Synthesis, Optical and Electrochemical Properties of Rubicene Derivatives

IPRIME Presentation

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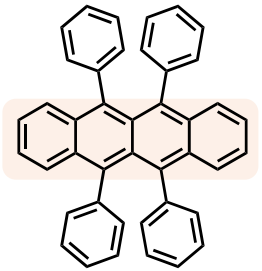
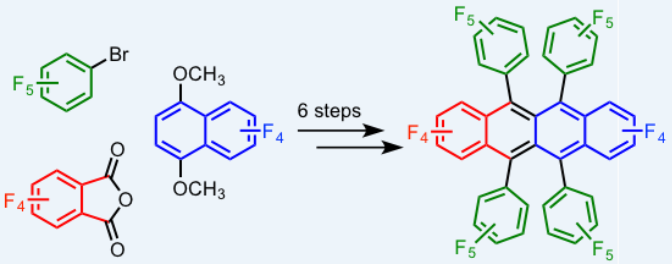
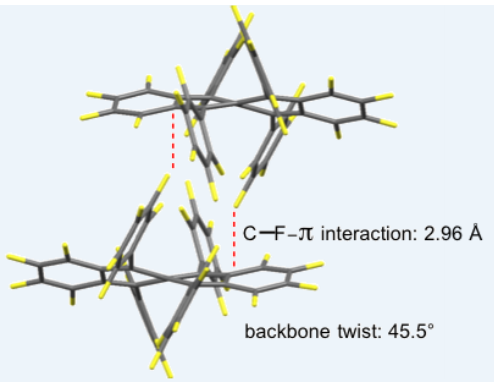
General Research Interest in Acene-based Molecules



rubrene

Perfluorination

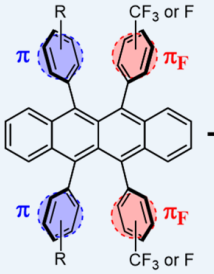




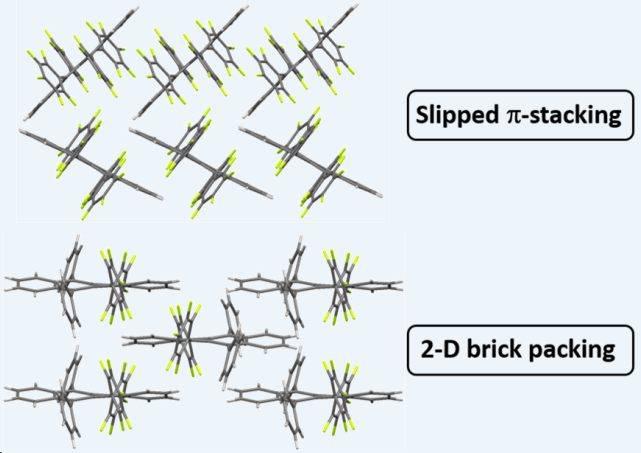
Chem. Commun., **2016**, *52*, 8127-8130

Diversification

12 fluorinated rubrenes examined



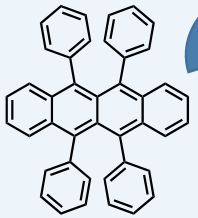
Tuning non-covalent interactions via fluorination



Transfer integral around 60 meV for 2-D brick packing

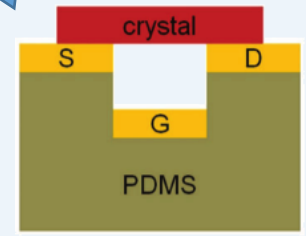
Cryst. Growth Des., **2017**, *17 (2)*, pp 643–658

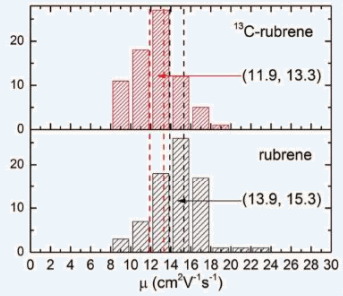
Isotope effect



All 42 carbons are ^{13}C labeled

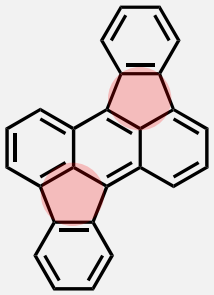
$^{13}C_{42}H_{28}$



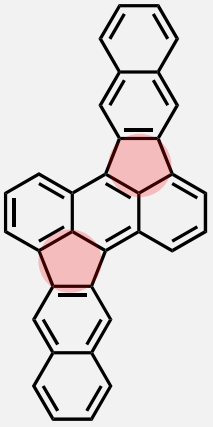


Adv. Electron. Mater. **2017**, *3*, 1700018

Cyclopenta-fused Polycyclic Aromatic Hydrocarbons (CP-PAH)

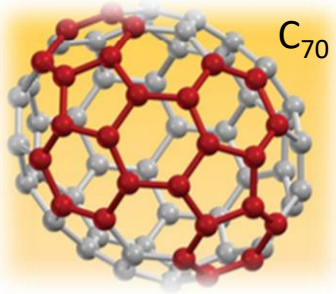


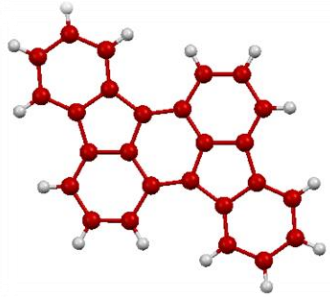
Rubicene

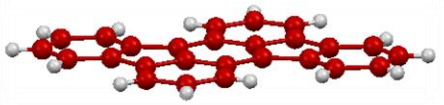


Dibenzo[*g*,*s*]rubicene

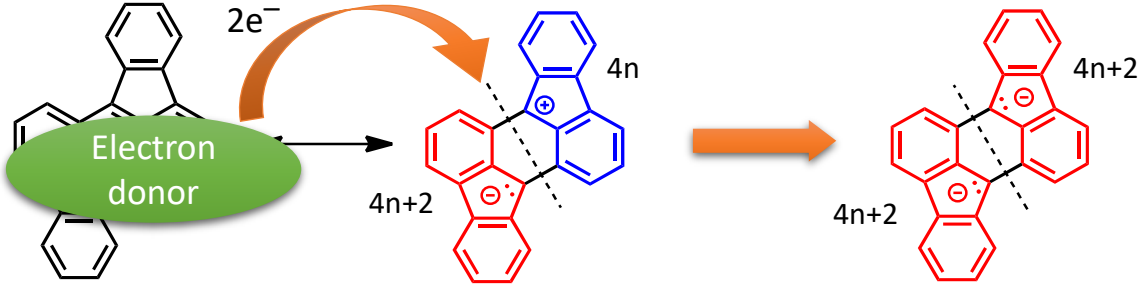
➢ Fullerene subunit — buckyball vs. planar



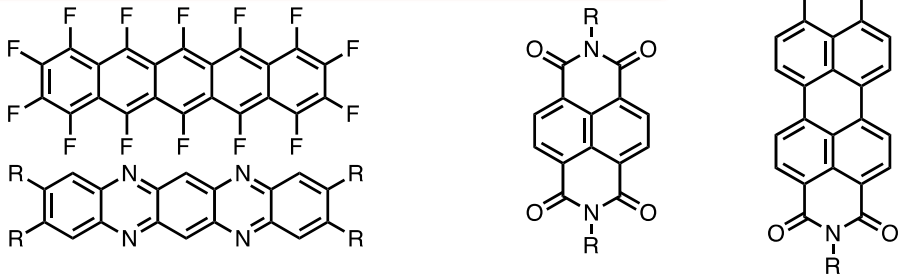




➢ Electron acceptor stabilized at "*charged state*"

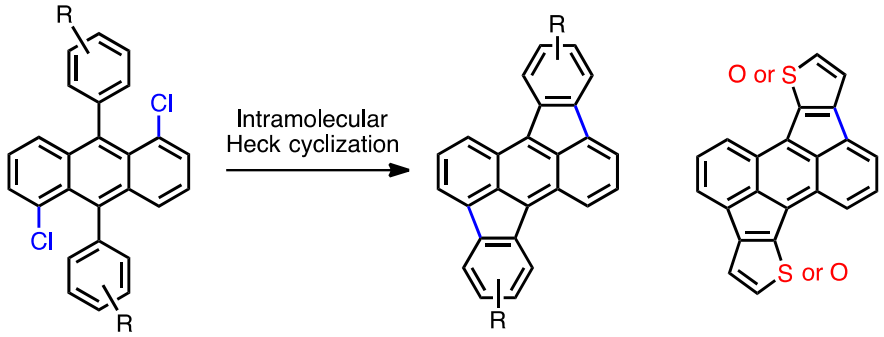


➢ Electron-deficient without EWG

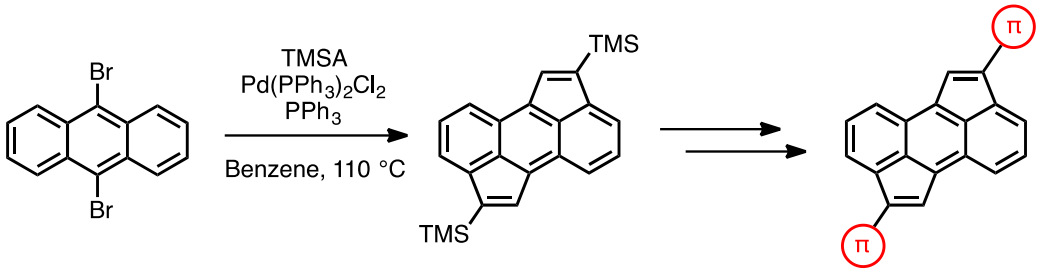


Synthetic Methods toward Five-membered Ring Formation

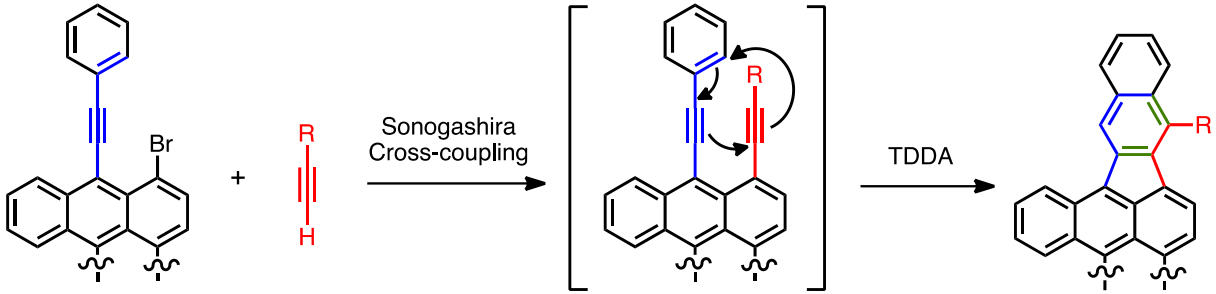
General method:

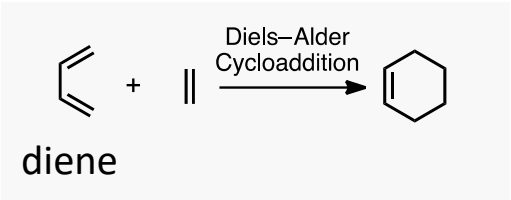


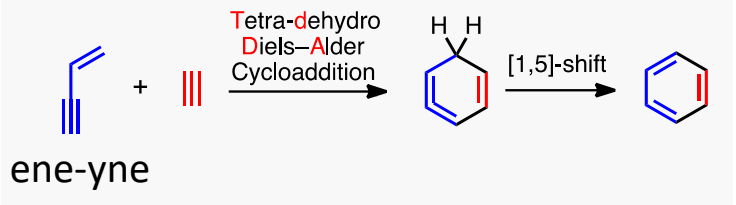
Plunkett's work:



In this work:



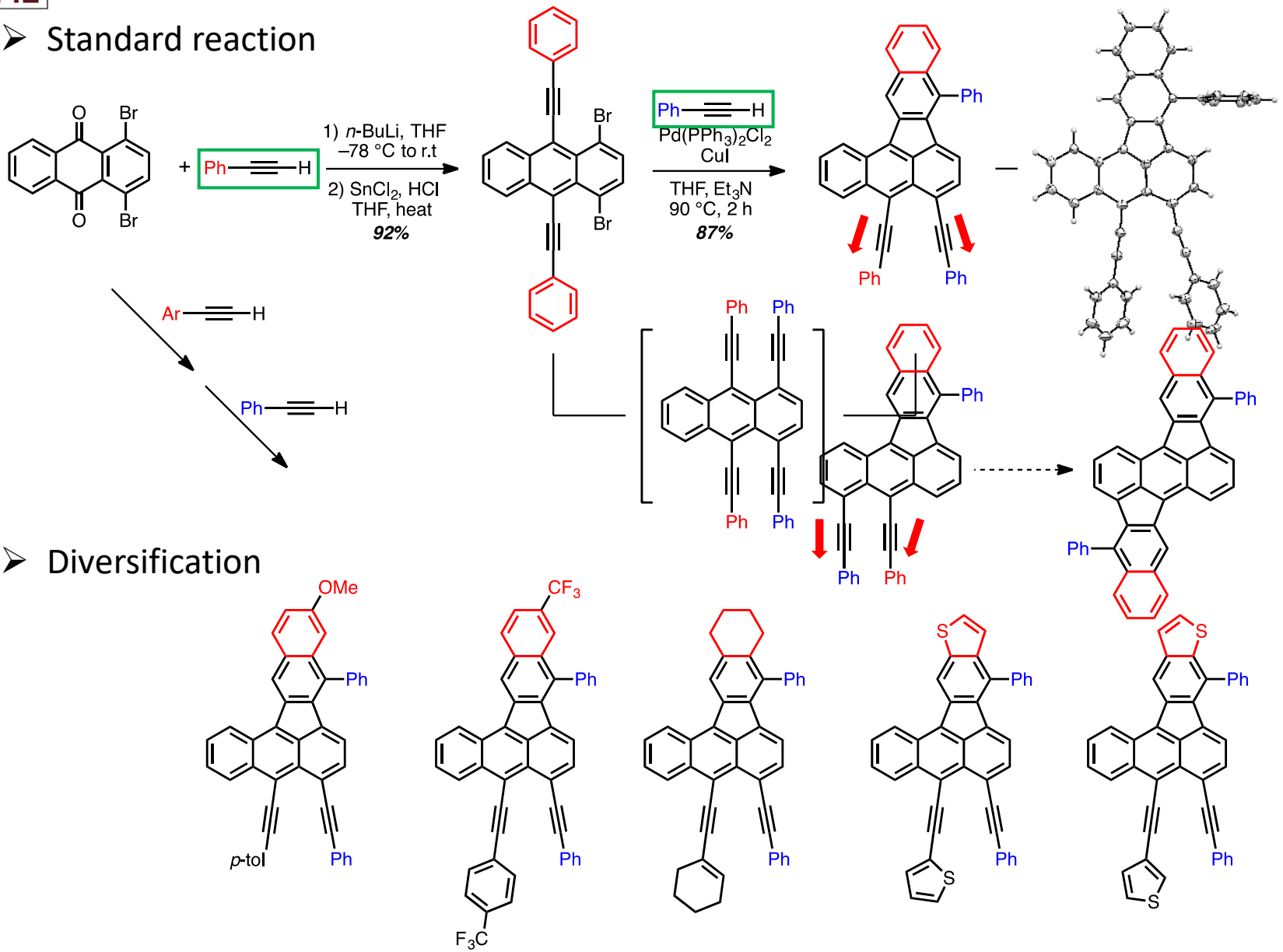




(1) Smet, M.; Van Dijk, J.; Dehaen, W. *Synlett*, **1999**, *4*, 495–497.
(2) Wood, J. D.; Jellison, J. L.; Finke, A. D.; Wang, L.; Plunkett, K. N. *J. Am. Chem. Soc.*, **2012,** *134*, 15783–15789.
(3) Mohebbi, A. R.; Wudl, F. *Chem. Eur. J.*, **2011**, *17*, 2642–2646.

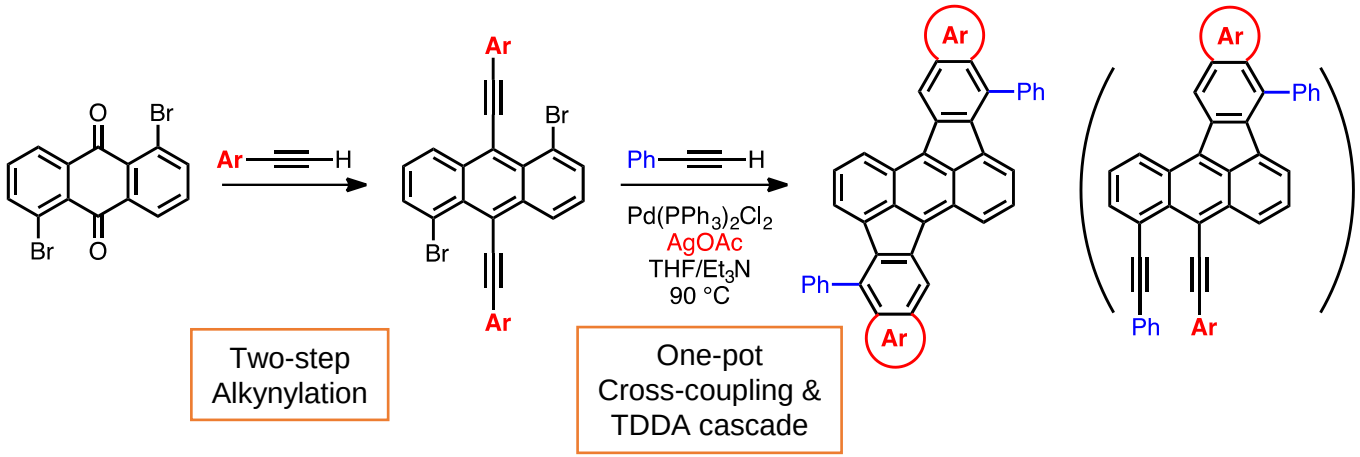
Synthesis of Half-rubicene Unit

- Standard reaction



- Diversification

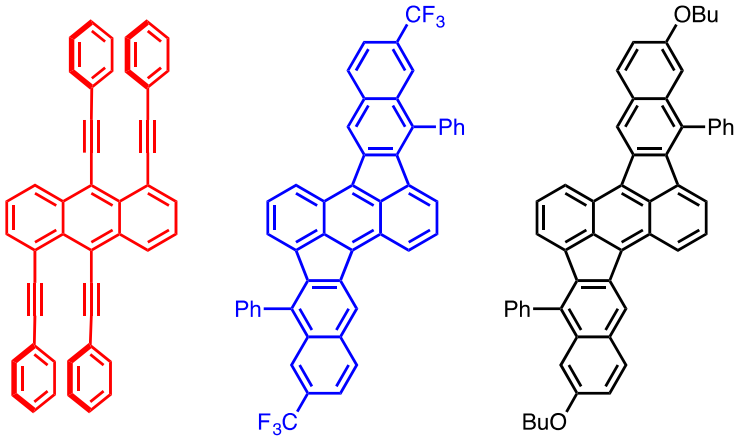
Synthesis of Diaryl[g,s]rubicene

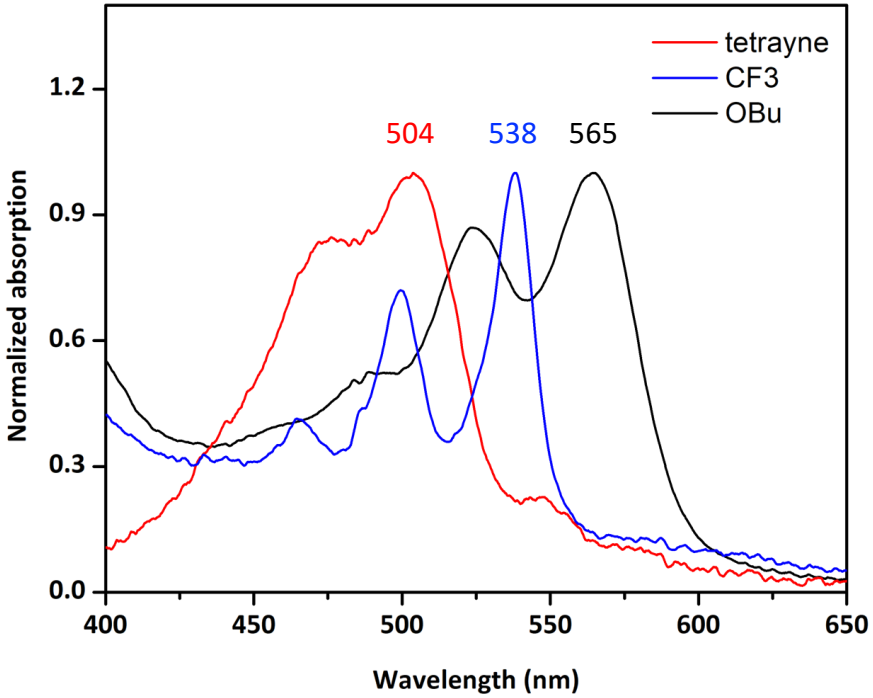


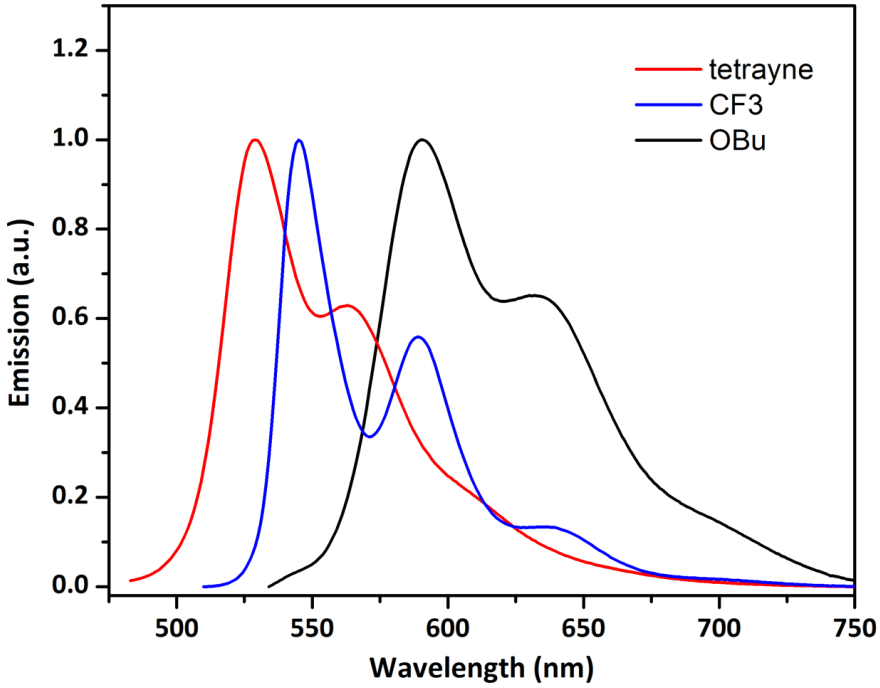
Ar Group		OBu	CF_3		S	S
Rubicene Yield	83%	89%	42%	94%	97%	92%

- e-rich substrates work well, e-poor substrates give moderate conversion
- Ene-yne + alkyne
- Compatible with heterocycles

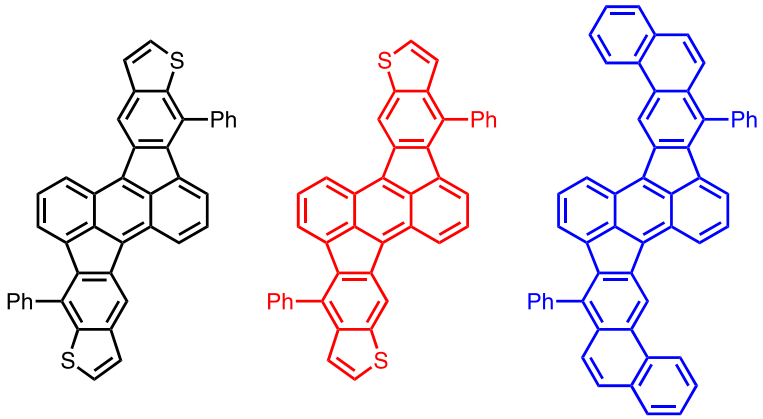
Absorption and Emission Spectra of Diaryl[g,s]rubicenes

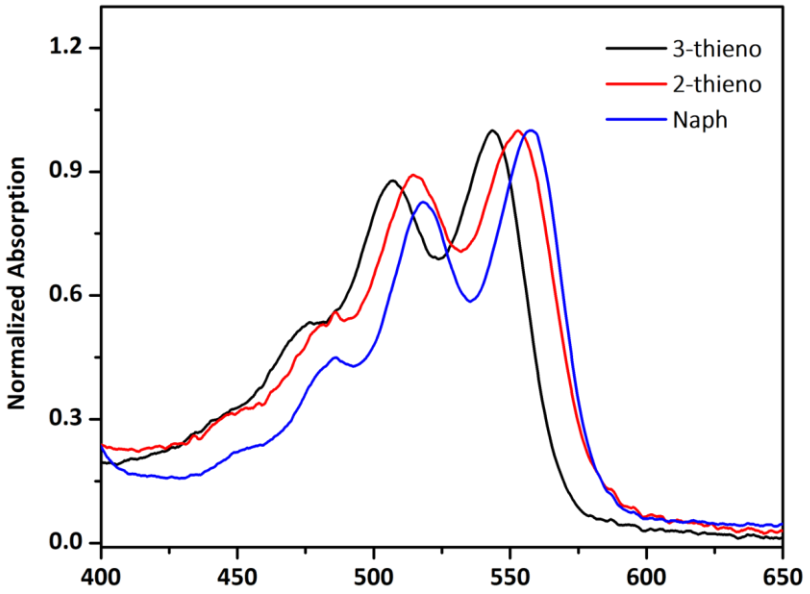


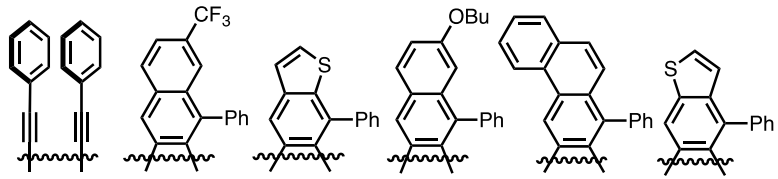


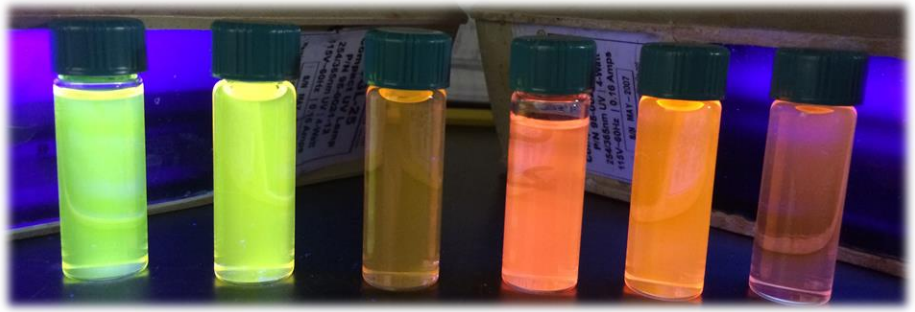


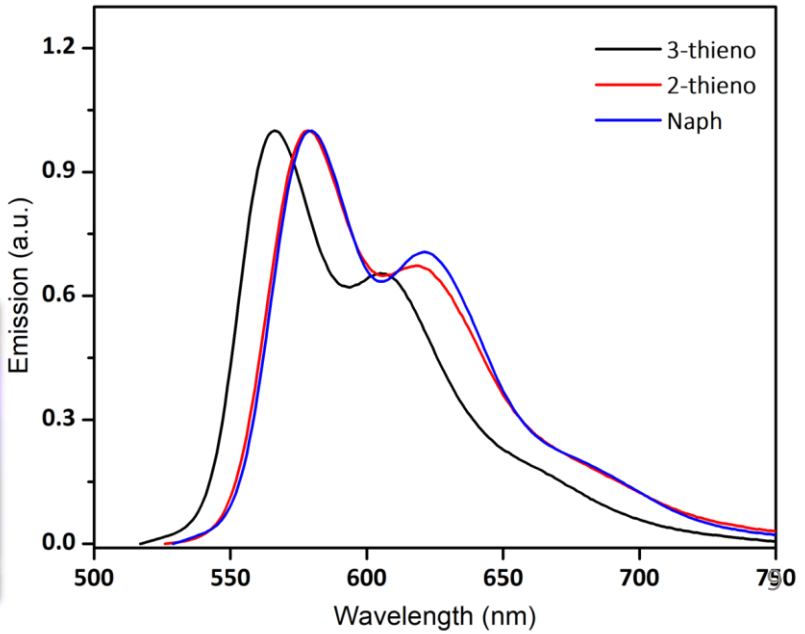
Absorption and Emission Spectra of Diaryl[g,s]rubicenes



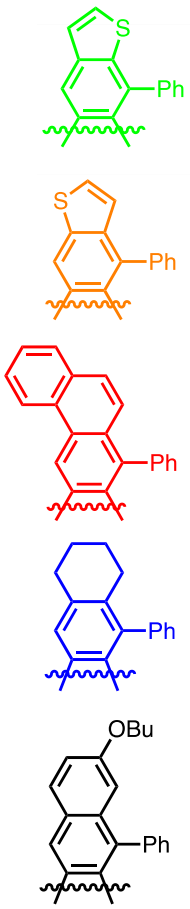


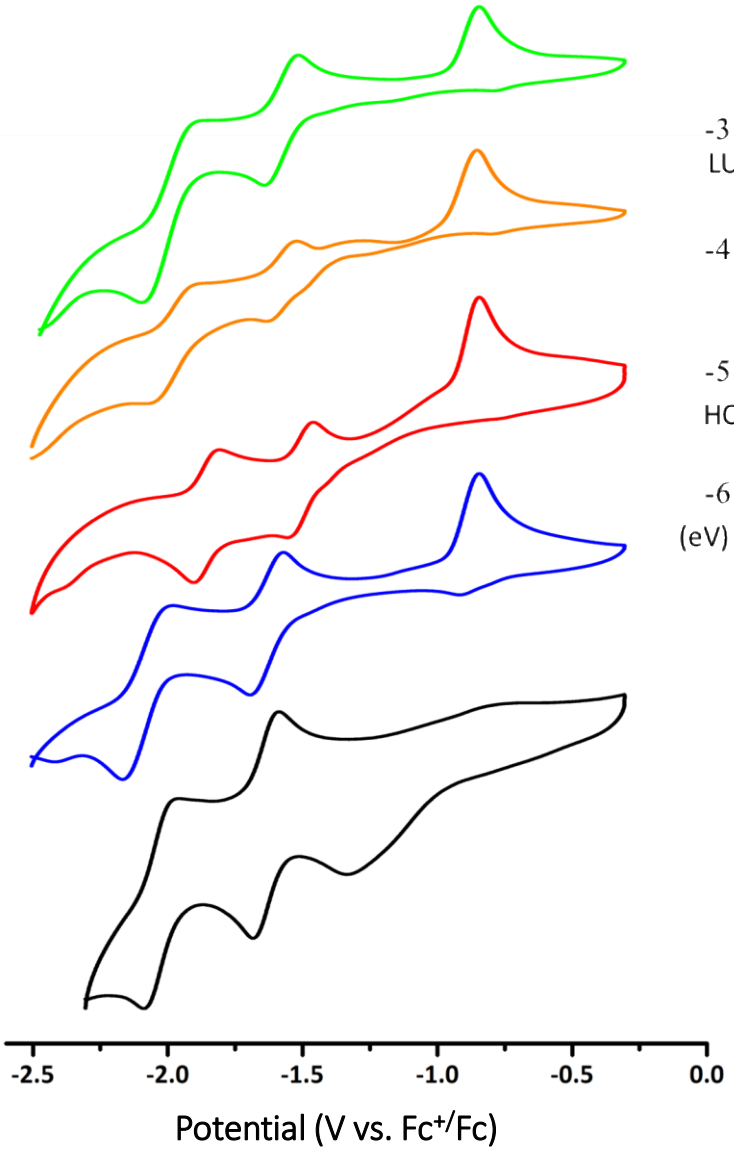
Ar Group						
Quantum Yield	88%	75%	17%	66%	79%	30%

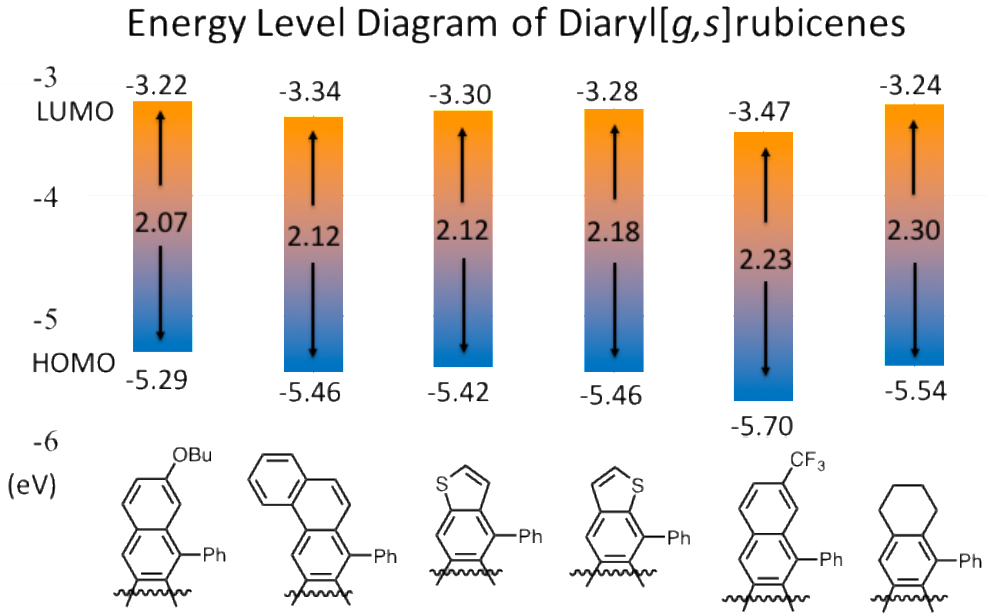




Electrochemical Properties







Compd	HOMO (eV)	LUMO (eV)	Bandgap (eV)
anthracene	–5.49	–2.25	3.24
tetracene	–5.18	–2.61	2.57
perylene	–5.34	–2.55	2.79

(1) Wood, J. D.; Jellison, J. L.; Finke, A. D.; Wang, L.; Plunkett, K. N. *J. Am. Chem. Soc.*, **2012,** *134*, 15783–15789.

Acknowledgements

- Prof. Christopher J. Douglas
- Shengyang Wang and Dr. Yong Guan for substrate synthesis
- Haynes group for optical characterization
- Buhlmann group for cyclic voltammetry experiments
- All Douglas group members

Thank you!