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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*-$PdCl_2[PPh_2(OEt)]_2$.

Autorzy

Anna M. Trzeciak

Hubert Bartosz-Bechowski

Zbigniew Ciunik

Katarzyna Niesyty

Józef J. Ziółkowski

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Streszczenie

PdCl2L2-type complexes with phosphines (L = PPhx(C6F5)3–x(x= 0–3)), phosphites (L = P(OMe)3, P(OPh)3,P(OEt)3), and phosphinites (L = PPh2(OC6F5), PPh2(O-3,5-F2C6H3), PPh2(OEt), PPh2(O-n-Bu), PPh2(O-t-Bu)) were syn-thesized and characterized by UV–vis and31P NMR methods. PdCl2L2complexes with less sterically demandingphosphines (Θ< 140°) exist ascisisomers, which is confirmed by the X-ray structure ofcis-PdCl2[PPh2(OEt)]2. Thesecomplexes react with CO in the presence of NEt3forming Pd(CO)xLy(x+y= 4) type carbonyls characterized by IRspectra. All PdCl2L2complexes studied are active as precursors of benzyl bromide carbonylation catalysts at 40°C and1 atm CO; however, the activity of thecisisomers is higher than that of thetransisomers. The highest yields of thecarbonylation product, phenylacetic acid methyl ester, were obtained usingcis-PdCl2[P(OMe)3]2(92%),cis-PdCl2[P(OPh)3]2(89%), andcis-PdCl2[PPh2(O-n-Bu)]2(78%) as catalyst precursors.

Słowa kluczowe

palladium complexes, fluorinated phosphines, benzyl bromide carbonylation

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