UV Study of Copper (Ii) Mixed Ligand Complexes Having Pyrazole as One of the Ligand

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Abstract

In the present investigation, UV data of four copper (II) mixed ligand pyrazole complexes, i.e., complex **I** - $[Cu(C_3H_8N_2O_2)Cl_2]$, complex **II** - $[Cu(C_3H_{14}N_2O_5)(SO_4)]$ complex **III** - $[Cu(C_3H_8N_2O_2)I_2]$ and complex **IV** - $[Cu(C_3H_{16}N_2O_6)(NO_3)_2]$ have been analysed. The analysed studies of the complexes represent the direct and indirect band gap energy of all studied complexes. The UV data have been analysed using Origin 2019 software. The band gap energy of all studied complexes has been same by direct and indirect band gap energy determination procedure. The results of the study revealed that the presence of SO_4 ion enhances the band gap energy in complex II whereas the presence of Cl, I and NO_3 ligand suppresses the band gap energy of complex I, III and IV.

Keywords: UV, pyrazole, direct, indirect and band gap energy.

Introduction

Spectroscopy is one of the most powerful tools available for the study of atomic and molecular structure and is used in the analysis of a wide range of samples [1-2]. UV-Vis (ultraviolet visible) spectroscopy is frequently used to provide characterization data for a variety of materials. Inorganic or organic, solid or liquid groups, such as organic molecules and functional groups, can be observed using UV-Visible spectroscopy, as can reflectance measurements for coatings, paints, textiles, biochemical analysis, dissolution kinetics, band gap measurements, etc. Depending on the degree of absorbance or transmittance of a different wavelength of beam light and the various responses of samples, the UV-Vis provides these details [3]. In this research work, we have studied and analysed UV data of 4 mixed ligand copper (II) complexes having pyrazole as one of the ligand.

Material and methods

Chemical were procured from renowned companies like E. Merck, Fluka and Aldrich and used without further purification. All solvents were A.R. grade and used as received for synthetic work. Metal salt were procured from Aldrich and pyrazole and pyrazole were procuredfrom E. Merck [4].

First of all copper and pyrazole (as a ligand) chemicals are taken in powder form. Now weighting both chemical separately with the help of weighting machine and we take both chemical in 1:2 molar ratio, (i.e., 1 part of metal and its double part of ligand). Now take a complete dry conical glass flask and mix both chemical pyrazole and metal in it and after that we have mix 10% ethanol in it well. Now this solution was refluxed for about 5 hours at 100°C with the help of a magneto stirrer machine. After this,

taking it out of the machine, this solution is filtered with the help of filter paper in another flask. On filtering we get precipitate from the solution. Now take out this precipitate on some other paper to remove its moisture and left it for 24 hours. Now after that keep it in the oven to completely dehumidify it. In this way we finally get the required sample [5-7].

Results and discussion

Except for the substance concentration, the band gap value of materials could also be calculated based on the absorption edge in steady-state absorption spectroscopy. In 1966, Tauc et al. put forward a classical method to determine the energy of forbidden width based on the absorbance signal [8]. The calculated formula is shown as equation

$$(\alpha h\nu)^{1/n} = A^* (h\nu - E_g)$$

in which h is the Planck constant, v is the photon frequency, α is the absorption coefficient, E_g is the forbidden bandwidth, and A* is the slope of the Tauc graph in the linear region [9]. It should be noted that the value of parameter n is related to the type of semiconductor. When the semiconductors adopt direct and indirect band gap types, the parameter *n* is fixed as 0.5 and 2, respectively [10],Table 1 represent the calculated value of the band gap energy for each sample.

UV-Vis studies of the 4 complexes were recorded, the prominent lines were indexed. Figure 1 to 8 represents the energy patterns of the studied samples. The UV results of all samples have been shown in table 1 in terms of complex number, direct band gap energy and indirect band gap energy.

Fig. 1 to 8 shows the different absorption and band gap energy graphs of Complex I to IV. First graph of each sample represent the absorption vs. energy graph, i.e., direct band gap energy graph and second graph of each sample also represent the absorption vs. energy graph, i.e., indirect band gap energy graph. Complex I, II. III and IV are mixed ligand copper complexes as shown in table 1. The order of band gap energy from direct band gap energy values are –

Complex III > Complex I > Complex II > Complex IV

and the order of band gap energy from indirect band gap energy values are –

Complex III > Complex I > Complex II > Complex IV

On comparing direct and indirect values of energy band gap of complexes I to IV (from table 1), we have same orders in both methods. The above order of band gap energy shows that when we introduce Cl, I, SO_4 and NO_3 as ligands in (copper + pyrazole) complexes we have different values of band gap energy in both methods but in same order. The above order shows that the presence of SO_4 ion enhances the band gap energy of (copper + pyrazole) complex whereas the presence of Cl, I and NO_3 ligand suppresses the band gap energy of (copper + pyrazole) complexes. The same order of all three complexes also represent that the band gap energy of mixed ligand (copper + pyrazole) complexes does not depends on the methods to find the values of band gap energy. The band gap energy value of complex III (copper + pyrazole + SO_4) is maximum and of complex IV (copper + pyrazole + NO_3) is minimum.

Conclusion

 The order of band gap energy shows that when we introduce Cl, I, SO_4 and NO_3 as ligands in (copper + pyrazole) complexes we have different values of band gap energy in both methods but in same order. The presence of SO_4 ion enhances the band gap energy of (copper + pyrazole) complex whereas the presence of Cl, I and NO_3 ligand suppresses the band gap energy of (copper + pyrazole) complexes.

Table 1 - Band gap energy values of copper complexes having pyrazole as one of the ligand.

S. No.	Complex	Chemical formula	Direct band gap energy (eV)	Indirect band gap energy (eV)
1.	Complex I	[Cu(C3H8N2O2)Cl2]	2.246	2.139
2.	Complex II	[Cu(C3H14N2O5)(SO4)]	1.807	1.915
3.	Complex III	[Cu(C3H8N2O2)I2]	2.315	2.219
4.	Complex IV	[Cu(C3H16N2O6)(NO3)2]	1.411	1.395

Figure 1 to 8 – Band gap energy values by direct and indirect method of copper complexes having pyrazole as one of the ligand.
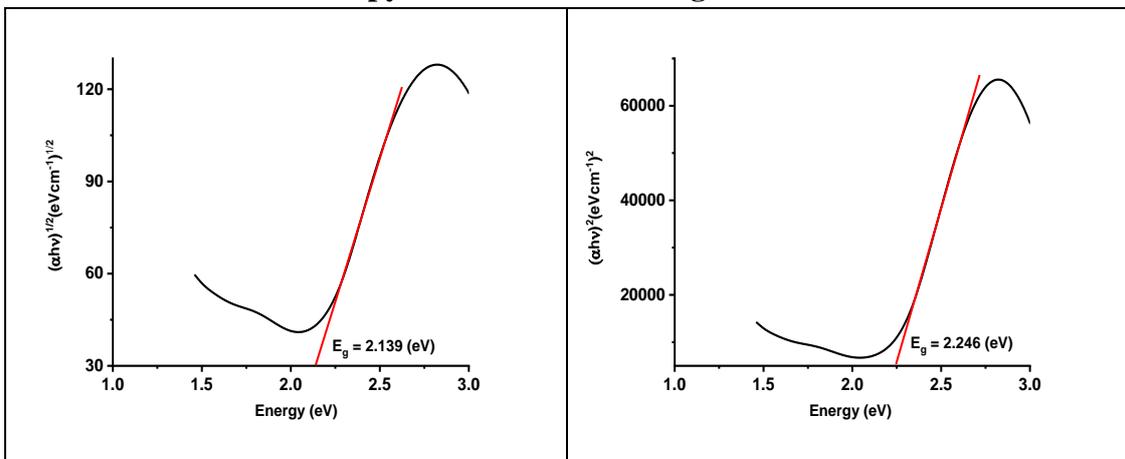

Fig. 1 – Complex I - Direct band gap (absorption factors vs. energy)

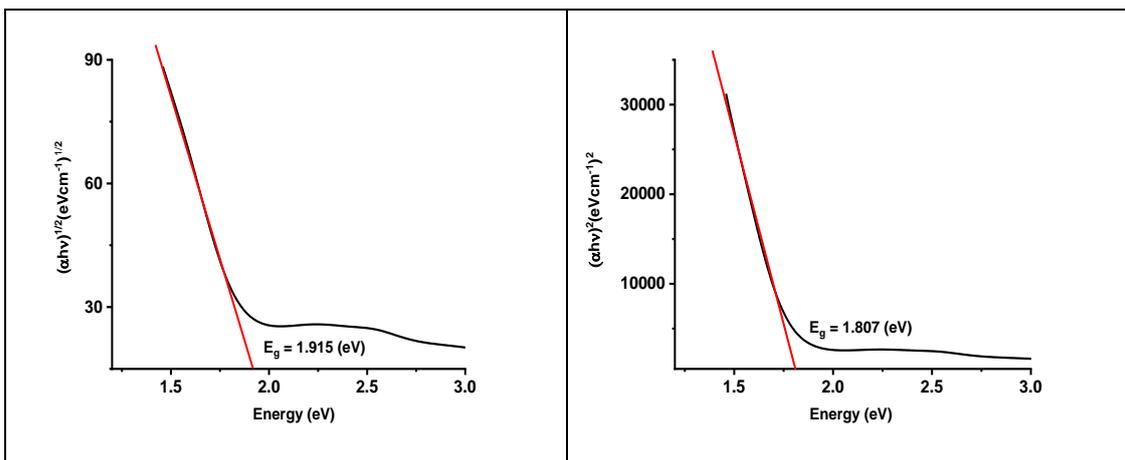**Fig. 2 – Complex I - Indirect band gap (absorption factors vs. energy)**

Fig. 3 – Complex II - Direct band gap (absorption factors vs. energy)

Fig. 4 – Complex II - Indirect band gap (absorption factors vs. energy)

Fig. 5 – Complex III - Direct band gap (absorption factors vs. energy)

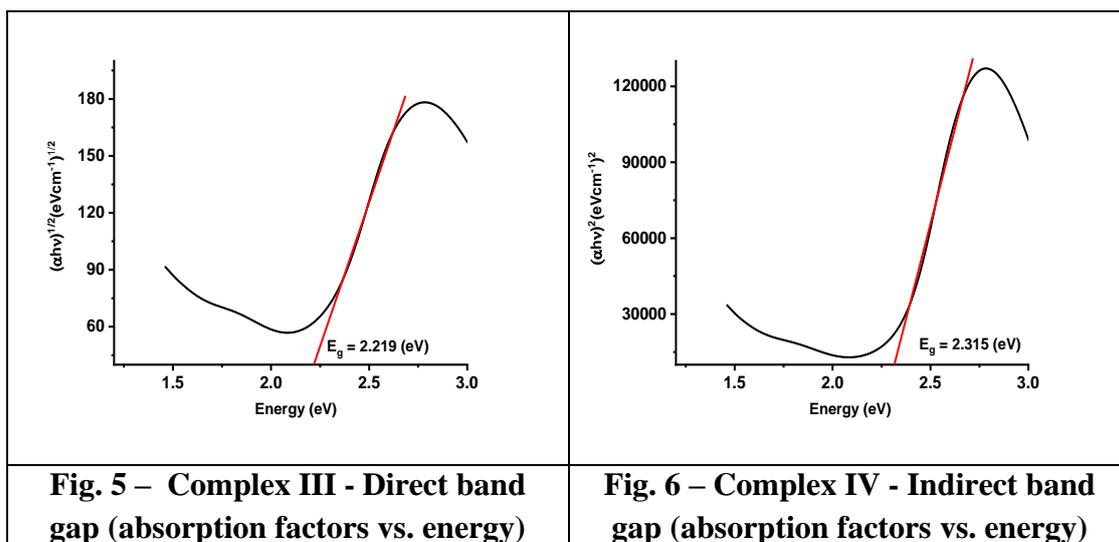**Fig. 6 – Complex IV - Indirect band gap (absorption factors vs. energy)**

Fig. 7 – Complex IV - Direct band gap (absorption factors vs. energy)

Fig. 8 – Complex IV - Indirect band gap (absorption factors vs. energy)
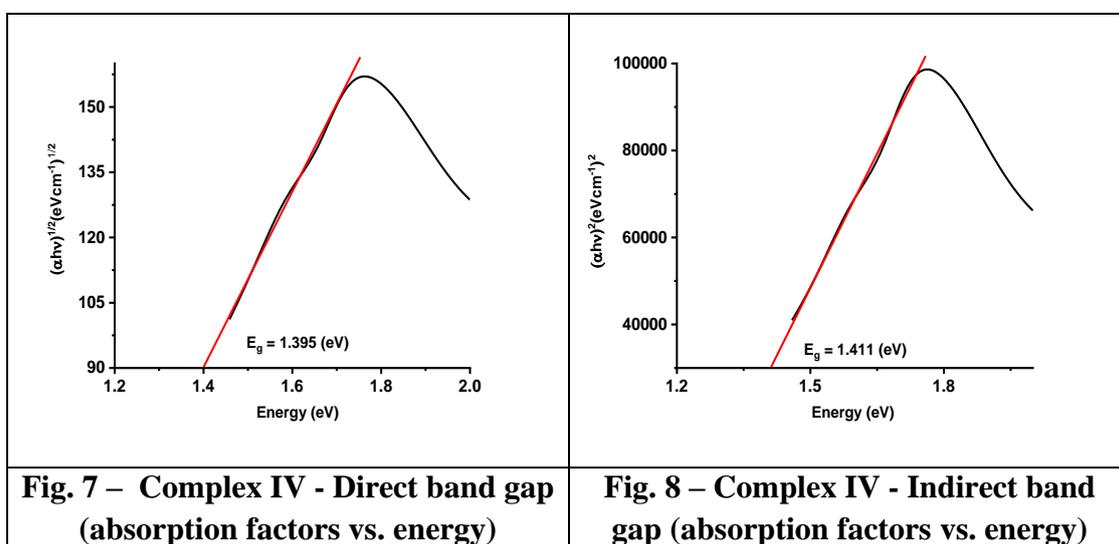
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