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A Study on Synthesis and Characterization of Organic Compound

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Abstract – A ligand-H2L complex, with a general formula [M (HL2)2] (M(II)=co, Ni, Cu) was synthesized and characterized for its elementary microelement, metal material, magnetic momentum and molar path measured (M(M)-IR), Fourier-infra-round infrarspectroscopic measurements (MI-IR), ultraviolet-visible spectroscopy (Uv-Vis), molar pathway, and Chl. Tetrahedral geometry for preparing change bases complexes was suggested on the basis of experimental proof. The ligand geometry and its complexes have been verified by their optimized computer studies architectures. A radical of 1.1-diphenyl-2-picrylhydrazyl (DPPH) antioxidant activity was tested and contrasted to the usual natural ascorbic acid, antioxidant. So compounds displayed outstanding radical behavior of scavenging.

Keywords: Synthesized, Characterized, Compounds

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INTRODUCTION

Following the arrival of the hypervalent-iodine electromethylation reagents 1 and 2 in 2006, organic synthesis have been commonly used[1-4]. The photocatalytic one-electron reduction of such compounds was recently based on increasing attention to produce strongly electrophilic trifluoromethyl radical[5-7]. For example, Governor et al. have highlighted the use of reagent 2, [Ru(bpy)3] Cl2, and allylsilanes as substrates[7] for regioselective allylic trifluoromethylation. In this sense also, numerous Electrophilic Trifluoromethylating Agents now have detailed electrochemical characterization [8]. In these tests, cathodic peak potential was recorded relative to the Ag/Ag+ pair of −1,82V and −1,10V for 1 and 2. Therefore, we envisaged increasing the reactivity of reagent 2 by growing the volume of electron in its scaffold. This was accomplished by adding a highly electron removal substitute in paraposition to the iodine atom, which may also lead to a more positive reduction potential. Therefore, the reagent scaffold nitration to include the latest 5-nitro-1-(trifluoromethyl)-3H-1α 3-2-benziodaoxol3-one(3) derivatives is taken into account on a recent paper [9].

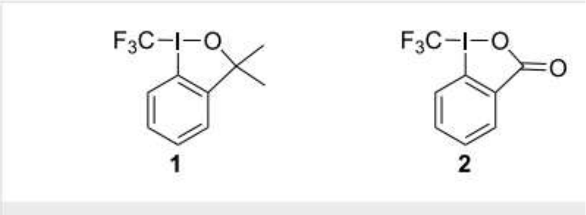


Figure: Electrophilic trifluoromethylating agents 1 and 2.

TECHNIQUES USED FOR CHARACTERIZATION OF COMPOUNDS

Elemental analysis

A comparatively limited number of elements form the bulk of organic compounds. Carbon, hydrogen, oxygen, nitrogen, sulphur, chlorine, etc. are the most essential. Eliminating the content of the carbon, hydrogen, nitroge and other elements in the organic compound molecule shall be used as a basic quantitative organic analysis. Ligands L-1 to L-7 has general properties:

The capillary process calculated the melting points (o C) of all substances. Uncorrected all the Melting Points. There is a crystallised yield of all compounds described. The extracted and dryed solvents were both included. Analyzed by its elemental contents was the whole of Ligand L-1 to L-7 synthesised and defined in the next part. Elemental analyzer Thermofinigan flash 1101 EA was used to measure the elements C, H and N of all samples. Carius method can be used to determine the halogen content in such cases[1]. A dry Carius tube was inserted in the 100 mg sample (80 cm in total, 1 cm diameter). The procedure was followed as follows. Approximately 25 mg nitrate was then added. Furthermore five or seven drops of nitric acid were applied and the tube was sized and stored into the oven for 6 hours with the temperature kept at 300 0 C. The tube was opened and the obtained silver halide precipitates transferred into the pre-wound G-4 funnel and weighed the precipitates.

Infrared spectroscopy

Instead of being rigidly attached like the bonds of an assembly model, the atoms of a molecule work as if they were linked by a fluid spizing. Their components may vary from rocking, scissors, turns, wags to symmetrical and asymmetric extensions in various vibrational modes. When a sample of a given compound transmits red radiation, its molecules will absorb the energy (and frequency) required to switch between vibrational ground states and vibration-excited states. For eg, a 90-billion-fold C-H bond requires to consume only this frequency's infraroad radiation to leap into its first vibration excited condition. The sum of the infrarot radiation emitted by the sample as a function of the frequency (or wavelength) of a radiation may be determined by the infraround energy absorption of different wavelengths. A comparatively wide absorption band consisting of an infrarot spectrum, rather than sharp spikes such as NMR. A band are often usually “INVERTED,” and is not a high plateau, but a wide valley. The consistency measurement is especially useful for infrared spectroscopy [2-6]. It may also be used to diagnose the presence from belt locations and intensities of particular functional groups and of other structural characteristics and to distinguish an uncertain compound with a established norm. It is better to display two similar substances, since in this field the properties of the fingerprint area of the infrared continuum are typically defined by the entire molecule, and not separated, as two substances are the same.

Proton nuclear magnetic resonance spectroscopy

Spectroscopy of nuclear magnetic resonance (NMR) is additional to IR spectroscopy for information on organic compounds structure. The proton is the most commonly observed centre which is then referred to as PMR spectroscopy. The functional community is told by IR spectra while the NMR Spectra offer details regarding the precise structure and atmosphere of the proton. This method is therefore more effective for clarifying an organic compound. The IR spectrum may seem similar but its NMR spectrum may vary greatly.

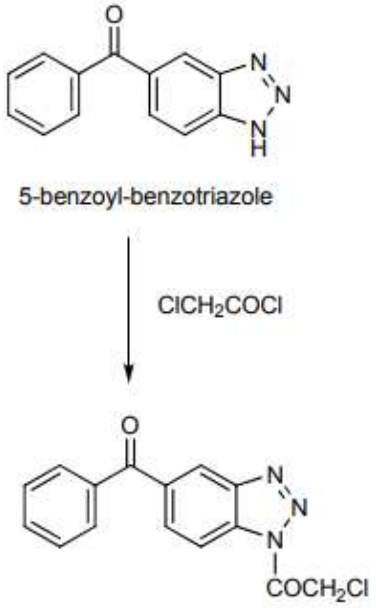
The nuclear magnet resonance phenomenon was first recorded independently by two phenomenon groups in 1946: at Stanford University Block, Hansen and Packard found a signal in water protons, and at Harvard University, Purcell, Torrey and Pund observed a signal in paraffin wax from the protons. The finding was co-hosted by Block and Purcell with the 1952 Nobel Prize in physics. The Nobel Prize for chemistry was won in 1991 with the developments of NMR technologies, which contributed to the broad implementation of different research industries. The uses of NMR are really wonderful in clinical, sound and biophysical sciences. The most important method used for characterization of organic compounds is the proton magnetic resonance (PMR) spectroscopy. It includes details on the numerous forms of molecule protons. In other terms, it talks of the numerous forms of conditions in the molecule of the hydrogen atoms. In addition to this, PMR offers details on the amount and ratio of various proton forms in a molecule. Every nucleus has a positive charge, it's well known. This load spins on the nuclear axis in some nuclei, and this atomic charge circulation produces a magnetic dipole along the axis. The nucleus thus represents a small bar magnet. In terms of spin number (I), the angular momentum of the rotating charge is defined. In terms of nuclear magnetism, magnitude of the induced dipole is expressed (μ). The most basic and frequently present in organic compounds is the rotating nucleus of a hydraulic atom (1H or proton). There is a magnetic moment of the hydrogen nucleus μ = 2.79268 and a number of spins (I) + 1⁄2. Thus, the magnet moment can have two potential orientations in an applied external magnetic field.

The position of the magnetic moment to the applied magnetic field is more stable (low energy) than the magnet moment to the field (high energy). The energy required to reverse a proton from the lower energy alignment to a higher energy alignment depends on the disparity in energy (aE) in both states. The substance can be positioned, in principle, in a magnetic field of constant strength and the spectrum can be obtained by passing the radiation of a changing frequency through the substance and the frequency at which radiations are absorbed in the same way as infrarot or ultra-violet spectrums. However, the usage of a steady radiation frequency and the power of the magnetic field were considered to be more convenient in operation. The energy needed to rotate the proton meets the energy of radiation, it absorbs and it receives a signal at any value of the field power. A nuclear magnetic resonance spectrum(NMR) is the so-called.

SYNTHESIS AND CHARACTERIZATION OF LIGANDS

Synthesis of N-(1-chloro acetyl)-5-benzoyl benzotriazole

The literature documenting process of the synthesis of N-(1-chloroacetyl)-5-benzoyl benzotriazole made from 5-benzoyl-1H-benzotriazole reactions with chloroacetyl chloride[2]. Below is the likely reaction scheme,



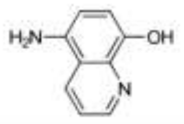
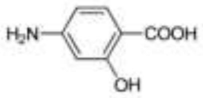
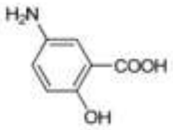
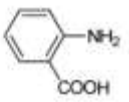
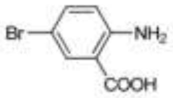
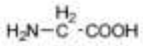
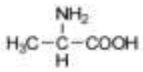
Scheme

General procedure for synthesis of N-(1-chloro acetyl)-5-benzoyl-1H-benzotriazole

The minimal volume of THF dissolved was 5-benzoyl-1H-benzotriazole (0.01 mole) and chloroacetyl chloride (0.01 mole) was then applied. And apply sodium bicarbonate (0.01 mole), all blended together well. For around 4 hours the mixture was flushed and refreshed by a water wash. The resultant liquid has been washed and dried. The result was ethanol recrystallized.

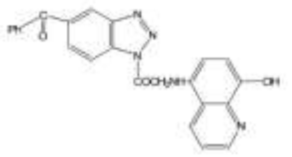
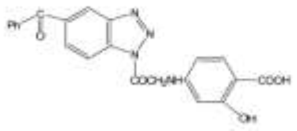
Synthesis of various ligands i.e. L-1 to L-7

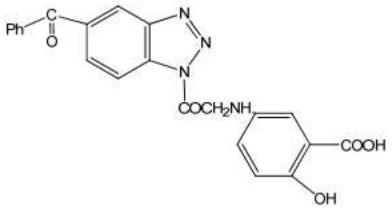
Upon synthesis of the target molecule i.e., L-1 via L-7, N-(1-chloro-acetyl)-5%-benzotriazol was previously prepared. The following table contained a variety of dynamic forming reagents used.

No.	Raw material	Structure
1.	5-amino-8-quinolinol	
2.	4-amino salicylic acid	
3.	5-amino-salicylic acid or Mesalazine	
4.	Anthranilic acid	
5.	5-bromo-anthranilic acid	
6.	2-amino-acetic acid (Glycine)	 $H_2N-\overset{H_2}{C}-COOH$
7.	2-amino propanoic acid (Alanine)	 $H_3C-\underset{H}{\overset{NH_2}{C}}-COOH$

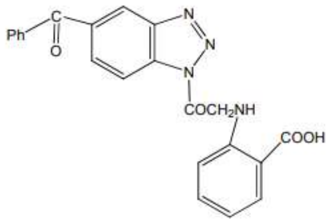
Synthesis of metal chelate of ligands L-1 to L-7

The transition metal chelates based on the benzotriazole-containing ligands mentioned are synthesised as heterocyclic movement. Also presented in this chapter are the preliminary characteristics of these transition metal chelates. Different metal ions of transition were used: Cu+2, Ni+2, Mn+2, Co+2 and Zn+2. These ligands are organised and designated accordingly:

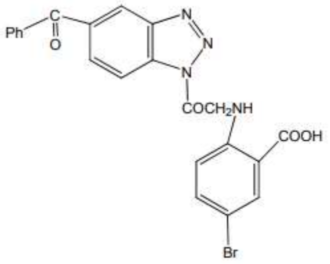
Structure	Designation
	L-1
	L-2



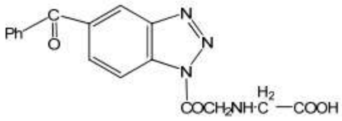
L-3



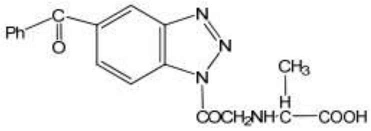
L-4



L-5



L-6



L-7

Characterization of metal chelate of ligands

The characterization of Ligands L-1 to L-7 metal chelates mentioned in a previous chapter. Both metal chelates have been distinguished by IR spectral tests and magnetic moments.

Infrared Spectroscopy

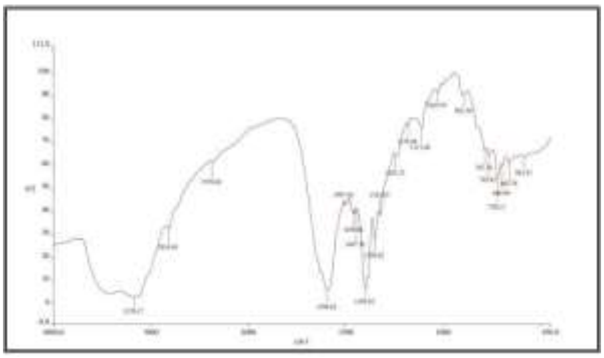


Figure: IR Spectrum of Ligand (L-1)2-Cu+2

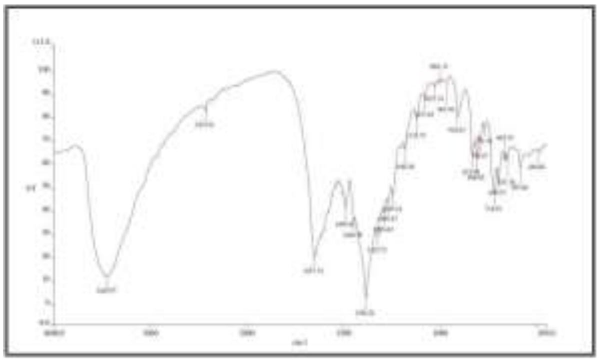


Figure: IR Spectrum of Ligand (L-2)2-Co+2

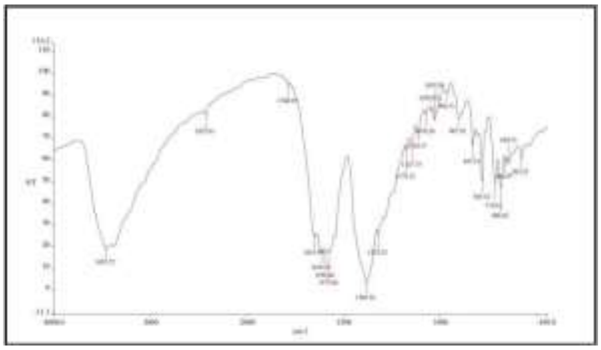


Figure: IR Spectrum of Ligand (L-3)2-Zn+2

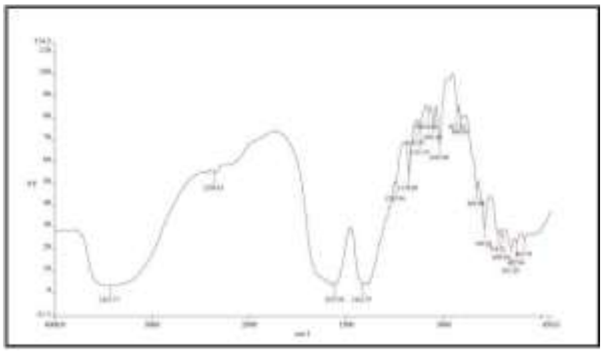


Figure: IR Spectrum of Ligand (L-4)2-Co+2

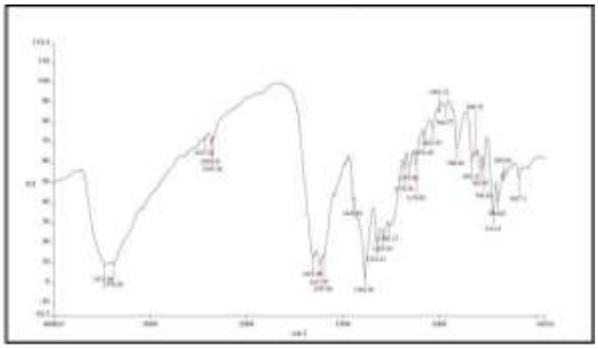


Figure: IR Spectrum of Ligand (L-5)2-Co+2

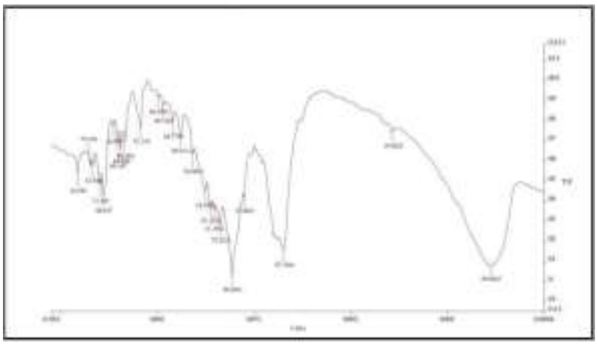


Figure: IR Spectrum of Ligand (L-6)2-Ni+2

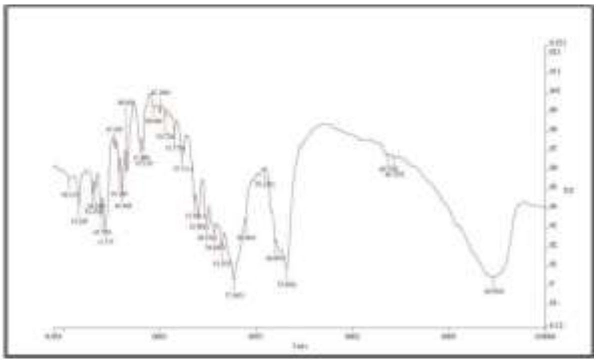


Figure: IR Spectrum of Ligand (L-7)2-Mn+2

Guidelines for Characterization of Organic Compounds

A. Sample Quality

The purified sample should be included in new substances as evidence of homogeneity. Appropriate elemental research. If no study has been carried out, supplementary data should be provided in the Supporting Material , for example, 1H NMR, 13C NMR, hplc, glpc, gel electrophoresis, etc.

B. Molecular Weight

Molecular weight proof should be given, in particular if there hasn't been elementary research. Low-resolution MS information is appropriate under conditions mitigating fragmentation. If alternative formulations with the same molecular mass (within one amu) need to be separated, HRMS data are required.

C. Miscellaneous

Numerical lists should be included of standard spectroscopic details to endorse allocated systems, functional improvements, uncommon chromophores, characteristics etc. Cleaning procedures used to prepare characterization samples should be identified. Details on the process of crystallisation (solvents; mp; etc.) should be used for crystalline samples. Data should be provided for non-racemic, chiral substances, including preferably [α]D values for allowing correlation of absolute configuration. Where correlation statistics based on Hplc or GLPC methods are provided, retention times for all enantiomers, solvent and flow rates statistics must be provided and chiral help recognition established.[10]

D. Intermediates on Solid Phase; Combinatorial Chemistry

A statistically meaningful sampling can allow for replication of the methodology and characterisation of new compounds. Intermediates resin bound should not be described if appropriate end product quality is demonstrated (as specified in A-C above).

CONCLUSION

Synthesis, separation, the analysis of the properties and reactivity of molecules are also important measures in the development of modern chemistry. This research section focuses mainly on the synthesis and characterization of biologically important organic molecular systems , particularly studies which seek the development, synthesis and structural characterization of functional organic molecular systems and systems such as proteins and other macromolecular systems.

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