



Structural studies of PdCl_2L_2 complexes with fluorinated phosphines, phosphines, and phosphinites as precursors of benzyl bromide carbonylation catalysts, and and X-ray crystal structure of *cis*- $\text{PdCl}_2[\text{PPh}_2(\text{OEt})]_2$.

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Streszczenie

PdCl_2L_2 -type complexes with phosphines ($\text{L} = \text{PPh}_x(\text{C}_6\text{F}_5)^{3-x}$ ($x = 0-3$)), phosphites ($\text{L} = \text{P}(\text{OMe})_3$, $\text{P}(\text{OPh})_3$, $\text{P}(\text{OEt})_3$), and phosphinites ($\text{L} = \text{PPh}_2(\text{OC}_6\text{F}_5)$, $\text{PPh}_2(\text{O}-3,5\text{-F}_2\text{C}_6\text{H}_3)$, $\text{PPh}_2(\text{OEt})$, $\text{PPh}_2(\text{O}-n\text{-Bu})$, $\text{PPh}_2(\text{O}-t\text{-Bu})$) were synthesized and characterized by UV-vis and ^{31}P NMR methods. PdCl_2L_2 complexes with less sterically demanding phosphines ($\Theta < 140^\circ$) exist as *cis* isomers, which is confirmed by the X-ray structure of *cis*- $\text{PdCl}_2[\text{PPh}_2(\text{OEt})]_2$. These complexes react with CO in the presence of NEt_3 forming $\text{Pd}(\text{CO})_x\text{L}_y$ ($x+y = 4$) type carbonyls characterized by IR spectra. All PdCl_2L_2 complexes studied are active as precursors of benzyl bromide carbonylation catalysts at 40°C and 1 atm CO; however, the activity of the *cis* isomers is higher than that of the *trans* isomers. The highest yields of the carbonylation product, phenylacetic acid methyl ester, were obtained using *cis*- $\text{PdCl}_2[\text{P}(\text{OMe})_3]_2$ (92%), *cis*- $\text{PdCl}_2[\text{P}(\text{OPh})_3]_2$ (89%), and *cis*- $\text{PdCl}_2[\text{PPh}_2(\text{O}-n\text{-Bu})]_2$ (78%) as catalyst precursors.

Słowa kluczowe

palladium complexes, fluorinated phosphines, benzyl bromide carbonylation

Adres publiczny

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