

烯基取代环戊二烯基钌配合物的合成及晶体结构

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摘要 本文通过环戊二烯基钠(茂钠)与溴丙烯反应制得单取代的环戊二烯,茂钠与氯丙烯得到双取代的环戊二烯。利用这两个配体合成了烯基取代的环戊二烯基(双三苯膦)氯化钌(1,2)并对化合物(2)进行了晶体结构分析。

关键词 [环戊二烯P](#) [钌化合物](#) [络合物](#) [晶体结构](#) [金属氢化物](#) [三苯基膦](#) [手征性](#) [元素有机化学](#)

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The synthesis and crystal structure of alkenyl-substituted cyclopentadienyl ruthenium complexes

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Abstract Two alkenyl-substituted cyclopentadienyl ruthenium complexes (1, 2) were synthesized. The diallylcyclopentadiene was obtained by a one-pot reaction of sodium cyclopentadienide and allyl chloride. The complex (2) with this ligand is chiral and characterized by X-ray analysis. It belongs to the triclinic space group P1(#2) with $a=1.1257(6)\text{nm}$, $b=1.8525(7)\text{nm}$, $c=1.0134(4)\text{nm}$, $\alpha=90.89(3)^\circ$, $\beta=102.77(4)^\circ$, $\gamma=106.93(3)^\circ$. $V=1.964(1)\text{nm}^3$, $Z=2$, $D_c \sim a \sim b \sim c=1.363\text{g}\cdot\text{cm}^{-3}$, $F(000)=832.00$. The X-ray structure of complex (2) reveals that geometry around the ruthenium can be considered as distorted tetrahedral. The distance of Ru-C, Ru-P and Ru-Cl is greatly different from that in $\text{CpRu}(\text{PPh}_3)_2\text{Cl}$. It can be concluded that the introduction of diallyl group into the cyclopentadienyl ligand results in the redistribution of electron around the ruthenium. The donation from diallyl group to cyclopentadienyl ligand weakens the back-donation from ruthenium to cyclopentadienyl ligand. Hence, the electron is transferred to PPh_3 , Cl ligands.

Key words [CYCLOPENTADIENE P](#) [RUTHENIUM COMPOUNDS](#) [COMPLEX COMPOUNDS](#) [CRYSTAL STRUCTURE](#) [METAL HYDRIDE](#) [TRIPHENYLPHOSPHINE](#) [CHIRALITY](#) [ELEMENTARY ORGANIC CHEMISTRY](#)

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