



Rhodium(I) N-heterocyclic carbene complexes as highly selective catalysts for 1-hexene hydroformylation.

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Streszczenie

Rhodium(I) carbene complexes of the type $[\text{Rh}(\text{NHC})(\text{cod})\text{X}]$ (where NHC = N-heterocyclic carbene obtained from dialkylimidazolium cation; cod = 1,5-cyclooctadiene; X = Cl, Br, I, SCN) with $\text{P}(\text{OPh})_3$ as a modifying ligand have been found to be very active catalysts for 1-hexene hydroformylation under mild conditions (80 °C, 10 atm of H_2/CO , 4 h). Even at a low rhodium concentration ($[\text{1-hexene}]/[\text{Rh}] = 2000$), aldehydes have been obtained in yields of up to 90% with a high n/iso ratio of ca. 7. During the catalytic process, rhodium(I) carbene complexes, $[\text{Rh}(\text{NHC})(\text{P}(\text{OPh})_3)_2\text{X}]$, reacted with H_2/CO , giving a catalytically active rhodium(I) hydrido complex containing an N-heterocyclic carbene ligand. The presence of $[\text{HRh}(\text{CO})(\text{P}(\text{OPh})_3)_3]$ and $[\text{Rh}(\text{NHC})(\text{P}(\text{OPh})_3)(\text{CO})\text{X}]$ complexes in the catalytic system has been confirmed. When $\text{P}(\text{OCH}_2\text{CF}_3)_3$ was used as modifying ligand with $[\text{Rh}(\text{NHC})(\text{cod})\text{Br}]$ as catalyst precursor, formation of $[\text{HRh}(\text{CO})(\text{NHC})(\text{P}(\text{OCH}_2\text{CF}_3)_3)_2]$ with a square-pyramidal structure was evidenced by ^1H and ^{31}P NMR.

Adres publiczny

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Strona internetowa wydawcy

<https://www.acs.org/content/acs/en.html>