

CHAPTER - VIII

SUMMARY AND CONCLUSION

INTRODUCTION

In the present investigations, PMR relaxation studies and chemical shift measurements have been carried out in five different systems. The systems chosen are (i) Cancerous tissues and bio-fluids, (ii) Aqueous solutions of Amino acids and Proteins, (iii) Aqueous sugar solutions with alkali halides (NaCl, KCl), (iv) Glycerine-Water and Dioxan-Water with paramagnetic ions, (v) Some carboxylic acids in dioxan. The relaxation times are measured using Bruker PC 120 NMR process analyser, and chemical shifts are recorded using Varian EM 390 NMR spectrometer.

STUDY OF NORMAL AND CANCEROUS TISSUES

The relaxation times (T_1 and T_2) were measured over 400 tissue samples of cancerous and normal tissue such as breast, penis, cervix, stomach etc of patients of Indian origin. The relaxation time (T_1) is found to be longer in cancerous tissues when compared to normal tissue, whereas the values of (T_2) do not seem to have any correlation. The percentage of water content is found to be higher in cancerous tissue as compared to normal tissue. The observed increase in the relaxation time in cancerous tissue may be due to the increased water content. The relaxation times were also measured in normal and Dolton's lymphoma

cells injected in mice by Air Pouch Technique. The results reveal that the relaxation time is found to be longer in cancerous tissue as compared to normal tissues. This is explained in depth on the basis of two state fast exchange model for the water molecules proposed by Zimmerman and Brittin. Atomic absorption studies were also carried out to find the trace elements in the above tissue. These studies indicate that cancerous tissue have more potassium content as trace element and the sodium content is more in normal tissue.

AQUEOUS SOLUTIONS OF AMINO-ACIDS AND PROTEINS

The relaxation times (T_1 and T_2) are measured in aqueous solutions of amino-acids (glycine, L-proline, tyrosine, tryptophan) and proteins (bovine serum albumin) in different percentage concentration and at different temperatures. Relaxation times are also measured in body pH and isoelectric pH range. The results of aqueous solutions of amino acids are explained in terms of flickering cluster model of water. The results of protein solution are explained as due to the formation of hydration shells between the solute and solvent molecules. The research work in aqueous solutions of tyrosine and tryptophan indicate the possibility of micelles in these solutions.

AQUEOUS SUGAR SOLUTIONS WITH ALKALI HALIDES

The relaxation times are measured in aqueous solutions of sucrose, glucose, fructose, maltose and galactose. The concentrations chosen are 2% and 5% by weight. The alkali halides (NaCl, KCl) are added in these solutions in the concentration range 1 M/L to 4 M/L. The result indicates that the relaxation times in aqueous solutions of sugars are found to decrease with increase of sodium chloride concentration whereas the addition of potassium chloride increases the relaxation times. This is generally discussed in terms of water structure making and breaking properties of alkali halides.

GLYCERINE-WATER AND DIOXAN-WATER WITH PARAMAGNETIC IONS

The relaxation times (T_1 and T_2) were measured in glycerine-water (highly viscous) and dioxan-water (less viscous) mixtures of several compositions. The paramagnetic ions were added to the solutions of the above highly viscous and less viscous systems in the form of copper nitrate and chromium nitrate in the concentration range of $(0.1 \text{ to } 0.4) \times 10^{20}/\text{cc}$. The results indicate that the possibility of anti parallel bonding of the paramagnetic ions is more in highly viscous solutions as compared to low viscous systems and the association in the above mixtures appears to be weak.

CHEMICAL SHIFT

Relaxation times (T_1 and T_2) and chemical shift studies were carried out in solutions of O-hydroxy benzoic acid (OHBA), P-hydroxy benzoic acid (PHBA) and M-toluic, O-toluic acids in dioxan at various solute concentrations. The NMR spectra corresponding to OH and COOH protons could be distinguished in solutions of OHBA in dioxan whereas solutions of PHBA in dioxan shows only one peak in the range of chemical shifts attributable to OH and COOH protons. In the solutions of OHBA in dioxan, the chemical shift of the proton of the hydroxyl group increases with increase of solute concentration and attains a maximum at a solute concentration of 0.04 mf and then decreases with further increase of solute concentration. For the carboxyl group, the chemical shift increases with increase of solute concentration and attains a maximum at 0.08 mf solute concentration. In solutions of PHBA in dioxan the chemical shift of the single line observed increases with increase of solute concentration and attains a maxima at a solute concentration of 0.05 mf. The results are interpreted as due to the formation of hydrogen bonds between the molecules of OHBA and PHBA and dioxan. The relaxation studies in the above solutions also confirm the above findings. The chemical shift of M-toluic and O-toluic acids in dioxan is recorded in the range of 0.01 mf to 0.13 mf of solute

concentration. The chemical shift of COOH proton of M-toluic acid increases with increase of solute concentration and attains a maximum at 0.08 mf and then decreases with increase of solute concentration whereas in solutions of O-toluic acid in dioxan, the chemical shift shows a broad maxima around 0.08 mf. This is interpreted as due to the formation of hydrogen bonds between solute and solvent molecules. The relaxation studies also confirm the above findings.