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Evaluation of molecular interactions between *o*-methoxy nitrobenzene and certain alcohols in *n*-hexane medium using ultrasonic sound at 303K

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The parameters like ultrasonic velocity, density and viscosity of ternary liquid mixtures containing di-substituted benzene [*o*-methoxynitrobenzene (*o*-MNB)] with 1-alkanols (1-propanol/1-butanol/1-pentanol) in *n*-hexane medium have been measured experimentally at 303K for the equimolar concentration of 1:1 ratio and the concentration ranges from 1×10^{-3}M to 1×10^{-2}M. The normal acoustical properties and their excess properties such as excess ultrasonic velocity (U^E), excess acoustic compressibility (κ^E), excess free length (L_f^E), excess free volume ($V^E{}_f$) and excess internal pressure ($\pi^E{}_i$) have been computed. The molecular interactions and their strength have been quantitatively assessed and the cyclic structure is proposed from the determination of thermodynamic parameters like formation constant (K), free energy of formation (ΔG_F), enthalpy change (ΔH) and entropy change (ΔS) through the formation of the hydrogen bonded complexes. The results are discussed in terms of intermolecular interaction based on existence of carbon profile between the components present in the ternary liquid mixtures.

Keywords: Ultrasonic velocity, Primary alcohols, Interaction, Ternary liquid mixtures, *o*-Methoxy nitrobenzene

Ultrasonication is a simple and convenient non-destructive tool that is extremely useful in the study of intermolecular interaction and helps to develop molecular sciences significantly. The structural arrangement of molecules in pure liquids and liquid mixtures is changed by the presence of intermolecular attraction in these systems[1,2]. Extensive investigation of molecular interactions (strong as well as weak) in binary and ternary liquid mixtures is useful in understanding various physical properties of such systems[3-6]. Hydrogen bond is thought to be a kind of weak dipole-dipole attraction and it plays a significant role in strengthening of molecular interactions and stabilizing supra-molecular complexes where non-covalent assemblies of molecules held together by various weak interactions, including hydrogen bonds. These systems are important in the study of chemical, physical and biological processes[7-9]. The three ternary liquid mixtures which are under investigation namely *o*-MNB+1-Pro/1-But/1-Pen in *n*-hexane can act as electron donors in the formation of charge transfer complexes and hydrogen donor in the formation of hydrogen bonded complexes which permit them to interact with other molecules with specific interactions. Understanding of intermolecular attraction in pure liquids and mixtures through thermodynamic and other acoustical properties including excess parameters are useful in industrial and pharmaceutical research.

The present study deals with the ultrasonic investigation of hydrogen bonded complexes formed between *o*-methoxy nitrobenzene (hydrogen acceptor) and aliphatic alcohols (1-pro/1-but/1-pen) in non-polar *n*-hexane solution at 303K. The compounds are so chosen in such a way that influence of strong electron withdrawing nitro group in anisole and the increase in the length of the alkyl chain in alcohols on the stability of H-bonded complexes can be assessed. The type and strength of the interaction between like and unlike molecules in the system have been discussed in terms of different types of molecular interaction. *o*-Methoxy nitrobenzene is used primarily as a precursor to *o*-anisidine which is used extensively in the synthesis of azo dyes[10]. It has also been used as an intermediate for various pharmaceuticals[11]. *n*-hexane, one of the components used as a solvent in the present investigation is an un-branched alkane, non-polar, volatile solvent and a colourless liquid with petroleum like odour, used as a solvent, paint thinner, made from crude oil. *n*-Hexane is used for the extraction of vegetable oils (soya beans), as a solvent in coordination complex catalysed polymerization of olefins and in adhesive formulations. The uses of *n*-hexane in industries are abundant as corrosive inhibitors, anti-scaling agent, fuel and fuel additives. On the other hand, aliphatic primary alcohols are one of the components in the current study which contain a hydroxyl group attached with carbon atom, which exhibit different behaviour due to different numbers of hydrogen atoms on hydroxy bearing carbon atom. Solubility of alcohols attributed to association of other component by intermolecular hydrogen bonding. In gasoline formulation alcohols are used as octane booster or antiknock additives[12].

In continuation of our earlier studies[13-15], in order to investigate the influence of increase in the length of the alkyl chain of the aliphatic mono hydroxy alcohols in carbon one with *o*-MNB, and to establish cyclic structure to the compound, the thermodynamical parameters in addition to usual acoustical parameters and excess parameters are evaluated for *o*-MNB+1-PRO/1-BUT / 1-PEN in *n*-hexane medium at 303K.

Experimental Section

Materials used

The mixture (*o*-methoxy nitrobenzene +1-propanol/1-butanol / 1-pentanol+*n*-nexane) of various concentrations (1×10^{-3}M to 1×10^{-2} M) of equal ratio 1:1 were prepared by taking analytical reagent grade and spectroscopic reagent grade chemicals. The procurement about the chemicals is provided in Table S1. All the component liquids were purified by the standard methods.

Instruments and techniques

Ultrasonic velocity measurements were made using an ultrasonic interferometer (Model F-81, supplied by M/S Mittal Enterprises, New Delhi, India) with the accuracy of $\pm0.1\text{ms}^{-1}$. Water at desired temperature is circulated through the outer jacket of the double-walled measuring cell containing the experimental liquid. The densities of the mixture were measured using a 10 mL specific gravity bottle by relative measurement method with an accuracy of ±0.01 $\text{Kg}\cdot\text{m}^{-3}$. An Oswald viscometer (10 mL) with an accuracy of ±0.001 $\text{Ns}\cdot\text{m}^{-2}$ was used for the viscosity measurement. The flow time was determined using a digital racer stopwatch with an accuracy of ±0.1s.

Derived Parameters

The following acoustical and thermodynamics parameters were calculated from the experimental data:

(i) Adiabatic compressibility (β) has been calculated from the ultrasonic velocity (U), and the density (ρ) of the medium using the Newton- Laplace equation[15] as follows:

$$\beta = 1/U^2\rho \qquad ...(1)$$

(ii) Intermolecular free length (L_f) has been determined as[16] follows:

$$L_f = K_T\beta^{1/2} \qquad ...(2)$$

Where K_T is the temperature – dependent constant known as Jacobson's constant ($K_T = 2.131\times10^{-6}$), and β is the adiabatic compressibility.

(iii) Free volume (V_f) in terms of ultrasonic velocity (U) and the viscosity (η) of liquid is as follows:

$$V_f = (M_{eff}\,U/\,k\eta)^{3/2} \qquad ...(3)$$

Where M_{eff} is the effective molecular weight of the mixture ($M_{eff} = \Sigma m_iX_i$, where m_i and X_i are the molecular weight and mole fraction of individual constituents, respectively), k is temperature independent constant which is equal to 4.281×10^9 for all liquids.

(iv) Internal pressures ($\prod_i$) can be calculated using the relation as follows:

$$\prod_I = bRT\,(k\eta/U)^{1/2}\,(\,\rho^{2/3}\,/\,M_{eff}^{7/6}) \qquad ...(4)$$

Where b stands for cubic packing, which is assumed to be 2 for all liquids, k is a dimensionless constant independent of temperature and nature of the liquids, its values is 4.281×10^9. T is the absolute temperature in Kelvin, M_{eff} is the effective molar weight, R is the universal gas constant.

(v) The Gibbs free energy can be determined using the relation as follows:

$$\Delta G = k_{B,}T.\ln(k_B.T.\tau/h) \qquad ...(5)$$

Where τ is viscous relaxation time, T is the absolute temperature, k_B is Boltzmann's constant, and h is Planck's constant.

6. Acoustic impedance (Z) is given as follows:

$$Z = U.\rho \qquad ...(6)$$

Excess Parameters

In order to study the non-ideality of the liquid mixtures, the difference between the values of acoustic and thermodynamic parameters of real mixtures (A_{exp}) and those corresponding to the ideal mixtures(A_{id}) were computing using the following equation:

$$A^E = A_{exp} - A_{id} \quad ...(7)$$

Where A^E represents excess parameters, $A_{id} = \Sigma A_i X_i$, i=1to n, A_i any parameter, X_i mole fraction of the components.

Thermodynamical Properties

$$\Delta G_F \text{ (free energy change)} = -RT \ln K \quad ... (8)$$

$$\Delta S \text{ (entropy)} = (\Delta G_F + 26604)/T \quad …(9)$$

The viscous relaxation time was obtained using the relation

$$\tau = (4/3)\, \beta\, \eta \quad …(10)$$

Where η is the viscosity and β is the adiabatic compressibility that can be calculated from the ultrasonic velocity (u) and the density of the system (ρ) as

$$\beta = (u^2 \rho)^{-1}$$

The value of enthalpy change ΔH is obtained from the graph.

Results and Discussion

Acoustical parameters and its role

The measured ultrasonic velocity (u), density (ρ) and dynamic viscosity (η) for *o*-methoxy nitrobenzene + 1-propanol (1-Pro)/1-butanol (1-But)/1-pentanol (1-Pen) in *n*-hexane medium at 303Kare listed in Table S2. The calculated values of adiabatic compressibility (κ), free volume (V_f), internal pressure (π_i), acoustic impedance (Z) and free length (L_f) for this system are also given in Table S3 and Table S4. Fig. (a) represents plot of 'u' against molar concentration for three different aliphatic alcohols along with *o*-MNB and *n*-hexane at 303K. Fig. S1 indicate that there is increase in ultrasonic velocity with concentration for all the three systems. However, there is linear increase in velocity with concentration at a given temperature. The solute-solvent interaction in these systems cannot be neglected due to carbon profile of interaction though *n*-hexane (solvent) which is non-polar. This can be validated by changing another non-polar solvent. In fact, that is going to be the test of carbon profile involvement in these ternary systems. The trend in 'u' values suggests that there is specific solute-solute interaction between *o*-MNB and alcohol molecules. Further, there is regular increase in 'u' value with increasing concentration at the temperature. This indicates that the interaction between unlike molecules of the solute increases with concentration. If we consider the trend in 'u' with temperature at a given molarity we find that there is decrease in 'u' suggesting the inter-molecular attraction between *o*-methoxy nitrobenzene and the alcohol molecules weakens when the temperature is increased. This is due to thermal agitation of the molecules in the system which affects the strength of intermolecular interaction. The uniform increase in density and viscosity with concentration in the systems at a given temperature also suggests that the extent of complex formation increases with the increase in concentration. The existence of specific interaction such as H-bond in the complex formed between *o*-MNB and alcohols can be established from the trend in the adiabatic compressibility (κ) with concentration in the ternary liquid mixtures. It is observed that 'κ'decreases with increasing concentration (Table S3) in all three systems. Plots of κ against concentration at three alcohols at 303K are depicted in Fig. (b). It may be pointed out here that it is the compressibility that changes with structure which results in the variation in in ultrasonic velocity. The decrease in adiabatic compressibility (κ) in liquid mixtures shows that there is certainly contraction on mixing of the components and the considerable variation is attributed to H- bonded complex formation in the systems. This conclusion may be further established through the variation in free length (L_f) with concentration. It may be seen from the data given in the above mentioned tables that free length (L_f) also decreases with concentration just as the behaviour of adiabatic compressibility. The molecules are brought close and the close packing is indicated by the decrease in compressibility as well as L_f values. It may be seen that there is regular decrease in L_f with increase in concentration in the liquid mixture at constant temperature. The internal pressure (πi) and acoustic impedance (Z) values for ternary mixtures are calculated at different concentration and presented in Table S3 and Table S4. Plots of (πi) against concentration are depicted in Fig. S3. The data presented in the tables and the plots indicate that πi values are significantly high in the liquid mixtures and it increases with concentration showing the presence of specific solute-solute interactions between unlike molecules. Further, there is non-linear variation in the πi values with concentration which supports the formation of H-bonded complex in the system. It can be seen there is increase in πi value with concentration which indicates that the degree of complex formation increases with concentration.

It can be observed from Table S2, the density of ternary mixture decreases from propanol to pentanol. It is in contrast to the values of individual alcohols where density increases. The carbon value increases from propanol to pentanol and nearing optimal value. This may be explained in terms of carbon one as there are network of carbon one plays the structural dealing[17]. In this regard, it is the network formation may be crucial in taking density and accordingly the acoustic one. With this it is important to take carbon one in the dealing of material preparation.

Fig. S4 shows plot of free length against concentration. When the temperature is raised there is breaking of molecular interactions and makes the molecules to move apart. Consequently, the system becomes less close-packed and more compressible. This is clearly reflected in the values of L_f' and 'κ' with increase of concentration at a given temperature.

The strength of inter-molecular interaction in binary and ternary liquid mixtures can be assessed from the trend in free volume with concentration. In the present investigation, the free volume (V_f) is found to show a reverse trend as that of internal pressure which indicates that there is a specific interaction existing between the unlike solute molecules. The decreasing trend in V_f with concentration shows that the close packing of the molecules inside the shield is due to larger magnitude of existing interactions. Another acoustic parameter that can be used to establish the intermolecular interactions in binary and ternary liquid mixtures is acoustic impedance (Z). Acoustic impedance values at the temperature and at various concentrations are computed for the ternary mixtures and the values are listed in Table S2. Generally, large values of 'Z' indicate the presence of specific interaction between solute molecules. It can be seen from the values of 'Z' increases with concentration indicating the formation of H-bonded complex between ethereal oxygen and alcohol molecules. The strength of intermolecular attractions in the H-bonded complexes in the liquid mixtures can be measured by available volume. In the present systems, the available volume decreases with increase of concentration which shows that the interaction increases with increase of concentration. Molar cohesive energy (MCE) in a liquid mixture is a measure of cohesive force of attraction between the molecules of the components. It is calculated from internal pressure and effective molar volume in liquid mixtures. These values are calculated for the systems and they are listed in Table S4. It can be seen that these values are relatively high and there is increase in cohesive energy with increases in concentration indicating that the molecular interaction between *o*-methoxy nitrobenzene and 1-alkanols increases with concentration. Plots of MCE against concentration for the ternary mixtures of the three systems are depicted in Fig. S5. Molecular interaction parameter (χ) is a useful acoustic parameter employed in the assessment of molecular interaction in binary and ternary liquid mixtures. The magnitude and sign of the χ values are used in assessing the strength of molecular interactions. These values are calculated and they are presented in Table S4. Plots of χ *vs*. concentration are given in Fig. S6. The data in the above mentioned tables and the plots in Fig. S6 indicate that the χ values are negative at all the investigated concentrations and temperatures showing that there are strong intermolecular attractions between ether and alcohol molecules.

Lennard-Jones Potential is also used to detect the strength of molecular interactions in binary and ternary liquid mixtures. These values are computed for the present system and given in Table S4. These values increase with concentration indicating the increase in the strength of molecular interaction between *o*-MNB and 1-alkanols with concentration.

Excess thermo-acoustic properties

In order to understand the nature of molecular interaction coherently between the components in the liquid mixtures it is better to study the excess thermo-acoustic properties of the liquid mixtures. The following excess properties are investigated in the three systems at different concentration and temperature 303K. Excess values of ultrasonic velocity (u^E), excess adiabatic compressibility (κ^E), excess free length (L_f^E), excess free volume (V_f^E), excess internal pressure (π_i^E) and excess acoustic impedance (Z^E). The positive values of excess properties show the presence of dispersive forces, while the presence of dipole – dipole, dipole induced dipole, charge transfer interaction and hydrogen bonding between unlike molecules are responsible for possessing negative values[18,19]. The values of excess parameters for the *o*-MNB + PRO, *o*-MNB + BUT and *o*-MNB + PEN systems are listed in Table S5 and

Table S6 in *n*-hexane solution at 303K respectively. In the present study, the values of excess ultrasonic velocity are negatives at all the concentrations and at the investigated temperatures for *o*-MNB + PRO, *o*-MNB + BUT and *o*-MNB + PEN systems in *n*-hexane solution. The negative values of excess ultrasonic velocity (Table S5) indicate the presence of strong attractive forces between the components in all three systems. The plots of excess ultrasonic velocity against concentration are depicted in Fig. S7.

Increase in Jacobson's due to loss of dipolar association and breaking up of H-bonding and difference in molecular size of the component molecules and decrease in free length due to dipole-dipole interactions, H-bond association and complex formation between unlike molecules in liquid mixtures determine the sign and magnitude of excess compressibility (κ^E), values[20,21]. The first effect results in increase in inter space between molecules in the mixture consequently sound waves cover small distances in mixtures than in pure components. This would result in positive deviation in both isentropic compressibility and free length. The decrease in free length is due to the decrease in interspace between molecules and sound waves cover larger distances in the mixtures. This would result in positive deviation in ultrasonic velocity and negative deviation in compressibility and free length. The excess compressibility for the systems *o*-MNB+PRO, *o*-MNB + BUT and *o*-MNB+PEN in *n*-hexane medium is negative at all the concentrations (Table S5) which indicate the presence of strong interactions between unlike molecules which may result in the formation of H-bond between *o*-MNB and PRO/BUT/PEN molecules[22]. In other words, negative values of excess adiabatic compressibility show the structure forming tendency and positive values is the structure breaking tendency[23]. Plots of κ^E against concentration at three systems are given in Fig. S8. Negative values of excess internal pressure and excess free length also indicate the existence of strong molecular interaction of H-bond type in the present systems. The study of excess internal pressure plays a vital role in the interaction of the components in the liquid mixtures. A positive value of excess internal pressure indicates the existence of weak interaction between the components in the liquid mixture and negative value shows the existence of strong interaction in the liquid mixture. In the present investigation, excess internal pressure is negative at all concentrations (Table S6 and Fig. S9) and the values are increasing with increase of concentration. This shows that there is strong interaction between ether and 1-alkanols molecules which may be of H-bond type. The values of excess free length are negative in the ternary liquid mixtures of *o*-MNB+alkanols systems and according to Fort and Moore[24], negative value of excess free length predicts the existence of strong interaction in the ternary liquid mixture due to charge transfer, dipole-dipole, dipole induced dipole interaction, interstitial accommodation and orientation ordering. In our present study, the negative value of excess free length (Table S5, Fig. S10) supports the presence of hydrogen bonding. This observation is further supported by negative values of excess adiabatic compressibility due to structural formation tendency. Adgaonkar *et al.*[25] shows the positive values of excess free volume indicates the presence of weak molecular interaction and negative values shows the strong molecular interaction between the component in the ternary liquid mixtures. In the case of *o*-MNB-ALKANOLS system the values of excess free volume are positive and increase with the increase of concentration (Table S6, Fig. S11). It shows that of the interaction increases with concentration.

The excess acoustic impedance values are calculated for *o*-MNB-ALKANOLS systems at various concentrations and they are listed in Table S6. Plots of excess acoustic impedance against concentration are given in Fig. S12. The positive excess value of acoustic impedance indicates the presence of strong interaction in the liquid mixtures. In the present study, values of excess acoustic impedance increases with increase of concentration but decrease with increase of temperature. The values of excess acoustic impedance also prove the strong molecular interaction between components in the ternary liquid mixtures.

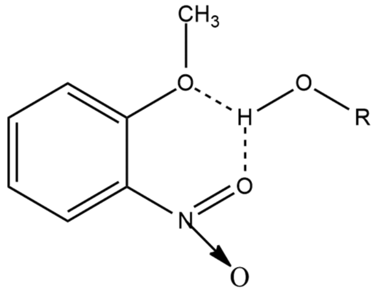
It may be seen from the data, in the above mentioned Table S5 and Table S6 that the trends in excess properties with concentration are similar to those observed in *o*-MNB+PRO system indicating the presence of strong intermolecular attraction between *o*-MNB and BUT molecules. However, if we compare magnitude of the values obtained in the two systems they are less in *o*-MNB + BUT system than in *o*-MNB + PRO system showing that the hydrogen bond is weaker in *o*-MNB + BUT system than in *o*-MNB + PRO system.

It is observed from the data in Table S5 and Table S6 that the trends in excess properties with concentration are similar to those observed in *o*-MNB+PRO and *o*-MNB+BUT systems showing the presence of strong intermolecular attraction between *o*-MNB and PEN molecules. However, comparing the magnitude of the values obtained in the three systems, they are less in *o*-MNB+PEN system than in *o*-MNB+BUT system which are less than in *o*-MNB+PRO system showing that the strength of hydrogen bond in the three systems is in the order *o*-MNB+PRO>*o*-MNB+BUT>*o*-MNB+PEN at 303K.

Thermodynamic properties

The main aim of the present study is to study the effect of increasing chain length of alkyl group of 1-alkanols on the strength of the H-bonding between aromatic substituted ether (o-methoxy nitrobenzene) and aliphatic alcohols. This can be quantitatively assessed by the determination of formation constant (K), free energy of formation (ΔG_F), enthalpy change (ΔH) and entropy change (ΔS) for the formation of the hydrogen bonded complex. The equilibrium constant for the formation of 1:1 stoichiometric complex can be calculated from the ultrasonic velocity using the Kannappan equation[26,27]. This method gives constant K values independent of concentration and it can be used for weak as well as strong complexes. It has been used for the formation of several charge transfer and hydrogen bonded complexes[28-31]. K values are calculated for the three systems at 303Kand they are given in Table S7. These are mean values computed at different concentrations.

Enthalpy of formation and entropy change values are calculated from the K values for three different systems which are under investigation using thermodynamic relations[32,33]. Analysis of K values provided in Table S7 clearly indicate that the stability of H-bonded complex between NA and alcohols is in the order *o*-MNB+PRO>*o*-MNB+BUT>*o*-MNB+PEN in *n*-hexane medium. It has been reported that 1-alkanols form H-bonded complexes with cyclohexanone in dimethyl acetamide (DMA) and the order is reported as PRO > PEN> BUT. The reason for the reverse in BUT and PEN is given as due to the proton abstracting ability of DMA. But in the present work, non-polar *n*-hexane medium is used and hence the role of solvent on the stability of complex is negligible. Therefore, it may be concluded that the strength of hydrogen bond in these complexes decreases with increase in chain length. It is observed that the formation of H-bonded complex is exothermic for which the K value plays a vital role. The values of ΔH listed in Table S7 shows that the formation of the complexes in the three systems is exothermic. It is found that the entropy change for the formation of complex is negative in the three systems indicating the orderliness increases during the formation of the complex. Based on the above facts, the following cyclic structure (Fig. 1) may be proposed for the H-bonded complex.



Where, R = $-CH_2-CH_2-CH_3$/ $-CH_2-CH_2-CH_2-CH_3$ / $-CH_2-CH_2-CH_2-CH_2-CH_3$

Fig. 1 — Cyclic structure of the H-bonded complex

It may be seen that the hydrogen of alcohol may be accepted by either etherial oxygen or oxygen of $–NO_2$ group. Thus, formation of H-bonded complexes in these three systems is also supported by the negative entropy values. Further, these H-bonded complexes are thermodynamically stable as indicated by the negative ΔG_F values for all the complexes. Relaxation time values for the three complexes are found to constant (Table S7) which indicates the similar type of complex is formed in all the three systems.

Compared to existing ternary one, there may be another one with same molecular identity will produce equivalent structural one provided there is adequate linearity in structure and available for flexible one. Accordingly, it is important to take carbon one in the discussion of ternary one and all[34,35]. With this we demonstrate here in that ternary one may be another way of dealing individual small molecules to club together in the event of necessary preparation of ever wanted carbon profile based system to deal the atmospheric one where there is no evidence of other molecules exist to interact. In the event of design in space it is to be considered that everlasting informed carbon may be crucial in design and all. In this connection it is considered here the deal of increase in temperature in the event of mass molar concentration and all. It is only the aromatic one where there is enough carbon to mould in to other molecular system where there is no adequate carbon and all. With this we arrive at values that may be taken for further development in the era of space research and all.

Conclusions

Ultrasonic studies are made on three ternary systems containing *o*-methoxy nitrobenzene as hydrogen acceptor and three structurally different primary alcohols in *n*-hexane solution at 303K. The variation in acoustic properties with concentration at a given temperature establishes the existence of specific interaction (H-bonded attraction) between *o*-MNB and alcohol molecules and the carbon profile that is crucial in dealing this ternary system of material one. Excess thermo-acoustic properties are reported for the three systems which also support the existence of H-bond between *o*-MNB and alcohols and carbon one. Thermodynamic properties such as stability constant (K), free energy change (ΔG_F), enthalpy change (ΔH) and entropy change (ΔS) for the complex formation are determined. These parameters are used to assess the stability of complexes and to study the influence of chain length of the alcohols on the stability of the complex. Negative values of free energy of formation show that these complexes are thermodynamically stable. The formation of these complexes involve exothermic as evident from the negative enthalpy values. These complexes have similar structure as shown by the relaxation time values for all the three systems.

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Supplementary Information

Supplementary information is available in the website http://nopr.niscpr.res.in/handle/ 123456789/ 58776.

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