Preface

Minerals are naturally occurring inorganic compounds. These are widely used in medicine, chemical industries, and agriculture and in daily life. They exhibit different colours due to the presence of transition metal ions. A detailed study of a few minerals has been carried out using EPR, Optical absorption, Chemical analysis and IR studies for the present thesis.

This thesis is spread over into six chapters.

Chapter -1

In chapter -1, theoretical principles of optical absorption, EPR and IR spectroscopy are described and a brief outline of the instruments and experimental techniques used by the author during the course of study is also presented.

Chapter – 2

This chapter describes the results of investigations with optical absorption, EPR and IR spectral studies on renierite mineral originated from Congo, generously donated by Prof. Dr. Michel Delines, Head, Dept. of Mineralogy, Institut Royal des Sciences, Naturelles, de Belgique, Bruxelles. It contains 9.78 and 7.10 wt% FeO and copper (copper or CuO) respectively. The optical absorption spectrum recorded at room temperature shows the presence of Fe(III) and Cu(II) ions in tetrahedral coordination. The crystal field splitting parameters evaluated for Fe(III) and Cu(II) are: Dq = 480, B = 520, C = 2500 cm⁻¹ and Dq = 430, Ds = - 620, Dt = 472 cm⁻¹ respectively. EPR spectrum was recorded in powdered form both at RT and LNT. g values are calculated for ferric
ion and divalent copper and they are found to be 2.03 and 2.40 respectively in the mineral. IR spectrum is characteristic of sulphate and hydroxyl groups.

Chapter – 3

The results of Optical and EPR investigations on tenorite mineral from Mexico, donated by Dr. Michel Delines, Head, Dept. of Mineralogy, Institut Royal des Sciences, Naturelles, de Belgique, Bruxelles are discussed in this chapter. The mineral contains 54.4 wt% of CuO. Tenorite is quite an interesting compound. The EPR spectrum exhibits the characteristic of d² configuration (two unpaired electrons) but not of d⁹ (single unpaired electron). The EPR parameters of bi-nucleus Cu(II) in d² system are evaluated and it is found that \( g = 2.160 \) and the zero-field splitting parameter, \( D = 125 \) G. The optical absorption spectrum shows a series of bands which are attributed to d⁹ system of Cu(II) in two independent sites of tetragonal C₄ᵥ symmetry.

Chapter - 4

The results of optical absorption and EPR studies on fuchsite mineral from Nellore district of India, gifted by Prof. K.V.R Chari, Head, Department of Geology, S.V.U.P.G. Centre, Kadapa, India are discussed in this chapter. Chemical analysis of the sample indicates that chromium is present to the extent of 3.37 wt%. EPR spectrum recorded in powdered form of the sample reveals the presence of the two Cr(III) sites having same g value of 1.98, but different D values of 270 G and 160 G. Optical absorption spectrum is clearly characteristic of Cr(III) in octahedral site symmetry. The EPR and optical absorption results are correlated. The covalency parameter \( \beta \) evaluated as 0.55 and is compared with other chromium bearing compounds. NIR spectrum is mainly due to well-defined OH bands.

Chapter - 5
The results obtained from the optical and EPR investigations on magnesite mineral of Mysore, India are presented. Its chemical analysis indicates that FeO is 1.60 wt%. The optical absorption spectrum is exhibiting only two bands around 10000 cm\(^{-1}\) that is attributed to Fe(II) in distorted octahedral symmetry. EPR spectrum clearly exhibits a six transitions indicating the presence of Mn(II) in the sample, with the parameters as: \(g = 2.007\) and \(A = 90 \text{ G}\). Even though Mn(II) could not be detected by optical absorption studies, it could be identified by EPR studies due to the high sensitivity of EPR technique.

Chapter – 6

The results of investigations on antlerite mineral collected from Chuquicamata, Chile presented by Prof. Dr. Michel Delines, Head, Dept. of Mineralogy, Institut Royal des Sciences, Naturelles, de Belgique, Bruxelles form the basis for this chapter. The elemental analysis indicates that the transition metal ion copper is present to the extent of 67.3 wt% in the mineral. Optical absorption spectrum carried out at room temperature confirms the presence of Cu(II) in rhombically distorted octahedral coordination. NIR spectrum reveals the presence of water fundamentals. EPR spectrum of the sample recorded at RT and LNT in powdered form shows \(g_1 = 2.36\), \(g_2 = 2.16\) and \(g_3 = 2.07\).