Ir-Catalyzed Preparation of SF$_5$-Substituted Potassium Aryl Trifluoroborates via C–H Borylation and Their Application in the Suzuki–Miyaura Reaction

**Abstract**

A novel method for the preparation of pentafluorosulfanyl-substituted potassium aryl trifluoroborates via iridium-catalyzed C–H borylation is reported. The corresponding products were obtained in high yields and have been submitted to Suzuki–Miyaura cross-couplings furnishing 3,5-disubstituted pentafluorosulfanylbenzenes.

**Significance:** A novel method for the preparation of pentafluorosulfanyl-substituted potassium aryl trifluoroborates via iridium-catalyzed C–H borylation is reported. The corresponding products were obtained in high yields and have been submitted to Suzuki–Miyaura cross-couplings furnishing 3,5-disubstituted pentafluorosulfanylbenzenes.

**Comment:** The described protocol is very versatile since the prepared compounds are potential important building blocks for drug discovery and agrochemicals. Moreover, the reaction proceeds under relatively mild conditions and tolerates various functional groups.

**Key words**

C–H borylation, potassium aryl trifluoroborates, iridium

**Selected examples:**

- R$^1$ = OMe, CN, CO$_2$Me, NMe$_2$, Cl, Br, I  
  R$^2$ = Ar  
  X = Br, I  
  dbtpy = 4,4′-di-tert-butyl-2,2′-dipyridyl  
  dppf = 1,1′-bis(diphenylphosphino)ferrocene

- 1. pin$_2$B$_2$ (1 equiv)  
  [Ir(OMe)(cod)]$_2$ (0.75 mol%)  
  THF, 80 °C, 24 h

- 2. KH$_2$F$_5$ (5.7 equiv)  
  THF–H$_2$O (5:3)  
  25 °C, 6 h

- R$^1$BF$_3$K (1 equiv)  
  R$^2$X (1.2 equiv)  
  PdCl$_2$(dppf) CH$_2$Cl$_2$ (2 mol%)  
  EtOH, 85 °C, 12–16 h

- or:  
  R$^1$BF$_3$K (1 equiv)  
  R$^2$X (2 equiv)  
  Pd(OAc)$_2$ (5 mol%)  
  K$_2$CO$_3$ (3 equiv)  
  MeOH, 80 °C, 16 h

**Yields:**

- 89% yield
- 81% yield
- 76% yield
- 93% yield
- 41% yield
- 57% yield
- 83% yield
- 46% yield
- 95% yield