CHAPTER-6
Correlations and Conclusions

PART-A Correlations

In this section the correlations among the parameters determined in the previous chapters (chapters 3, 4 and 5) are discussed in detail in order to understand the underlying physics.

6.1 Correlations in System 1 and System 2

In Chapter-3, different dielectric and thermodynamical parameters, like static permittivity ($\varepsilon_{\text{static}}$), high frequency permittivity ($\varepsilon_\infty$), effective Kirkwood correlation factor ($\theta_{\text{eff}}$), corrective Kirkwood correlation factor ($\theta_r$), excess Helmholtz free energy ($\Delta F^E$), dipole moment ($\mu$), excess dipole moment ($\Delta \mu$) and Hydrogen bonding energy ($\Delta E$) are determined for propan-2-ol + methyl benzoate (system 1) and propan-2-ol + ethyl benzoate (system 2).

In chapter-4, various dielectric, thermodynamic and conformational parameters like excess permittivity ($\varepsilon^E$), Bruggeman factor ($f_B$), relaxation times ($\tau$), excess inverse relaxation time ($\left(\frac{1}{\tau}\right)^E$), activation free energy ($\Delta G^*$), molar enthalpy of activation ($\Delta H^*$), molar entropy of activation ($\Delta S^*$) and FT-IR spectra (experimental and theoretical) are determined for system 1 and system 2.

6.1.1 Correlation between dielectric permittivity and Kirkwood parameters in System 1 and System 2

In system 1 and system 2 the static permittivity ($\varepsilon_{\text{static}}$) value of mixture is decreasing as the mole fraction of benzoates (MB and EB) is increasing (Tables 3.1 and...
3.2). This phenomenon indicates that the alignment of dipoles along the field is changing from parallel orientation to anti parallel orientation. This effect should decrease the effective Kirkwood correlation factor ($g_{\text{eff}}$) which depends on the dipoles orientation. In the case of pure MB the values of $g_{\text{eff}}$ are more than pure EB due to the high orderliness of dipoles. From Tables 3.3 and 3.4, one can clearly observe that the values of $g_{\text{eff}}$ are decreasing with increasing mole fraction of benzoates. This trend has been observed at all temperatures (303K, 308K, 313K, 318K and 323K).

The corrective Kirkwood correlation factor ($g_\tau$), which is an indicator for hetero interaction of the components in the mixture, is less than unity if the dipoles of both compounds are oriented in such a way that the number of effective dipoles is less than the corresponding average value of the pure liquids and is greater than unity if the dipoles of both compounds are oriented in such a way that the number of effective dipoles is more than the corresponding average value of the pure liquids. In the present Chapter 3, for both the systems, the alignment of dipoles from parallel orientation to anti parallel orientation indicates that the number of effective dipoles is less than the corresponding average value of the pure liquids and correspondingly $g_\tau$ must be less than unity. From Tables 3.3 and 3.4, it is clearly observed that the value of $g_\tau$ is less than unity for all mixture concentrations and temperatures. Further it is observed that $g_\tau$ values deviate more from unity, in system 2 than in system 1, at all temperatures indicating stronger hetero interaction in the case of system 2.
6.1.2 Correlation between excess Helmholtz free energy and excess dipole moment in System 1 and System 2

The positive values of excess Helmholtz free energy ($\Delta F^E$) for the mixture systems indicate the formation of $\beta$ – clusters with anti-parallel alignment. Due to the formation of $\beta$ – clusters the effective dipole moment will be decreased when compared to the sum of individual systems and thereby it destructs the angular correlation between non ideal molecules which may decrease its internal energy. The higher positive values of $\Delta F^E$, in the case of system 2 compared to that of system 1, indicate that the formation of $\beta$ – clusters is high in system 2. The negative values of $\Delta F^E$ indicate the formation of $\alpha$- clusters. Due to the formation of these $\alpha$- clusters the effective dipole moment will be increased which increases the internal energy. In the present case, for both the systems (system 1 and 2), it is observed that the orientation of dipoles has been changed from parallel to anti-parallel which should form $\beta$ – clusters with positive values of $\Delta F^E$. From the high positive values of $\Delta F^E$ (Table 3.8), it is evident that $\beta$ – clusters are formed in both the systems up to 0.7 mole fraction of benzoates in mixture. For 0.8 and 0.9 mole fraction of benzoates in mixture, negative values of $\Delta F^E$ are observed which predicts the formation of $\alpha$- clusters and accordingly $g_\tau$ values are increased for these two mole fractions (Tables 3.3 and 3.4). This effect is witnessed for all temperatures.

The formation of $\beta$ – clusters, for equimolar mixture in both the systems, decreases the effective dipole moment of the mixture when compared to the sum of individual systems. Due to this the excess dipole moment ($\Delta \mu$) value, for equimolar
mixture, must be negative. It has been observed, experimentally and theoretically, that
the values of $\Delta\mu$ are negative for equimolar mixture in both the systems (Tables 3.10).
The same phenomenon has been observed experimentally for all temperatures (Tables
3.10).

6.1.3 Correlation between excess permittivity and Bruggeman factor in System 1
and System 2

The negative value of excess permittivity ($\varepsilon^E$) indicates that the interaction
between the mixture components may form multimers through hydrogen bonding in
such a way that the effective dipole moment gets reduced whereas the positive value of
$\varepsilon^E$ indicates that the interaction is in such a way that the effective dipole moment
increases. In the present study the negative values of $\Delta\mu$, for both the systems (system
1 and 2), suggest that the effective dipole moment gets reduced and simultaneously
negative $\varepsilon^E$ values must be obtained. The Figures 4.1 and 4.2 are clearly shows the
negative values of $\varepsilon^E$, for all temperatures.

The non-linear variation of Bruggeman factor ($f_B$) with volume fraction ($\phi_2$)
indicates the interaction between the components of the liquid mixtures. In both the
systems, the negative values of $\varepsilon^E$ suggest the existence of multimers through hydrogen
bonding which must result in non-linear variation of $f_B$ with $\phi_2$. From the Figures 4.3
and 4.4, the non-linear variation of $f_B$ with $\phi_2$ can be clearly observed for both the
systems at all temperatures.
6.1.4 Correlation studies from dielectric relaxation, thermodynamic parameters and FT-IR spectra in System 1 and System 2

The low value of the effective Kirkwood correlation factor for benzoates explains the non-associative nature of the compounds which results in low value of relaxation time. The relaxation times of pure EB are greater than that of pure MB due to increase in molecular size and effective radius of the rotating unit. The high value of the effective Kirkwood correlation factor for IPA shows the associative nature (the formation of intra molecular hydrogen bonding between one alcohol molecule and another) of the compound which results in high value of relaxation time. The increase in the mole fraction of associative (IPA) liquid in non associative (benzoates) liquid increases the value of $g^{\text{eff}}$, which intern must increase the value of relaxation time of the binary mixture. Table 4.1 shows the increment in the relaxation time as the mole fraction of IPA increases in the binary mixture at all temperatures. Further, this effect leads to slower rotation of the dipoles, giving negative excess inverse relaxation time $\left( \frac{1}{\tau} \right)^e$ (shown in Figures 4.7 and 4.8).

The increasing positive values of activation free energy ($\Delta G^*$) suggest the existence of molecular associations between unlike (associative and non-associative) molecules in the mixture and the positive value of molar enthalpy of activation ($\Delta H^*$) gives [115], the amount of heat liberated in the process of dielectric reorientation and accordingly negative values of Hydrogen bonding energy ($\Delta E$). Further, The negative values of molar entropy of activation ($\Delta S^*$) indicate that there are fewer configurations
possible in the activated state and for these configurations and the molecules are ordered to higher extent than in the normal state suggesting a stable bond formation.

The variations in the above parameters with mole fraction and temperature predict the presence of hydrogen bonding between the compounds in system 1 and system 2. The conformation of hydrogen bonding in the equimolar binary mixtures, in system 1 and 2, is confirmed through FT-IR spectra, experimentally and theoretically (Table 4.4).

**6.2 Correlations in System 3 and System 4**

In Chapter-5, different dielectric, thermodynamical and conformational parameters like static permittivity ($\varepsilon_{\text{static}}$), high frequency permittivity ($\varepsilon_\infty$), effective Kirkwood correlation factor ($g_{\text{eff}}$), corrective Kirkwood correlation factor ($g_\tau$), excess Helmholtz free energy ($\Delta F^E$), dipole moment ($\mu$), excess dipole moment ($\Delta \mu$), excess permittivity ($\varepsilon^E$), Bruggeman factor ($f_\beta$), relaxation times ($\tau$), excess inverse relaxation time ($\left(\frac{1}{\tau}\right)^E$), excess activation free energy ($\left(\Delta G^*\right)^E$), excess molar enthalpy of activation ($\left(\Delta H^*\right)^E$), excess molar entropy of activation ($\left(\Delta S^*\right)^E$) and FT-IR spectra (experimental and theoretical) are determined for system 3 (1PN + MB) and system 4 (1PN + EB).

**6.2.1 Correlation between dielectric permittivity and Kirkwood parameters in System 3 and System 4**

In systems 3 and 4 the static permittivity ($\varepsilon_{\text{static}}$) value of mixture is decreasing as the mole fraction of benzoates (MB and EB) is increasing (Tables 5.1 and 5.2) as in the case of IPA. This phenomenon indicates that, in 1PN also, the alignment of dipoles
along the field is changing from parallel orientation to anti parallel orientation. This effect should decrease the effective Kirkwood correlation factor \( g^{\text{eff}} \). From Tables 5.3 and 5.4, it is observed that the values of \( g^{\text{eff}} \) are decreasing with increasing mole fraction of benzoates. This phenomenon has been observed at all temperatures.

### 6.2.2 Correlation among excess Helmholtz free energy, excess dipole moment, excess permittivity and Bruggeman factor in System 3 and System 4

In the present systems, the alignment of dipoles from parallel orientation to anti parallel orientation indicates that the number of effective dipoles is less than the corresponding average value of the pure liquids and correspondingly \( f_g \) must be less than unity. From Tables 5.3 and 5.4, it is clearly observed that the value of \( f_g \) is less than unity at all mixture concentrations and temperatures. Further, for both the systems (system 3 and 4), it is observed that the orientation of dipoles has been changed from parallel to anti parallel which should form \( \beta \) – clusters with positive values of \( \Delta F^E \) [116]. From the high positive values of \( \Delta F^E \) (Table 5.8), it is evident that \( \beta \) – clusters are formed in both the systems up to 0.7 mole fraction of benzoates in the mixture. For 0.8 and 0.9 mole fraction of benzoates in the mixture, negative values of \( \Delta F^E \) are observed which predicts the formation of \( \alpha \)- clusters and accordingly \( f_g \) values are increased for these two mole fractions (Tables 5.3 and 5.4). This effect is witnessed for all temperatures.

It has been observed, experimentally and theoretically, that the values of \( \Delta \mu \) are negative for equimolar binary mixtures in both the systems (Tables 5.9 and 5.10) due to the formation of \( \beta \) – clusters. The same phenomenon has been observed experimentally
for all temperatures. The negative values of $\Delta \mu$, for both the systems (system 3 and 4), suggest that the effective dipole moment gets reduced and simultaneously negative $\varepsilon^E$ values must be obtained. The Figures 5.5 and 5.6 clearly show the negative values of $\varepsilon^E$ and Figures 5.7 and 5.8 show the non-linear variation of $f_\beta$ with $\phi_2$, in consequence with negative values of $\varepsilon^E$.

### 6.2.3 Correlation studies from dielectric relaxation, excess thermodynamic parameters and FT-IR spectra in System 3 and System 4

The low value of the effective Kirkwood correlation factor for benzoates explains the non-associative nature of the compounds which results in low value of relaxation time. The high value of the effective Kirkwood correlation factor for 1PN shows the associative nature of the compound which results in high value of relaxation time. Further, it is observed that the relaxation times of pure 1PN are greater than that of pure IPA due to larger effective radius of the rotating unit. Table 5.11 shows the increment in the relaxation time as the mole fraction of 1PN increases in mixture systems 3 and 4, at all temperatures, due to increasing associative nature. This effect leads to slower rotation of the dipoles, giving negative excess inverse relaxation time $\left( \left( \frac{1}{\tau} \right)^E \right)$ (shown in Figures 5.11 and 5.12).

The positive value of excess activation free energy $\left( \left( \Delta G^* \right)^E \right)$ is due to the formation of $\beta$ – clusters, because $\beta$ – clusters are characterized by reduced internal energy making excess activation free energy positive (shown in Figures 5.13 and 5.14). With increase in the temperature the thermal agitation increases and the dipole requires more energy in order to attain the equilibrium with the applied field and results
in negative excess molar entropy values (shown in Figure 5.15). This indicates that the activated state is more ordered than the normal state, which is true because in the activated state the dipoles try to align with the applied field.

Thus the parameters determined, in the present Chapter 5, correlate with one another and at the same time each parameter supports the formation of hydrogen bonding in the mixture systems. The existence of hydrogen bonding in the equimolar binary mixtures, in case of system 3 and 4, is confirmed through FT-IR spectra, experimentally and theoretically (Table 5.12).

All the data provided in chapters 3, 4 and 5 gives information regarding interaction between the components in the liquids as well as the orientation of the dipoles in the mixture. From this information it has been strongly concluded that there exists hydrogen bonding between the compounds in systems (1, 2 and 3). The following Table 6.1 can be used as a ready reference to reckon the conclusions made in chapters 3, 4 and 5.
Table 6.1: Comparison of various experimental dielectric and thermodynamical parameters for pure and equi molar binary mixture systems at 303K temperature

<table>
<thead>
<tr>
<th>Compound</th>
<th>$\varepsilon_{static}$</th>
<th>$\varepsilon_\infty$</th>
<th>$g_{eff}$</th>
<th>$\tau$</th>
<th>$\Delta F^E$ (Joule/mole)</th>
<th>$\mu$  (Debye)</th>
<th>$\Delta \mu$ (Debye)</th>
</tr>
</thead>
<tbody>
<tr>
<td>propan-2-ol</td>
<td>18.1621</td>
<td>1.9079</td>
<td>3.1316</td>
<td>1.0000</td>
<td>0.0000</td>
<td>173.19</td>
<td>1.63</td>
</tr>
<tr>
<td>(IPA)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>propan-1-ol</td>
<td>20.2783</td>
<td>1.9293</td>
<td>3.3959</td>
<td>1.0000</td>
<td>0.0000</td>
<td>246.23</td>
<td>1.57</td>
</tr>
<tr>
<td>(1PN)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>methyl benzoate</td>
<td>06.8000</td>
<td>2.3070</td>
<td>1.0280</td>
<td>1.0000</td>
<td>0.0000</td>
<td>12.82</td>
<td>1.81</td>
</tr>
<tr>
<td>(MB)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>ethyl benzoate</td>
<td>06.1333</td>
<td>2.2755</td>
<td>0.9432</td>
<td>1.0000</td>
<td>0.0000</td>
<td>13.42</td>
<td>2.05</td>
</tr>
<tr>
<td>(EB)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>System 1</td>
<td>10.1333</td>
<td>2.1609</td>
<td>1.6093</td>
<td>0.7261</td>
<td>136.9287</td>
<td>68.61</td>
<td>3.08</td>
</tr>
<tr>
<td>(IPA+MB)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>System 2</td>
<td>08.8666</td>
<td>2.1785</td>
<td>1.4158</td>
<td>0.5079</td>
<td>186.764</td>
<td>71.12</td>
<td>3.57</td>
</tr>
<tr>
<td>(IPA+EB)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>System 3</td>
<td>12.0000</td>
<td>2.1726</td>
<td>1.9170</td>
<td>0.8054</td>
<td>101.0238</td>
<td>117.13</td>
<td>2.96</td>
</tr>
<tr>
<td>(1PN+MB)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>System 4</td>
<td>10.1333</td>
<td>2.1623</td>
<td>1.6116</td>
<td>0.6810</td>
<td>180.9495</td>
<td>121.24</td>
<td>3.21</td>
</tr>
<tr>
<td>(1PN+EB)</td>
<td></td>
<td></td>
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</tr>
</tbody>
</table>
PART-B Conclusions

- The Dielectric and Thermodynamic studies have been done on four individual systems i.e., propan-2-ol (IPA), propan-1-ol (1PN), methyl benzoate (MB), ethyl benzoate (EB) and four binary systems i.e., propan-2-ol + methyl benzoate (System 1), propan-2-ol + ethyl benzoate (System 2), propan-1-ol + methyl benzoate (System 3) and propan-1-ol + ethyl benzoate (System 4) for various mole fractions at different frequencies and temperatures (303K, 308K, 313K, 318K and 323K).

- Semiempirical - AM1, PM3, MNDO and ab initio - Hartree-Fock (HF) Hamiltonian quantum mechanical calculations have been carried out and the geometry optimization calculations have been performed on pure compounds - propan-2-ol, propan-1-ol, methyl benzoate, ethyl benzoate and the equimolar binary mixture systems - propan-2-ol + methyl benzoate, propan-2-ol + ethyl benzoate, propan-1-ol + methyl benzoate and propan-1-ol + ethyl benzoate.

- In system 1 and system 2 (CHAPTER 3) non-linear variation of \( \varepsilon_{\text{static}} \) and \( \varepsilon_{\infty} \) is observed with mole fractions, at all temperatures. This non-linearity indicates the interaction between the compounds in the systems.

- The values of \( g^{\text{eff}} \) are greater than unity for IPA, MB at all temperatures, indicating parallel orientation of the electric dipoles and the values of \( g^{\text{eff}} \) are less than unity for EB, at all temperatures, indicating anti-parallel orientation of the electric dipoles. The decrement of \( g^{\text{eff}} \) value, as the mole fraction of MB, EB increases in mixture, indicates that the alignment of dipoles along the field is changing from parallel orientation to anti parallel orientation in both systems 1 and 2.
➢ The deviation of $g_f$ from unity, in the binary mixtures of system 1 and system 2 indicates the magnitude of hetro interaction between the compounds in the mixture.

➢ The high positive values of $\Delta F^E$, in system 1 and system 2, up to 0.7 mole fraction of benzoates in mixture at all temperatures, indicate the formation of $\beta$ – clusters with anti-parallel alignment. Due to the formation of these $\beta$ – clusters the effective dipole moment will be decreased. For 0.8 and 0.9 mole fraction of benzoates in mixture, negative values of $\Delta F^E$ are observed which predicts the formation of $\alpha$-clusters and accordingly $g_f$ values are increased for these two mole fractions. This effect is witnessed for all temperatures.

➢ In system 1 and system 2, the increase in the dipole moment, of equimolar mixture when compared to the individual systems indicates the hydrogen bond formation. Further, the negative excess dipole moment values indicate the absence of any contribution from ionic structure. The theoretical dipole moment values are in reasonable agreement with the experimental values.

➢ The hydrogen bonding energies for the systems 1 and 2 are found to be negative, in all theoretical models, indicating the formation of hydrogen bonding.

➢ The negative values of $\varepsilon^E$ and the non-linear variation of $f_g$ with volume fraction $\phi_2$, in system 1 and system 2 (CHAPTER 4), suggest the formation of multimers through hydrogen bonding.

➢ The relaxation times of pure propan-2-ol are high due to the formation of intramolecular hydrogen bonding between one alcohol molecule and another (R-O-H…O-H-R), which leads to the formation of self-associated groups.
The relaxation times of pure methyl and ethyl benzoates are less compared to propan-2-ol. This is due to the non-existence of self-associated groups.

The relaxation times are found to increase, in the binary mixture of system 1 and system 2, as the concentration of propan-2-ol increases in mixture at all temperatures indicating the formation of hydrogen bonding between hydroxyl group (-OH) of propan-2-ol and –CH group of methyl and ethyl benzoates, which restricts the free internal rotation of the molecules.

The values of excess inverse relaxation time are negative for the systems 1 and 2. These negative values indicate the slower rotation of dipoles due to the formation of hydrogen bonded structures producing a field, which hinders the effective dipole rotation.

The increasing positive values of activation free energy, for systems 1 and 2, suggest the existence of molecular association between unalike molecules in the mixture. In the present study activation free energy values in system 2 are greater than that of system 1, which indicates the strength of bond formation in system 2 is high compared to system 1.

The molar enthalpy values for both the systems (1 and 2) are positive indicating the bond formation. The molar enthalpy of activation of dielectric reorientation for system 2 is observed to be greater than system 1, indicating the strength of bond formation.

The negative values of molar entropy of activation, in both the systems (1 and 2), indicate that the activated complexes have lower entropy than the reactants, since entropy is a measure of disorder or chaos of the reaction. These values also indicate
that there are fewer configurations possible in the activated state and for these configurations the molecules are ordered to higher extent than in the normal state.

- The FT-IR analysis convinces intermolecular hydrogen bonding of the equi molar binary mixtures (system 1 and system 2) effectively with proportionate variations in stretching frequencies of –OH and –CH compared to their respective pure systems. The theoretical FT-IR values are in reasonable agreement with the experimental values.

- In systems 3 and 4 (CHAPTER 5) also the non-linear variation of $\varepsilon_{\text{static}}$ and $\varepsilon_{\infty}$ is observed with mole fractions at all temperatures, as in system 1 and system 2, indicating the interaction between the compounds.

- The values of $g^{\text{eff}}$ are also greater than unity for 1PN, at all temperatures, indicating parallel orientation of the electric dipoles. But in both the mixture systems (3 and 4), the parameter $g^{\text{eff}}$ exhibits a steadily decreasing tendency as the concentration of MB, EB goes on increasing in mixture at all temperatures. This tendency leads to the conclusion that there exists heterogeneous interaction between the compounds in the mixture systems.

- As the concentration of MB, EB increases in mixture, $g_f$ values deviate more from unity indicating the hetero interaction between the compounds. Further it is observed that $g_f$ values deviate more from unity in system 4 than in system 3, at all temperatures, indicating stronger hetero interaction in case of system 4.

- The high positive values of $\Delta F^E$, in systems 3 and 4 (chapter 5), indicate that $\beta$ – clusters are formed up to 0.7 mole fraction of MB, EB in mixture. For 0.8 and 0.9
mole fraction of MB, EB in mixture, negative values of $\Delta F^E$ are observed which predicts the formation of $\alpha$- clusters same as in case of system 1 and 2.

- In systems 3 and 4 the increase in the dipole moment of equimolar mixture when compared to the respective individual systems indicates the hydrogen bond formation. Further, the negative excess dipole moment values, in both the systems, indicate the absence of any contribution from ionic structure.

- The negative values of $e^E$ suggest the formation of multimers through hydrogen bonding. The more negative deviations in $e^E$ values of system 4 compared to system 3 indicate that the strength of hydrogen bond formation is more in system 4 than in system 3.

- The relaxation times of pure 1PN are greater than that of MB and EB. The relaxation times increase as the concentration of 1PN increases in mixture, indicating the bond formation probably between –OH group of 1PN and –CH group of benzoates. The values of excess inverse relaxation time are negative for the systems 3 and 4 as in case of system 1 and system 2. Further it is observed that the negative deviations of excess inverse relaxation time are more in case of system 4 than in system 3 which shows greater strength of intermolecular hetero interaction in system 4.

- The values of excess activation free energy are positive, in both the systems (3 and 4), indicating the presence of interaction between the molecules of the mixtures.

- The negative values of excess molar enthalpy, for both the systems, show that strong attractive interactions are present between unlike molecules of the mixtures. The formation of hydrogen bonding between the components in system 3 and system 4 is also justified by the negative values of excess molar entropy.
The analysis of experimental FT-IR convinces the intermolecular hydrogen bonding of the binary mixtures propan-1-ol + methyl benzoate (system 3) and propan-1-ol + ethyl benzoate (system 4) effectively with proportionate variations in stretching frequencies of –OH and –CH compared to their respective pure systems. The theoretical FT-IR values are in reasonable agreement with the experimental values.

The correlations among the various dielectric and thermodynamic parameters, determined experimentally and theoretically, are discussed comprehensively in CHAPTER 6 (Part – A). Interestingly all the parameters determined in the present work correlate one another and at the same time each parameter supports the formation of hydrogen bonding between the mixture systems.

**Future Work**

- Wide frequency measurements can be taken up using coaxial probe technique.
- Neutron diffraction technique will be helpful for a better understanding of the complexes formed through hydrogen bonding. Temperature variation FT-IR spectra analysis can be focused.
- Study of $^1$H NMR spectra is useful to support the existence of hydrogen bonding in the binary mixture systems.
- Molecular polarizability studies can be taken up.
- Computational analysis with Density Functional Theory (DFT) and Moller - Plesset (MP2) calculations can be performed to obtain more accurate results.