イプチセン型合成ブロックの反応集積化による プロペラ状π電子系中分子の創製

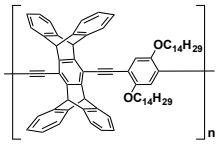
（関西学院大理工）羽村季之

Iptycene

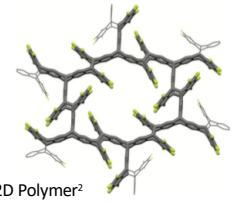
triptycene

- ✓[2.2.2] Bridgehead system
- ✓Rigid geometry
- ✓D_{3h} Symmetry with three-blade geometry

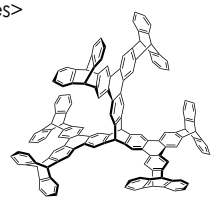
< Examples of π-extended Iptycene Derivatives>



TNT Quenching[1]



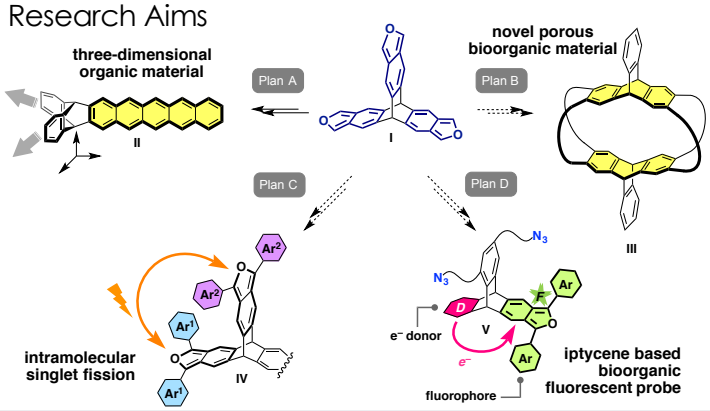
2D Polymer[2]



supertriptycene[3]

[1]T. M. Swager *et al. J. Am. Chem. Soc.* **1998**, *120*, 5321–5322; [2]B. King *et al. J. Am. Chem. Soc.* **2013**, *135*, 14134–14141; [3]M. Mastalerz *et al. J. Org. Chem.* **2015**, *80*, 9342–9348.

Research Aims

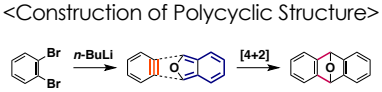


Isobenzofurans

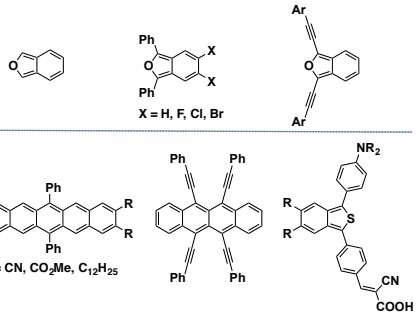
isobenzofuran

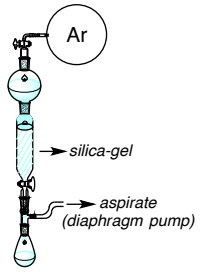
- ✓10π Quinoid Structure
- ✓High Reactivity
- ✓[4+2] Cycloaddition

<Construction of Polycyclic Structure>



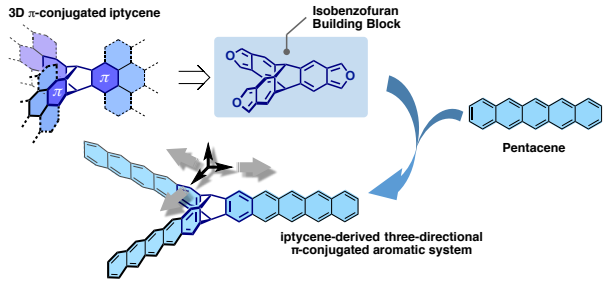
<Previously Prepared Isobenzofuran Derivatives>





T. Hamura *et al. Org. Lett.* **2014**, *16*, 286–289, *Org. Lett.* **2015**, *17*, 3094–3097, *Chem. Lett.* **2017**, *46*, 25–28.

Design of a novel Isobenzofuran Building Block



Synthesis of Iptycene Derived Tris-Pentacene

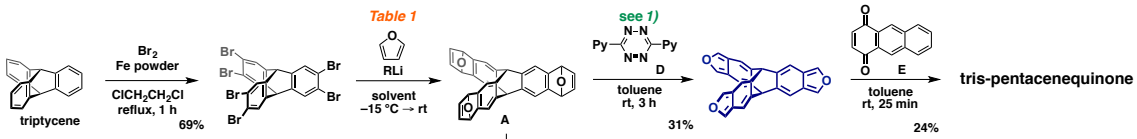
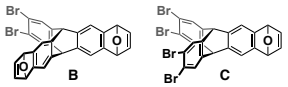
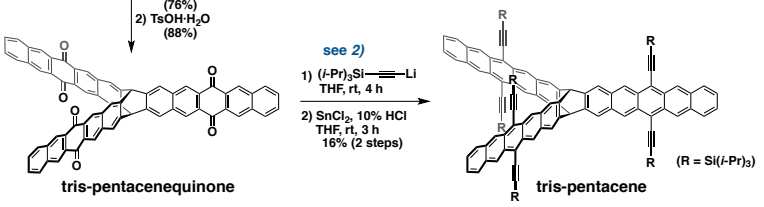


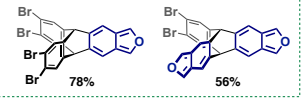
Table 1

RLi	solvent	A / %	B / %	C / %
n-BuLi (1.5 eq)	PhCl	3	20	50
n-BuLi (2.5 eq)	PhCl	20	33	6
PhLi (4.0 eq)	toluene/THF (v/v 1/1)	41	20	4

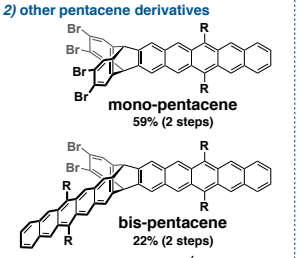




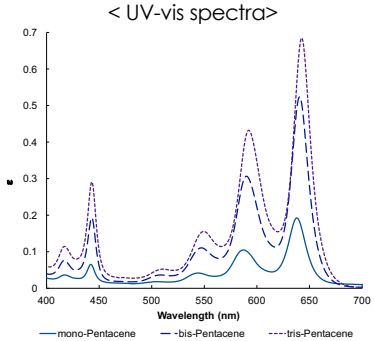
1) other isobenzofuran building blocks



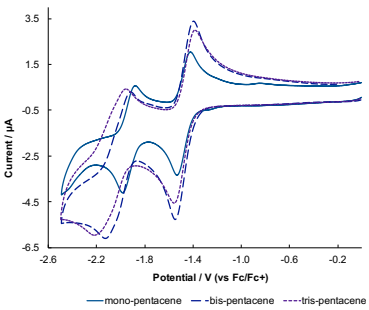
2) other pentacene derivatives



< UV-vis spectra>



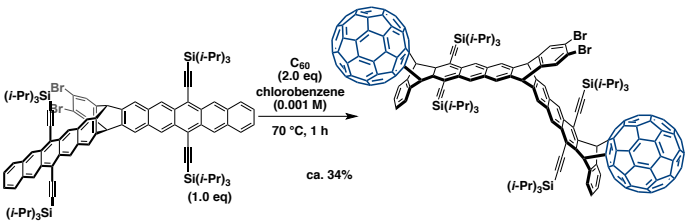
< Cyclic Voltammograms>



	λ_{abs} (nm)[a]	$E^{1/2ox}$ (V)[b]	$E^{1/2red}$ (V)[b]	E^{HOMO} (eV)[c]	E^{LUMO} (eV)[c]	E_g^{EChem} (eV)
mono-Pentacene	638, 588, 545	0.52	-1.47	-5.32	-3.32	2.00
bis-Pentacene	641, 590, 548	0.51	-1.46	-5.31	-3.34	1.97
tris-Pentacene	643, 593, 550	0.50	-1.47	-5.30	-3.33	1.97

a 1.0×10^{-5} M in CH_2Cl_2. b Recorded $E_{1/2}$ values vs Fc/Fc^+ in THF with $TBAPF_6$ as supporting electrolyte. c HOMO and LUMO energy levels were calculated from half-wave potentials for respective first redox according to the equations $E_{HOMO} = -(4.8 + E_{1/2}^{ox})$ eV and $E_{LUMO} = -(4.8 + E_{1/2}^{red})$ eV.

< Initial Study of Cycloaddition with 3D Pentacene with C_{60}>



< Potential Applications of 3D Pentacene>