

多硅基取代 π -苯基羰基钼化合物的合成和结构

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摘要 芳基二硅烷 $\text{RC}_6\text{H}_4\text{SiMe}_2\text{SiMe}_3$ 与 $\text{Mo}(\text{CO})_3\text{Py}_3$ 在 BF_3 存在下反应,生成 π -苯基羰基钼化合物($\eta^6\text{-RC}_6\text{H}_4\text{SiMe}_2\text{SiMe}_3$) $\text{Mo}(\text{CO})_3$ (R = p-Me和p-OMe)。在同样条件下,二芳基二硅烷 $\text{RC}_6\text{H}_4\text{SiMe}_2\text{SiMe}_2\text{C}_6\text{H}_4\text{R}$ 与两倍摩尔的 $\text{Mo}(\text{CO})_3\text{Py}_3$ 反应,得到双钼化合物($\eta^6,\eta^6\text{-RC}_6\text{H}_4\text{SiMe}_2\text{SiMe}_2\text{C}_6\text{H}_4\text{R}$) $[\text{Mo}(\text{CO})_3]_2$ 和单钼化合物($\eta^6\text{-RC}_6\text{H}_4\text{SiMe}_2\text{SiMe}_2\text{C}_6\text{H}_4\text{R}$) $\text{Mo}(\text{CO})_3$ (R = H, o-Me, m-Me, p-Me和p-OMe)。不对称二芳基二硅烷 $\text{R}^1\text{C}_6\text{H}_4\text{SiMe}_2\text{SiMe}_2\text{C}_6\text{H}_4\text{R}^2$ 进行上述反应,得到类似的化合物($\eta^6,\eta^6\text{-R}^1\text{C}_6\text{H}_4\text{SiMe}_2\text{SiMe}_2\text{C}_6\text{H}_4\text{R}^2$) $[\text{Mo}(\text{CO})_3]_2$ 和($\eta^6\text{-R}^1\text{C}_6\text{H}_4\text{SiMe}_2\text{SiMe}_2\text{C}_6\text{H}_4\text{R}^2$) $\text{Mo}(\text{CO})_3$ (R¹,R² = H, p-Me和p-OMe; R¹ \neq R²)。该单核化合物是由钼原子配位于不同苯基的异构体组成的混合物。利用 IR,¹H NMR和元素分析鉴定了所有产物,并利用单晶X射线衍射法对化合物 ($\eta^6,\eta^6\text{-RC}_6\text{H}_4\text{SiMe}_2\text{SiMe}_2\text{C}_6\text{H}_4\text{R}$) $[\text{Mo}(\text{CO})_3]_2$ (R = p-Me)的分子结构进行了测定。

关键词 羰基化合物 钼化合物 X射线衍射分析 苯 P 硅烷 P 红外分光光度法 质子磁共振谱法

分类号 [O621](#)

Synthesis and Molecular Structure of Polysilanyl-substituted η^6 - Phenylcarbonylmolybdenum

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Abstract Aryldisilane $\text{RC}_6\text{H}_4\text{SiMe}_2\text{SiMe}_3$ reacted with $\text{Mo}(\text{CO})_3\text{Py}_3$ in the presence of BF_3 , giving ($\eta^6\text{-benzene}$) tricarbonylmolybdenum complex $\eta^6\text{-RC}_6\text{H}_4\text{SiMe}_2\text{SiMe}_3$) $\text{Mo}(\text{CO})_3$ (R = p-Me and p-OMe). Under the same condition, diaryldisilane $\text{RC}_6\text{H}_4\text{SiMe}_2\text{SiMe}_2\text{C}_6\text{H}_4\text{R}$ reacted with two equivalents of $\text{Mo}(\text{CO})_3\text{Py}_3$ to afford di-molybdenum complex ($\eta^6,\eta^6\text{-RC}_6\text{H}_4\text{SiMe}_2\text{SiMe}_2\text{C}_6\text{H}_4\text{R}$) $[\text{Mo}(\text{CO})_3]_2$ as well as mono-molybdenum complex ($\eta^6\text{-RC}_6\text{H}_4\text{SiMe}_2\text{SiMe}_2\text{C}_6\text{H}_4\text{R}$) $\text{Mo}(\text{CO})_3$ (R = H, o-Me, m-Me, p-Me and p-OMe). Unsymmetric diaryldisilane $\text{R}^1\text{C}_6\text{H}_4\text{SiMe}_2\text{SiMe}_2\text{C}_6\text{H}_4\text{R}^2$ underwent the above reaction to produce similarly the complexes ($\eta^6,\eta^6\text{-R}^1\text{C}_6\text{H}_4\text{SiMe}_2\text{SiMe}_2\text{C}_6\text{H}_4\text{R}^2$) $[\text{Mo}(\text{CO})_3]_2$ and ($\eta^6\text{-R}^1\text{C}_6\text{H}_4\text{SiMe}_2\text{SiMe}_2\text{C}_6\text{H}_4\text{R}^2$) $\text{Mo}(\text{CO})_3$ (R¹,R² = H, p-Me和p-OMe; R¹ \neq R²). This mononuclear complex was a mixture of isomers with molybdenum coordinated to different phenyl groups. All complexes obtained were characterized by elemental analyses, IR and ¹H NMR spectra. The molecular structure of ($\eta^6,\eta^6\text{-RC}_6\text{H}_4\text{SiMe}_2\text{SiMe}_2\text{C}_6\text{H}_4\text{R}$) $[\text{Mo}(\text{CO})_3]_2$ (R = p-Me) has been determined by means of X-ray diffraction analysis.

Key words [CARBONYL COMPOUNDS](#) [MOLYBDENUM COMPOUNDS](#) [XRD](#) [SILANE P](#) [IR](#) [¹H NMR](#)

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