Bis(tri-tert-butylphosphine)palladium(0) \([\text{Pd}(t\text{-Bu}_3\text{P})_2]\)

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Introduction

The catalyst bis(tri-tert-butylphosphine)palladium(0) \([\text{Pd}(t\text{-Bu}_3\text{P})_2]\), 1, CAS: 53199-31-8 is a colorless, air-sensitive solid. It must be manipulated in a glove box or under inert gas. \([\text{Pd}(t\text{-Bu}_3\text{P})_2]\) (1) contains bulky, electron-rich tertiary phosphine ligands \([t\text{-Bu}_3\text{P}].\) In a palladium-catalyzed cross-coupling reaction, they promote the oxidative addition as they can stabilize higher oxidation states. Reductive elimination is also facilitated because of the bulky ligands. Thus 1 has been shown to be superior in transition-metal-catalyzed cross-coupling reactions compared to the classical \([\text{Pd}($\eta^5$-C_5H_5)$]_2\) catalyst. \([\text{Pd}(t\text{-Bu}_3\text{P})_2]\) is not only efficient for typical cross-coupling reactions, such as Stille, Negishi, Suzuki, Heck, Sonogashira, or Buchwald–Hartwig aminations, with electrophiles R-X (X = Cl, Br, I, OTf, SO_2Cl and others), but also for cross-coupling of organolithium reagents, alkynylgermanes, alkali-metal silanolates, triorganogano-indium reagents and others. Moreover, it has been used for arylations of hydro-siloxanes, decarboxylative cross-coupling reactions, carboxylations and amino-carboxylations, carboiodinations, C-H functionalizations, cyanations, methylation of olefins and annulation reactions. In recent years, 1 has become one of the best new-generation catalysts and plays an important role in organic synthesis.

\[\text{Pd}(t\text{-Bu}_3\text{P})_2\] is commercially available and can also be prepared by treating \([\text{Pd}($\eta^5$-C_5H_5)$][\text{P}(t\text{-Bu}_3\text{P})_2]\) with the ligand \([t\text{-Bu}_3\text{P}].\) in n-hexane at room temperature for 3 h. The pale red crude product can be recrystallized from n-hexane at −20 °C to give pure colorless crystals.

**Figure 1** Bis(tri-tert-butylphosphine)palladium

<table>
<thead>
<tr>
<th>Table 1 The Use of Bis(tri-tert-butylphosphine)palladium(0) ([\text{Pd}(t\text{-Bu}_3\text{P})_2])</th>
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<tr>
<td>([\text{Pd}(t\text{-Bu}_3\text{P})_2])-Catalyzed Cross-Coupling of Organolithium Reagents</td>
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<td>([\text{Pd}(t\text{-Bu}_3\text{P})_2])-Catalyzed Cross-Coupling of Alkali-Metal Silanolates</td>
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<td>([\text{Pd}(t\text{-Bu}_3\text{P})_2])-Catalyzed Amination of Hydrosiloxanes</td>
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[Pd(t-Bu₃P)₂]-Catalyzed Decarboxylative Cross-Coupling Reaction

Forgione, and Bilodeau and coworkers developed a procedure for highly selective Pd-catalyzed decarboxylative cross-coupling reactions between heteroaromatic carboxylic acids and various aryl halides in the presence of a reactive C-H group. This process provides a valuable alternative for other cross-coupling reactions, in cases where appropriate cross-coupling partners are not commercially available and hard to be synthesized.

[Reference List]

References