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Inversion of Kirkwood-Buff theory and evaluation of preferential solvationparameters for binary liquid mixtures

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Abstract:

The Kirkwood- Buff Integrals for binary liquid mixtures of N-Methylacetamide + hydrocarbons and Formamide + Isomeric Butanol have been calculated using thermodynamic data at 308.15 K. The similar Inversion theory as proposed by A. Ben Naim has been used to evaluate the K-B parameters of the binary liquid mixtures. The self and mutual interactions of the component are then discussed. The Preferential Solvation Parameters and Local Mole Fractions have also been evaluated for the above mentioned binary mixtures. The Preferential Solvation Parameters of these mixtures are discussed in terms of the molecular interaction that occurs.

Keywords: Binary liquid mixtures, Kirkwood-Buff integrals, molecular interaction, preferentialsolvation parameters

1. Introduction:

The Kirkwood-Buff (KB) theory is the most important statistical mechanical theory of solutionswhich is applicable to all types of intermolecular interaction [1]. It is valid both classically and quantum mechanically. The KB theory of solutions was originally formulated to obtain thermodynamic quantities from molecular distribution function and is useful whenever distribution functions are available either from analytical calculations or from computer simulation [2]. This theory links macroscopic (thermodynamic) properties of solution with microscopic description, given the radial distribution function g_{ij} (r). It seems that the KB theory gives valuable tools for the investigation of solution. This theory allows one to receive information about molecular interaction inits 'global' form for mixtures for which the description in terms of associated constant is very difficult or impossible [3]. Our previous work included the study of intermolecular interactions of amides with alcohols [4-7].

The KB Inversion theory allows the evaluation of integrals over the pair correlation functions from the thermodynamic quantities. In 1977, A. Ben Naim [8] proposed KB inversion theory using the thermodynamic properties of mixtures such as partial molar volumes, partial vapor pressure and isothermal compressibility for the calculation of $G_{\alpha\beta}$ (KB integrals) for binary liquid mixtures. Much interest has been developed by this inversion theory over the last few years. J. Zielkiewicz [3] evaluated the K-B integrals for some binary and ternary mixtures. Pandey *et al.* [9] and A. K. Nain
[10] have computed KB integrals using the experimental values of ultrasonic velocity and density.

The preferential solvation takes place in a concentric region around each molecule in the mixtures designated as the correlation volume V_{cor} [11]. Marcus [12-15] evaluated KB parameters and volume corrected preferential solvation parameter for mixed solvents. E. Matteoli evaluated KB parameter and preferential solvation for some binary mixtures [16]. To the best of our knowledge, very few studies have been made available in literature for amides. J. Zielkiewicz [17, 18] evaluated KB parameter and preferential solvation parameters for binary mixtures of amides + water/alcohol and their ternary mixtures. Nain has studied solutions of acetonitrile + amide using the KB theory [19].

In the present study, KB inversion theory has been applied to the binary mixtures of N- Methylacetamide + hydrocarbons and formamide + isomeric Butanol at 308.15 K (*Table 1*). Volume corrected preferential solvation parameter (V_{cor}) and local mole fractions for the above mentioned binary mixtures have also been evaluated and discussed in terms of the intermolecular interactions.

Amides are chosen for the present study because they are convenient model system for investigating peptides and protein-solvent interactions [20]. On the other hand, alcohols are of interestin their own right and serve as simple example of biologically and industrially important amphiphilic materials [21] and hydrocarbons are growing as the most important chemicals used in hydrocarbons processing industries [22]. The favorable dielectric solvent and optical properties of acetonitrile and propane nitrile have permitted it to be used widely in spectrophotometric and electrochemical experiments and in peptide chemistry [23].

The experimental data required for the calculations have been taken from the different sources [20, 22, 24].

2. Theory:

A direct relationship between thermodynamic properties such as compressibility, partial volume and derivatives of chemical potentials, in terms of the so-called KB integrals (KBI) [1] defined by

$$G_{ij} = \int_0^\infty \left[g_{ij}(R) - 1 \right] 4\pi R^2 dR \qquad (1)$$

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where $g_{ij}(R)$ is the pair correlation function defined in the open, or the T, V,μ system for the two species i and j.

KB theory of solution is used to obtain thermodynamic quantities from molecular distributionfunction. KB inversion theory of solution allows the evaluation of integrals from thermodynamic quantities [2]. KB equation [8] for binary mixtures can be written as

$$\eta = \rho_A + \rho_B + \rho_A\rho_B\left(G_{AA} + G_{BB} - 2G_{AB}\right) \quad (2)$$

$$\xi = 1 + \rho_A G_{AA} + \rho_B G_{BB} + \rho_A\rho_B\left(G_{AA} + G_{BB} - G_{AB}^2\right) \quad (3)$$

The isothermal compressibility and partial molar volumes are given by [8]:

$$\kappa_T = \xi / \kappa T\eta \quad (4)$$

$$\bar{V}_A = \left[1 + \rho_B\left(G_{BB} - G_{AB}\right)\right]\eta / \quad (5)$$

$$\bar{V}_B = \left[1 + \rho_A\left(G_{AA} - G_{AB}\right)\right]\eta / \quad (6)$$

The derivatives of the chemical potentials were obtained using the vapor pressure data, assuming that the vapor above the mixture at room temperature may be treated as an ideal gas [10]. Thus, for component A, we may write as:

$$\mu_A = \mu_A^0 + \kappa T \ln p_A \quad (7)$$

If x_A is the mole fraction of A in the mixture, then we get the relation

$$x_A\left(\partial p_A / \partial x_A\right) = \rho^* / \eta \quad (8)$$

The number density ρ*, of the mixture is calculated from the partial molar volumes in the mixtures.

$$\rho^* = \rho_A + \rho = \left(x\bar{V}_A + x\bar{V}_B\right)^{-1} \quad (9)$$

From Eq. 5 we can obtain η from the data on partial vapor pressures of either A or B in the entire composition range. The partial vapor pressures are calculated from the activity coefficients, which arerelated to the excess Gibbs energy of the mixture. On the basis of the theory of absolute reaction rate, the excess Gibbs free energy (ΔG^E) was calculated [25] by using the following equation:

$$\Delta G^E = RT\left[\ln(\eta V) - \sum_{i=1}^{2} x_i\left(\eta_i V_i\right)\right] \quad (10)$$

The excess Gibbs free energy in the form of Redlich - Kister equation is expressed as:

$$\Delta G^E(x_A) \quad \text{or} \quad V^E(x_A) = x_A\left(1 - x_A\right)\sum_{i=0} a_i(2x_A - 1)^i \quad (11)$$

The systems undertaken are assumed to be 'regular' mixtures and the excess Gibbs energy for aregular mixture is given by

$$G^E = x_A x_B N w \quad (12)$$

where, w is a constant and is depend on temperature but independent of composition.

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The activity coefficients in a regular mixture are given by:

$$\ln\gamma_A = x_B w\ \kappa T, \qquad \ln\gamma_B = x_A w\ \kappa T \tag{13}$$

The partial vapor pressures were evaluated using the activity coefficients. As the isothermal compressibility (κ_T) of the mixtures is not known, they can be estimated from semi empiricalrelationship [26]:

$$\kappa_T = \left(1.71\times10^{-3}\right)\left(T^{4.9}U^{2}/\ \ _{mix}\right)\rho^{\frac{4}{3}}_{mix} \tag{14}$$

Using the value of η,ξ, V_A and V_B, the value of G_{AB} is calculated using the relation:

$$\overline{V}_A\overline{V}_B = (\xi - \eta G_{AB})/\eta^2 \tag{15}$$

Once G_{AB} is obtained, the values of G_{AA} and G_{BB} can be easily calculated using Eqs. (5) & (6), respectively.

Another quantity proposed by Ben Naim [8], Δ_{AB}, which is a measure of the "degree of similarity " between the two components of the mixtures, has also been calculated by using the following equation:

$$\Delta_{AB} = G_{AA} + G_{BB} - 2G_{AB} \tag{16}$$

The condition Δ_{AB}= 0 signifies symmetrical ideal solutions. The magnitude of Δ_{AB} can be used toindicate the extent of deviation from ideal behavior.

Using the G_{ij} quantities, it is possible to estimate values of the so-called linear coefficients ofpreferential solvation: [17, 18, 27]

$$\delta_{AB} = x_A G_{AB} - x_A \sum_K x_K G_{KB} \tag{17}$$

Information on preferential solvation can be obtained by using this quantity. A positive value of δ_{AB} means that species B is preferentially solvated by species A, but no quantitative estimate of the excess local composition around the central molecule B is obtained. It should be remembered that $\delta_{BA} = -\delta_{AA}$ and $\delta_{BB} = -\delta_{AB}$.

The linear coefficients of preferential solvation are useful to evaluate the local mole fractions ofspecies A around the central B molecule [17, 27, 28]:

$$x_{AB} = x_A + \frac{\delta_{AB}}{V_{cor}} \tag{18}$$

where, $V_{cor} = 4\pi/\left(3R_{cor}^3\right)$ is the correlation volume of solvation shell sphere with the radius R_{cor} [8,17, 18].

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3. Results and discussion:

The values of the various parameters of pure liquids used in the calculations are listed in *Table 1*.

N-Methylacetamide (NMA) + Hydrocarbons

The variation of KB parameter viz. G_{AB}, G_{AA} and G_{BB} against mole fraction of N-methylacetamide (x_A) for binary mixtures of N-methylacetamide+ benzene, N-methylacetamide + toluene and N-methylacetamide + mesitylene at 308.15 K are shown graphically in *Figs. 1-3*. The values of 'degree of similarity' $\Delta_{AB,}$ linear coefficients of preferential salvation (δ_{AB} and δ_{AA}) and local mole fraction (x_{12} and x_{21}) for each system are listed in *Table 2*.

Fig. 1(a) indicates that the G_{AB} values are negative and initially increases and attain a maximum at $x_A \approx 0.44$ which suggest an increasing correlation between NMA and benzene molecules on increasing the concentration of NMA. G_{AB} values are then decrease after $x_A \approx 0.44$ with increase in mole fraction of NMA, suggest a decreasing correlation between these two molecules.

Fig. 1(b) shows that G_{AA} values are positive and decrease sharply with increase in mole fraction of NMA until $x_A \approx 0.33$ and then become negative, showing a decreasing correlation between NMA molecules. G_{AA} values then slightly increase after $x_A \approx 0.33$ on increasing the mole fraction of NMA.

Fig. 1(c) shows that G_{BB} values are negative and decrease initially with increase in mole fraction of NMA until $x_A \approx 0.63$. This suggests a decreasing correlation between benzene molecules. G_{BB} values are then increase after $x_A \approx 0.63$ and finally become positive, may be due the dipole-dipole interaction between the benzene molecules at higher concentration of NMA.

It is observed from Table 2 that the Δ_{AB} values are positive and decreases initially to a negative value, attaining a minimum at $x_A \approx 0.33$ and then again increases to a positive value, indicating the dissimilarity between the unlike molecules in the mixture and negative deviation from the ideal behavior [2].

The interactions that take place in the binary liquid mixtures based on KB integrals depend on the accuracy with which there integrals can be calculated from the thermodynamic data [29, 30]. Some abnormal features seen in the values are probably artifacts, but on the whole the values shown in *Tables 2 & 3* appear to be valid representations. Therefore the evaluated preferential salvation parameters are trustworthy, based as they are on the iterative calculation of correlation volume [11, 13, 31]. To study preferential salvation of amide in the investigated binary mixtures, the δ_{AB} values defined by Eq. (17) will be used. These values reflect changes in the local mole fraction of species *A* around the central *B* molecule, and they depend on two main factors: *the energy of intermolecular interaction*s [32] and *the differences in the molecular sizes* [17].

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It is seen from the *Table 2* that values of δ_{AB} are very small and the local mole fraction are close to bulk ones. The positive values of δ_{AB} denote favored mutual preferential salvation of NMA and benzene, concomitant with the disfavored self interaction of the benzene molecules; positive values of δ_{AA} denote favored self-preferential salvation of NMA, concomitant with the disfavored mutual interaction of NMA with the benzene molecule [11].

It is observed from *Table 2* that the NMA tends to aggregate near a benzene molecule with a maximum of δ_{AB}=1.88 near $x_A \approx 0.53$ and that it tends to avoid slightly the vicinity of NMA with a minimum of δ_{AA}= -1.88 near $x_A \approx 0.33$.

The values of G_{AB}, G_{AA}, G_{BB} , Δ_{AB} , δ_{AB} , δ_{AA} , x_{12} and x_{21} for binary mixtures of NMA+ toluene and NMA+ mesitylene shows similar trends as that for NMA+ benzene system. It is observed from *Table 2* that the NMA tends to aggregate near a toluene and mesitylene molecule with a maximum of δ_{AB}=2.66 and 3.06 near $x_A \approx 0.58$ and 0.55, respectively. It also tends to avoid slightly the vicinity of NMA with a minimum of δ_{AA} = -2.17 and -1.27 near $x_A \approx 0.34$ and 0.44 for NMA+ toluene and NMA+ mesitylene mixtures respectively. It is observed from *Figs. 1-3* that the values of G_{AB} vary in the order: *benzene* > *toluene* > *mesitylene*. It shows that the interaction between NMA and hydrocarbons follows the order: *benzene* > *toluene* > *mesitylene.*

Formamide (FA) + Isomeric Butanol

The variation of KB parameter viz. G_{AB}, G_{AA} and G_{BB} against mole fraction offormamide (x_A) for binary mixtures of formamide+ 1-butanol, formamide+ 2-methyl-1-propanol and formamide+ 2-methyl-2-propanol at 308.15 K are shown graphically in *Figs. 4-6*. The values Δ_{AB}, δ_{AB}, δ_{AA}, x_{12} and x_{21} for each system are listed in *Table 2*. These values show the similar trends as that for NMA+ benzene system.

It is observed from *Table 2* that the FA tends to aggregate near a 1-butanol molecule with a maximum of δ_{AB}=1.51 near $x_A \approx 0.49$ and that it tends to avoid slightly the vicinity of FA with a minimum of δ_{AA}= 0.47 near $x_A \approx 0.36$. Again FA tends to aggregate near a 2-methyl-1-propanol molecule with a maximum of δ_{AB}=1.64 near $x_A \approx 0.49$ and that it tends to avoid slightly the vicinity of FA with a minimum of δ_{AA}= 0.64 near $x_A \approx 0.49$ and FA tends to aggregate near a formamide+ 2-methyl-2-propanol molecule with a maximum ofslightly δ_{AB}=1.48 near $x_A \approx 0.61$ and that it tends to avoid the vicinity of FA with a minimum of δ_{AA}= 0.55 near $x_A \approx 0.70$.

It is observed that the values of G_{AB} vary in the order: *1-butanol < 2-methyl-1-propanol < 2- methyl-2-propanol*. This suggests that the strength of interaction between alcohol and FA molecules follows the order: *1-butanol < 2-methyl-1-propanol < 2-methyl-2-propanol* [20].

List of symbols

T	Absolute temperature
x_i	Mole fraction of i^{th} component
V	Molar Volume of binary mixture
V_i	Molar volume of i^{th} component
$\overline{V}_A$	Partial molar volume of component *A*
$\overline{V}_B$	Partial molar volume of component *B*
R	Universal gas constant
N	Avogadro number
MW	Molecular weight of mixture U
	Ultrasonic velocity of mixture
V^E	Excess molar volume
U_{mix}	Ultrasonic velocity of binary mixture p_A
	Partial vapor pressure of component *Ak*
	Boltzmann constant
p	Vapor pressure

Greek letters

ρ_A	Number density of component *A*
ρ_B	Number density of component *B*
κ_T	Isothermal compressibity
η	Viscosity of binary liquid mixtures
η_i	Viscosity of component *A*
γ_A	Activity coefficient of component *A*
ρ_{mix}	Density of binary liquid mixture.

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Table 1: Molecular quantities for pure liquids used in the calculation of KB parameters at 308.15 K.

Liquid	MW (10^{-3} kg)	ρ ($kg.m^{-3}$)	U ($m.s^{-1}$)	η ($N\text{-}m^{-2}$ s)	*p* ($N.m^{-2}$)
N-Methylacetamide (NMA)	73.10	945.9	1362.0	3.312	187.22
Formamide (FA)	45.04	1123.5	1580.0	2.648	2.13
Benzene	78.11	873.4	1252.6	0.480	13117.95
Toluene	92.14	862.2	1258.7	0.493	3927.12
Mesitylene	120.19	861.8	1303.5	0.548	344.48
1-Butanol	74.12	800.2	1206.1	1.975	851.56
2-Methyl-1-propanol	74.12	790.6	1172.0	2.261	1408.25
2-Methyl-2-propanol	74.12	770.2	1089.3	2.333	5784.58

Table 2: Experimental mole fraction (x_A), Δ, linear coefficients of preferential solvation (δ_{AB} & δ_{AA}) and local mole fractions (x_{12} & x_{21}) for NMA (1) + hydrocarbons (2) at 308.15 K.

x_A	Δ (10^{-4} m^3.$mole^{-1}$)	δ_{AB} (10^{-5} m^3.$mole^{-1}$)	δ_{AA} (10^{-5} m^3.$mole^{-1}$)	x_{12}	x_{21}
NMA (1)+ Benzene (2)					
0.0294	115.77	-0.75	32.28	0.02	0.71
0.2260	-1.09	0.63	-1.27	0.23	0.78
0.3310	-1.40	1.23	-1.88	0.34	0.68
0.4370	-1.36	1.66	-1.67	0.45	0.58
0.5349	-1.19	1.80	-1.16	0.55	0.48
0.6329	-0.78	1.38	-0.43	0.65	0.37
0.7301	0.74	-0.77	0.69	0.72	0.26
0.8230	14.55	-16.80	4.40	0.67	0.14
0.9747	85.64	-20.49	0.63	0.78	0.02
NMA (1)+ Toluene (2)					
0.0366	84.3	-0.63	29.10	0.03	0.99
0.1983	-1.07	0.77	-0.93	0.20	0.81
0.3436	-1.75	1.78	-2.17	0.36	0.67
0.4518	-1.71	2.34	-1.91	0.47	0.56
0.5799	-1.58	2.66	-1.20	0.60	0.43

0.6965	-1.28	2.31	-0.38	0.72	0.31
0.7868	-0.34	0.91	0.33	0.79	0.21
0.8882	8.38	-6.82	1.50	0.83	0.10
0.9825	58.47	-9.77	0.28	0.89	0.01
NMA (1)+ Mesitylene (2)					
0.0458	79.27	-0.62	34.02	0.04	0.79
0.3137	-1.54	2.02	-1.29	0.33	0.69
0.4362	-1.64	2.76	-1.27	0.45	0.57
0.5467	-1.50	3.06	-0.65	0.57	0.46
0.6460	-1.20	2.84	0.09	0.67	0.35
0.7315	-0.58	1.94	0.80	0.75	0.26
0.8095	1.18	-0.27	1.54	0.81	0.18
0.8779	8.09	-6.21	2.47	0.82	0.10
0.9874	68.60	-8.25	0.28	0.91	0.01

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Table 3: Experimental mole fraction (x_A), Δ, linear coefficients of preferential solvation (δ_{AB} & δ_{AA}) and local mole fractions (x_{12} & x_{21}) for FA (1) + Isomeric Butanol (2) at 308.15 K.

x_A	Δ (10^{-4} m^3.$mole^{-1}$)	δ_{AB} (10^{-5} m^3.$mole^{-1}$)	δ_{AA} (10^{-5} m^3.$mole^{-1}$)	x_{12}	x_{21}
FA (1) + 1-Butanol (2)					
0.0844	15.10	-0.03	11.64	0.08	0.82
0.1995	0.85	0.72	2.07	0.21	0.78
0.2727	-0.13	1.09	0.83	0.28	0.72
0.3642	-0.41	1.41	0.47	0.38	0.63
0.4911	-0.27	1.51	0.85	0.51	0.50
0.6006	0.29	0.98	1.68	0.61	0.38
0.6912	1.81	-0.80	3.07	0.68	0.27
0.7699	9.55	-9.13	7.78	0.63	0.11
0.8467	19.45	-17.20	8.05	0.55	0.02
FA (1) + 2-Methyl-1-propanol (2)					
0.1092	11.9	-0.02	11.56	0.11	0.79
0.2053	1.85	0.60	3.62	0.21	0.76
0.3677	-0.2	1.35	0.89	0.38	0.62
0.4992	-0.4	1.64	0.64	0.52	0.49
0.6079	-0.35	1.60	0.77	0.63	0.38
0.6993	-0.17	1.28	0.93	0.72	0.29
0.7772	0.22	0.67	1.05	0.79	0.21
0.8440	1.06	-0.30	1.09	0.84	0.14
0.9029	3.31	-1.89	1.02	0.87	0.08
FA (1) + 2-Methyl-2-propanol (2)					
0.1112	10.52	-0.08	10.32	0.11	0.81
0.2296	1.83	0.47	3.70	0.23	0.74
0.3735	0.44	0.90	1.94	0.38	0.61
0.5054	-0.17	1.32	0.90	0.52	0.48
0.6138	-0.38	1.48	0.58	0.63	0.38
0.7045	-0.40	1.37	0.55	0.72	0.29
0.7815	0.22	0.49	0.87	0.79	0.21
0.8476	1.00	-0.42	0.88	0.84	0.14
0.9051	7.20	-4.80	1.39	0.82	0.07

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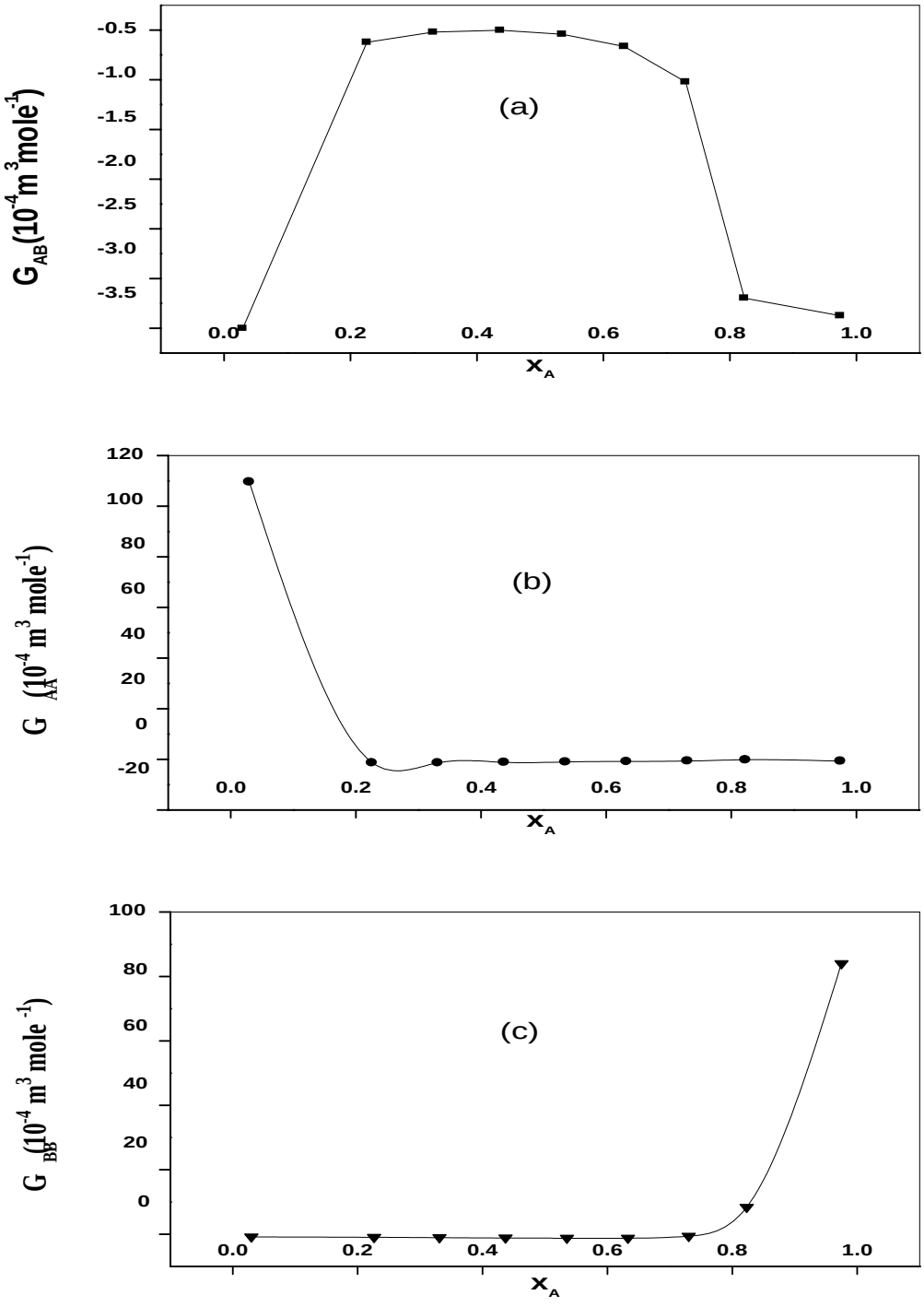

Fig.1 Plots of G_{AB}, G_{AA} and G_{BB} against mole fraction, x_A, of N-Methylacetamide for N-Methylacetamide + Benzene mixture at 308.15 K.

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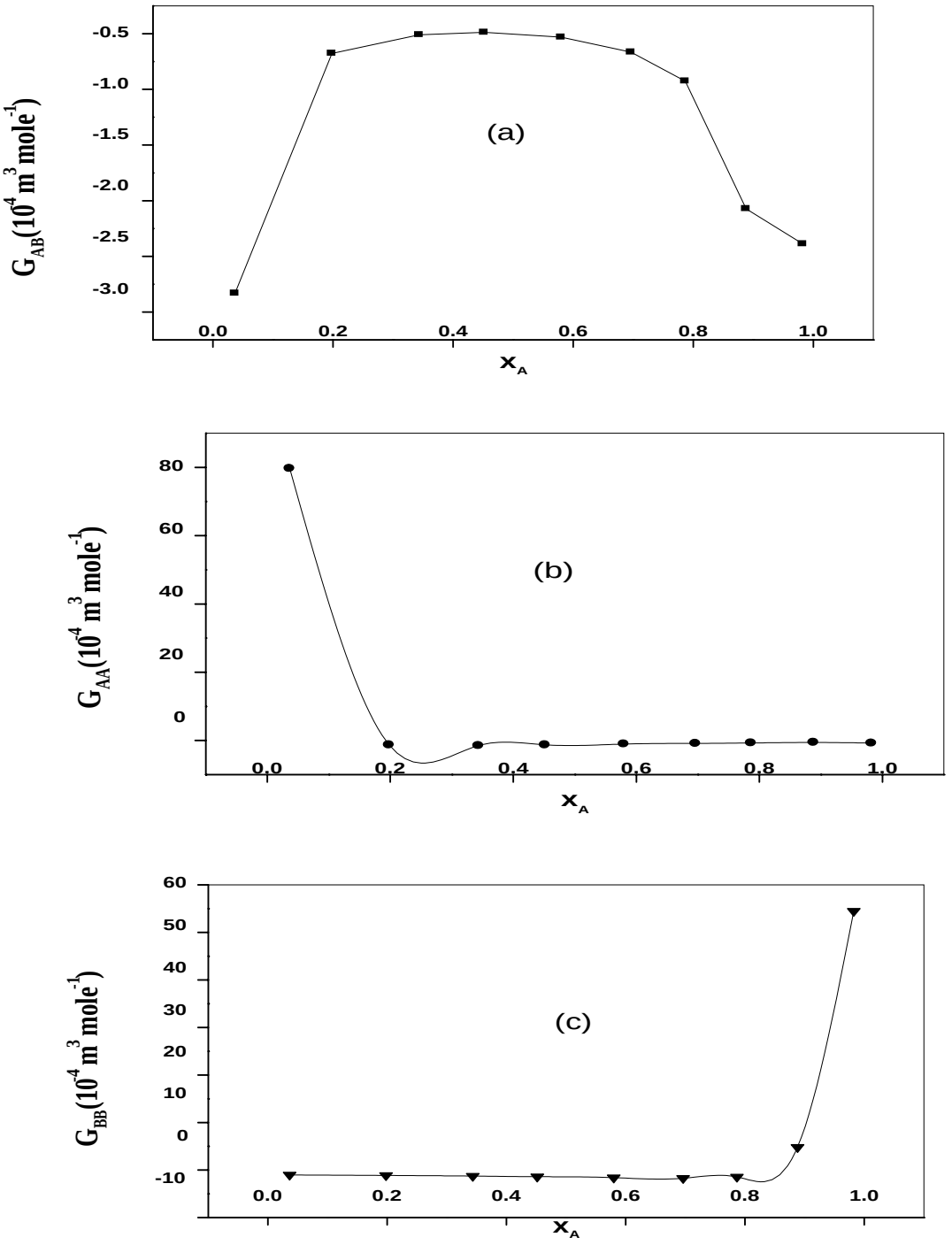

Fig.2 Plots of G_{AB}, G_{AA} and G_{BB} against mole fraction, x_A, of N-Methylacetamide forN-Methylacetamide + Toluene mixture at 308.15 K.

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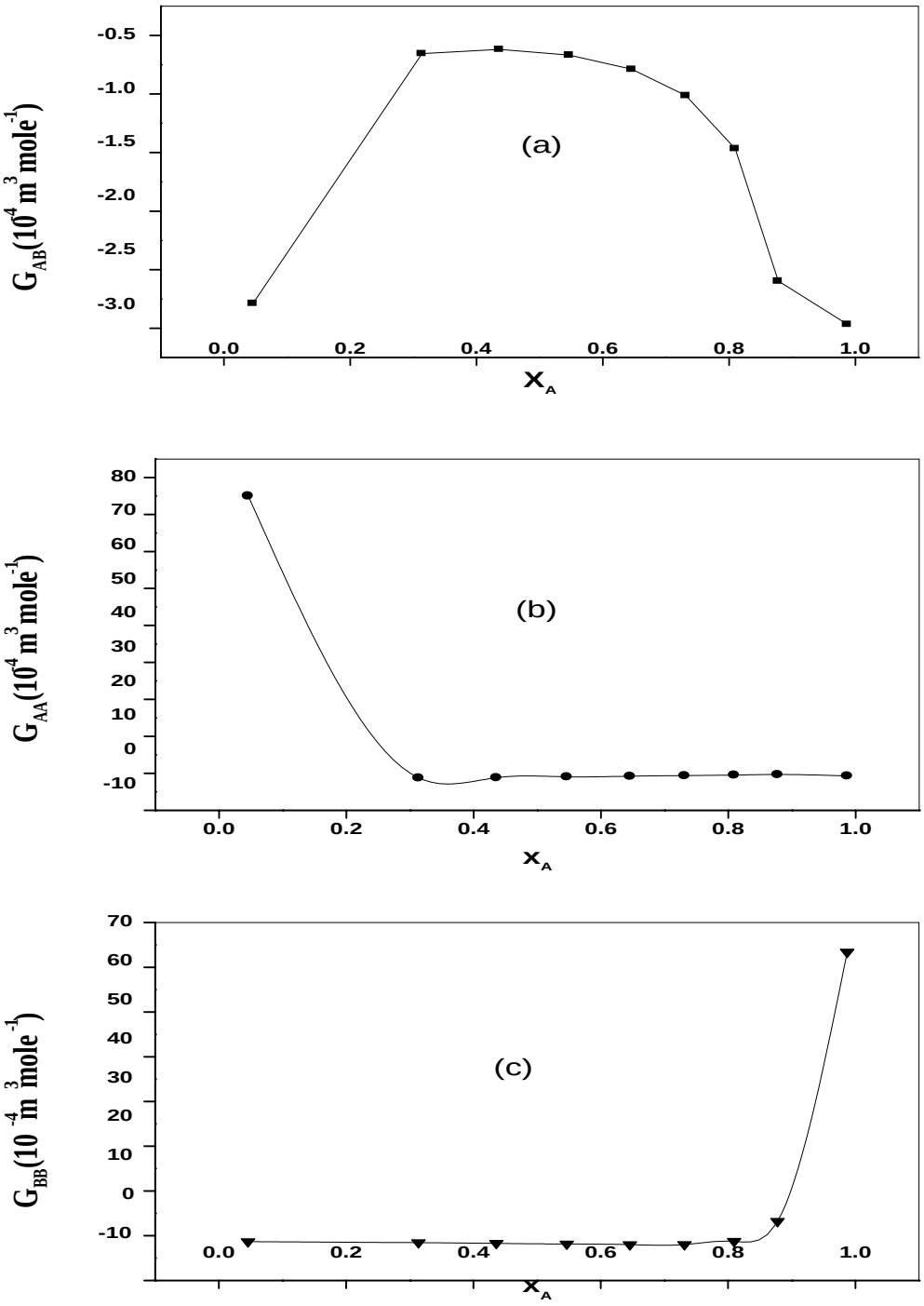

Fig.3 Plots of GAB, G_{AA} and G_{BB} against mole fraction, x_A, of N-Methylacetamide for N-Methylacetamide + Mesitylene mixture at 308.15 K.