

Rhodium pyrrolylphosphine complexes as highly active and selective catalysts for propene hydroformylation: the effect of water and aldehyde on the reaction regioselectivity.

Autorzy

Ewa Mieczyska

Ryszard Grzybek

Anna M. Trzeciak

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Streszczenie

The hydroformylation of propene catalyzed by $\text{Rh}(\text{acac})(\text{CO})_2$ (acac =acetylacetonate) with a 13-fold excess of *N*-pyrrolylphosphine ligands PPyr_3 , PPh_2Pyr , or $\text{PPh}(\text{Pyr})_2$ ($\text{Pyr}=\text{NC}_4\text{H}_4$) was investigated under a pressure of 15 bar ($\text{propene}/\text{H}_2/\text{CO}=5:5:5$) at 80 °C. The *N*-pyrrolylphosphine ligands facilitated an excellent regioselectivity towards *n*-butanal aldehyde, significantly better than PPh_3 and PCy_3 under the same conditions. In the presence of the strongest π -acceptor, PPyr_3 , the linear-to-branched aldehyde (l/b) ratio was 8.6, which increased to 27.1 if water was added to the system. The application of a pure aldehyde as a solvent instead of toluene caused a significant increase in the aldehyde yield but with a decreased l/b ratio (2.9–7.6). The regioselectivity parameter l/b increased to 19.3 after the introduction of water as a cosolvent.

Słowa kluczowe

aldehydes, alkenes, hydroformylation, phosphane ligands, rhodium

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