An Overview of Statistical Thermodynamic Consideration of Binary Mixtures Composed of Molecular Fluids: A Special Instance to The Heats of Mixing of Binary Mixtures of Organic Fluids Over The Whole Composition Range With Graphical Representation

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Abstract

The excess enthalpy of most binary liquid mixtures is calculated through numerous models. This research uses the 'Hard-Fluid Model' under various thermodynamic parameters. This research encompasses the application of the model to instigate the excess enthalpy of Binary Liquid Mixtures. A statistical thermodynamic approach is applied to the system of mixtures. This treatment is applied to organic fluids like Benzene, Carbon Tetrachloride n-hexane, Cyclohexane, etc., and their mixtures over the whole composition range and thermodynamic systems.The calculated results are shown as a function of molefraction graphically. Hence, the calculated results of the research are compared to the experimental results of the binary mixtures in a thermodynamic system. The results are then calculated from other existing methods in research. The results from the corresponding mixture of binary liquids are found to be satisfactory in certain cases that are discussed in the research. This research motivated researchers and physicists to study the excess enthalpy of different binary liquid mixtures through the methods and approaches of existing thermodynamic systems.

Keywords: Heats of Mixing (Excess Enthalpy),Statistical Thermodynamics, Thermodynamic Systems for Binary Liquids, Hard-Fluid Model,Binary Liquid Mixtures, Whole Composition Range, Molefraction, Graphical Representation.

Introduction

Data of some systems related to thermodynamic enthalpies and the excess enthalpy of binary liquid mixtures are Benzene + Carbon Tetrachloride, Cyclohexane + Carbon Tetrachloride, Cyclohexane + Benzene, Cyclohexane + n-hexane, n-hexane + Benzene, etc. [1].

These binary liquid mixtures hold to be quite useful in testing existing thermodynamic systems for theoretical solutions of non-electrolyte and binary organic and dense liquid mixtures. The non-electrolytes and the liquids that are components in thermodynamic systems consist of molecules that have relatively simple shapes and structures. These binary mixtures can further be prepared at good purity and compositions [2].

The thermodynamic systems along with the binary liquid mixtures enable the chemists and chemical engineers to rely on the data provided by the thermodynamic systems and obtain reliable data for process designing and estimation of the thermodynamic system. The data obtained from the system helps researchers and physicists provide information on the relationship between the binary liquid mixtures, their macroscopic properties, and the functions of the thermodynamic systems for fundamental research considerations. However, these research considerations are relatively rare and do not appreciate research studies of phase behaviors [3].

Literature Review

Calculations on the excess enthalpy of the thermodynamic functions related to binary liquid mixtures of non-polar liquids have been carried out by various thermodynamic models that are reported in literature [4]. In some instances, the thermodynamic system is held specifically for mixtures containing Benzene and Acetonitrile. However, insufficient data has been found on generalizing the theoretical equation that may co-relate with the experimental results yet produced by researchers and existent in literature. Researchers have used the results of the theory of scale particles to calculate and mitigate the heat of vaporization of pure liquids [5, 6.] The scale particle theory is also used to calculate the excess entropy of binary liquid mixtures. Researchers [7] have also incorporated the results of the heat of vaporization to calculate the molar heat of the mixing of non-ionic binary solutions. This work reports an extension of the theory of thermodynamic properties of solutions of non-ionic liquids, previously deduced by the author [8].

The thermodynamic properties of the solutions of non-ionic liquids aim to correlate the experimentally deduced heat of the mixing of binary liquid mixtures. The role of the thermodynamic properties is to produce experimental results through integrated models that relate the heat of the mixing of ionic solutions in such a way that the molecular structure and the intermolecular attractions are attainable [9]. These interactions will help deduce equations that give a quantitative agreement compared to the experimental values published in research. The equations thus deduced have been derived through previously existing theoretical equations in literature. In the current study, the researchers have reported the results of the heat of mixing of some systems from statistical thermodynamic consideration. The 'hard sphere model' for a mixture of liquids is used and the contact area (a) has been calculated from various physico-chemical properties. Finally, the reported results have been discussed based on molecular structure and intermolecular interactions of the equations involved [10, 11].

Methodology

Calculations

The interactions of the intermolecular energies that exist in liquids and binary solutions are related to the surface areas of the segments of liquids that have intermolecular binding. The segments are composed of molecules for the energies (per unit area) to come in contact with the surfaces and develop a constant that is in equilibrium. The segments related to different contact areas have different contact energies due to differences in the type of bonding and surface interactions [12]. The researchers and physicists have come up with equations that have been based on these ideas. Thus, the ideological theories of the researchers are used to understand and develop the magnitude of the properties and parameters that are taken into consideration when understanding the heat of vaporization and the head of mixing of binary liquid mixtures. Thus, the parameters involved can be incorporated into other thermodynamic systems and functions that contain similar segments. Eventually, these parameters can help understand the nature of the thermodynamic functions and also predict the heat of vaporization and mixing curved through quantities and properties that are derived for theoretical implications and understandings [13].

The molecules and ions in atoms consist of interaction energies that pair the ions together to form atoms. However, due to under-compensated interaction energies, the ions tend to fall apart quite rapidly. In generalized form, it creates an increased distance in the interatomic energies between constituted atomic particles. However, in liquids, the largest part of the energies of the intermolecular interactions come from between pairs of atoms and ions with whom the connected and adjacent molecules are even closer [14]. The average sum of the weaker intermolecular interactions is due to the atomic interactions being weak. Hence, they have weaker efficiencies and bonding capacity between different molecules, pure liquids, and binary mixtures. Consequently, they have smaller summation averages as compared to different liquids that have similar types of bonding and mixing concentrations.

The structure of liquids, except for those that contain monoatomic molecules is highly complex and cannot be used to calculate the average intermolecular energies. The energy summation can also be a result of the total intermolecular energies or through the atom-atom interaction energies. Research shows that the interaction energies of the interatomic distance are co-dependent, except for the insufficient interactions between simple ions [15, 16.] However, this is unfortunately quite true in H-H interactions as well.

To avoid discrepancy due to the above-discussed factors, researchers need to use thermodynamic models to attain an approximately sufficient yield that can also be applied to numerous theoretical approaches and experimental measurements, involving pure liquids or binary mixtures. However, the model used by the researchers in this study tends to meet the requirements and parameters to make the thermodynamic system function properly [17].

The molecular surfaces are composed of different segments. Molecules have numerous active reaction sites and molecular surfaces that are readily available for mutual contact with neighboring surfaces. However, if the molecules contain segments that are chemically different, then these segments will interact differently with other segments and surfaces of different molecules [18].

Most molecular surfaces and segments do not tend to connect or bind with other surfaces. As normally assumed, molecules that develop intermolecular interactions, also have long, flexible chains that work as active sites for reactions to be performed. With molecules that do not bind with other surfaces naturally have rigid molecular chains and active sites for reaction. It must also be noted that with each segment type, the average, intermolecular segment has an optimum temperature that is acceptable and needed for the reaction to take place [19]. The temperature is constant regardless of any variations that happen due to the nature and property of the connecting segment. Thus, segmental surfaces can interact with different or the same segments. Furthermore, the different types of segments and their relative contact areas should help to minimize the free energy. Henceforth, the surface area of the molecule is governed by one, or more than one equilibrium constants for the interaction energies per unit contact area[20].

Researchers have derived equations that relate to the cohesive energies in a thermodynamic system. The thermodynamic system involves active sites for reaction, segments, and different types of molecules. The intermolecular surface area for contact appreciates a segment-segment contact. The parameters thus set for the thermodynamic functions and systems are applicable for all other systems that contain similar segments or segment-segment contact. In liquids, the energies of the intermolecular interaction are related to the contact surface of the segments. However, equations based on these interactions and the thermodynamic system conform to the curves for the heat of mixing which is also confirmed through the quantitative analysis of theoretical equations [21].

The segment of the contact surface is designated through subscripts i, j, etc., additionally, the segment-segment contact is designated by subscripts ii, ij. jj, etc. $a_{i,}$ and a_j denote the intermolecular contacting surface in one mole of substance or mixture. The average intermolecular area per mole is Avogadro's number of single segments of the i (or j, etc.) that is designated by a_i^o (or a_j^0, etc.). The average areas of intermolecular contact per mole for contact surface areas of different types are designated by a_{ii}, a_{ij}, $a_{jj,}$ etc. Additionally, the average energy per unit contact area for different types of intermolecular contact can be designated ε_{ii}, ε_{ij}, $\varepsilon_{jj,}$ etc. These attraction energies are negative by conventional theories.

If there is one type of segment with one type of contact, then the sum (negative of cohesive energy) per mole is obviously

$$\mathbf{E_i = n_i\, a_i^0\, \varepsilon_u /2 \qquad (1)}$$

$$\mathbf{E_j = n_j\, a_j^0\, \varepsilon_u /2 \qquad (2)}$$

Where n_i, (or n_j) is the number of i (or j) types of segments per molecule.

In the case of benzene, cyclohexane, and carbon tetrachloride only one type of segment C-H (or C-Cl) is present and these molecules can be considered as a single segment. So $n_i = n_j = 1$.

Researchers have formulated the following expression for surface tension 'y' of fluids about the theory of rigid sphere liquids that is given by equation (3),

$$\gamma i = KT/4\pi\sigma_i^2\, [12\eta/1- \eta + 18\eta^2/ (1- \eta)^2] - P\sigma_i/2 \qquad (3)$$

Where P is the pressure, η is the packing fraction and it is expressed as $\pi/6\rho_i\sigma_i^3$ ρ_i is the number density and σ_i is the rigid-sphere diameter, also known as the hard-core diameter of the molecule that comprises the fluid. T is absolute temperature, and K is Boltzmann constant.

By rearranging equation (3) to a more convenient form, we obtain equation (4)

$$\gamma i = ½\, KT\, \sigma_i\, p_i\, [2 - \eta - \eta^2)\, /1(- \eta)^3] - ½\, P\sigma_i \qquad (4)$$

The energy vaporization per hard-core molecules from the rigid-sphere theory of liquids is given as equation (5)

$$E' = KT^2\alpha\, [(1 + 2\eta)^2/ (1- \eta)^3]$$

Where a thermal expansivity is given in equation (6)

$$\alpha = (1- \eta)^3/ T\, (1+2\eta)^2$$

Substituting equation (6) into equation (5) yields

$$E'= KT\, (1- \eta^3)/ (1- \eta)^3 \qquad (7)$$

Eliminating $(1- \eta)^3$ from equations (4) and (7), we get equation (8),

$$\gamma i = ¼\ \sigma_i\, p_i\, [2 - \eta - \eta^2/ (1- \eta)^3]E' - ½\, P\sigma_i \qquad (8)$$

Since $p_i = N/Vi$ and $NE' = E_{i'}$ gives equation (9),

$$\gamma i = ¼\ \sigma_i\, [2 - \eta - \eta^2/ (1- \eta^3)\, (E'/V_i) - ½\, P\sigma_i \qquad (9)$$

The molar hard-core volume is given by 'V'.

Thus, equation (9) is related to the surface tension (γ_i) of the liquid and the cohesive energy (E_i)

The molar energy change of mixing is equal to per mole of excess enthalpy or mole of molar heat of mixing of binary liquid mixtures. The excess enthalpy also denoted the difference between the actual enthalpy of one mole of solution [22]. The summation of the molar enthalpies of the components involved in the thermodynamic function, each, is multiplied by the mole fraction of the incorporated solution in the thermodynamic function. The equation is given by equation (10)

$$H^E = H- X_i\, H_i - X_i\, H_j = E - X_i\, E_i - X_j\, E_j \qquad (10)$$

Again the expression for heat of mixing previously deduced by the author is,

$$H^E = \grave{a}_i{}^{\circ}\Delta\varepsilon/2\, [r\, (X_j - X_j{}^2)\, /\, 1+ X_j\, (r-1)] \quad (11)$$

The attraction energy of the binary mixture is given by $\Delta\varepsilon$. The equation that denoted the energy is given by,

$$\Delta\varepsilon = 2\varepsilon_{ij} - \varepsilon_j - \varepsilon_i \qquad (12)$$

$$r=a_j^0/a_i^0 \qquad (13)$$

$$\varepsilon_{ij} = \sqrt{}\varepsilon_i\, \varepsilon_j \qquad (14)$$

The mole fraction of one of the components of the thermodynamic function is given by x_j.

The cohesive energy can be calculated from equation (9) since other parameters are known. The attraction energies of the single component are known. So, from equations (1) and (2) ai0 and a_j^0 can be calculated. The heat of mixing works as a function of mole fraction that can be calculated from equation (11).

Results and Discussion

Table 1 lists the parameters required for the inclusion of pure components. Cohesive energies and their values are calculated by the determination of the surface tension of pure liquids. The thermodynamic system studies the use and composition of small spherical molecules. Hence, the potential of Lennard-Jones comes in quite handy to determine the adequate representation of interactions of the molecular structures of the components added in the binary liquid mixture. Hence, the mixtures involved suit best to critically assess the theory behind the model and to take full access to the intricacies related to the theory. Moreover, Table 3 presents the results computed under the impression of Lorentz-Bertholet [23] that combines that the results are valid. The interaction between unlike molecular species and the Lennard Jones parameters are given by.

$$\varepsilon_{ij} = \sqrt{}\varepsilon_i\, \varepsilon_j \qquad (15)$$

Hence comparing the results with the data acquired from the experimental setup, the agreement holds to be unsatisfactory. The discrepancy in the excess enthalpies is quite small. This fact is attributed to the unsatisfactory nonadherence to the rules of Lorentz-Bertholet theory. This also connects with the uncertainties related to the chosen parameters that were potential for the theory. There is no set proof or justification that the validity of the combining rules is correct to be used for realistic molecules. The effects that deviate from the rules set on the properties of mixing should be thoroughly investigated. Equation (15) ε_{ij}, tells about the depth of the potential energy curve for a thermodynamic system. All the above equations are correct and can be used for gaseous states that follow Lennard-Jone's theory, its nature, and its potential. As compared to gaseous states, the interactions between the molecules are not simple in the case of liquids. Equation (15) can be used when the fluids that are mixed and the depth of the potential of the binary liquid mixture are different. On the foundations of quantum mechanics, the interactions between the molecules i, and j are to be studied in detail. This is essential to establish the relation between theory and practice. Thus, the following ad-hoc relation is proposed.

$$\varepsilon_{ij} = \sqrt{\varepsilon_i \varepsilon_j}\,(1+\beta) \qquad (16)$$

The adjustable parameter is ß. It is allowed to vary from +5 % to -5%. To obtain satisfactory results, the different types of thermodynamic systems and their approximate values are given in Table (2). Table (3) represents the heat of mixing fur equimolar binary liquid mixtures. Three sets of data are given that represent the heat of mixing calculated from equation (11). This is done for each system A, B, and C, respectively. Huggin's and the experimental data help investigate the physical properties of the thermodynamic system.

Hence, it is generally easier to select a combination rule that is in agreement with the experimental results of the model used in the research. It is interesting to note that the optimum choice of (1+ ß) in equation (16) for all the systems approximately corresponds to the diameter ratios of hard spheres in the mixture. Thus the equation can be written as equation (16)

$$\varepsilon_{ij} = \sqrt{\varepsilon_i \varepsilon_j}\,\sigma_i \geq \sigma_j \qquad (17)$$

Where $\sigma_i \geq \sigma_j$

However, the results are not satisfactory with the results obtained from using equation (16). Furthermore, the appropriate choice of hardcore diameter may also give satisfactory results.

Figure (1-5) shows a graphical comparison of the mixing properties that behave as the function of mole fractions. The optimum parameters have helped to construct the curves. These curves also help determine and predict the change of properties of other mole fractions.

Component	**γ (dynes/cm)**	**σ (A°)**	**E/K (^{0}K)**	**E Cohesive Energy (KCal/Mole)**
Carbon Tetrachloride	25.5	5.18	497	7.18
Benzene	27.5	5.02	308	6.81
Cyclohexane	23.7	5.33	313	6.21
n-Hexane	17.4	5.51	413	6.35

Table 1: Parameters for pure components surface tension and hardcore diameters at 25°C

Systems	**r**	**ß**	**σ_i / σ_j**	**$\grave{a}_i \Delta \varepsilon$**
$C_6H_6 + CCl_4$	1.53	0.037	1.032	0.1706
c-C_6H_{12}+CCl_4	1.37	0.037	1.03	0.250
C_6H_6 + c-C_6H_{12}	1.131	0.05	1.055	1.2127
C_6H_6 + n-C_6H_{14}	1.44	0.05	1.097	0.8580
n-C_6H_{14}+c-C_6H_{12}	1.29	0.027	1.033	0.3823

Table 2: Parameters for Different Mixtures

Systems	**Heat of Mixing (Cals/Mole), X_2= 0.5**		
	A	**B**	**C**
C_6H_6 + CCL_4	27.2	27.4	27.0
c-C_6H_{12} + CCL_4	35.05	35.1	35.0

C_6H_6 + c-C_6H_{12}	181.1	185.7	195±5
C_6H_6 + n-C_6H_{14}	128	-	205.0
n-C_6H_{14} + c-C_6H_{12}	52.8	-	51±1

Table 3: Enthalpy of mixing at 25°C

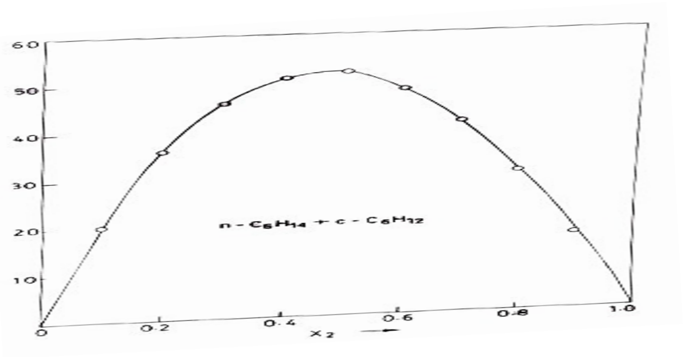

Figure 1: Heat of Mixing: For n-Hexane + Cyclohexane System

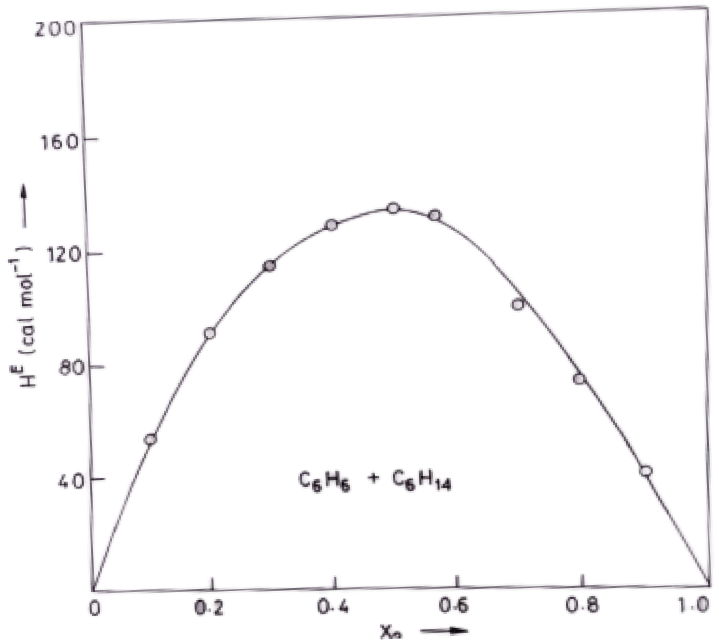

Figure 2: Heat of Mixing: For Benzene + n-Hexane System

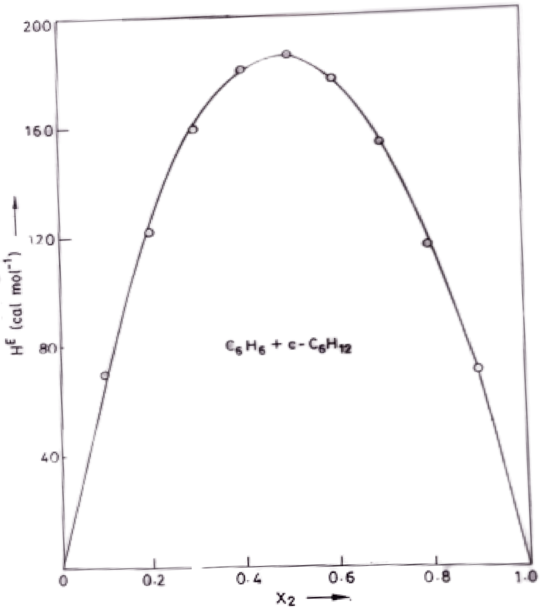

Figure 3: Heat of Mixing: For Benzene + Cyclohexane System

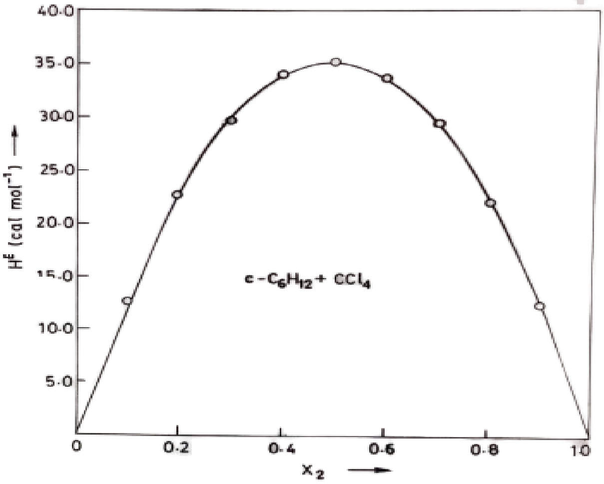

Figure 4: Heat of Mixing: For Cyclohexane + Carbon Tetrachloride System

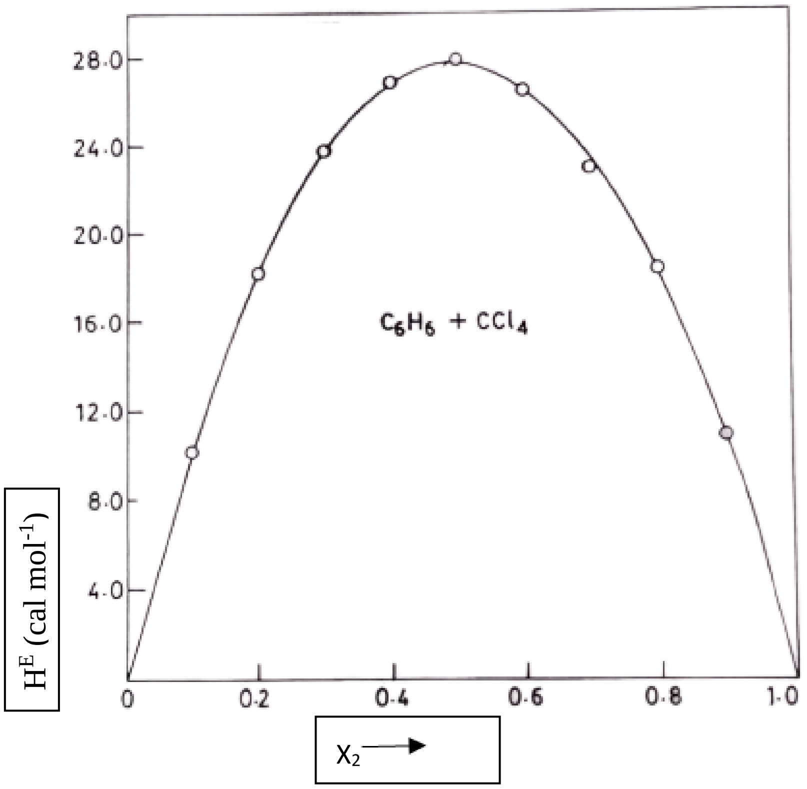

Figure 5: Heat of Mixing: For Benzene + Carbon Tetrachloride System

Conclusion

Binary liquid mixtures hold to be quite useful in testing existing thermodynamic systems for theoretical solutions of non-electrolyte and binary organic and dense liquid mixtures. This research constitutes the use of the 'Hard-Fluid Model' under various thermodynamic parameters. Hence, the calculated results of the research are compared to the experimental results of the binary mixtures in a thermodynamic system. The results from the corresponding mixture of binary liquids are found to be satisfactory in certain cases that are discussed in the research. This research motivated researchers and physicists to study the excess enthalpy of different binary liquid mixtures through the methods and approaches of existing thermodynamic systems. Table 1 lists the parameters required for the inclusion of pure components. The different types of thermodynamic systems and their approximate values are given in Table (2). Table 3 presents the results computed under the impression of Lorentz-Bertholet that combines that the results are valid. Table (3) also represents the heat of mixing fur equimolar binary liquid mixtures. Figure (1-5) shows a graphical comparison of the mixing properties that behave as the function of mole fractions. The optimum parameters have helped to construct the curves. These curves also help determine and predict the change of properties of other mole fractions.

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