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Synthesis, Characterization and Theoretical Investigation of the Complex [(C5H7O2)3SiFe(CH3)3Cl]

The recognition of the importance of transition metal compounds containing metal carbon σ bonds has been the subject of past three decades, due to their extensive application as homogenous catalysis in industrial processes. However, transition metal-carbon sigma bonds are less common due to the kinetically facile reactions they undergo such as α, β and γ eliminations, oxidative reduction, homolysis etc. The reactivity of the Grignard reagent CH3MgBr towards metal salts [(C5H7O2)3SiFeCl4], [Cr(C5H5N)3Cl3] and [Mn(C5H7O2)3] was investigated in order to synthesize complexes with metal carbon sigma bonds.

The reaction of $[(C_5H_7O_2)_3SiFeCl_4]$ and CH_3MgBr in ether at 0 °C for 24 h, under N_2, yields the complex $[(C_5H_7O_2)_3SiFe(CH_3)_3Cl]$ **1**. The reaction of CH_3MgBr with $[Cr(C_5H_5N)_3Cl_3]$ and $[Mn(C_5H_7O_2)_3]$ under conditions similar to those used with $[(C_5H_7O_2)_3SiFeCl_4]$ yields an intractable yellow and brown mixture respectively. The complex **1** (Fig 1) has been characterized by IR, UV, PDMS and NMR spectroscopy.

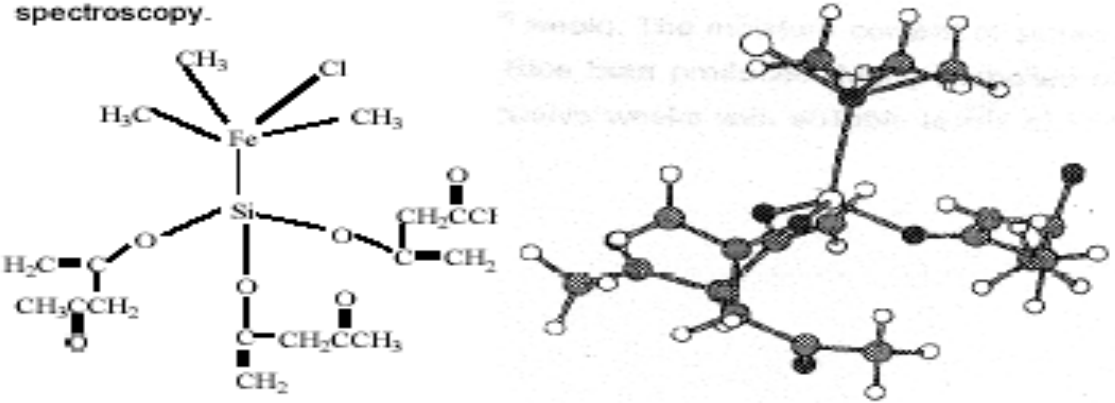

Fig 1: The structure of the complex 1 (a) With atom labeling (b) Ball & stick model

Hyperchem Pro 6.0 computational chemistry package was used for the modelling of the complex. The MM+ model shows the perfect terahedral geometry at the silicon centre where all bond angles are approximately 1090. Slightly distorted square pyramid is obtained at the Fe center. The energy calculation also shows that the molecule is very stable as it has a moderate heat of formation (11 kcal/ mol).