

Carbonylation of benzyl bromide to benzeneacetic acid and its esters catalysed by water-soluble palladium complexes.

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Rok wydania

2000

Czasopismo

Journal of Molecular
Catalysis A-Chemical

Numer woluminu

154

Strony

93-101

DOI

10.1016/S1381-
1169(99)00390-8

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

A catalytic system containing $\text{PdCl}_2(\text{cod})$ ($\text{cod}=1,5$ -cyclooctadiene) and a water-soluble phosphine PNS ($\text{PNS}=\text{Ph}_2\text{PCH}_2\text{CH}_2\text{C}(\text{O})\text{NHC}(\text{CH}_3)_2\text{CH}_2\text{SO}_3\text{Li}$) in water/toluene solution exhibits activity in the carbonylation of benzyl bromide to benzeneacetic acid (87% yield) at 130°C and 10 atm of CO. In a reaction carried out in water/alcohol solution, corresponding esters were obtained in yields dependent on the kind of alcohol used: 24% for BuOH, 62% for i PrOH, 78% for EtOH, and 85% for MeOH. In the synthesis of benzeneacetic acid methyl ester $\text{C}_6\text{H}_5\text{CH}_2\text{C}(\text{O})\text{OCH}_3$ at 50 – 100°C under 5–10 atm of CO, TOF ca. 300 was achieved. The contribution of palladium(0) phosphine complexes was proved using the $^{31}\text{P}\{^1\text{H}\}$ NMR and IR methods. The complex $\text{Pd}(\text{PNS})_4$, obtained in the reaction of $\text{PdCl}_2(\text{cod})$ with PNS and NaBH_4 , reacts with $\text{C}_6\text{H}_5\text{CH}_2\text{Br}$ yielding an oxidative addition product, $\text{PdBr}(\text{C}_6\text{H}_5\text{CH}_2)(\text{PNS})_2$, identified using the $^{31}\text{P}\{^1\text{H}\}$ NMR method. In CD_3OD solution containing $\text{Pd}(\text{PNS})_4$ and $\text{C}_6\text{H}_5\text{CH}_2\text{Br}$ saturated with CO, the ester described by the formula $\text{C}_6\text{H}_5\text{CH}_2\text{C}(\text{O})\text{OCD}_3$ was identified. This suggests that the reaction of CO-insertion into $\text{Pd}-\text{C}$ bonding is relatively fast.

Słowa kluczowe

Palladium, Water soluble catalyst, Carbonylation, Benzyl bromide, Benzeneacetic acid

Adres publiczny

[https://doi.org/10.1016/S1381-1169\(99\)00390-8](https://doi.org/10.1016/S1381-1169(99)00390-8)

Strona internetowa wydawcy

<http://www.elsevier.com>