Dimerization and Rearrangement of Fluorene Based Dialkynes

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Circumazulene is a polycyclic aromatic hydrocarbon, consisting of an upper half with a fivemembered ring and a lower half with a seven membered ring.^[1] During our attempted synthesis of the upper half, we serendipitously discovered a rearrangement reaction of fluorene based dialkynes as well as an expanded scope for their dimerization.^[2] To study electronic effects on these competing reactions, several substituents were introduced. To further elucidate the underlying reaction mechanism of the rearrangement, pathways leading to the benzannulation and rearrangement were calculated by DFT-methods. Both the rearranged and dimerization products were studied for their optoelectronic properties.^[3]



Figure 1: Fluorene based dialkynes and their reactivity under platinum catalyzed benzannulation conditions.

References:

- [1] F. Wu et al., Chemistry 2023, 29, e202301739.
- [2] H. Hopf et al., Angew. Chem. Int. Ed. Engl. 2003, 36, 1187-1190.
- [3] Our work, manuscript in preparation.