Synthesis, Structure and Reactivity of the Molybdenum Cycloheptatrienyl Tetrahydroborate Complex \{(\eta^7\text{-C}_7\text{H}_7)\text{Mo}(\eta^2\text{-BH}_4)[\text{P(cyclo-C}_6\text{H}_{11})_3]\}\n
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Dedicated to Professor Wolfgang Jeitschko on the occasion of his 70\textsuperscript{th} birthday

The reaction of the cycloheptatrienyl-toluene sandwich complex \{(\eta^7\text{-C}_7\text{H}_7)\text{Mo(\eta^6\text{-C}_6\text{H}_5\text{Me})}\text{BF}_4\} with tricyclohexylphosphine in acetonitrile furnishes the cationic half-sandwich cycloheptatrienyl complex \{(\eta^7\text{-C}_7\text{H}_7)\text{Mo[\text{P(C}_6\text{H}_{11})_3](CH}_3\text{CN})_2\}\text{BF}_4 (1). Treatment of 1 with NaBH\textsubscript{4} in ethanol results in the formation of the tetrahydroborate complex \{(\eta^7\text{-C}_7\text{H}_7)\text{Mo(\eta^2\text{-BH}_4)[\text{P(cyclo-C}_6\text{H}_{11})_3]}\} (2), in which the borohydride ligand is coordinated to the molybdenum atom through two three-center, two-electron bonds. The complex is stable in ethanol and water. The expected formation of a metal trihydride of the type \{(\eta^7\text{-C}_7\text{H}_7)\text{MoH}_3[\text{P(cyclo-C}_6\text{H}_{11})_3]\} as a hydrolysis product could not be observed. Since this behaviour differs from the reactivity reported for related cyclopentadienyl-ruthenium complexes, a comparative computational study on the model complexes \{(\eta^5\text{-C}_5\text{Me}_5)\text{RuH}_3(\text{PMe}_3)\} (4) and \{(\eta^7\text{-C}_7\text{H}_7)\text{MoH}_3(\text{PMe}_3)\} (5) was performed revealing that the classical trihydride form [MH\textsubscript{3}] represents the global minimum for the ruthenium complex 4, whereas the dihydrogen-hydride form [MH(\eta^2\text{-H}_2)] is more stable for the molybdenum counterpart.

Key words: Cycloheptatrienyl Ligands, Hydride Ligands, Dihydrogen Complexes, Density Functional Calculations