Transition Metal Complexes Of [Methyl 2-((4-Chlorophenyl) (Hydroxy)Methyle) Acrylate]: - An Important Biologically Active Mbh Adduct

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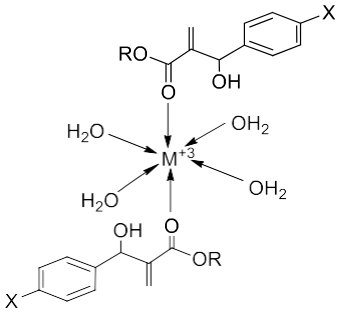
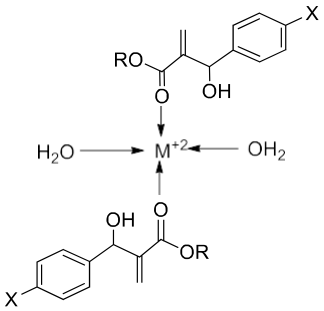
ABSTRACT

The establishment of synthetic chemistry have excessive sophistication to modernize associated drug discovery and designing. Most of the drug designing firms have recently encouraged the synthesis potentiality due to inspiring the field as vital for medication discovery innovations. In the present research, by utilizing single-pot reaction, Morita-Baylis-Hillman (MBH) adduct was synthesized and purified via column and thin layer chromatography. Adduct was further reacted as ligand with five different transition metal salts (Co(III), Ni(II), Cu(II), Cr(III), Mn(II)) under reaction conditions and amorphous metal complexes were purified. The molecular and structural formulae of the metal complexes were predicted through spectral and elemental analysis. The IR spectra were also generated computationally by the Hartree Fock (HF) B3LYP technique in combination with the 3-21G (d,p) theoretic study based set, which were found in good agreement with the experimental data and hence verified the predicted structural formulae. Moreover, to recognize crystal class of these complexes, powder XRD was accomplished. In addition, the antibacterial, antioxidant as well as antifungal potential of MBH- Adduct and its metal complexes were determined and it was observed that ligand with its metal complexes are active antioxidants. The antibacterial activity was studied against bacterial strains of Staphylococcus aureus, Escherichia coli, Bacillus pumilis and Salmonella typhi. It was found that in contrast to ligand and other complexes, the Co(III) complex possesses a superior potential against these bacterial strains. Our research demonstrates, application of MBH-Adduct in metal complex synthesis as a first example. In addition, the novel compounds of transition metals have great strength in against numerous infective disorders and may prove as inexpensive and effectual drugs as well.



M= Cr, Co

Fig 1. Proposed Complexes of $CrL_2(H_2O)_4$ & $CoL_2(H_2O)_4$



M= Ni, Cu, Mn

Fig 2. Proposed Complexes of $NiL_2(H_2O)_2$, $CuL_2(H_2O)_2$ & $MnL_2(H_2O)_2$

INTRODUCTION

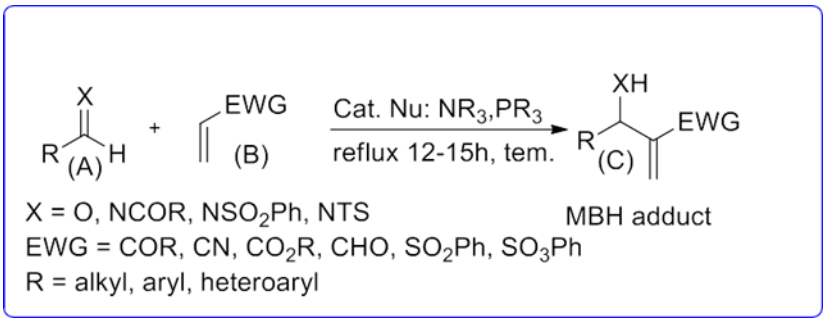
Transition metals perform imperative characters in living processes and the area of information in close relation to the inorganic chemistry applications. Furthermore, binding significance of metal ions for the cure of the diseases in the biological system is one of the major characteristic in the field of bio-inorganic chemistry [1]. The transition elements are very important metals due to the strong inter-atomic bonding, formation of colored compounds, high mechanical properties, and variety of biological activities. Complexes of organic based ligands with transition metals have a great importance in centers of enzymatic activity, and act as biological redox facilitators [2]. A synthetic novel compound containing spatiality of utilization in drugs represent atom-economy, cheap and commercially available starting reagents, execution simplicity and chemo specified elements in product, next synthetic modifications is a major concern of research theme. Therefore, the C-C bond formation is a major consequence in the ease of diverse mode of reaction, to prepare the required product. One of the C-C bond formation reaction is MBH reaction for building up of miscellaneous entities in the heterocyclic as well as natural product chemistry [3]. Most of organic compounds possessing carboxylic group (aldehydes, ketones and alcohols), halogen and thio-aromatic are very important class of ligands due to the variety of bonding sites. Typically the MBH molecules can be synthesized rapidly in high yields, via a single step route and by means of ecofriendly synthetic conventions. MBH adducts and their derivatives are inexpensive, effective, possessing high potentiality bioactive compounds. Furthermore, when a ligand have ester functionality, C=C bond and donor functional group, then its chelating ability must be increased because such ligand compound now have more binding possibilities towards the central metal ion [4].

OBJECTIVES

- To synthesize the Methyl 2-((4-chlorophenyl)(hydroxy)methyle) acrylate (a MBH adduct)
- To characterized the MBH adduct by UV-visible, FTIR, Mass spectrometry
- To synthesize novel MBH adduct based transition metal complexes
- To characterized the novel metal complexes by UV-visible, FTIR, XRD powder diffraction and comparative computational DFT
- To construct the molecular models of the novel metal complexes
- To investigate biological activity (antibacterial, antifungal, antioxidant) of the synthesized complexes

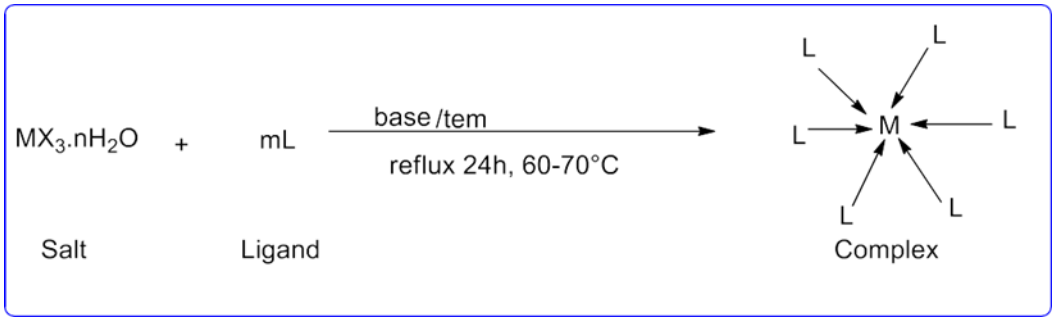
METHODOLOGY

MBH adduct was synthesized by the procedure adopted by Basavaiah, D. in 2007 [5]. The general method, employed in this work is outlined in Scheme **1**.



Scheme 1. Preparation of MBH adduct

After required characterization, the pure adduct was subjected to reaction with various transition metal salts, using well established method [6] with few modifications, for the preparation of desired complexes.



Scheme 2. Preparation of MBH adduct based transition metal complexes.

Finally, the products were subjected to investigation of biological activities.

RESULTS

It is concluded from the aforementioned research study that Methyl 2-((4- chlorophenyl) (hydroxy)methyle) acrylate-based Metal Complexes with octahedral and tetrahedral geometries can successfully be synthesized. Moreover, the resultant biological activities (antibacterial, antifungal and antioxidant) of few complexes are higher than their corresponding ligand, and hence prove their efficacy to be used as drug for certain ailments.

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