Application in the Suzuki-Miyaura Reaction

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Iridium-Catalyzed Preparation of SF₅-Substituted Aryl Trifluoroborates

Ir-Catalyzed Preparation of SF5-Substituted Potassium Aryl Trifluoroborates via C-H Borylation and Their

$$\begin{array}{c} \text{1. pin}_2B_2 \text{ (1 equiv)} \\ \text{[Ir(OMe)(cod)]}_2 \text{ (0.75 mol\%)} \\ \text{dtbpy (1.5 mol\%)} \\ \text{THF, 80 °C, 24 h} \\ \hline \\ \text{2. KHF}_2 \text{ (5.7 equiv)} \\ \text{THF-H}_2O \text{ (5:3)} \\ \text{25 °C, 6 h} \\ \end{array} \\ \begin{array}{c} \text{R}^1 \\ \text{EtOH, 85 °C, 12-16 h} \\ \hline \\ \text{or:} \\ \text{R}^2\text{X (2 equiv)} \\ \text{or:} \\ \text{R}^2\text{X (2 equiv)} \\ \text{or:} \\ \text{R}^2\text{X (2 equiv)} \\ \text{MeOH, 80 °C, 16 h} \\ \end{array} \\ \text{up to 94\% yield} \\ \\ \text{R}^1 = \text{OMe, CN, CO}_2\text{Me, NMe}_2, \text{CI, Br, I} \\ \text{R}^2 = \text{Ar} \\ \text{X = Br, I} \\ \text{dtbpy = 4,4'-di-tert-butyl-2,2'-dipyridyl} \\ \end{array}$$

Selected examples:

dppf = 1,1'-bis(diphenylphosphino)ferrocene

CI BF₃K
$$Me_2N$$
 BF_3K Br BF_3K BF_5 BF_5

Significance: A novel method for the preparation of pentafluorosulfanyl-substituted potassium aryltrifluoroborates 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.

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