Der erste verbrückte, bifunktionelle Cyclopentadienyl-Imidazolyliden-Ligand und Komplexe mit Titan und Zirconium

The First Bridged, Bifunctional Cyclopentadienyl-Imidazolylidene Ligand and Complexes with Titanium and Zirconium

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Starting from imidazole, 1-[2-(cyclopenta-2,4-dienyl)ethyl]-3-methylimidazolium iodide (**3**) was obtained as a mixture of isomers by a simple three-step synthesis. The reaction of **3** with $Ti(NEt_2)_4$ or $Zr(NEt_2)_4$ by double deprotonation of the imidazolium salt led to the isomerically pure cationic complexes $[\{\eta^5\text{-}C_5H_4\text{-}(CH_2)_2\text{-}NHC\}M(NEt_2)_2]^+I^-$ (NHC = N-heterocyclic carbene) **4a** (M = Ti) and **4b** (M = Zr), respectively, in which a cyclopentadienyl and a methylimidazol-2-ylidene unit are linked by an ethylidene-1,2 bridge to form a novel chelating ligand system. In the case of the reaction of **3** with $Zr(NEt_2)_4$ the neutral compound $[\{\eta^5\text{-}C_5H_4\text{-}(CH_2)_2\text{-}NHC\}Zr(NEt_2)I_2]$ (**5**) is formed as an additional product. According to the X-ray structure analyses, the titanium atom of **4a** is tetra-coordinated while no coordinative interaction exists with the iodide anion; on the other hand, in **5** the zirconium centre is pentacoordinated.

Key words: Titanium, Zirconium, Bridged Cyclopentadienyl N-Heterocyclic Carbene Ligands, Crystal Structures, Agostic Interaction