MOLECULAR INTERACTIONS IN BINARY LIQUID MIXTURES CONTAINING BENZYL BENZOATE

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ABSTRACT

Speeds of sound, densities and viscosities of the binary mixture of Benzyl benzoate with mole fractions of amides - Formamide (FA), N-Methyl formamide (NMF) and Di methyl formamide (DMF) have been estimated utilizing the standard strategies at 303.15, 308.15 and 313.15K. From these deliberate values, different thermo-dynamic parameters such as isentropic compressibility (K_s), intermolecular free length (L_f), molar volume (V_m), Gibbs free energy (ΔG), enthalpy (H) and their excess properties were determined. The figured qualities have been fitted to the Redlich-Kister type polynomial condition utilizing least squares technique to assess the twofold coefficients and standard deviations.

Keywords: Speed of Sound, Density, Molar Volume, Free Length, R-K polynomial.

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INTRODUCTION

Changes in physicochemical properties of fluid mixtures with mole fractions and temperatures are important for understanding their thermodynamic behaviour. Amides are very interesting compounds as they possess the very common in *nature* -CO-NH- peptide bond having great importance in molecular biology. Another important application of amides is that they can act as oxygen and /or nitrogen donors and can be used as extractant carriers for numerous radioactive elements. On the other hand, Benzyl Benzoate is an anti-parasitic *insecticide*, a plasticizer in *cellulose*, a food additive and fixative in fragrances and used for killing the mites responsible for scabies.^{1,2} So the thermo physical study of esters as one of the components in the binary system is of increasing interest due to their wide range of applications in flavouring, perfumery, artificial essences, cosmetics and medicines. Benzyl benzoate (BB) is a non polar aprotic *solvent* having low dipole moment 2.06D and dielectric constant 4.90 respectively. Amide mainly consists of the chain-like hydrogen-bonded structure by combining through -NH₂.....O = CH- interactions.³ As abiding the discussion on amides and benzyl benzoate the experimental results of measured density (ρ), viscosity (η) and speed of sound (U) values were used to calculate the excess properties as well as fitted to the reduced Redlich-Kister (R-K) equations, through the Legendre polynomials, and are interpreted in terms of *molecular* interactions and structural effects. A brief survey of literature has shown that the trends found in our results are in good agreement with the results reported by earlier workers.⁴⁻⁸ having similarity in the components of the system. Additionally, FTIR analysis explains the shifting of principal bands also supports the breaking as well as forming of new H-bonding between the components for the binary system of Benzyl benzoate with formamide, NMF and DMF⁹⁻¹⁴ at different mole fractions.

EXPERIMENTAL

The samples were prepared very soon to start the experiment with the assistance of mass disparity and uncertainty in the mole fraction was projected to be less than ± 0.0001 . The purity analysis of substances was reported in Table-1.

Table-1: Purity Analysis

Chemical Name	CAS Number	Source	Initial Mole Fraction	Purification Method	Final Mole Fraction	Analysis Method
Benzyl benzoate	120-51-4	Hi Media Laboratories Pvt. Ltd. Mumbai, India	0.99	Distillation	0.995	GLC
Formamide	75-12-7		0.99	Distillation	0.997	GLC
DMF	68-12-2		0.99	Distillation	0.997	GLC
NMF	123-39-7	Tokyo Industries.co. Ltd, Japan	0.99	Distillation	0.997	GLC

GLC-Gas Liquid Chromatography

Table-2: Comparison of Experimental Densities (ρ), Viscosities (η) and Speed of sound (U) of pure liquids with literature values.

Liquid	Temp (K)	Density(ρ) kg m ⁻³		Viscosity(η) mPa s		Speed of sound(U) m s ⁻¹		C_p J K ⁻¹ mol ⁻¹	α K K ⁻¹
		lit	expt	lit	expt	lit	expt		
Benzyl benzoate	303.15	1.1193 ^a	1.1196	6.532 ^a	6.536	1506.0 ^a	1504.8	215.92 ^g	0.9966 ⁱ
	308.15	1.1145 ^b	1.1144	6.261 ^b	6.342	1493.1 ^b	1492.6	223.60 ^g	0.9931 ⁱ
	313.15	1.1097 ^a	1.1098	5.021 ^a	5.045	1471.4 ^a	1474.8	231.52 ^g	1.0036 ⁱ
Formamide	303.15	1.1257 ^c	1.1241	2.877 ^c	2.782	1588.0 ^c	1582.6	107.11 ^h	0.9967 ⁱ
	308.15	1.1198 ^d	1.1189	2.500 ^d	2.468	1577.2 ^d	1580.4	105.20 ^h	0.9961 ⁱ
	313.15	1.1183 ^c	1.1174	2.273 ^c	2.225	1568.0 ^c	1574.0	108.56 ^h	0.9998 ⁱ
NMF	303.15	0.9946 ^c	0.9934	1.585 ^e	1.563	1408.5 ^c	1408.2	124.95 ^h	0.9989 ⁱ
	308.15	0.9903 ^e	0.9908	1.462 ^e	1.478	1400.6 ^e	1402.6	126.05 ^h	0.9960 ⁱ
	313.15	0.9861 ^e	0.9855	1.352 ^e	1.383	1382.2 ^e	1392.2	129.47 ^h	1.0047 ⁱ
DMF	303.15	0.9476 ^f	0.9462	0.767 ^f	0.772	1459.6 ^f	1452.2	152.00 ^h	1.0037 ⁱ
	308.15	0.9421 ^f	0.9417	0.726 ^f	0.735	1434.7 ^f	1428.8	153.02 ^h	1.0014 ⁱ
	313.15	0.9351 ^f	0.9333	0.679 ^f	0.688	1420.8 ^f	1414.6	157.14 ^h	1.0020 ⁱ

Standard uncertainties 'u' are $u(X_1+X_2)=0.0001$, $u(\rho)=0.01$ kg m⁻³, $u(\eta)=0.001$ mPa s, $u(U)=0.56$ m s⁻¹

^a Reference[9] ^b Reference[10] ^c Reference[11] ^d Reference[12] ^e Reference[13]

^f Reference[14] ^g Estimated from NIST web book ^h Reference[23] ⁱ From density data

Interferometer (M-81S, M/s Mittal Enterprises, New Delhi, India) may use to measure the speed of sound at 2 MHz frequency with an exactness of ± 0.1 m.s⁻¹ for benzyl benzoate with formamide, NMF and DMF and uncertainty in the speed of sound to be established by ± 0.56 m.s⁻¹. The density of mixtures was measured with standard technique (specific gravity bottle) and uncertainty in density is ± 0.01 kg m⁻³. The viscosities were measured with Ostwald viscometer. The viscometer was calibrated at different temperatures using redistilled water. The flow time has been measured after the attainment of bath temperature by each pure compound and mixtures. The flow time has been measured with an electronic stop watch (Winner digital stopwatch W-999, Ravi scientific industries, New Delhi, India) with a precision of ± 0.01 s. The uncertainty in viscosity measurement is up to ± 0.001 mPa s. For all the measurements, the temperature was maintained by circulating water from an electronically controlled

thermostatic bath (M/s Mittal Enterprises, New Delhi) with a precision of ± 0.01 K. The infrared spectra for all systems have been recorded using (Alpha-2, M/S Bruker, Germany) at Chalapathi Institute of Pharmaceutical Sciences -drug testing Lab, Guntur, India. The comparison of experimental densities (ρ), viscosities (η) and speed of sounds (U) of pure liquids with literature values are given in Table-2.

RESULTS AND DISCUSSION

Excess thermodynamic properties: The values of excess properties with mole fraction for the studied binary system at three different temperatures have been calculated by using equations (1) to (6) and are presented in Figures (1) to (5).

$$\text{Excess isentropic compressibility } K_s^E = K_s - K_s^{id}, K_s = \frac{1}{\rho \cdot U^2} \text{ Kg}^{-1} \text{ ms}^{-2} \quad (1)$$

Where K_s^{id} is the ideal isentropic compressibility relation recommended by Benson & Kiyohara.¹⁵

$$K_s^{id} = \sum \phi_i \left\{ K_{s,i}^o + \frac{T V_i^o (\alpha_i^o)^2}{C_{p,i}^o} \right\} - T \left(\sum X_i V_i^o \right) \left(\frac{\sum \phi_i \alpha_i^o}{\sum X_i C_{p,i}^o} \right) \quad (2)$$

In which $K_{s,i}^o$, V_i^o , α_i^o , $C_{p,i}^o$ are the isentropic compressibility, molar volume, isobaric thermal expansion coefficient and molar isobaric heat capacity of pure component i , T represents temperature and ϕ_i is volume fraction.

$$\text{Excess molar volume } V_m^E = X_1 M_1 + X_2 M_2 / \rho - (X_1 M_1 / \rho_1 + X_2 M_2 / \rho_2) \quad (3)$$

$$\text{Excess free length } L_f^E = L_f - K_T (K_s^{id})^{1/2} L_f = K_T \sqrt{K_s} \text{ \AA}^o \quad (4)$$

K_T represent a temperature dependent constant where $K_T = (91.368 + 0.3565 T) \times 10^{-8}$

$$\text{Excess Gibb's free energy } \Delta G^E = RT [\ln (\eta V / \eta_2 V_2) - X_1 \ln (\eta_1 V_1 / \eta_2 V_2)] \quad (5)$$

Where R represents gas constant, T is absolute temperature

$$\text{Excess Enthalpy } H^E = H - (X_1 H_1 + X_2 H_2) H = \pi_i V \text{ J. mol}^{-1} \quad (6)$$

$$\text{Where internal pressure } \pi_i = bRT \left[\frac{K\eta}{U} \right]^{1/2} \left[\frac{\rho^{2/3}}{M_{eff}^{7/6}} \right] \text{ Pa}$$

Where H represents the calculated value of enthalpy, V is the molar volume, η and ρ represent obtained viscosity and density for the mixture and H_1 , H_2 represents enthalpy X_1 , X_2 represents mole fractions ρ_1 , ρ_2 be the densities η_1 , η_2 represents viscosities V_1 , V_2 represents molar volumes and M_1 , M_2 represents molecular weights of pure components 1 and 2, respectively. b stands for the cubic packing factor which is assumed to binary liquids, K is temperature independent constant, R is the gas constant and T is the absolute temperature of binary mixtures.

The observed values of all the excess properties can be explained the chemical or specific interactions result due to forming and/or breaking of hydrogen bonds and other complex-forming interactions and the geometrical effect allowing the molecule of smaller size to fit into the other's structure that makes the negative values of L_f^E and K_s^E . Addition of BB with FA induces a gradual dissociation of hydrogen bonds in the FA molecule. At the same time, there is also the possibility of forming hydrogen bonds between FA and BB because FA possesses three hydrogen-bond donors in addition to a proton acceptor group C=O. The positive values of V^E , ΔG^E and H^E over the whole composition range for the BB + FA, NMF and DMF mixture may be due to the predominance of breaking up of the hydrogen-bonded structures of the pure amides over the formation of (weak) hydrogen bonding between BB and amide molecules into the voids created by the bigger BB molecules.

The values of K_s^E being negative for mixtures of BB with FA, NMA and DMF over the whole composition range, suggest that the interactions between BB and substituted amides are stronger than BB-BB or amide-amide interactions. This finding is in accordance with a view proposed by Fort and

Moore.¹⁶ The strength of the interaction between BB and the substituted amide *molecules* seems to be strongly dependent on the positions of the methyl groups in the amide *molecules*. The substituted amide molecules in their pure state have lesser H-bonding network than primary amides. Mixing BB with substituted amides may induce the formation of a (new) hydrogen bond between the hydrogen atom of the amides with the carbonyl group of the ester and vice versa. Moreover, there may be a possibility of weak $\pi \cdots \text{H}$ bonding between π -electrons of the benzene ring of BB and the H-atom of substituted amide molecule as may be found in the recent studies of Rodham et al.¹⁷ and Larsen and co-workers¹⁸ in which they have been reported the existence of weak $\pi \cdots \text{H}$ bonding between the π -electrons of the benzene ring and the hydrogen atoms of ammonia and that of the $-\text{OH}$ group of tert-butyl alcohol. This leads to the negative values of K_s^E and L_f^E in case of mixture of BB with substituted amides. The intermolecular free length is the distance between the surfaces of the neighbouring *molecules*. The variation of Speed of sound in a solution depends upon the increase or decrease of intermolecular free length after mixing the components. The interdependence of intermolecular free length and speed of sound was evolved from a model for sound propagation proposed by Kincaid and Eyring.¹⁹ The speed of sound for form amide mixtures found to be decreased with the mole fraction of BB whereas for the substituted amides it increases with the mole fraction of BB at three different temperatures. This effect shows the positive/negative deviation of intermolecular free length L_f^E for formamide and other substituted amides and is useful to assess the compactness in the liquid mixture. The rise in temperature makes the intermolecular free length to increase as expected due to thermal expansion of the liquid medium. Another thermodynamic function, which has also been investigated, is the excess molar free energy of activation of flow (ΔG^E). According to Reed and Taylor²⁰ and Meyers et. al²¹ the parameters may be considered as a reliable measure to detect the *nature* of interactions between unlike molecules. In all the present systems the ΔG^E values are found to be positive at all the compositions over the entire range of temperatures indicates the presence of specific interaction between the unlike components which is maximum for BB+FA/DMF/NMF due to the possibility of H-bonding as well as dipole and induced dipole interactions.

(A)

(B)

(C)

Fig.-1(A-C): Variation of Excess isentropic Compressibility with respect to mole fraction of Benzyl benzoate + Formamide/DMF/NMF at three different temperatures

(A)

(B)

(C)

Fig.-2(A-C): Variation of Excess molar Volume with respect to mole fraction of Benzyl benzoate + Formamide/ DMF / NMF at three different temperatures

Next, Redlich- Kister type polynomial²² a nonlinear regression method is done by:

$$Y^E = X_1 (1-X_1) \sum_{i=1}^n A_i (2X_1 - 1)^{i-1} \quad (7)$$

Where $Y^E = K_S^E, V^E, L_f^E$. The values of coefficient A_i were determined by least square and reported in Table-3.

$$\text{Standard deviation } (\sigma) \text{ written by } (\sigma) = [\sum_{i=1}^n (Y_{\text{exp}}^E - Y_{\text{cal}}^E) / (D-N)]^{1/2} \quad (8)$$

Where D is the number of experimental data points and N is the number of parameters.

(A)

(B)

(C)

Fig.-3(A-C): Variation of Excess free length with respect to mole fraction of Benzyl benzoate + Formamide / DMF / NMF at three different temperatures

(A)

(B)

(C)

Fig-4(A-C): Variation of Excess Gibbs free energy with respect to mole fraction of Benzyl benzoate + Formamide / DMF / NMF at three different temperatures

(A)

(B)

(C)

Fig-5(a-c): Variation of Excess enthalpy with respect to mole fraction of Benzyl benzoate + Formamide / DMF / NMF at three different temperatures

Table-3: Parameters (A_k) and Standard Deviation (σ) for Benzyl benzoate with Formamide, DMF and NMF at $T=303.15\text{ K}, 308.15\text{ K}$ and 313.15 K

Parameter	Temperature(K)	A0	A1	A2	σ
Benzyl benzoate + Formamide					
$10^{12}K_S^E/(\text{m}^2.\text{N}^{-1})$	303.15	-0.2921	0.1350	0.0668	0.0029
	308.15	-0.2131	0.0945	0.0969	0.0028
	313.15	-0.1426	0.0605	0.0782	0.0020

$10^6 V^E/(\text{m}^3.\text{mol}^{-1})$	303.15	0.5773	0.1577	-0.3636	0.1378
	308.15	0.6652	0.0289	-0.0944	0.1436
	313.15	0.2926	0.0798	-0.2721	0.0668
$10^{13} L_f^E/(\text{m})$	303.15	-0.0143	-0.0019	0.0049	0.0458
	308.15	-0.0197	-0.0042	0.0053	0.0310
	313.15	-0.0239	-0.0043	0.0082	0.0188
$\Delta G^E/(\text{J.mol}^{-1})$	303.15	28.6395	-8.9965	-7.6609	4.7352
	308.15	29.3934	-12.1845	1.1884	5.0328
	313.15	30.8436	-11.6963	6.2391	5.3669
$H^E/(\text{J.mol}^{-1})$	303.15	0.0339	-0.0010	-0.0187	0.0533
	308.15	0.0405	-0.0024	-0.0223	0.0404
	313.15	0.0278	-0.0026	-0.0148	0.0269
Benzyl benzoate + DMF					
$10^{12} K_S^E/(\text{m}^2.\text{N}^{-1})$	303.15	-2.6278	0.2923	1.8532	0.0431
	308.15	-3.0613	0.3084	0.9877	0.0498
	313.15	-3.4820	0.4105	0.0953	0.0610
$10^6 V^E/(\text{m}^3.\text{mol}^{-1})$	303.15	3.4327	0.5034	-3.3120	0.8991
	308.15	4.0993	0.5705	-2.1330	1.1268
	313.15	4.7453	1.0932	1.5322	1.4176
$10^{13} L_f^E/(\text{m})$	303.15	-0.0153	0.0002	0.0052	0.3962
	308.15	-0.0232	0.0040	0.0041	0.4864
	313.15	-0.0273	0.0044	-0.0032	0.5778
$\Delta G^E/(\text{J.mol}^{-1})$	303.15	16.1045	-1.8280	-9.7901	2.8781
	308.15	17.9153	-1.9977	-6.9849	3.3327
	313.15	19.2969	-4.0274	-1.0225	3.8062
$H^E/(\text{J.mol}^{-1})$	303.15	0.0724	0.0003	-0.0181	0.4102
	308.15	0.0673	0.0040	-0.0331	0.5007
	313.15	0.0578	0.0080	-0.0421	0.5910
Benzyl benzoate + NMF					
$10^{12} K_S^E/(\text{m}^2.\text{N}^{-1})$	303.15	-2.0022	-0.8225	3.1485	0.0409
	308.15	-2.6173	-0.5773	3.1322	0.0526
	313.15	-3.1030	-0.2168	2.3809	0.0532
$10^6 V^E/(\text{m}^3.\text{mol}^{-1})$	303.15	2.3712	-0.1227	-1.0137	0.6402
	308.15	2.7109	-0.0338	0.0471	0.8217
	313.15	3.0296	0.1104	1.0045	0.9956
$10^{13} L_f^E/(\text{m})$	303.15	-0.0215	-0.0047	0.0284	0.2708
	308.15	-0.0181	-0.0039	0.0276	0.3679
	313.15	-0.0276	-0.0064	0.0318	0.4595
$\Delta G^E/(\text{J.mol}^{-1})$	303.15	19.7545	-4.9526	-5.2590	3.4312
	308.15	21.7670	-4.9848	-2.8422	3.9231
	313.15	22.5661	-6.9109	5.7353	4.3637
$H^E/(\text{J.mol}^{-1})$	303.15	0.0245	0.0053	-0.0385	0.2770
	308.15	0.0293	0.0048	-0.0354	0.3745
	313.15	0.0193	0.0031	-0.0322	0.4660

FTIR Spectra

The observed principal bands are listed in Table-4. Partial band assignments of the *solvent* mixtures by comparing with the pure *solvents* have been made and are discussed accordingly. The main absorptions bands displayed by the esters are due to C=O (stretching) and C-O (stretching) and amides are due to C=O (stretching) and N-H (stretching) vibrations. The shifting of ester C=O (stretching) frequency of pure Benzyl Benzoate in the *solvent* mixtures with different amides may be due to the formation of hydrogen bonding between the unlike components.

The FT-IR spectra of these three mixtures with various compositions indicate that there are some variations in the peaks with compositions especially 30% BB with 70% FA then the other two compositions for BB+FA mixtures but for the other two mixtures there are no variations of peaks with

respect to compositions. It is due to the dissociations of intra or inter *molecular* H- bonding of FA *molecules* or formation of the same between BB and FA molecules. The absent of shifting of peaks with variations of compositions of NMF and DMF in their mixtures ruled out the possibility of formation of intermolecular H- bonding between the unlike *molecules*.

Table-4: Characteristic FT-IR Absorption Frequencies of Functional Groups in cm^{-1a}

S.No.	Functional Group	Pure Solvent				Solvent Mixtures		
		BB	FA	NMF	DMF	BB+FA	BB+NMF	BB+DMF
1	Ester C=O (stretching)	1638(s)				1714(s)	1717(m)	1717(m)
2	Ester C-O (stretching)	1261(s)				1265(s)	1269(vs)	1269(vs)
3	Amide C=O (stretching)		1682(vs)	1664(vs)	1669(vs)	1601(w)	1657(vs)	1667(vs)
4	Amide N-H (Stretching)		3310(vs)	3300(vs)		3065(vw)	3299(m)	

^a vs = very strong, s = strong, m = medium, w = weak, vw = very weak

CONCLUSION

The experimental values are used to compute various excess thermo dynamic parameters and also compared with the theoretical values obtained from the literature. The excess values of enthalpy and molar volume are found to be positive and small for all the binary systems also the values of excess properties K_s^E and L_f^E are found to be negative for the mixture of BB with FA, NMF and DMF in the whole mole fraction range at the three different temperatures. The results can be explained by the breaking of the intra and inter molecular H-bonding present in the pure amides *molecules* and there may be some dipole induced dipole interactions present in all the mixtures especially between secondary amide and benzyl benzoate, which is supported by the greater value of the thermodynamic function excess Gibbs energy. Further the values of the excess parameters are fitted to the Redlich-Kister polynomial equation and the results are also presented. Moreover, FTIR analysis of the pure *solvent* and their mixtures are also reported where the principal bands of the esters and amides are assigned. The spectra of various compositions of each of the three mixtures are compiled and presented in three different figures to understand the shifting of peaks for variations in mole fractions. The shifting of the principal bands also supports the breaking as well as forming of new H-bonding between the components of the mixture.

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