Acene-based Polycyclic Aromatic Hydrocarbons: Syntheses, Crystal Structures and Optical Characteristics

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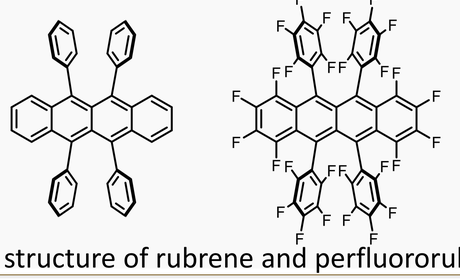
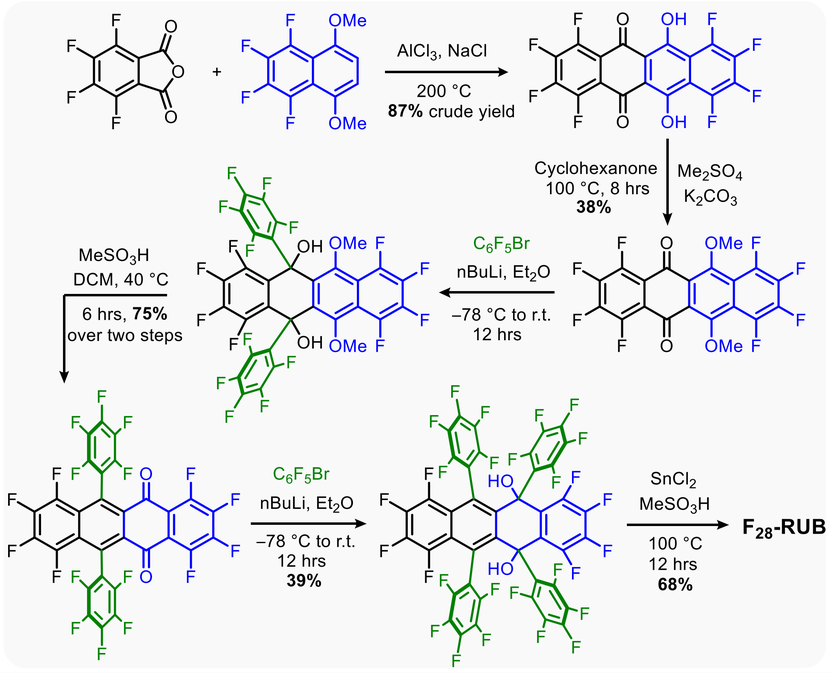
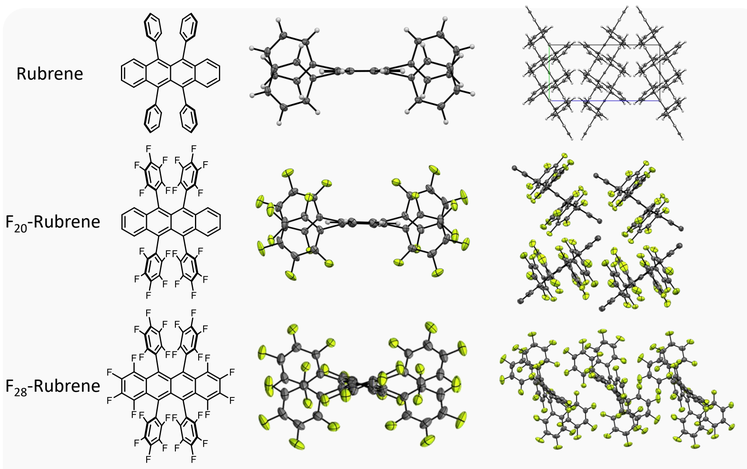
Perfluorinated rubrene : synthesis, crystal packing and electrochemical characterizations

Fluorination of an organic conjugated system can greatly impact its material properties in several aspects: It greatly lowers the LUMO energy level and increase the stability to O_2; It affects the packing motif in the solid states via fluorine-based intermolecular interactions. Rubrene and its derivatives has been widely studied as high-performance organic semiconductors. In this work, we established the synthesis of a perfluorinated analog of rubrene. The electro-chemical property and the crystal structure of perfluororubrene were studied to demonstrate the effects of fluorine introduction.



Chemical structure of rubrene and perfluororubrene





Summary of cyclic voltammetry results

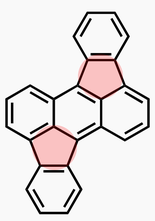
Compound	E_{ox} V	E_{red1} V	E_{red2} V	HOMO eV	LUMO eV
Rubrene	0.38	–1.44	–	–5.18	–3.36
F_{28}-Rubrene	–	–0.83	–1.60	–	–4.05

Cyclopenta-fused PAHs: studies into dibenzo[*g*,*s*]rubicenes

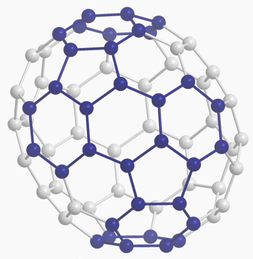
The Innovative design for small molecule organic semiconductors is crucial to the development of next-generation organic semiconductors. Though fullerenes are by far the most widely used electron acceptors in organic photovoltaics, the structure–property relationship is hard to establish due to the difficulty in chemical modifications. Thus, fullerene fragments are considered potential substitutes for fullerene as novel electron-acceptors because of a) the inheritance of the core structure; b) decent solution processing and c) convenient derivatization and on-demand tuning of frontier orbital energy levels.

Design and Synthesis

➢ Dibenzo[*g*,*s*]rubicene as the core structure of C_{70} fullerene

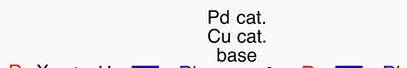


Rubicene

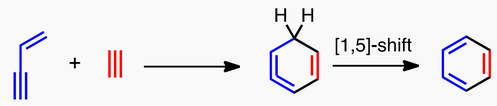


Dibenzo[*g*,*s*]rubicene within the structure of C_{70} fullerene

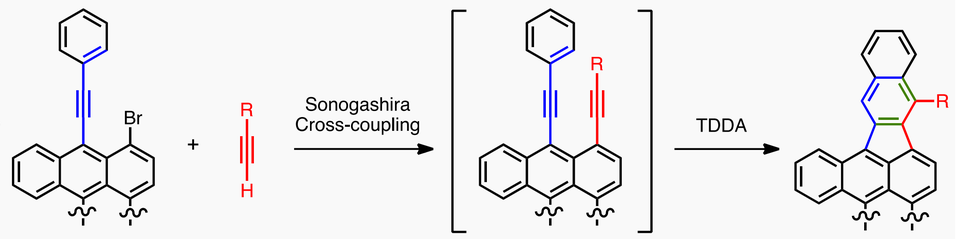
Sonogashira cross-coupling

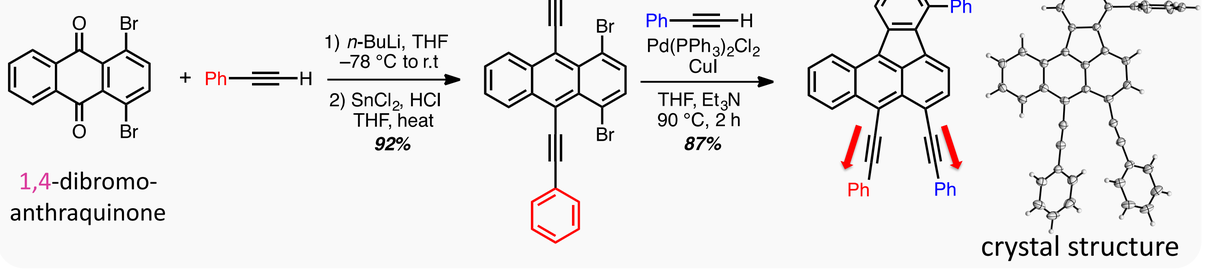


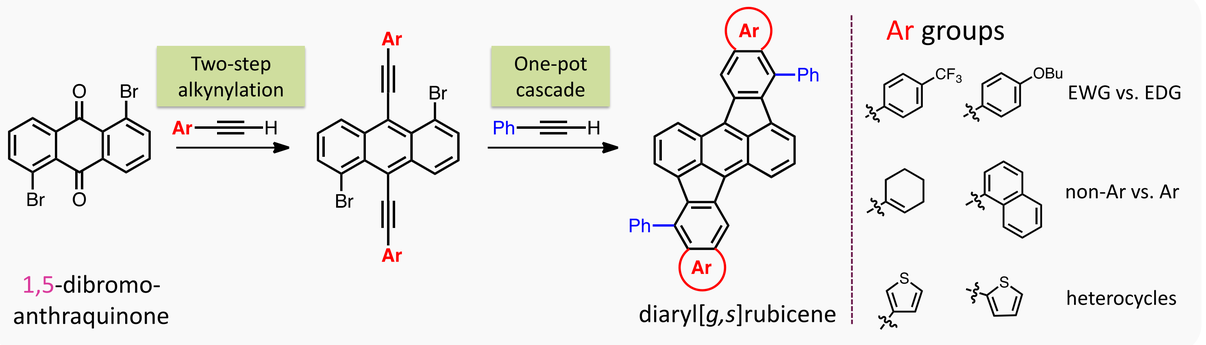
Tetra-dehydro Diels–Alder cycloaddition (TDDA)



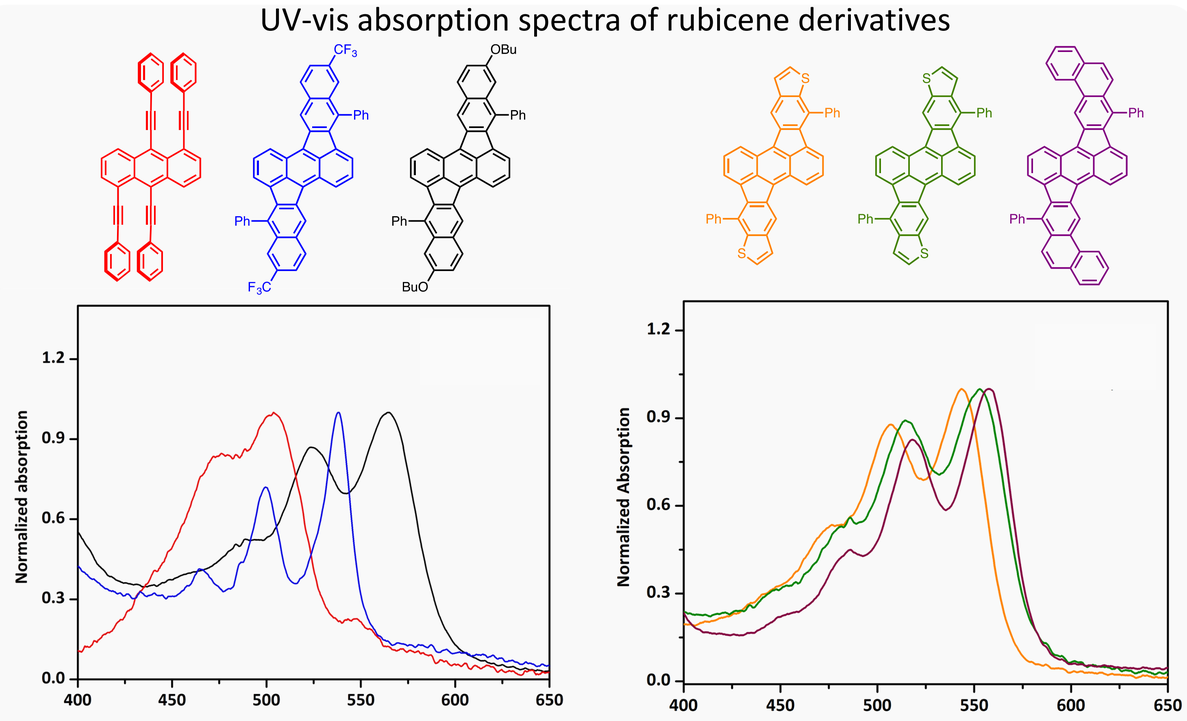
One–pot Sonogashira and TDDA cascade





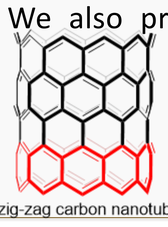


UV-vis absorption spectra of rubicene derivatives

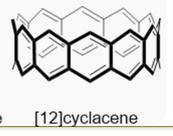


3D carbon nanobelts : synthesis towards a [12]cyclacene derivative

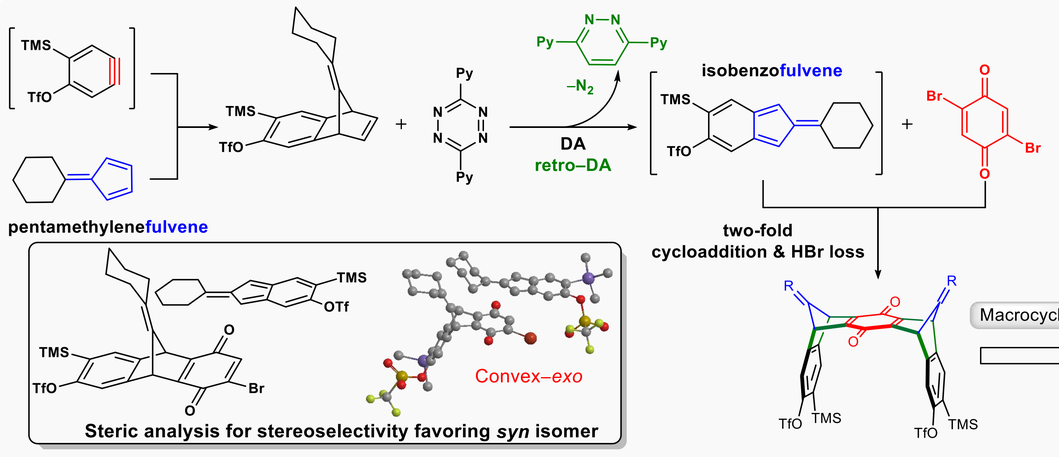
Carbon nanobelt represents the monolayer unit of carbon nanotubes. [n]Cyclacene is a typical form of carbon nanobelts that is highly strained and fully conjugated. Synthesis of such a cyclic structure requires a clever route to avoid the strain barrier. In this work, we present our strategy to construct a macrocyclic framework in a stereoselective fashion. We also proposed the end-game aromatization using a thermally-driven decarbonylation reaction.



zig-zag carbon nanotube



[12]cyclacene



End game strategy