

Iron-Catalyzed Tandem Cyclization of Diarylacetylene to a Strained 1,4-Dihydropentalene Framework for Organic Electronic Materials

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Keywords: Iron; Tandem Cyclization; 1,4-Dihydropentalene; Organic Electronic Materials

1,4-Dihydropentalene framework fused in pi-conjugated molecules flattens and rigidifies the system for development of new types of organic electronic materials.¹ The typical properties rely on the strained structure which helps to raise the highest occupied molecular orbital (HOMO) and lowers the lowest unoccupied molecular orbital (LUMO) energy levels.² To extend, we are further intrigued to fuse 1,4-dihydropentalene framework with heteroaromatic rings such as thiophenes which is expected to have high HOMOs along with narrow band gaps therefore serving as potential donor units in A-D-A type non-fullerene acceptor (NFA) materials to be utilized for near-infrared organic photodetector devices (NIR OPDs). However, there lacks efficient and flexible methods for making such a strained ring system. Herein we report a mild and versatile synthetic access using iron-catalyzed single-pot tandem cyclization of a diarylacetylene to synthesize a variety of substituted indeno[2,1-*a*]indenes and their thiophene congeners, as well as further elongated 1,4-dihydropentalene ladder structures (Figure 1a). Tandem cyclization allows construction of multiple rings in one pot, providing unprecedented carbon-bridged arylenevinylenes. Optoelectronic properties of newly synthesized molecules suggest their promising application in photovoltaic and light emitting devices (Figure 1b).

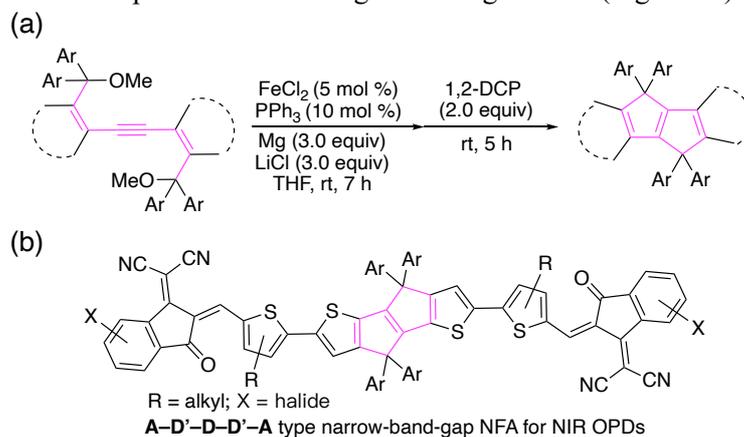


Figure 1

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