Iron-Catalyzed Aza-Annulative π-Extension using a Self-Oxidation Auxiliary

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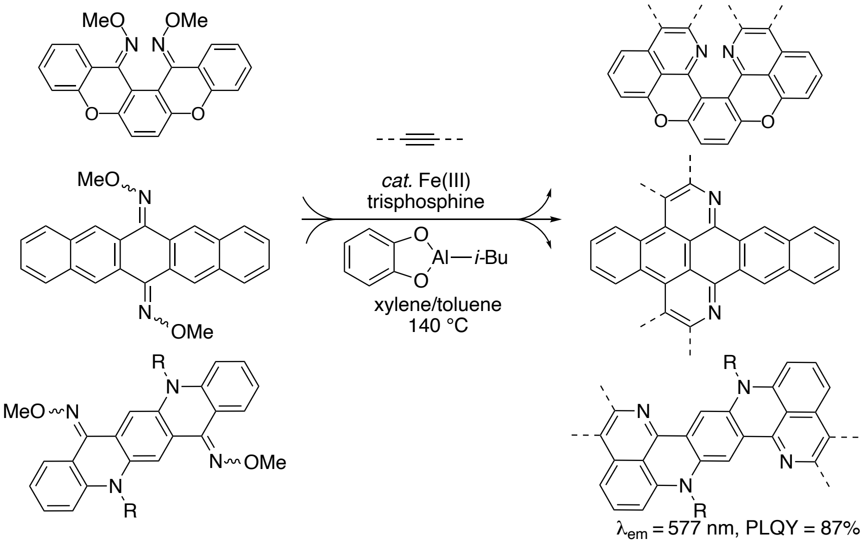
Aza-annulative π-extension (**AAPE**) reactions[1] offer a potent pathway to create novel donor-acceptor conjugated materials by integrating an imine moiety into the conjugated system, serving as an electron-accepting unit[2]. However, the affinity of late-transition metals for conjugated π-systems, coupled with their elevated cost, has posed significant challenges, restricting efficient **AAPE** reactions on straightforward C–H substrates for developing conjugated new materials. In this study, we unveil an iron-catalyzed C–H activation methodology[3], facilitating **AAPE** with diverse internal alkynes and employing oxime ether as both a self-oxidizing auxiliary[4] and nitrogen source, derived seamlessly from accessible carbonyl compounds. The **AAPE** reaction was enabled by using trisphosphine as a ligand, and isobutyl aluminum(III) catecholate as a base.[5] By using the reaction, we discovered an aza-oxa[5]helicene from dixanthone as a potential circularly polarized luminescence material and two narrow-band-emissive molecules from easily accessible pentacene-6,13-dione and quinacridone, which emit blue and yellow light with high color purity and high fluorescence quantum yield. These findings emphasize the potential of iron-catalyzed C–H activation in expanding the range of donor-acceptor-type conjugated materials for organic electronics.



λ_{em} = 577 nm, PLQY = 87%
FWHM = 25 nm

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