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The role of aluminiun chloride in the Fischer-Hafner synthesis of technetium and rhenium bisarenes

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Rhenium bis-arenes can be obtained by heating the corresponding potassium perrhenate ($KReO_4$) salt with an arene as a solvent and in the presence of aluminum chloride ($AlCl_3$) and zinc. Variations of this method, originally proposed by Fischer and Hafner, demonstrated that, in some cases, the reaction occurs without using Zn as a reductive agent, but also, that the presence of the Lewis acid is essential. The aim of this work is to study the interactions of $AlCl_3$ with benzene, as well as the reactivity of the system formed afterwards, in order to understand its role in the reaction pathway. Calculations at DFT/M06-2X and MP2 levels using 6-311G(2df,2pd) depicted that the association between $AlCl_3$ and benzene leads to the formation of a charge transfer adduct where the $AlCl_3$ is placed over one of the carbons of benzene. The charge is transfered from the aromatic π system to the Al atom. The analysis of this complex through local reactivity descriptors allowed locating the areas of the benzene's π system more susceptible to react with the Rhenium via electrophilic attack. Meta and orto positions are particularly reactive to that class of attack. Therefore, the initial association with rhenium should occur in these sites. Thus, results show that the formation of the $AlCl_3$-benzene adduct could be an important intermediate in the formation of $[Re(\eta^6\text{-benzene})_2]^+$ complex.

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