ABSTRACT

The work presented in this thesis is theoretical as well as experimental. The theoretical work is useful for the analysis of experimental data. The polarization and angular distribution measurements reveal unique properties of the Mossbauer radiation in the presence of nuclear hyperfine interactions. A general theory has been developed for the measurement of interaction parameters.

The polarization distribution measurements of the Mossbauer radiation could be an effective tool for probing the microscopic fields. Therefore, using the multipole radiation field theory, calculations have been extended to the mixture of magnetic and quadrupole interactions in the transitions $|3/2\rangle \rightarrow |1/2\rangle$ and $|7/2\rangle \rightarrow |5/2\rangle$, when asymmetry parameter ($\eta$) is non-zero and zero, respectively. Detailed calculations show that the polarization and angular distribution measurements of the Mossbauer $\gamma$-rays are extremely sensitive to hyperfine field parameters (viz: electric field gradient, asymmetry parameter ($\eta$), angles $\theta$, $\phi$ and Euler angles $\alpha$, $\beta$ and $\gamma$). We have applied D-matrix formalism to transform coherency matrix, intensity, degree of polarization and hence angular and polarization distribution function from the principal axis to the crystal fixed axis system. It is shown further that the results obtained with the polarization and angular
distribution measurements are unambiguous. The theory developed for the Mossbauer resonance is useful in the analysis of the Mossbauer spectra in single crystals.

In the experimental part, some model complexes (like biological complexes) have been prepared and their Mossbauer spectra have been studied with the help of Mossbauer spectrometer at room temperature. The electric field gradient and isomer shift acting at the Mossbauer nucleus have been calculated in each case and attempts have been made to understand the parameters related to the surrounding of the probe (Fe ion).

The study presented in this thesis is basically divided into five chapters, each chapter starting with an introduction and ends up with references.

**Chapter-I** : Review of Theory

**Chapter-II** : The Angular and Polarization Distributions of the Mossbauer Radiation $|3/2^+\rangle \rightarrow |1/2^-\rangle$ in the Single Crystals

**Chapter-III** : The Angular and Polarization Distributions of the Mossbauer Radiation $|7/2^+\rangle \rightarrow |5/2^-\rangle$

**Chapter-IV** : Instrumentation

**Chapter-V** : Mossbauer Study of Some Iron Complexes
Chapter-I gives background of the Mossbauer effect and its importance, hyperfine interactions and their origins and application of the Mossbauer effect to study insight of solids through interactions.

In Chapter-II a theory has been constructed, using the multipole radiation field to study angular and polarization distributions of Mossbauer radiation. The parameters which are involved in the interactions can be determined from the above measurements. When a Mossbauer nucleus has both the interactions - quadrupole as well as magnetic, simultaneously, then calculations are carried out for the evaluation of degree of polarization for each transition available between two nuclear states. The theory has been applied to Mossbauer nuclei, which decay from the excited state having spin 3/2 to ground state having spin 1/2, assuming the asymmetry parameter (η) non-zero. In the Chapter-III the same theory has been extended to those Mossbauer nuclei which have excited state spin 7/2 and ground state spin 5/2, when the asymmetry parameter (η) is zero.

Chapter-IV. This chapter deals with the instrumentation used to carry out Mossbauer investigations on iron complexes.

Chapter-V describes preparation of the iron samples and their characterization through XRD and Mossbauer studies.
Usefulness of the Work:

The work which has been presented in this thesis has following usefulness.

1. The theory provides a powerful tool to study those parameters, which are involved in the interactions. It provides a basis to analyse experimental data.

2. The theory is specially meant for single crystals. Computer analyses show that the intensity and angular and polarization distributions of Mossbauer gamma-rays are direction dependent which give information about the symmetry of the parameters.

3. Rotation matrices \([D_{m,m}^{l}(\alpha \beta \gamma)]\) transform the results from principal axis system to crystal fixed axis system because there is no \(a priori\) that the two systems must overlap each other. Thus correct information is obtained on the orientation of the two axes systems with respect to each other. The D-matrices also keep track of how angular momentum and projection quantum numbers change. However, people have already made use of cosine method to correlate the two axes. This method is cumbersome due to lengthy mathematical calculations and also it loses information on the above quantum numbers.
The iron complexes which we have studied have following usefulness:

1. Biologically
   (i) Nuclear magnetic resonance imaging agents (NMRI) in detecting tumour and cancer.
   (ii) Metal intoxication
   (iii) Anti-fungal

2. Industrially
   (i) Anti corrosive materials
   (ii) Paint industry