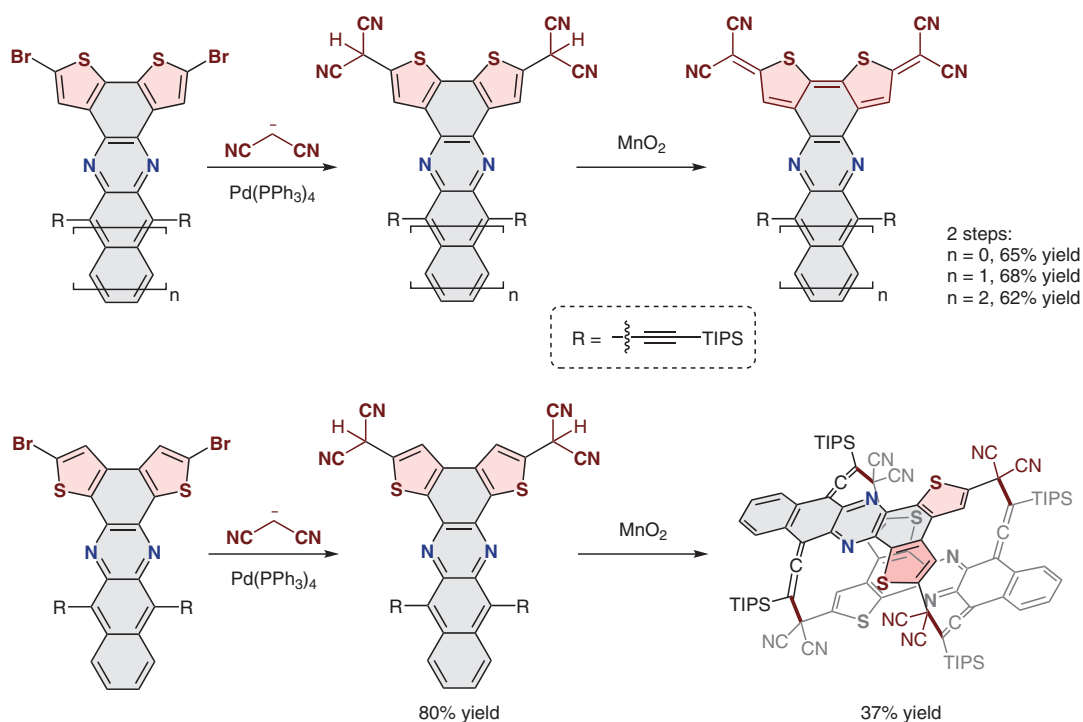


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Dimerization of a Reactive Azaacene Diradical: Synthesis of a Covalent Azaacene Cage
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Molecular Cage from Diradical Dimerization



Significance: Two series of regio-isomeric dicyanomethylene-substituted dithienodiazacenes are synthesized. Different orientations of the thiophene units are found to bring about different diradical character and chemo-stability. The *para*-isomers are stable, closed-shell quinoidal molecules, while the *ortho*-isomer dimerizes into a cage-like structure, presumably via the open-shell diradical state.

Comment: Uniquely, instead of forming covalent bonds directly between the radical sites mainly located with the dicyanomethylene carbons, the dimerization occurs by joining the ethynylene carbon adjacent to TIPS with the dicyanomethylene. This phenomenon suggests the diradicaloid character of the bis(TIPS-ethynylene)-substituted diazatetra-cene.

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Category

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