

Synthesis, Optical and Electrochemical Properties of Rubicene Derivatives

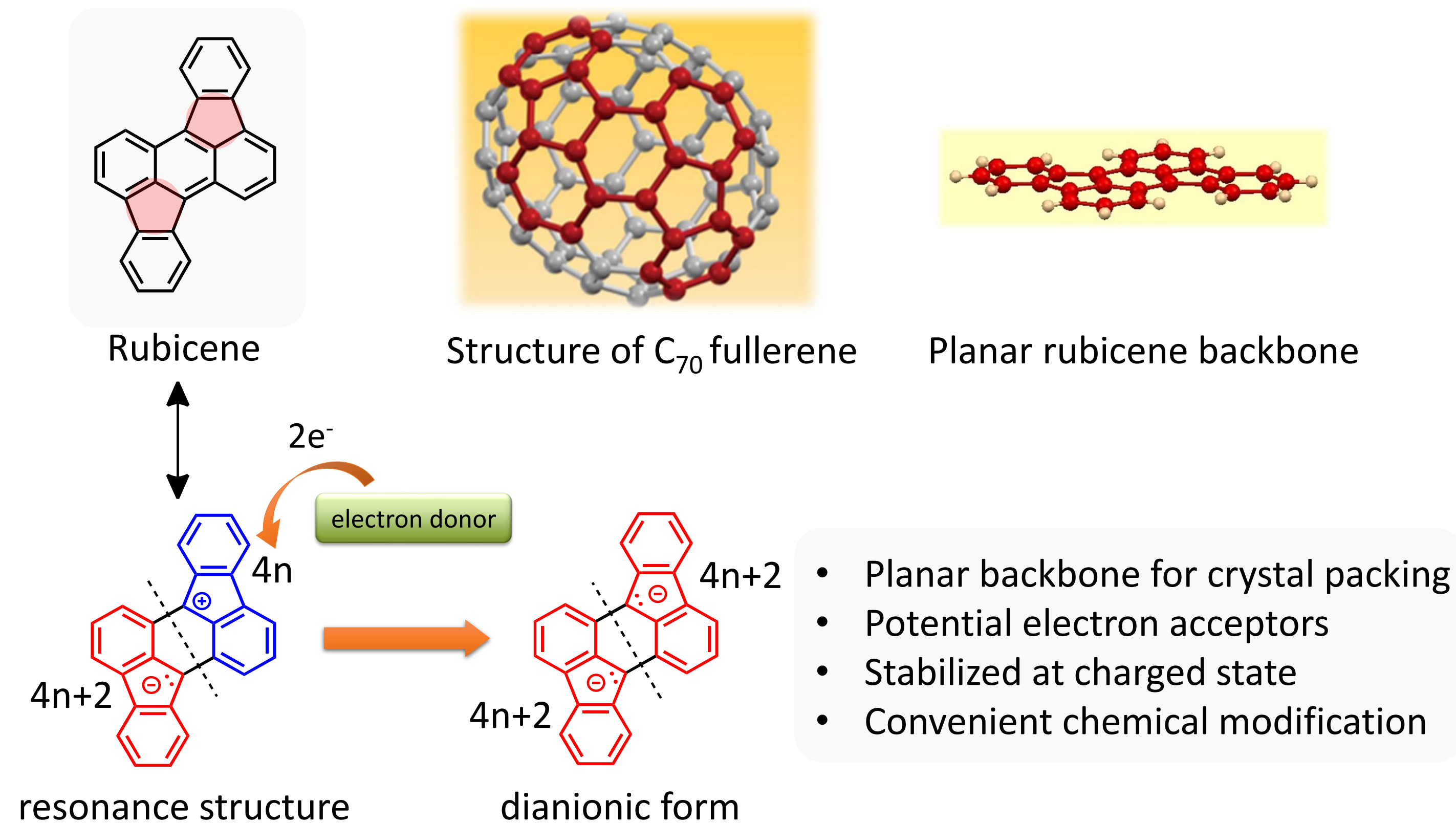
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Motivation

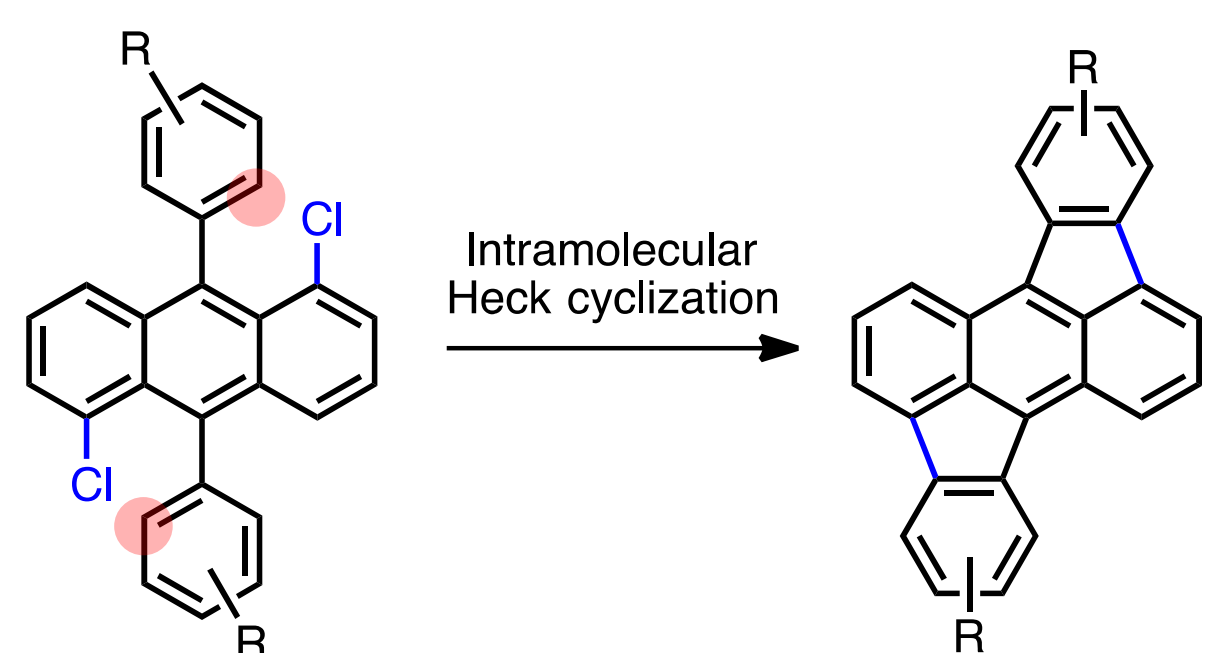
The Innovative design for small molecule organic semiconductors is crucial to the development of next-generation organic photovoltaics (OPVs). Fullerene derivatives are by far the most widely used electron acceptors in OPV devices. However, the challenge in chemical modifications limits the systematic studies to unravel the structure–property relationship. The molecular fragment of fullerenes are of particular interest as they serve as model systems for understanding the electronic structure, chemical reactivity and charge transport features.

➤ Rubicene as the core structure of C₇₀ fullerene



Synthetic Strategy

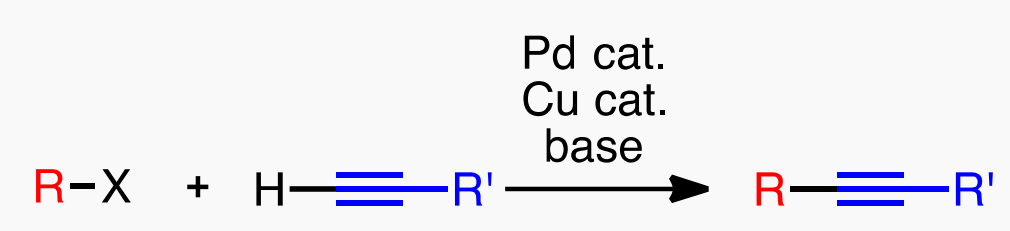
❖ General synthetic methods for cyclopenta-fused aromatic compounds



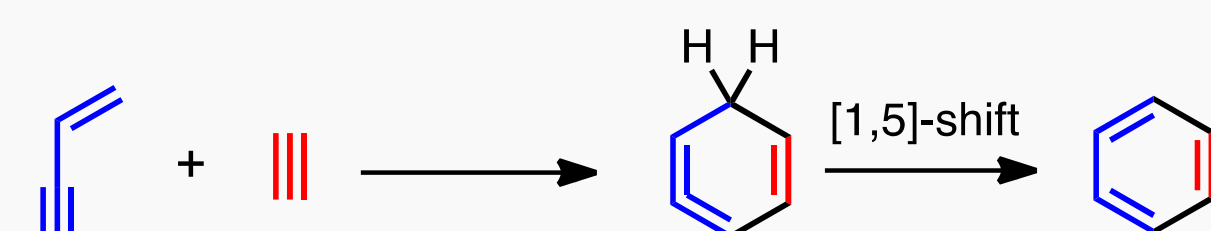
- Intramolecular cyclization via transition-metal catalyzed cross-couplings
- Lack of late-stage diversification
- Inefficient ring construction

❖ This work: large π -system synthesis via tandem cyclization

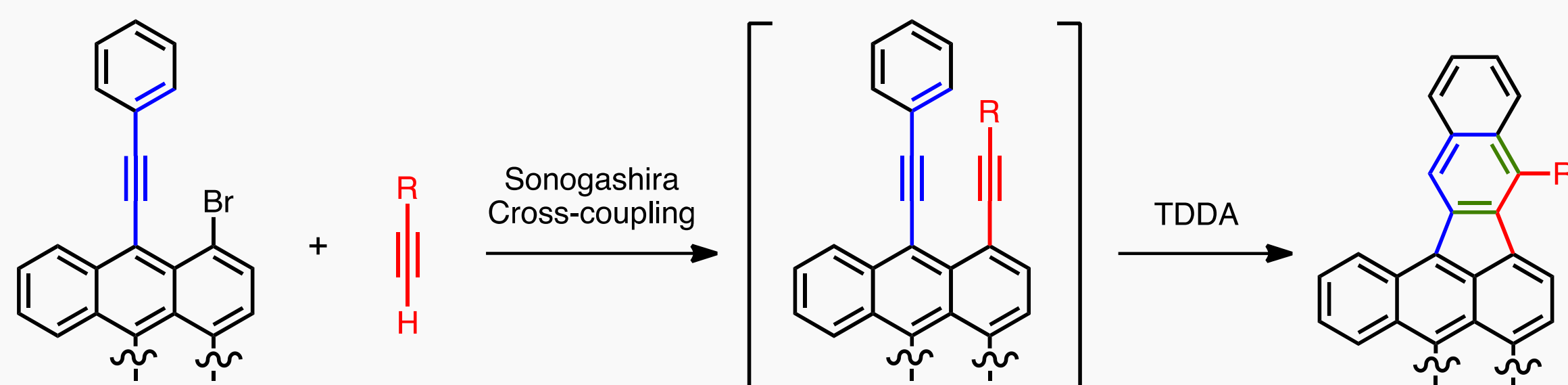
Sonogashira cross-coupling



Tetra-dehydro Diels–Alder cycloaddition (TDDA)



One-pot Sonogashira and TDDA cascade

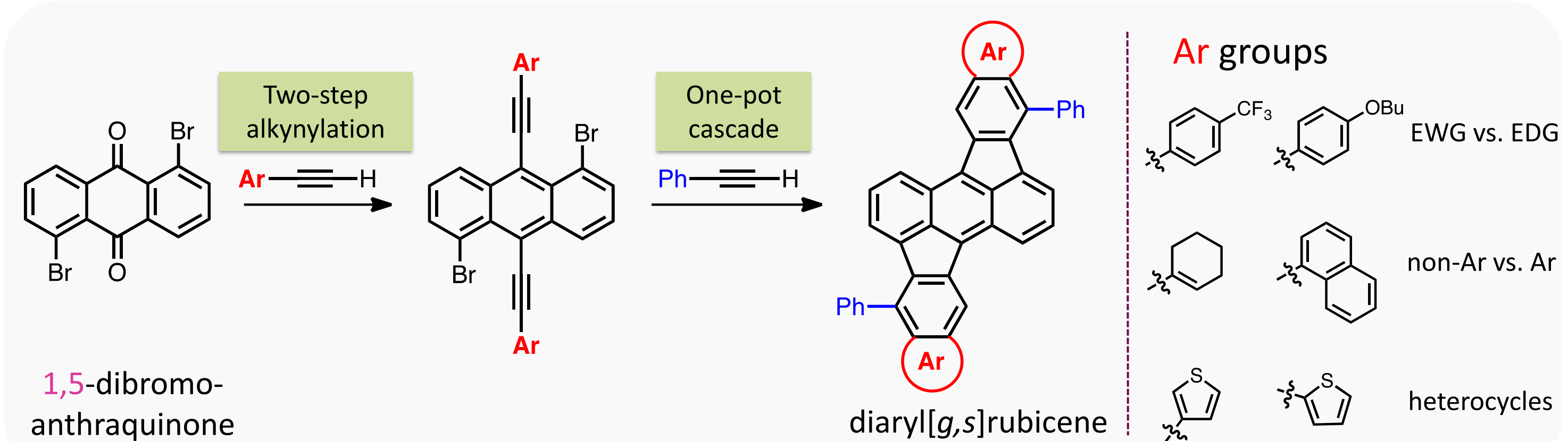
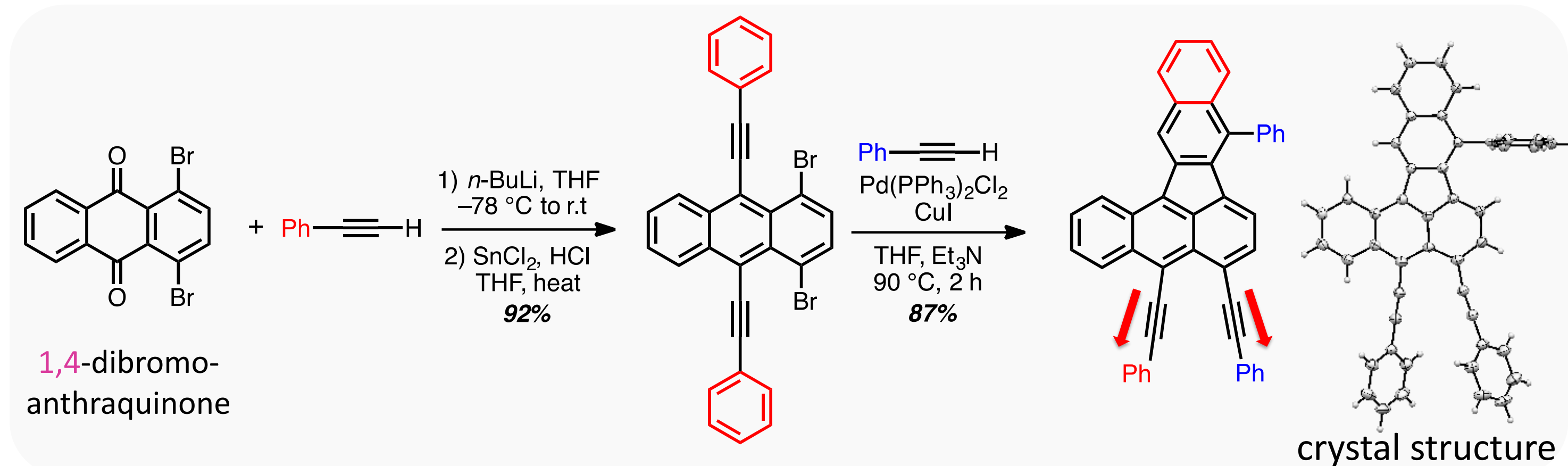


Acknowledgements & References

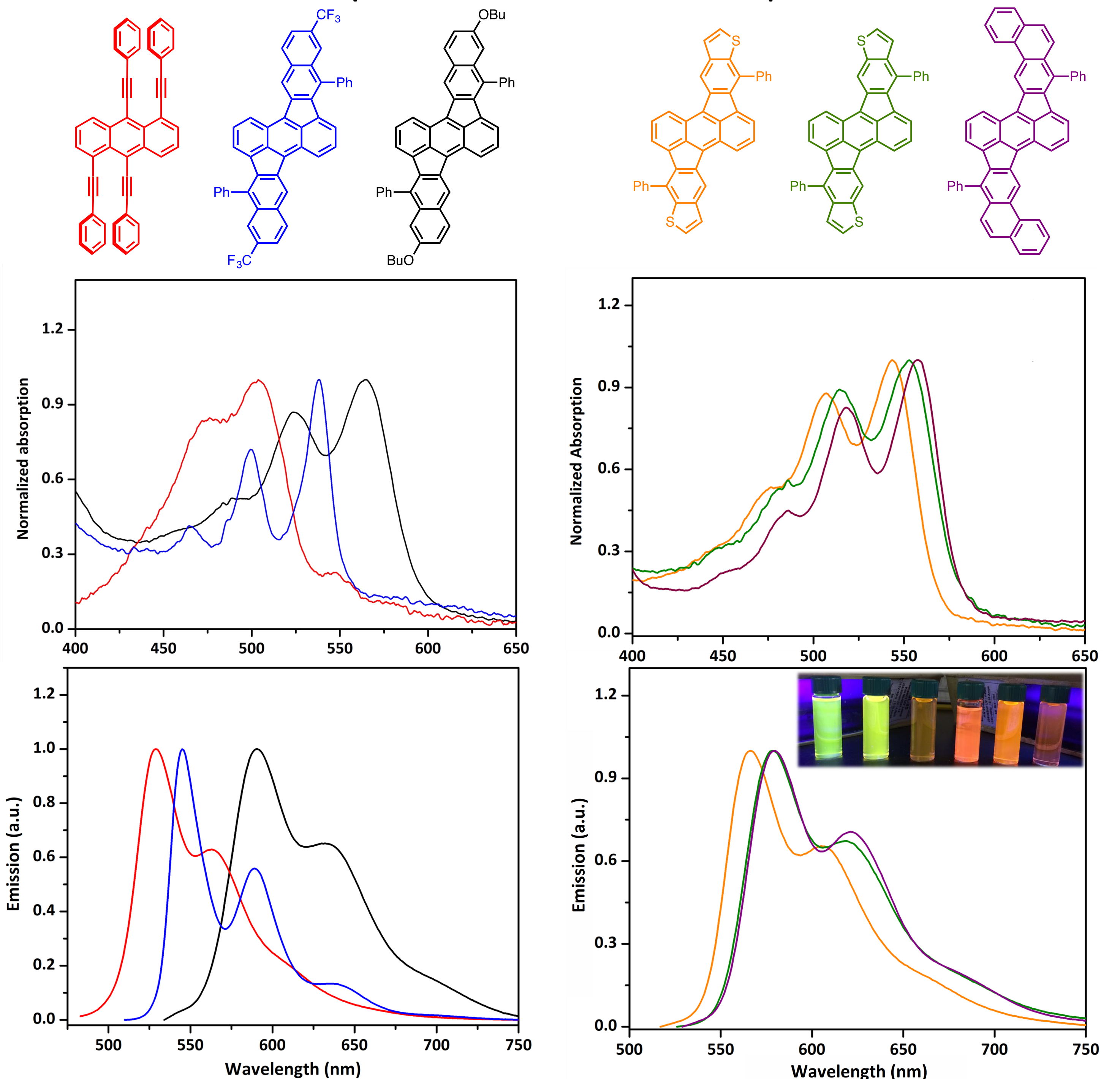
- Douglas research group members
- Dr. Victor Young Jr. and William (Billy) Ogden for the X-Ray crystal structure
- Bo Zhi from Haynes research group for optical characterizations
- Xue Zhen from Buhlmann Research group for cyclic voltammetry experiments

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Synthesis of Diaryl[g,s]rubicenes



Absorption and Emission Properties



Electrochemical Properties

