

# Synthesis, Structure and Reactivity of the Molybdenum Cycloheptatrienyl Tetrahydroborate Complex $\{(\eta^7\text{-C}_7\text{H}_7)\text{Mo}(\eta^2\text{-BH}_4)[\text{P}(\text{cyclo-C}_6\text{H}_{11})_3]\}$

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*Dedicated to Professor Wolfgang Jeitschko on the occasion of his 70<sup>th</sup> 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  $\{(\eta^7\text{-C}_7\text{H}_7)\text{Mo}[\text{P}(\text{C}_6\text{H}_{11})_3](\text{CH}_3\text{CN})_2\}\text{BF}_4$  (**1**). Treatment of **1** with  $\text{NaBH}_4$  in ethanol results in the formation of the tetrahydroborate complex  $\{(\eta^7\text{-C}_7\text{H}_7)\text{Mo}(\eta^2\text{-BH}_4)[\text{P}(\text{cyclo-C}_6\text{H}_{11})_3]\}$  (**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  $\{(\eta^7\text{-C}_7\text{H}_7)\text{MoH}_3[\text{P}(\text{cyclo-C}_6\text{H}_{11})_3]\}$  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  $[\text{MH}_3]$  represents the global minimum for the ruthenium complex **4**, whereas the dihydrogen-hydride form  $[\text{MH}(\eta^2\text{-H}_2)]$  is more stable for the molybdenum counterpart.

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