SUMMARY
The summary of the work presented in various chapters of the thesis is outlined below -

CHAPTER-I

This chapter deals with the role of thermodynamic excess functions in the study of molecular interactions in binary as well as ternary mixtures of non-electrolytes and contains a brief account of intermolecular forces, the sources of their information and the manner of representation of intermolecular potentials. This chapter also includes a brief description of various theories of solutions of non-electrolytes but special attention has been paid to Flory's theory and Sanches & Lacombe theory of fluid mixtures. Some graph theoretical concept has also been defined in this chapter.

CHAPTER-II

This chapter contains a review of literature on molar excess volumes, \( V^E \), molar excess enthalpies, \( H^E \), molar excess Gibbs free energies and spectroscopic studies on binary mixtures of non-electrolytes. It also includes a brief review of \( V^E \) and \( H^E \) of ternary mixtures of non-electrolytes.

CHAPTER-III

This chapter deals with the purification of materials, checking of their purity together with experimental techniques for measurements of molar excess volumes, molar excess enthalpies of binary and ternary mixtures (as a function of composition and temperature) and molar excess
Gibbs free energies and proton magnetic resonance studies of binary mixtures of non-electrolytes.

CHAPTER-IV

This chapter contains $V^E$ and $H^E$ data of 298.15 and 308.15 K of -

1) 1,2-dichloroethane (i) + pyridine (j)
2) 1,2-dichloroethane (i) + $\gamma$-picoline (j)
3) 1,2-dichloroethane (i) + n-hexane (j)
4) 1,2-dichloroethane (i) + n-heptane (j)
5) n-heptane (i) + pyridine (j)
6) n-heptane (i) + $\gamma$-picoline (j)
7) n-heptane (i) + $\beta$-picoline (j)
8) Aniline (i) + pyridine (j)
9) Aniline (i) + $\gamma$-picoline (j)
10) Aniline (i) + $\beta$-picoline (j)

$G^E$ data at 308.15 K for -

1) 1,2-dichloroethane (i) + pyridine (j)
2) 1,2-dichloroethane (i) + $\gamma$-picoline (j)
3) 1,2-dichloroethane (i) + n-picolin (j)
4) n-heptane (i) + $\gamma$-picoline (j)

$V^E$ and $H^E$ data at 298.15 and 308.15 K for -

a) 1,2-dichloroethane (i) + pyridine (j) + $\beta$-picoline (k)
b) 1,2-dichloroethane (i) + n-heptane (j) + pyridine (k)
c) 1,2-dichloroethane (i) + n-heptane (j) + $\beta$-picoline (k)
d) n-heptane (i) + pyridine (j) + $\gamma$-picoline (k)
e) Aniline (i) + pyridine (j) + $\beta$-picoline (k)
f) Aniline (i) + pyridine (j) + $\gamma$-picoline (k)
along with the manner of their representation by Redlick-Kister type equations. This chapter deals with an examination of $V^E$ and $H^E$ data of binary mixtures (1) to (x) in terms of

1) Graph theoretical approach

ii) Flory's theory; and

iii) Sanches and Lacombe theory,

and it has been shown that $V^E$ and $H^E$ values predicted from graph theoretical approach compare very well with the corresponding experimental values unlike the $V^E$ and $H^E$ values predicted by Flory's theory and Sanches and Lacombe theory. The cross interaction energies $6^E_{ij}$ of the binary mixtures obtained from Sanches and Lacombe theory have been utilized to see as to how these deviate from geometric mean law and this information has been employed to speculate the nature of binary interactions in these mixtures. The nmr studies on 1,2-dichloroethane + pyridine, 1,2-dichloroethane (1) + $\alpha$-picoline (j), aniline (1) + pyridine (j), aniline (1) + $\gamma$-picoline (j) have also been employed to lend credence to the nature and extent of interaction in these mixtures.

The graph theoretical approach has also been utilized to predict $V^E (T_2 = 298.15 K, x_1)$ and $H^E (T_2 = 298.15 K, x_1)$ data for binary mixtures (1) to (x) when their corresponding $V^E (T_2 = 308.15 K, x_1)$ and $H^E (T_1 = 308.15 K, x_1)$ data evaluated from $V^E (T_1 = 308.15 K, x_1 = 0.5)$ and $H^E (T_1 = 308.15 K, x_1 = 0.4$ and $x_1 = 0.5)$ data are known and it has been shown that values so predicted for $V^E$ and $H^E$ are of the right order of magnitude but qualitative agreement with the experimental values is not so impressive. This has been
attributed to be due to the $V^E_{\text{specific}}$ and $H^E_{\text{specific}}$ effects.

This chapter also examines $V^E$ and $H^E$ data of ternary mixtures (a-f) of non-electrolytes in terms of -

1) Lattice theory,  
2) Conformal solution theory,  
3) Sanchez and Lacombe theory; and  
4) "Graph theoretical" approach,

and it has been shown that while both the Sanchez and Lacombe as well as "Graph theoretical approach" describe well the $H^E$ data of the various ternary mixtures, the same is not true of the $V^E$ data of ternary mixtures so far as Sanchez and Lacombe's theory of fluids is concerned. The $V^E$ data of binary mixtures have also been utilized to predict $V^E$ data for ternary mixtures. The $V^E$ data on ternary mixtures have also been utilized to study the nature of molecular interaction between the $j$ th and $k$ th components of these $(i+j+k)$ mixtures in the presence of the $i$ th components.