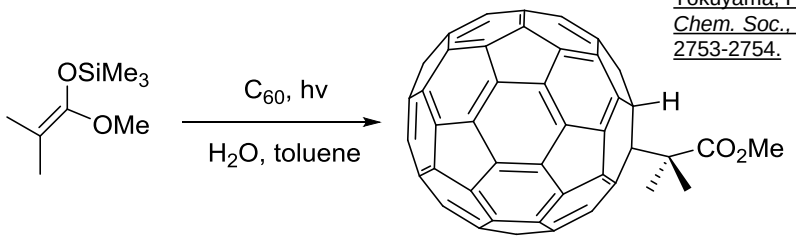
Isobe, H.; Ohbayashi, A.; Sawamura, M.; Nakamura, E. *J. Am. Chem. Soc.* **2000**, *122* (11), 2669-2670.

Hydrophosphorylation



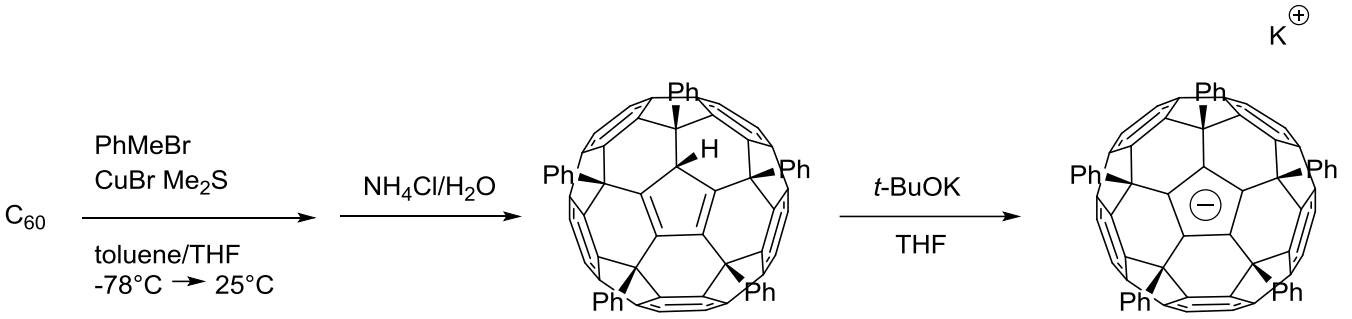
Isobe, H.; Chen, A.-J.; Solin, N.; Nakamura, E. *Org. Lett.* **2005**, *7*, 5633-5635.

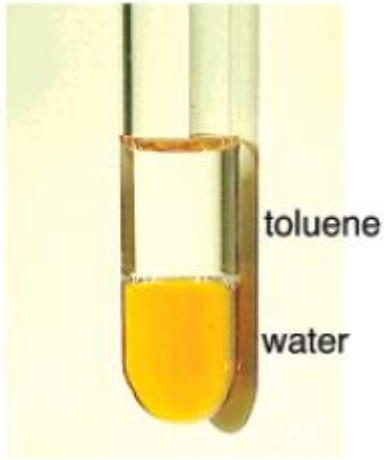
Carboxylic esters



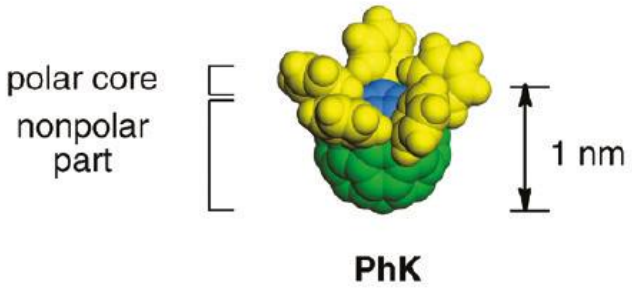
Tokuyama, H.; Isobe, H.; Nakamura, E. *J. Chem. Soc., Chem. Commun.* **1994**, *24*, 2753-2754.

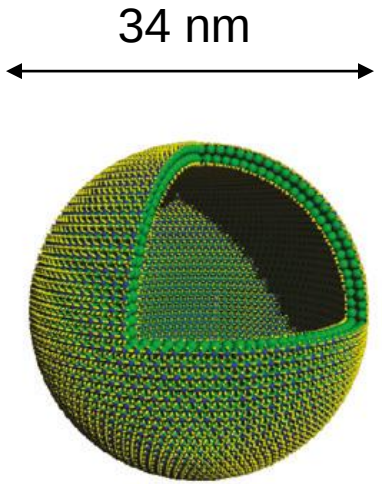
Water-soluble fullerene and bilayer vesicle formation

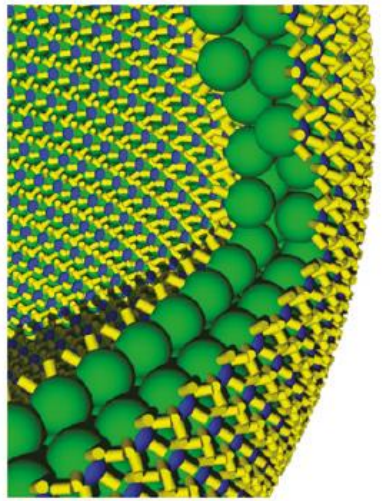


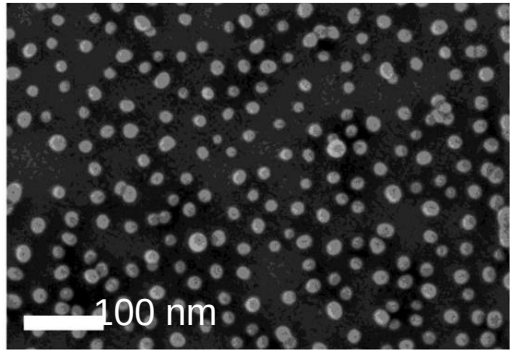


High stability because of the delocalization of negative charge



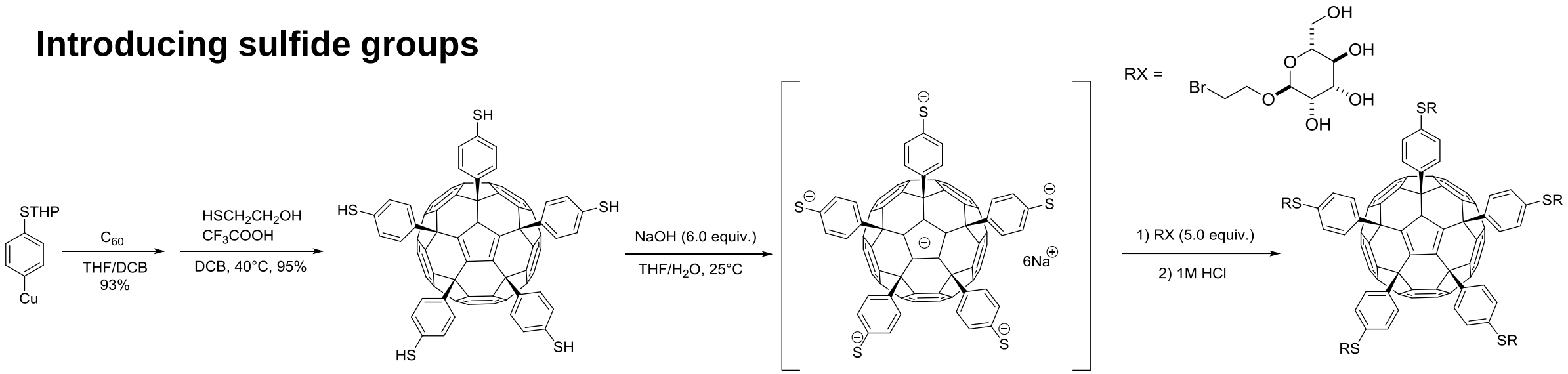






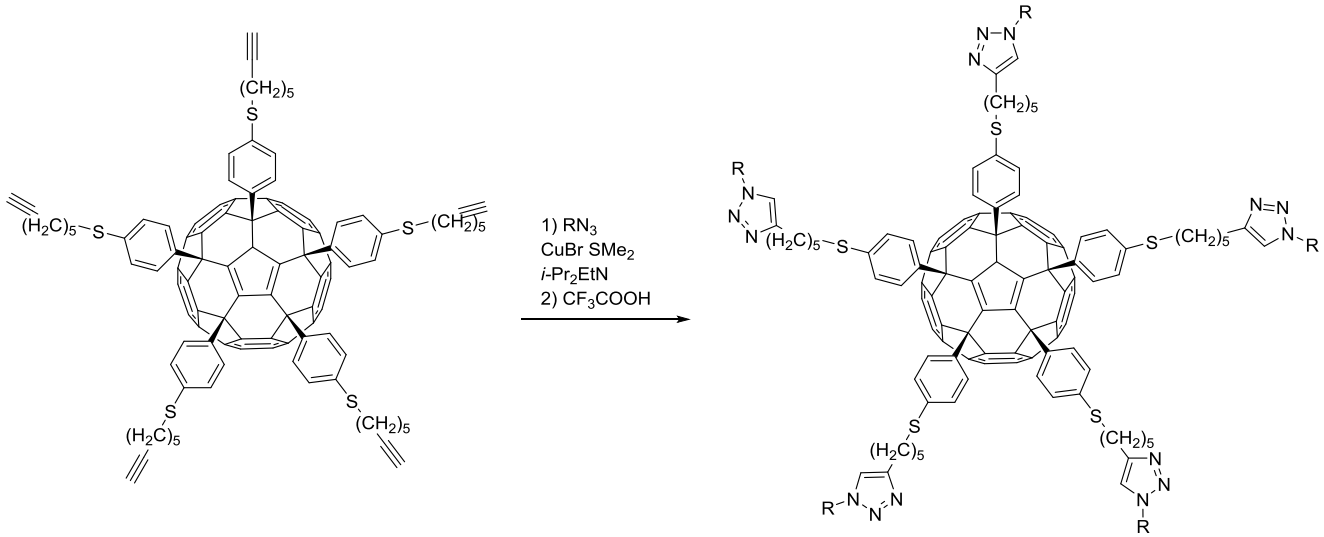
Zhou, S.; Burger, C.; Chu, B.; Sawamura, M.; Nagahama, N.; Toganoh, M.; Hackler, U. E.; Isobe, H.; Nakamura, E. *Science* **2001**, *291*, 1944-1947.
Sawamura, M.; Iikura, H.; Nakamura, E.; *J. Am. Chem. Soc*. **1996**, *118*, 12850-12851
Sawamura, M.; Nagahama, N.; Toganoh, M.; Hackler, U. E.; Isobe, H.; Nakamura, E.; Zhou, S.-Q.; Chu, B.; *Chem. Lett*. **2000**,1098-1099.

Introducing sulfide groups



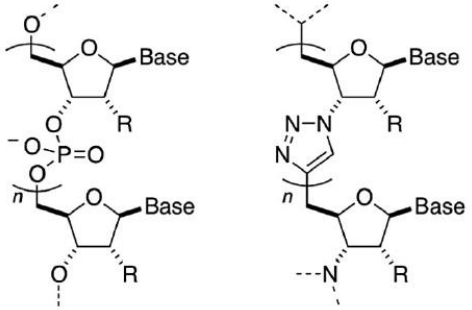
Isobe, H.; Mashima, H.; Yorimitsu, H.; Nakamura, E. *Org. Lett.* **2003**, *5*, 4461-4463.

„Click“-Chemistry Fullerene glycoconjugates

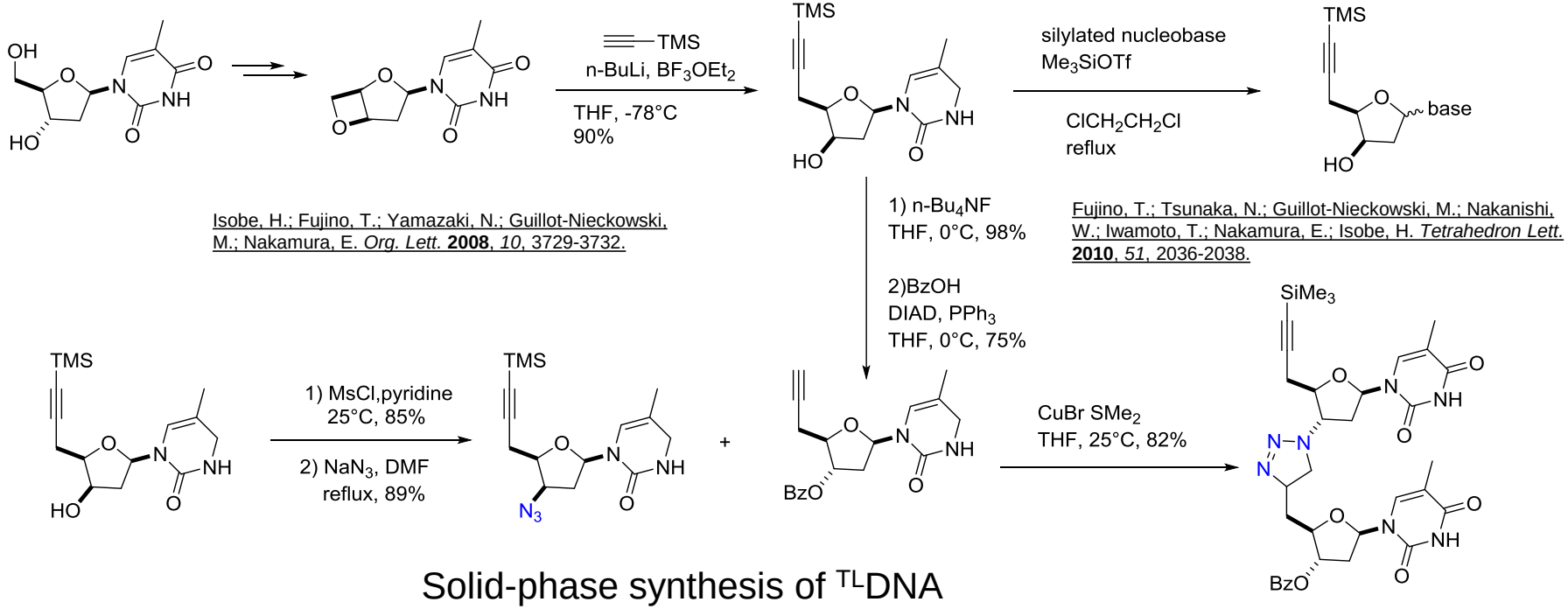


Isobe, H.; Cho, K.; Solin, N.; Werz, D. B.; Seeberger, P. H.; Nakamura, E. *Org. Lett.* **2007**, *9*, 4611-4614.

Triazole-linked analogues of DNA



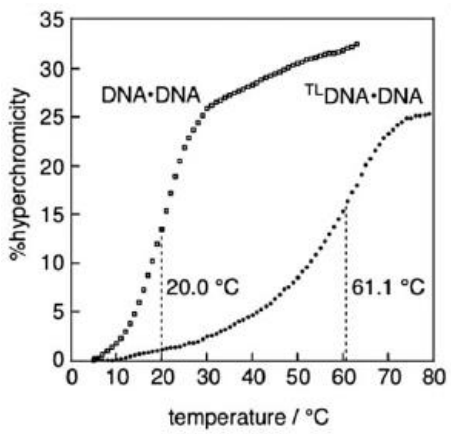
Solution-phase synthesis of ^{TL}DNA



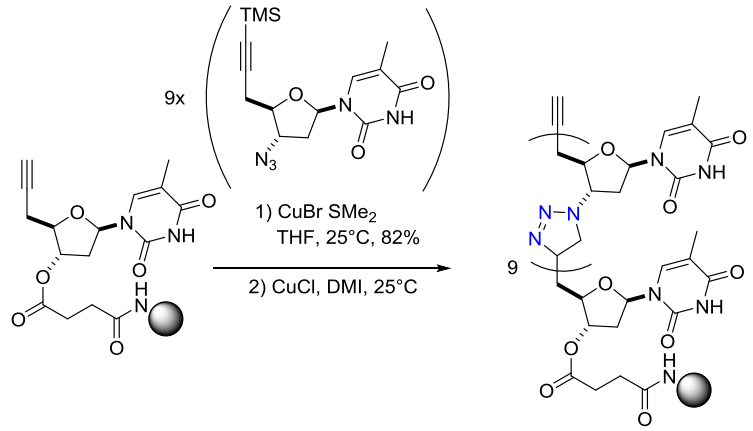
Isobe, H.; Fujino, T.; Yamazaki, N.; Guillot-Nieckowski, M.; Nakamura, E. *Org. Lett.* **2008**, *10*, 3729-3732.

Fujino, T.; Tsunaka, N.; Guillot-Nieckowski, M.; Nakanishi, W.; Iwamoto, T.; Nakamura, E.; Isobe, H. *Tetrahedron Lett.* **2010**, *51*, 2036-2038.

^{TL}DNA forms double-helix with DNA



Solid-phase synthesis of ^{TL}DNA



Postmodification

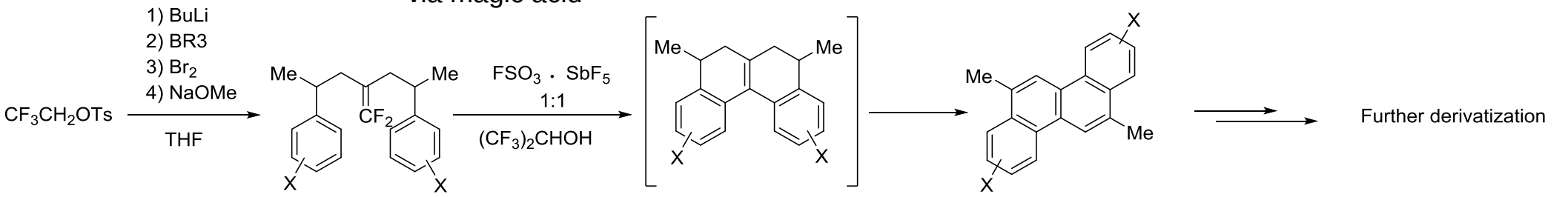
0.61% (19 steps)

Fujino, T.; Miyauchi, Y.; Tsunaka, N.; Okada, K.; Isobe, H. *Heterocycles* **2013**, *87*, 1023-1028.

First publication on polycyclic aromatic hydrocarbons:

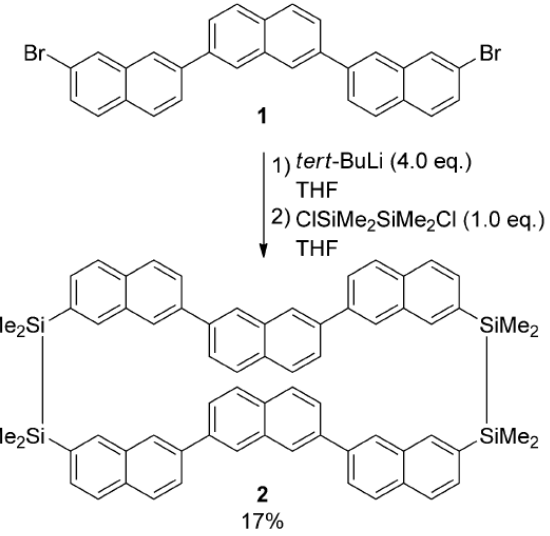
Synthesis of chrysene ([4]phenacene) derivatives

Friedel-Crafts-type Cyclization
via magic acid

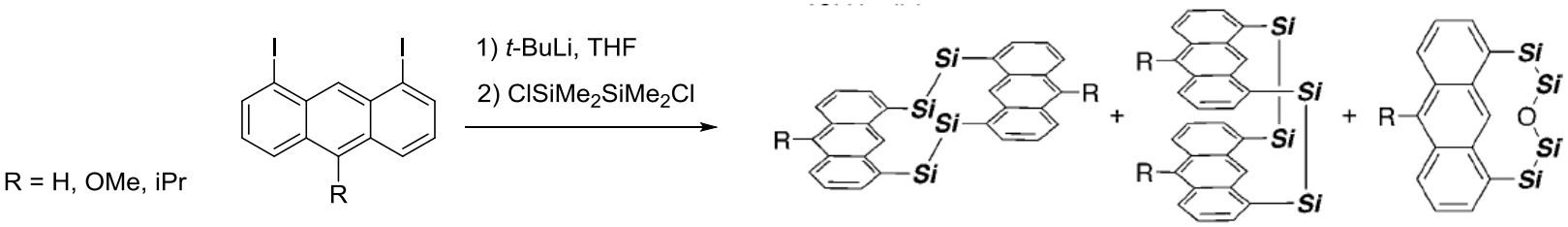


Isobe, H.; Hitosugi, S.; Matsuno, T.; Iwamoto, T.; Ichikawa, J. *Org. Lett.* **2009**, *11*, 4026-4028.

Disilanyl double-pillared bisternaphthyl



Synthesis of disilanyl double-pillared bisanthracene

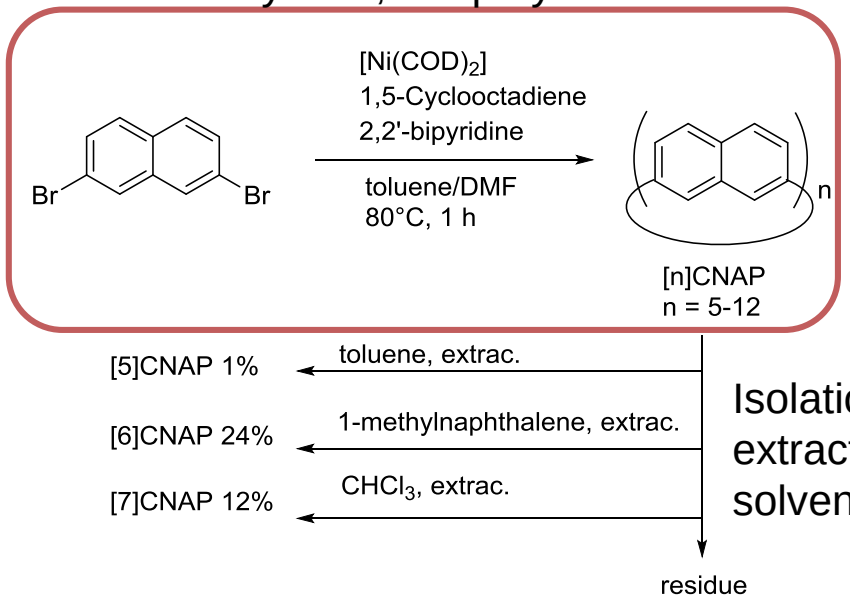


Nakanishi, W.; Hitosugi, S.; Piskareva, A.; Shimada, Y.; Taka, H.; Kita, H.; Isobe, H. *Angew. Chem. Int. Ed.* **2010**, *49*, 7239-7242.
Nakanishi, W.; Hitosugi, S.; Shimada, Y.; Isobe, H. *Chem. Asian J.* **2011**, *6*, 554-559.

Nakanishi, W.; Matsuyama, N.; Hara, D.; Saeki, A.; Hitosugi, S.; Seki, S.; Isobe, H. *Chem. Asian J.* **2014**, *9*, 1782-1785.

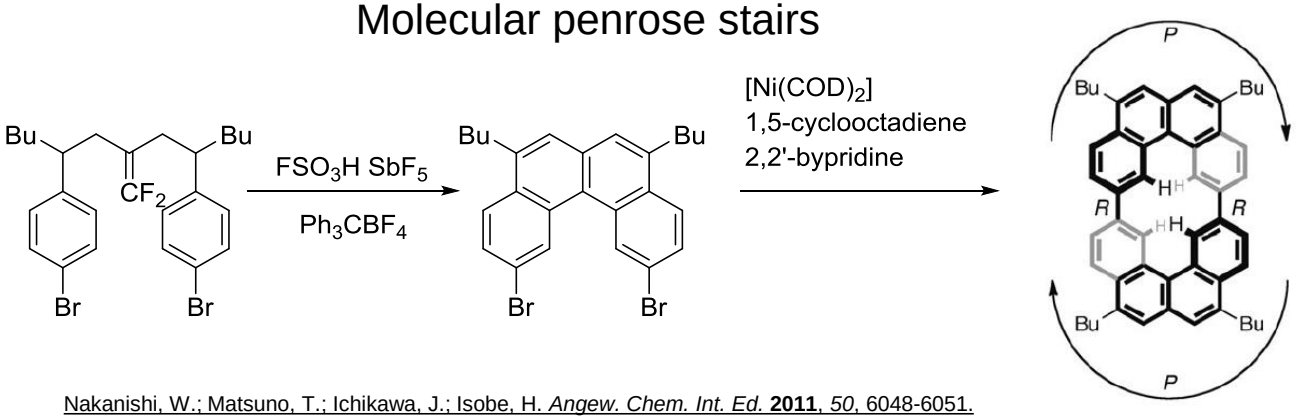
Synthesis of macrocyclic aromatic hydrocarbons

Cyclo-2,7-naphtylenes



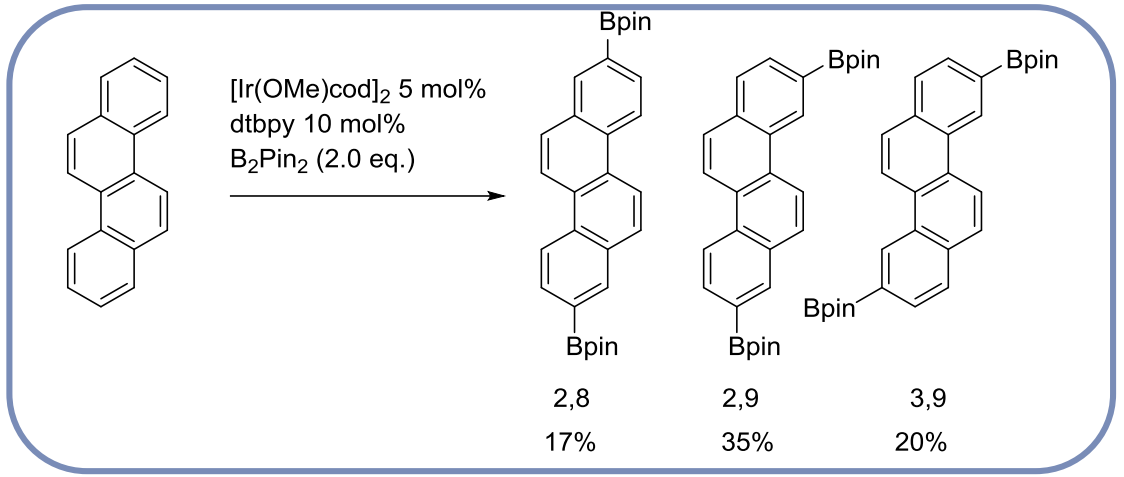
Nakanishi, W.; Yoshioka, T.; Taka, H.; Xue, J. Y.; Kita, H.; Isobe, H.; *Angew. Chem. Int. Ed.* **2011**, *50*, 5323-5326.

Molecular penrose stairs



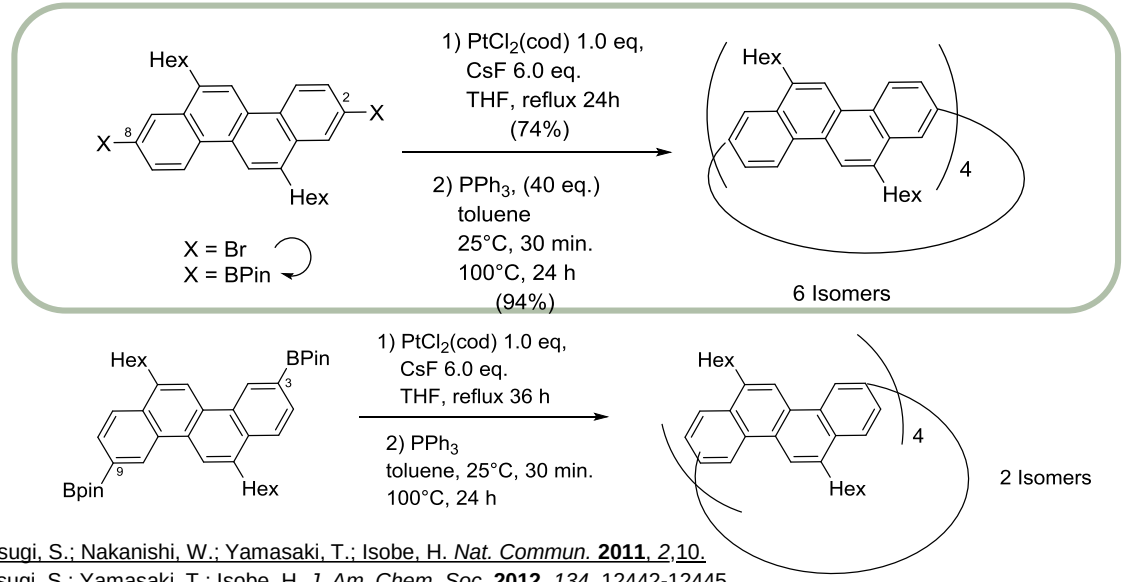
Nakanishi, W.; Matsuno, T.; Ichikawa, J.; Isobe, H. *Angew. Chem. Int. Ed.* **2011**, *50*, 6048-6051.

Iridium-catalyzed borylation



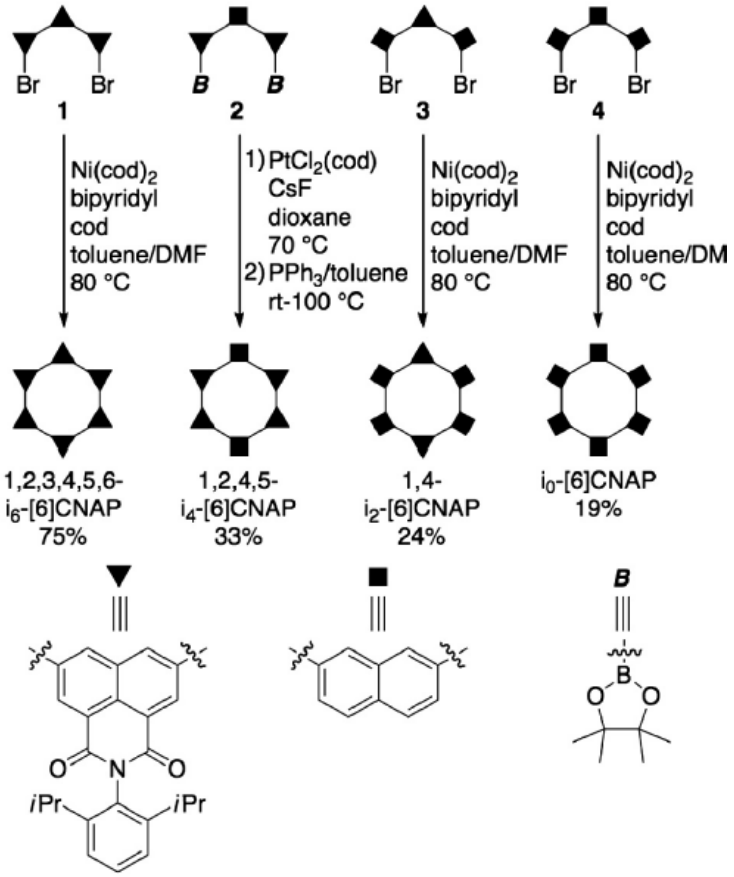
Hitosugi, S.; Nakamura, Y.; Matsuno, T.; Nakanishi, W.; Isobe, H. *Tetrahedron Lett.* **2012**, *53* , 1180-1182.

Bottom-up synthesis of chiral nanotube



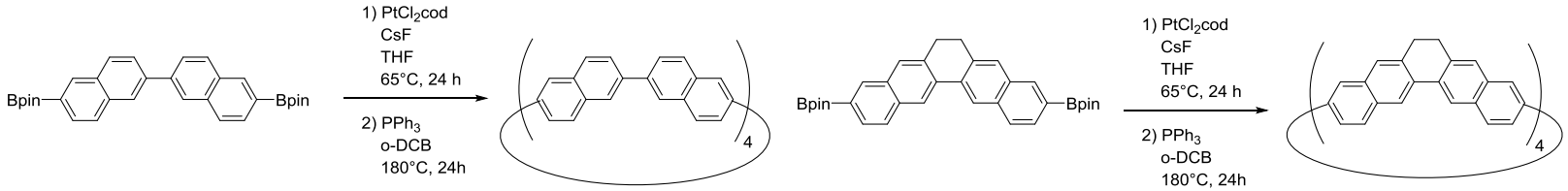
Hitosugi, S.; Nakanishi, W.; Yamasaki, T.; Isobe, H. *Nat. Commun.* **2011**, *2*,10.
Hitosugi, S.; Yamasaki, T.; Isobe, H. *J. Am. Chem. Soc.* **2012**, *134*, 12442-12445.

Synthesis of [6] Cyclo-2,7-naphtylene macrocycles with dicarbxylic imide



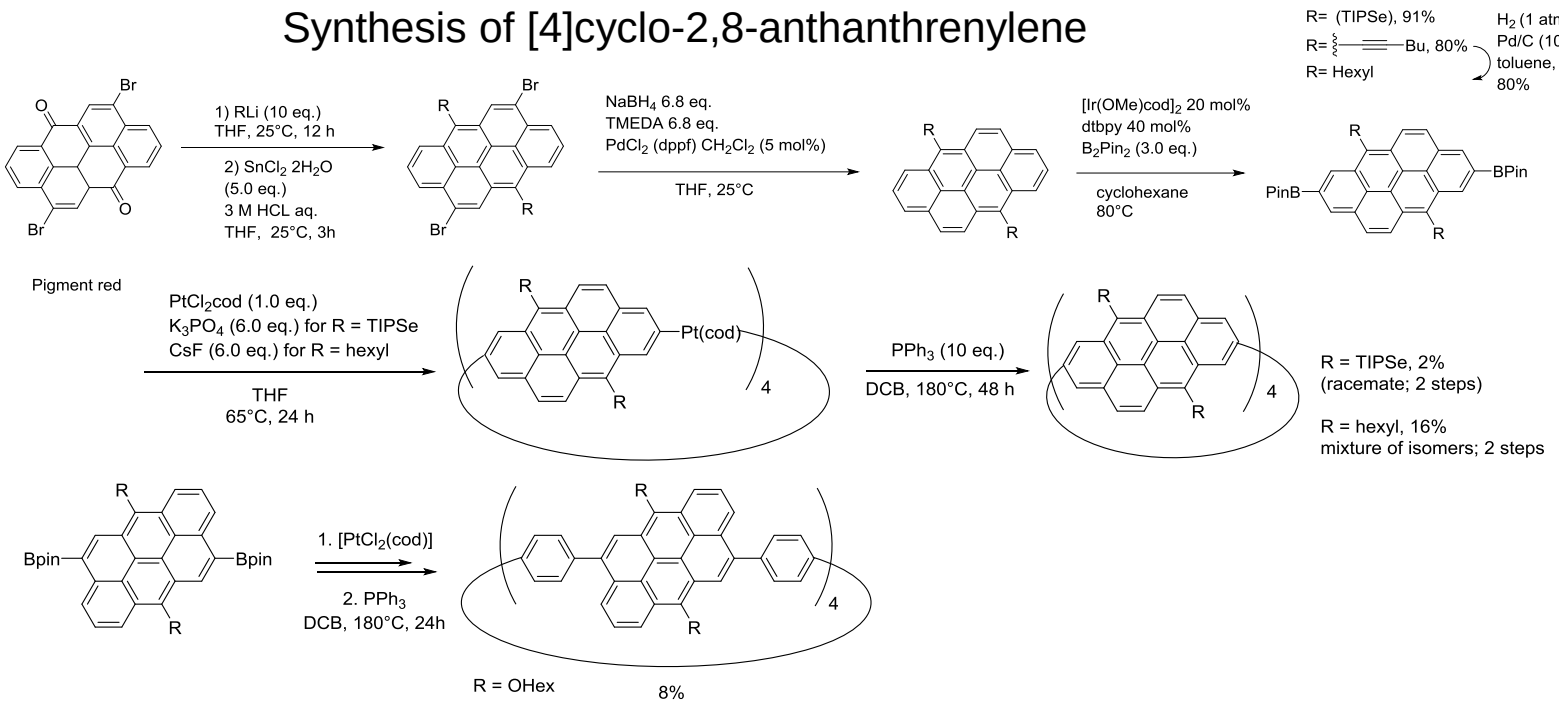
Xue, J. Y.; Nakanishi, W.; Tanimoto, D.; Hara, D.; Nakamura, Y.; Isobe, H. *Tetrahedron Lett.* **2013**, *54*, 4963-4965.

Belt-Shaped Cyclonaphthylenes



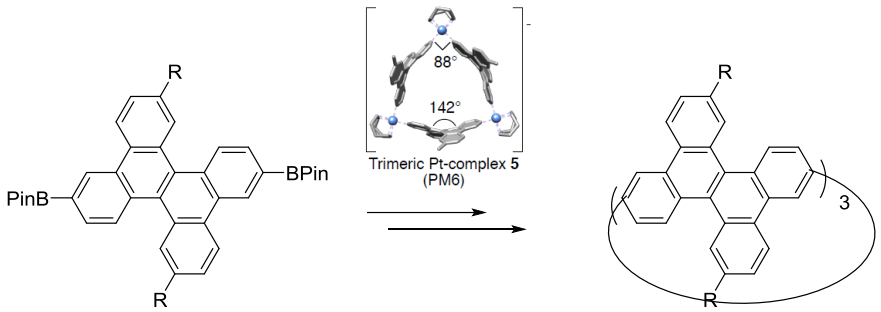
Sun, Z.; Sarkar, P.; Suenaga, T.; Sato, S.; Isobe, H. *Angew. Chem. Int. Ed.* **2015**, *54*, 12800-12804.

Synthesis of [4]cyclo-2,8-anthanthrenylene



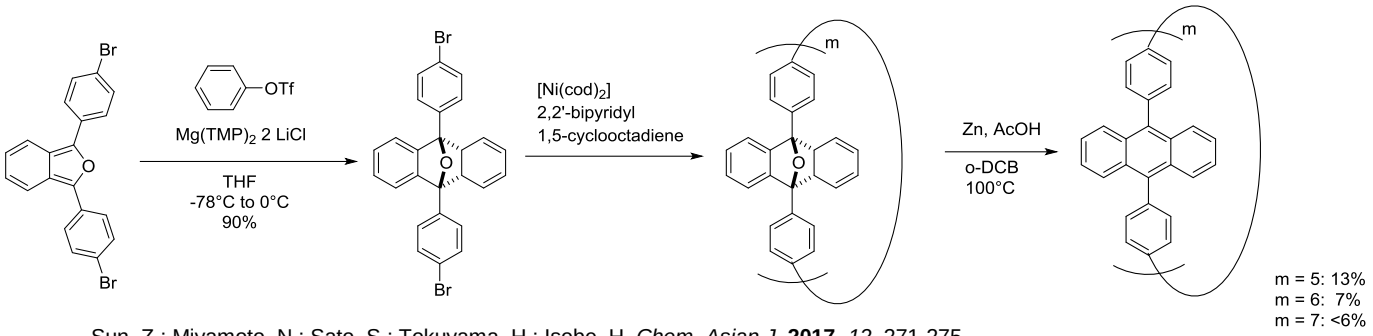
Matsuno, T.; Kamata, S.; Hitosugi, S.; Isobe, H. *Chem. Sci.* **2013**, *4*, 3179-3183.
Sarkar, P.; Sato, S.; Kamata, S.; Matsuno, T.; Isobe, H. *Chem. Lett.* **2015**, *44*, 1581-1583.

Trimer Pt-macrocycle

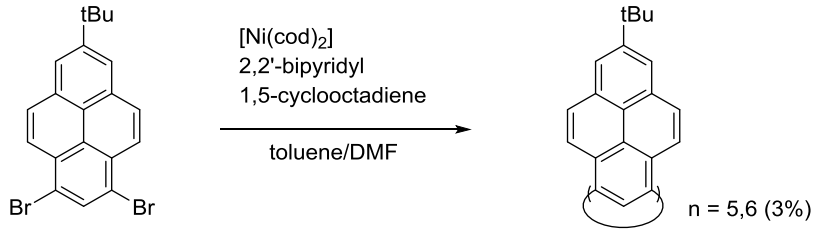


Kogashi, K.; Matsuno, T.; Sato, S.; Isobe, H. *Angew. Chem. Int. Ed.* **2019**, *58*, 7385-7389.

Obtuse-angled corner unit for the synthesis of CPP

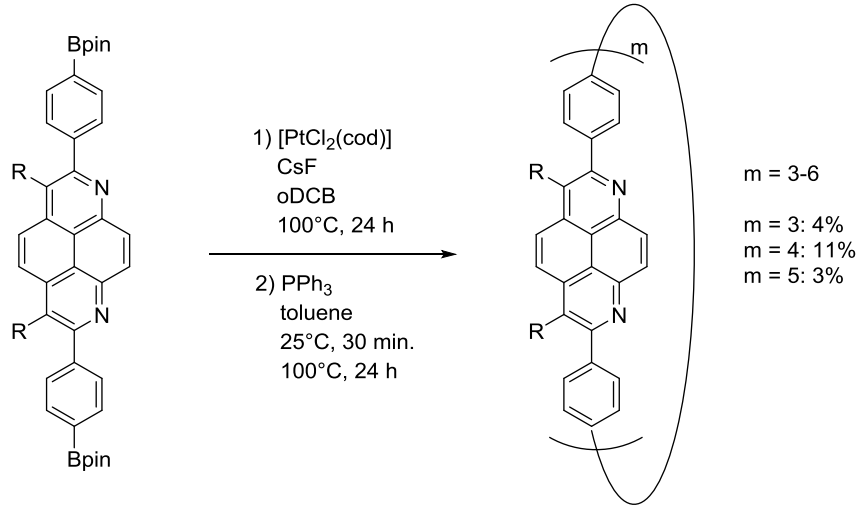


Sun, Z.; Miyamoto, N.; Sato, S.; Tokuyama, H.; Isobe, H. *Chem. Asian J.* **2017**, *12*, 271-275.



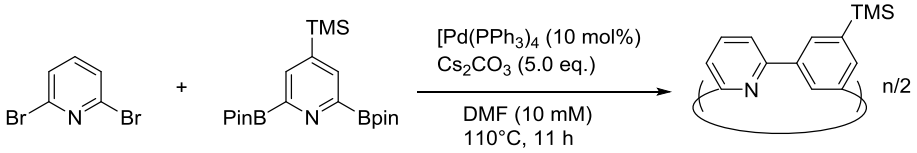
Ikemoto, K.; Sato, S.; Isobe, H. *Chem. Lett.* **2016**, *45*, 217-219.

Macrocyclization with heterocycles



Ikemoto, K.; Fujita, M.; Too, P. C.; Tnay, Y. L.; Sato, S.; Chiba, S.; Isobe, H. *Chem. Lett.* **2016**, *45*, 658-660.

Macrocyle formation via suzuki-cross coupling

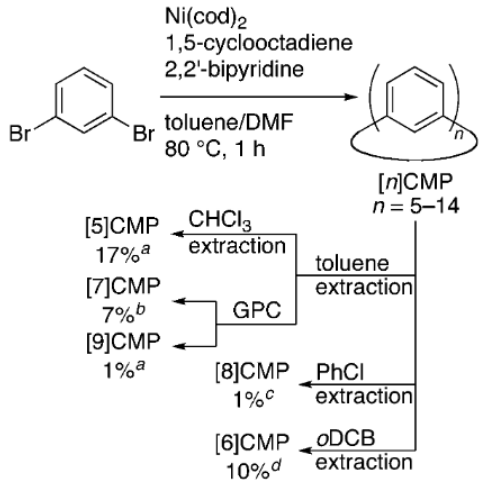


n = 6 13%
n = 8 5%
n = 10 7%
n = 12 5%
n = 14 4%

Xue, J. Y.; Ikemoto, K.; Sato, S.; Isobe, H. *Chem. Lett.* **2016**, *45*, 676-678

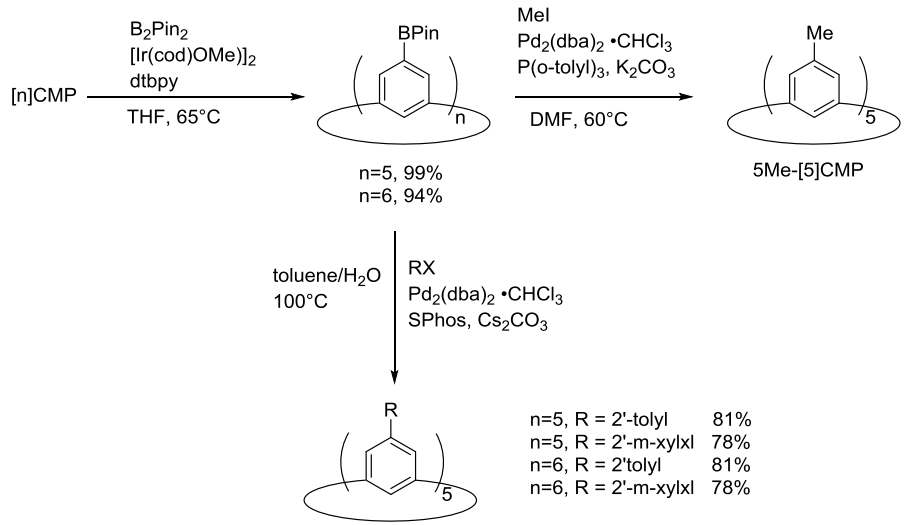
Phenine frameworks: trisubstituted benzene derivative as building block

Yamamoto-coupling



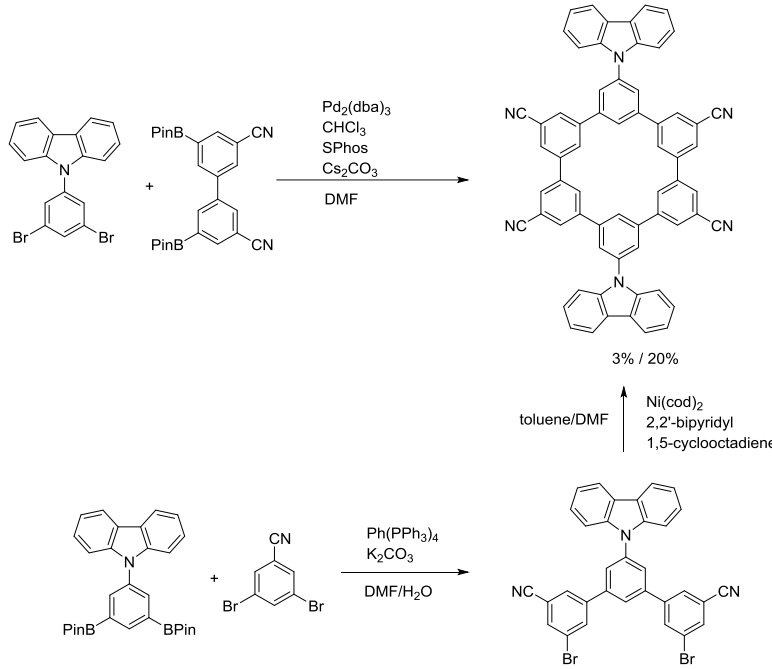
Xue, J. Y.; Ikemoto, K.; Takahashi, N.; Izumi, T.; Taka, H.; Kita, H.; Sato, S.; Isobe, H. *J. Org. Chem.* **2014**, *79*, 9735-9739.

Derivatization of CMPs



Ikemoto, K.; Yoshii, A.; Izumi, T.; Taka, H.; Kita, H.; Xue, J. Y.; Kobayashi, R.; Sato, S.; Isobe, H. *J. Org. Chem.* **2016**, *81*, 662-666.

Donor-acceptor-substituents



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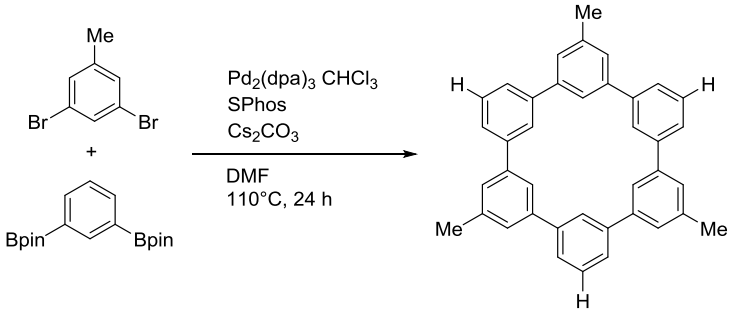
Suzuki-cross-coupling



3Me-[6]CMP

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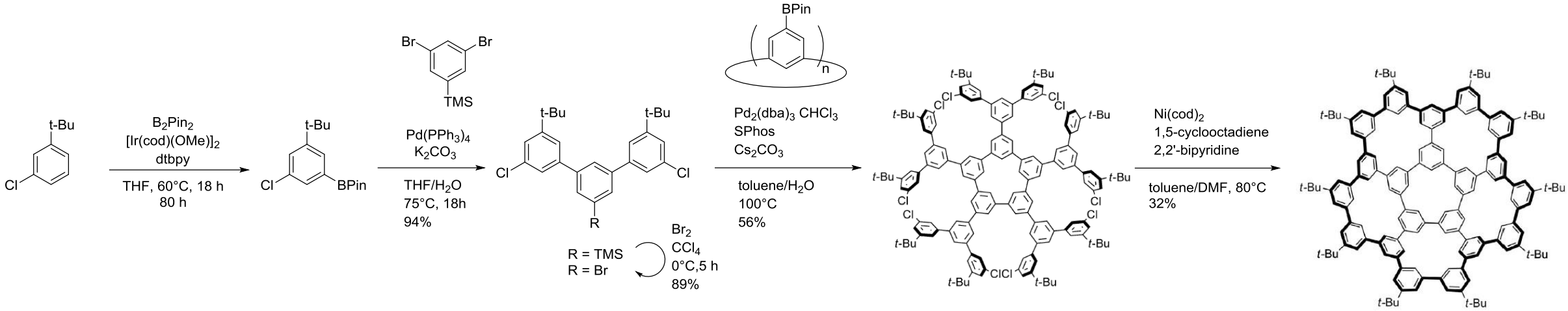
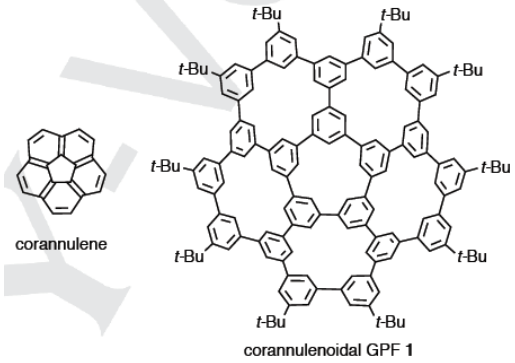
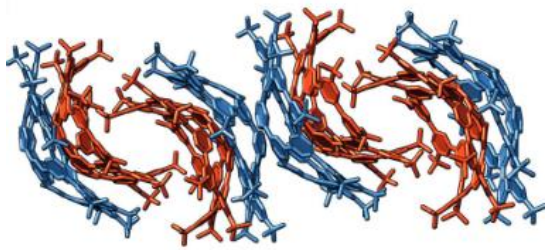
Phenine frameworks: Geodesic phenylene bowl, saddle and hemisphere

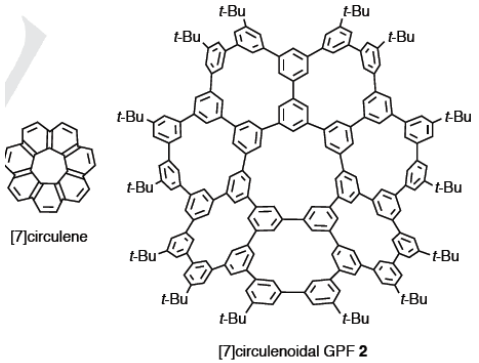


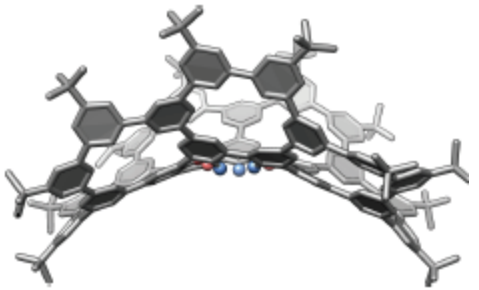
Geodesic phenylene bowl





Geodesic phenylene saddle





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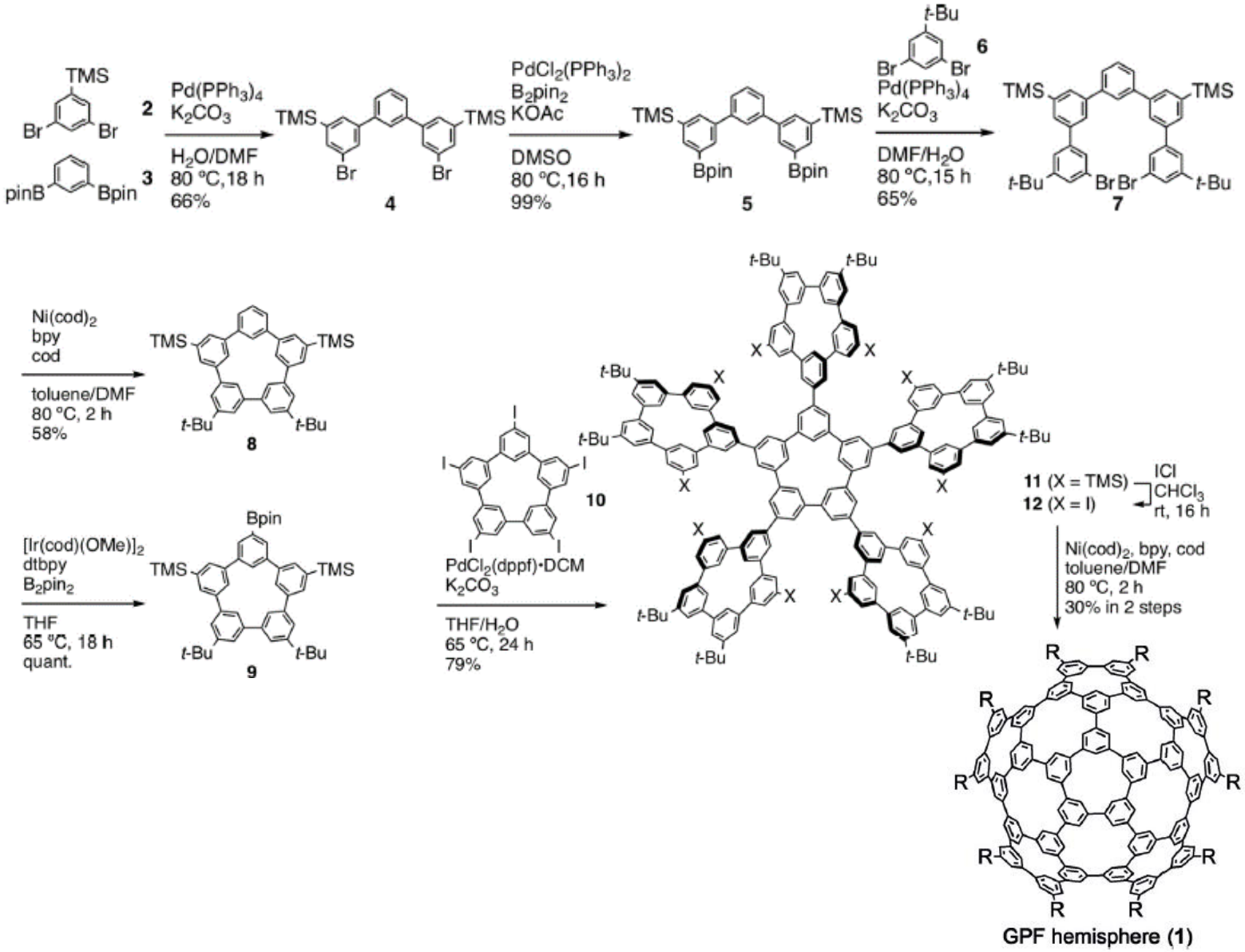
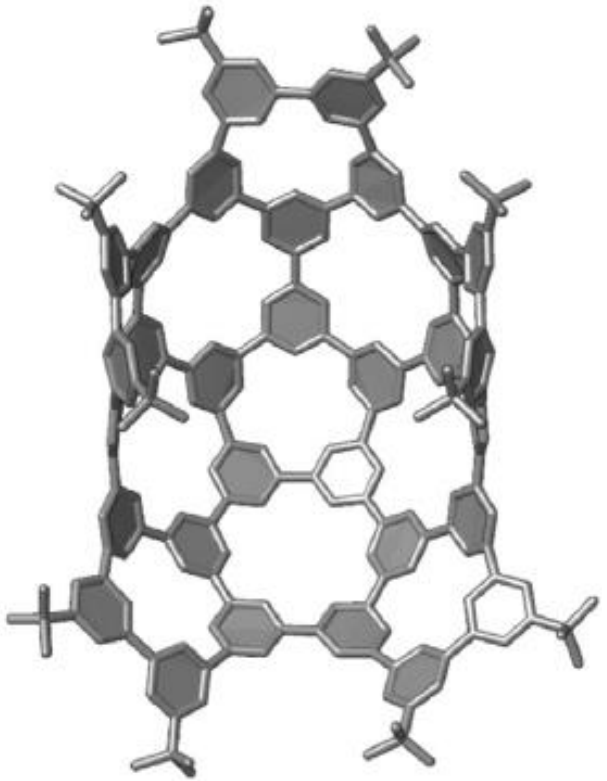
Phenine frameworks: Geodesic phenylene bowl, saddle and hemisphere





X-ray

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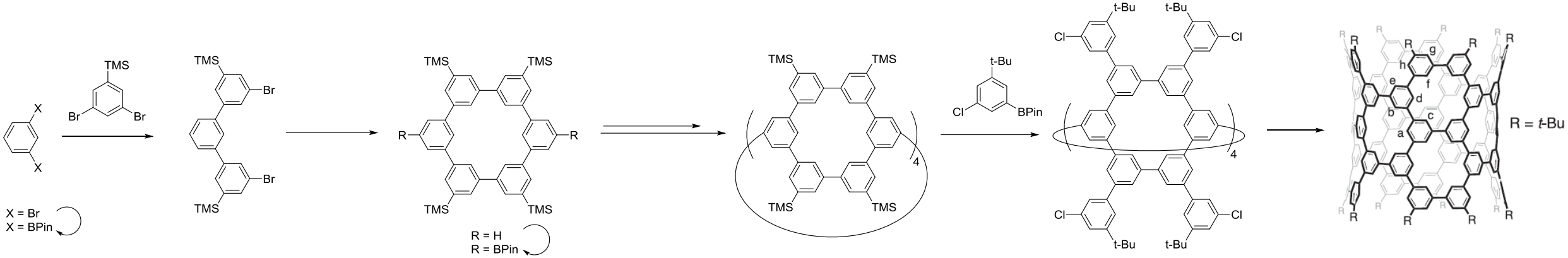
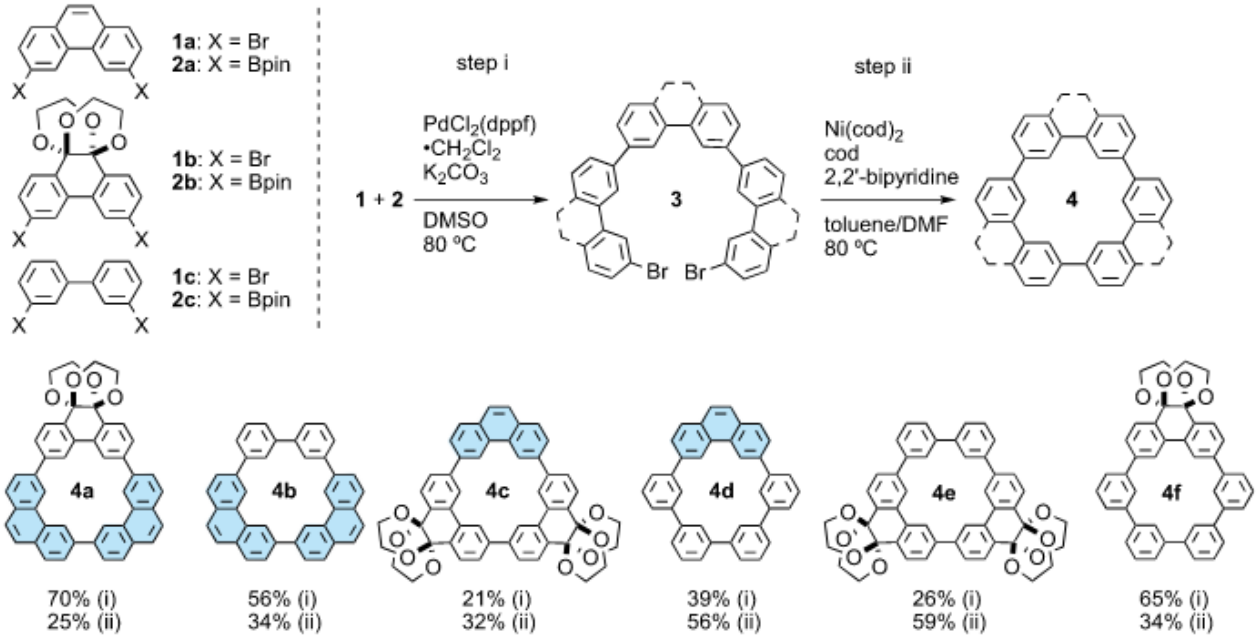
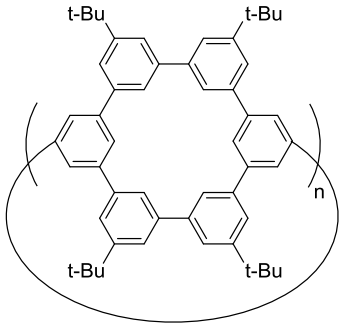
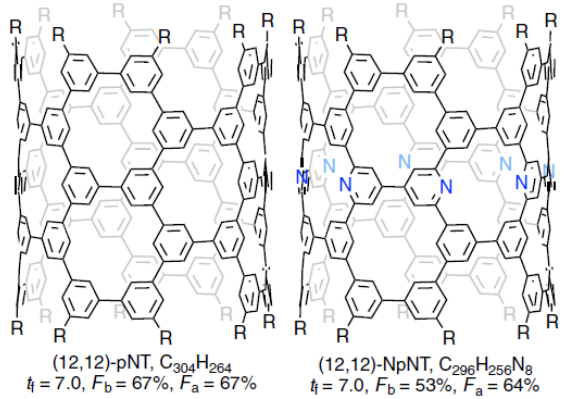
Phenine frameworks: nanotubes and CPP with periodic vacancy defects







[n]cyclo-para-phenylenoidal GPF
([n]-CPP-GPF; n = 3,4,5)



(12,12)-pNT, $C_{304}H_{264}$
t_f = 7.0, F_b = 67%, F_a = 67%

(12,12)-NpNT, $C_{296}H_{256}N_8$
t_f = 7.0, F_b = 53%, F_a = 64%

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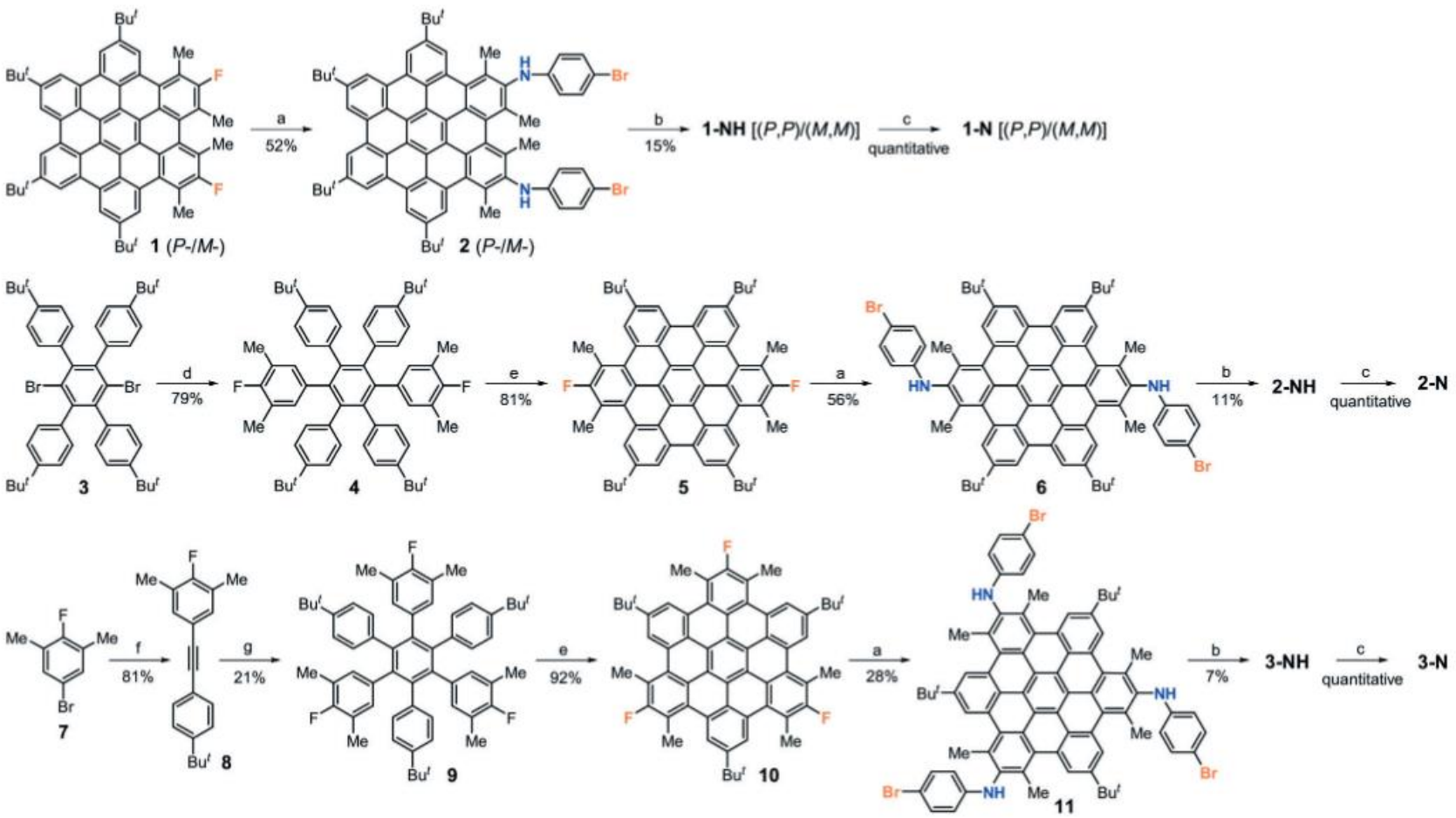
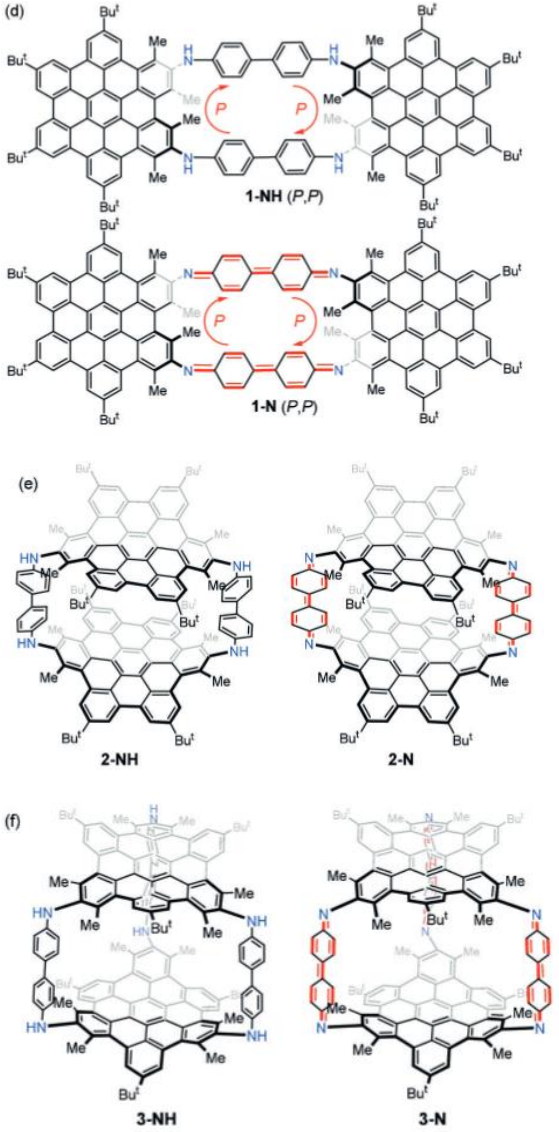
Superbenzene-Based-Conjugated Chiral Macrocycles and Cyclophanes



Scheme 1. Synthetic routes of benzidine/quinoidal benzidine-linked, HBC-based macrocycles (**1-NH/1-N**) and cyclophanes (**2-NH/2-N**; **3-NH/3-N**): a) 4-Bromoaniline, $KOBu^t$, toluene/DMSO, 80°C; b) $Ni(COD)_2$, THF, 65°C; c) PbO_2, $CHCl_2CHCl_2$ or THF, rt; d) 2-(4-fluoro-3,5-dimethylphenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane, K_2CO_3, $Pd(PPh_3)_4$, THF/H_2O, 90°C; e) $FeCl_3$, CH_2Cl_2, $MeNO_2$, rt; f) 1-(*tert*-butyl)-4-ethynylbenzene, CuI, $Pd(PPh_3)_2Cl_2$, Et_3N, 70°C; g) $Co_2(CO)_8$, 1,4-dioxane, 100°C.



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