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Dithioligand-based heterobimetallic complexes: synthesis and electrical behaviour

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ABSTRACT

New semiconducting materials with suitable band gap ranges are required by the semiconducting electronic material sector. There are numerous dithio compounds that have good semiconducting qualities. With a nanosecond layer pulse at 532 nm wavelength, they exhibit good optical limiting properties. Chemists are involved in a conjugated framework of hetero atoms for the synthesis of metal-based semiconducting molecular content. 1–9 Several studies have been published on complex related monometallic complexes with a band in the good semiconductor range. years 9 to 14. The objective of this study is to synthesise, characterise, and investigate the heterobimetallic complexes. UV-Visible and powder XRD spectra, and solid-state electrical conductivity. In these compounds, electrical conductivity can be observed.

Keywords: Heterobimetallic, Chalcone, Semiconductor, dithio complexes, Electrical conductivity

INTRODUCTION

It has been documented that chalcones have non-linear optical properties such as excellent blue light transmittance and crystallisation potential. With a nanosecond layer pulse at 532 nm wavelength, they exhibit good optical limiting properties. Chemists are involved in a conjugated framework of hetero atoms for the synthesis of metal-based semiconducting molecular content. 1–9 Several studies have been published on complex related monometallic complexes with a band in the good semiconductor range. years 9 to 14 The synthesis, characterization, and solid-state electrical conductivity of some new chalcones-based mono, bimetallic complexes of the type[M(CS3)2] are described in this paper. [M′(L)2(H2O)2] [M′(L)2(H2O)2] [M′(L)2(Hwhere [M= Cu(II), Zn(II) and M′= Fe(II), Ni(II), Co(II), CS32- = tri-thiocarbonate, L = chalcone based ligand. There structure aspects and electrical behavior were analyzed.

Experimentation

2.1 Chalcone-based ligand preparation:

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Benzaldehyde and 2-acetyl-1-naphthol were dissolved in 25 ml of ethanol, agitated at room temperature for an hour, and then 1.5 ml of a 40% KOH solution was added. The reaction mixture was then left at room temperature for the remainder of the day. The reaction mixture was then added to a bowl of ice-cold, diluted HCl-containing water. The resulting solid product was separated by filtering, recrystallized in ethanol, and then stored above CaCl2.

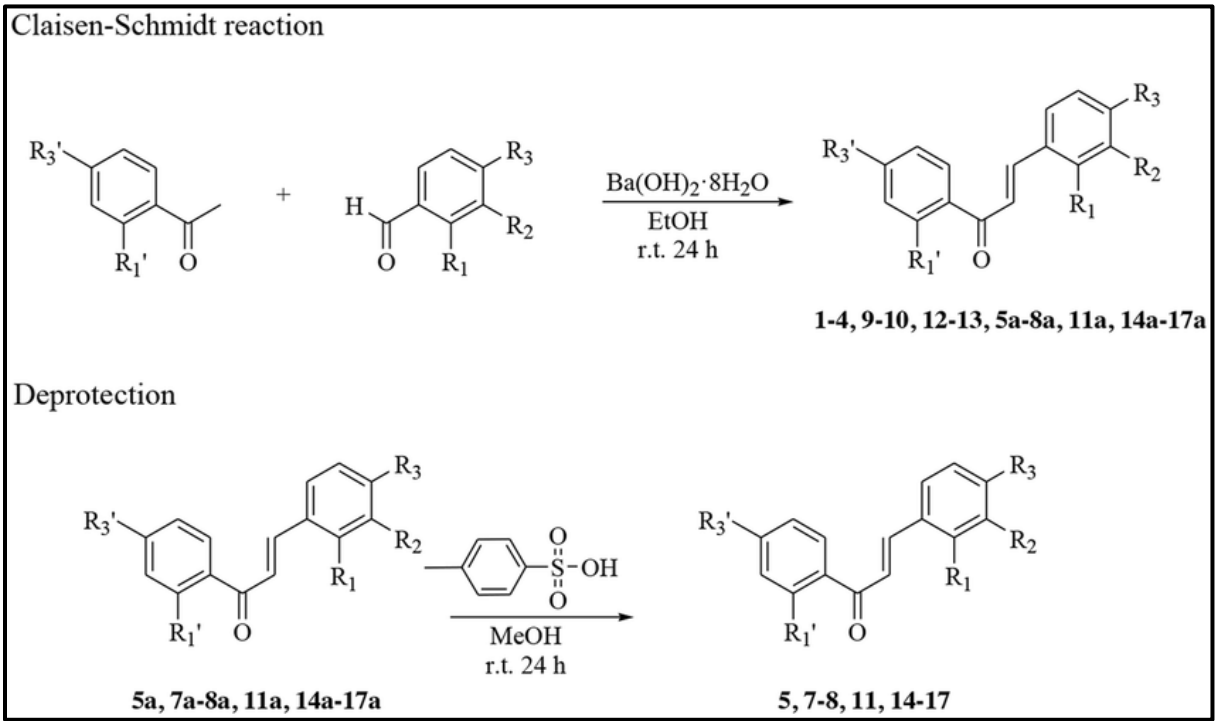

Figure. 1. Preparation of chalcone based ligand (Claisen- Schmidt condensation)

2.2 Preparation of tri-thiocarbonate ligand:

The carbon disulfide (CS2) solution in DMF was mixed with an aqueous solution of potassium hydroxide (KOH) at a temperature of 15-20 0C to create the potassium salt of K2CS3.

2.3 Preparation of complexes

By using standard methods, the chalcone ligand was complexed with metal salts (Ferrous sulfate/Cobalt Chloride/Nickel Chloride). To make the metal chalcone complex, metal salt solutions in ethanol-water (1:1, V/V) were slowly applied to the ethanolic chalcone ligand solution with stirring. By slowly adding a saturated ethanolic-water solution of copper sulfate/Zinc acetate to a solution of a tri-thiocarbonate ligand, the salts were formed. The resulting products were filtered and vacuum-dried.3.

Physical measurement and analysis

Elemental analyses (C, H, and N) were carried out on a Carlo Erba 1108 component analyzer. The complex's organic component was broken down using conc. HNO3, and the metal and sulphur were quantified using conventional gravimetric methods. Uncorrected measurements of the melting point were made in an open capillary. Purity and reaction progress were tested using TLC on silica gel

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plates. FT-IR spectra were collected on an FT-IR Nicolet 510 spectrometer using the standard KBr disc technique over the range of 500- 4000 cm-1 with a resolution of 4 cm-1, and 1H & 13C-NMR spectra were recorded 600 MHz models using DMSO-d6.

The complexes' powder XRD spectra were obtained at room temperature on a Seifert model ID-300 with a nickel channel (= 1.5406). The XRD designs were estimated to be 2 in the 20-90 scale. Using Bragg's condition n = 2dsin, where n is the order of reflection and is the angle of reflection, the interlayer dispersion d was identified. Using two test systems, the Keithley 236 source measure unit and the Schlumberger Impedance/Gain stage evaluation model (Si-1260), the electrical conductivity of packed pellets in the buildings was evaluated (SMU). The block was evaluated at a repetition rate of 1 kHz using a heap of 20 KN and a course of circular plate-shaped pellets secured with Elteck's silver paste for electrical contact. Inside, the temperature was kept at a controlled 1°C range.

RESULTS AND DISCUSSION

4.1 FT-IR SPECTRA

The Absorption band of aromatic (-OH) actually can be seen in IR spectra of ligand 3420 cm-1. This show that just one of the phenolic oxygen from every one of the ligand is deprotonated and engaged with coordination with metal moreover, the band showed up in IR scale 1307 - 1270 cm-1 because of IR phenolic C-O stretching in free chalcone ligand has been downward shifted and spectra of the complexes demonstrating the coordination through phenolic oxygen in the bonding of metal are upheld by the presence of new band □(C-O-M) in range of 865-988 cm-1. The complexes and ligand show IR bands stretching frequency in the range of 2933-3000 cm-1, 2467-2512 cm-1, and 1122-1618 cm-1corresponding for (=CH of Ar), (-CH=CH) and (-C=O) group of the chalcone based ligand and bands at 1287-1318 cm-1, 865-988 cm-1 and 765-795 cm-1 for (-C=S), (-C-O-M) and (-C-S-M) bands of a tri-thiocarbonate ligand. The presence of coordinates water is also supported by FT-IR spectra of the complexes.

4.2 NMR spectra

The NMR spectra of the complexes were recorded in DMSO-d6, 1H & 13C-NMR data are recorded as Table 3. The presence of aromatic proton is confirmed by the multiple in between 7.06 - 8.46 ppm, -CH=CH- band has been confirmed by the signal in a range of 7.10-8.38 ppm. While singlet peak of a hydroxyl group in the ligand (L) at 10.80 but due to complexation (-OH) peak not observed in complexes and 13C-NMR signals appears at the range of 128.00- 164, 114.16 – 148 and 180.02 - 198.48 of (Ar-C), (-C=C- of ethylene carbon) and α,β-unsaturated ketones (-C=O).

4.3 Electronic spectra

Due to the n-* transformation of,-unsaturated ketones, the UV-Visible spectra display absorbance in the range of 220-480 nm. Bathochromic shift causes a compound with a double bond moiety, i.e. a chromophoric group (-C=O), to absorb at a higher wavelength. The -* transition in aromatic 256 nm causes the B-band to appear.4.4

4.4 Magnetic susceptibility

The table shows the magnetic moment values of the complexes. 5. Magnetic susceptibility of complexes evidence indicates that Cu(II) has a square planar geometry, while Ni(II), Co(II), and Fe have octahedral geometry (II).

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4.5. Solid state electrical conductivity

The complexes' temperature-dependent solid-state electrical conductivity demonstrates their semiconducting existence. The conductivity of water increases as the temperature rises. This behaviour may be explained by the existence of exocyclic sulphur in CS32-, which forms short M—-S and S——S interactions.

4.6 Powder XRD Spectra

Figures 2-3 demonstrate the powder X-ray diffraction patterns of the complexes. Small variations in 2 and d-spacing, lattice strain, crystallite size, and peak intensity have been observed in the patterns. The crystallinity of the complexes is determined by contrasting background patterns to sharp peaks in the powder XRD diffraction of the sample. The complexes' crystalline existence is shown by their powder XRD patterns (Figures 2 and 3).

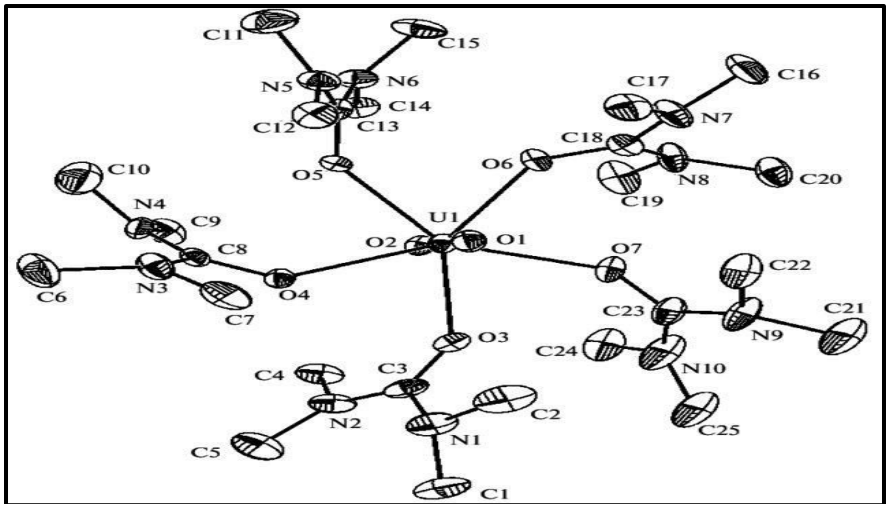

Fig. 2 [Cu(CS3)2][Ni(L)2(H2O)2]

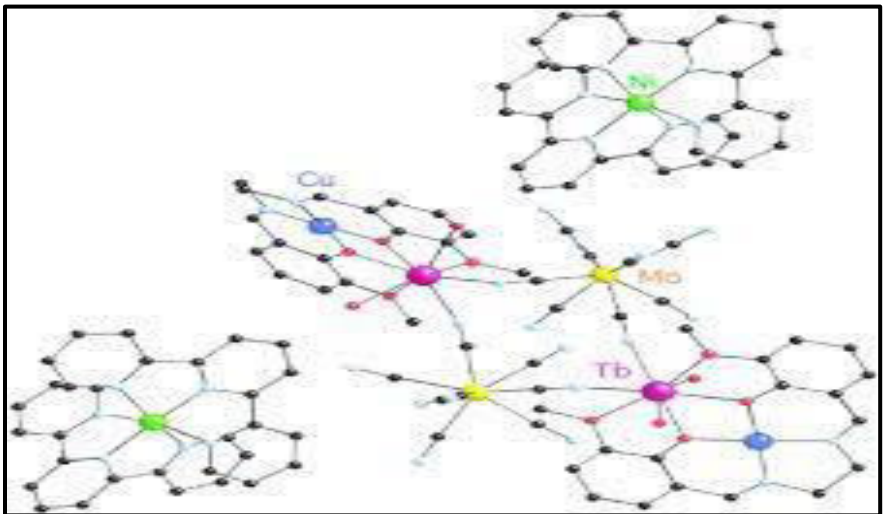

Fig. 3 [Zn(CS3)2][Ni(L)2(H2O)2]

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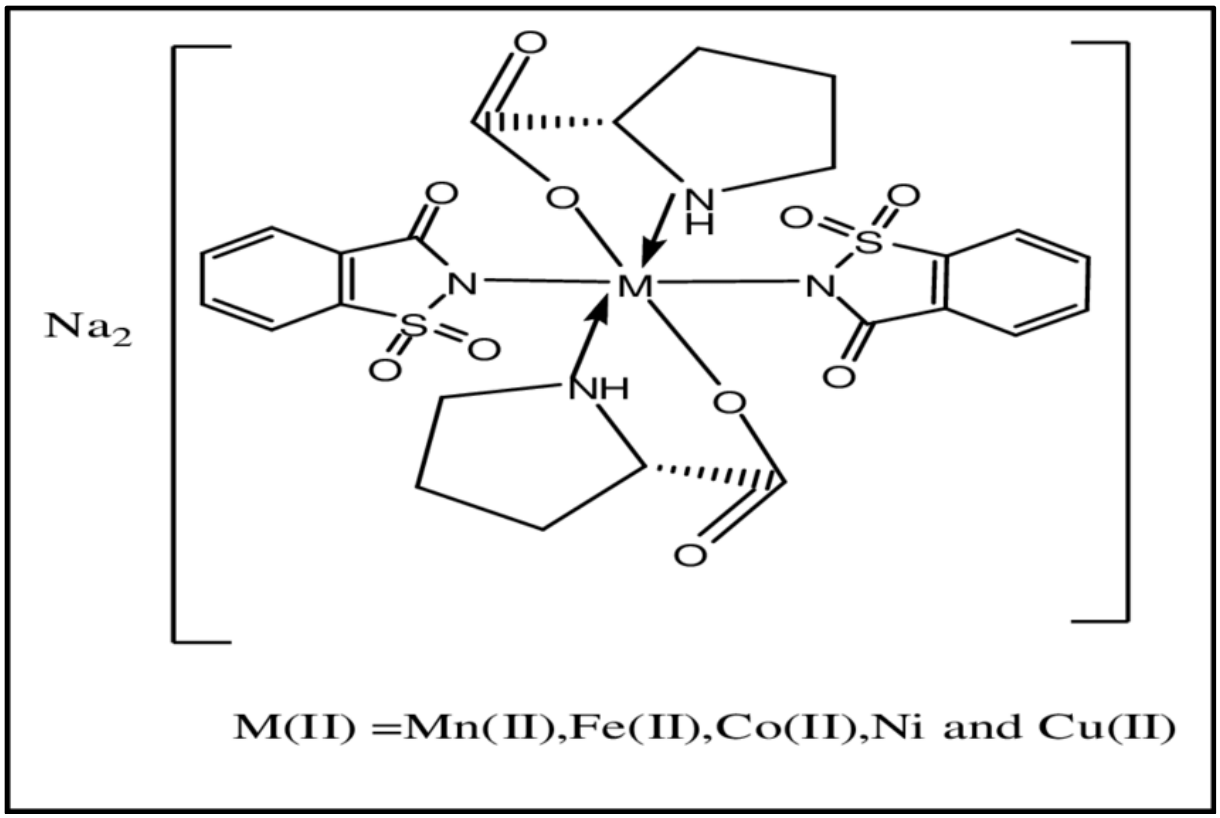

Figure. 4 Proposed structure of the complexes

Conclusion:

Electronic absorption specifications and magnetic susceptibility measurements are met by the anionic metallo ligand [M(CS3)2-]. The square planar shape of the core metal atom [M= Cu(II) or Zn(II)] is evident. In the cationic component of the complex salt, the central metal atom [Fe(II)/ Ni(II) or Co(II)] is assumed to be in octahedral geometry. An IR peak confirms the presence of organised water. According to studies on temperature-dependent solid-state conductivity, these substances are semiconductors. Stepwise temperature increases have been seen to increase conductivity. There is probably contact between M—-S and S—-S.

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