

## Iron-Catalyzed Regioselective Selenophenyl C–H/C–H Coupling and Polymerization

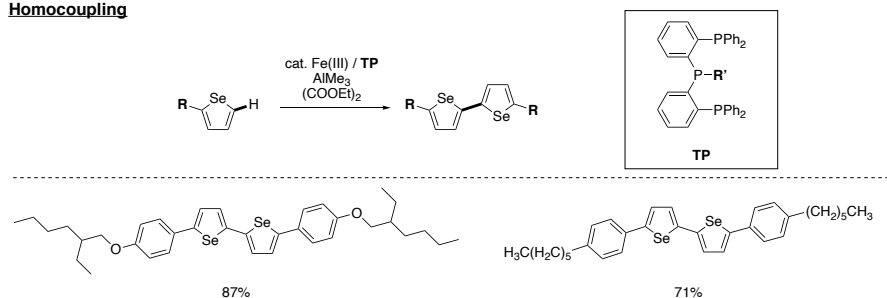
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**Keywords:** Iron Catalysis; C–H bond activation; Selenophene; Polymerization; Organic electronic materials

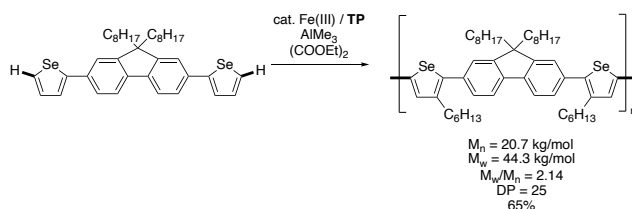
Selenophene-contained small molecules and polymers have attracted attention as efficient organic electronic materials for optoelectronic device applications because of their narrow band gap and high charge carrier mobility rendered by large and polarizable selenium atom.<sup>1</sup> Regioselective coupling of two selenophene moieties is currently using transition-metal catalyzed coupling reactions such as Suzuki couplings,<sup>2</sup> Stille couplings,<sup>3</sup> etc., which require tedious synthetic steps to access prefuctionalized starting materials and monomers (e.g. selenophenyl halides and organometallics).

Herein we report that a Fe(III)/AlMe<sub>3</sub>/diethyl oxalate catalytic system<sup>4</sup> with a newly designed tridentate phosphine ligand directly activates selenophenyl C–H bonds with high regioselectivity to allow facile synthesis of selenophene containing dimer, oligomer, and even polymers. The reaction uses diethyl oxalate as a mild oxidant and therefore is applicable to highly conjugated compounds such as those mainly use in organic electronic materials. The reaction will be useful for the flexible design of novel selenophene-containing semiconductive polymers.

### Homocoupling



### Polymerization



1) Fan, B. et al. *Acc. Chem. Res.* **2021**, 54, 3906. 2) Shabana, R. et al. *Phosphorus, Sulfur. and Silicon.* **1990**, 48, 239. 3) Shahid, M. et al. *Chem. Sci.* **2012**, 3, 181. 4) Doba, T. et al. *Nat. Catal.* **2021**, 4, 631.