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Excess Molar Volumes of 2-Furaldehyde with Ethanol, butan-1-ol and butan-2-ol

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ABSTRACT

Measurements have been made for excess molar volume, V^E at 303.15K and atmospheric pressure by using a dilatometer for the system of 2-Furaldehyde (C_4H_3O-CHO), +ethanol, or butan-1-ol or butan-2-ol. An appropriate polynomial equation was used to fit the experimental data for $\mathbf{V^E}$, and the results obtained have been deduced in context of specific interaction in the liquid state.

Keywords: Dilatometer, Excess Volume, Specific interaction, H- bonding, 2-Furaldehyde

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INTRODUCTION

2-Furaldehyde (C_4H_3O-CHO), top recognized constituent and starting place of the other precisely significant furans. Originated from polysaccharides and lignin biomass, C_4H_3O-CHO is recapturing interest as a bio-primarily based substitute for the production of numerous merchandise from antacids to composts, plastics, and varnishes.

Currently, it turned into diagnosed chemical substances for manufacturing of various chemicals in twenty first century (Bojell JJ et. al., 2010) [1]. It is pretended from sugars containing five-C (monosaccharide components of hemicelluloses) (Yan K et. al, 2014) [2]. The excess molar properties permit for the improvement of new relationships and representations.

This property is also useful for getting information on intermolecular interactions that could arise in liquid components, specially wherein H-bonding takes place. In the present work, we have continued to study excess properties of binary mixtures containing σ-acceptor and n-donor components in the liquid state (Tripathi et al. 2020, 2021) [3,4].We report data on excess molar volumes for the system of C_4H_3O-CHO+ethanol (C_2H_5OH),or butan-1-ol ($CH_3(CH_2)_3OH$) or butan-2-ol ($CH_3CHOHCH_2CH_3$) at 303.15K and the data have been fitted to smoothing equation with the help of an appropriate equation and discussed the results in context of donor-acceptor interactions.

EXPERIMENTAL

All the chemicals were obtained from Aldrich Chemicals. The stated purity of chemicals as measured by GC were more than 99%. They were used without further purification. Excess volumes were measured with the help of a dilatometer. The precision in the measurement and experimental procedure are described in our earlier publication (Tripathi et. al, 2021) [4]. All the chemicals were dried above molecular sieve, $4A^0$, before doing experimental work.

Method: A dilatometer having two-branches and a capillary, made of glass with reproducibility of ±0.002 $X10^3$ m^3 mol^{-1}, was used. Two liquid components were weighed and inserted into dilatometer through hypodermic syringe over Hg without air bubble in the two branches. The dilatometer with wooden stand in erected position was kept in a thermostat bath at desired temperature. The temperature of bath was adjusted to ±0.01 K. The mixing of the components was achieved by swinging the dilatometer backward and forward at some point in a defined angle, and the Hg levels in the capillary were read with the help of a cathetometer (reproducibility ±0.001 cm). Initially the dilatometer is kept for an hour in the thermostat and then mixing is done outside the bath. After that it is again kept in the bath for half an hour before taking reading in order to achieve thermodynamic equilibrium.

3. RESULT AND DISCUSSION

Experimental data at 303.15 K for V^E, in terms of C_4H_3O-CHO mole fraction x_1 , are collected in Table 1. Excess volume data for different mixtures were fitted to an appropriate equation as given below:

$$V^E = x_1 (1 - x_1) \sum_{i=1}^{N} A_i (2x_1 - 1)^{i-1} \quad \text{--(1)}$$

The values of the all coefficients arising from the fits and the corresponding standard deviations are summarized in Tables 2. Standard deviation is obtained with the method as given in our earlier paper. (Tripathi, AD et al. 2021) [4]. A graphical representation of excess molar volume Vs mole fraction is shown in Fig. 1.

Table 1 contains the experimental data for excess molar volume, V^E, for the system C_4H_3O-CHO(x1) + C_2H_5OH, or $CH_3(CH_2)_3OH$, or $CH_3CHOHCH_2CH_3$(x2). A graphical representation of V^E vs mole fraction of C_4H_3O-CHO is shown in Fig. 1. The data show that the values of excess volume are –ve for the systems C_4H_3O-CHO + C_2H_5OH, or $CH_3(CH_2)_3OH$ and both +ve and –ve for the system C_4H_3O-CHO(x1) + $CH_3CHOHCH_2CH_3$(x2). Broad studies have not been made for such type of the mixtures in the literature. The molecules of 2-Furaldehyde are recognized to be present as dipolar initially. When alcohols such as C_2H_5OH, or $CH_3(CH_2)_3OH$, or $CH_3CHOHCH_2CH_3$ are added to C_4H_3O-CHO, it results in infringement of these dipolar association. The negativity in V^E values of mixtures indicate that the dissimilar interactions are too effective and prime above the structure infringement effects in the mixtures (Radojkovic N, 1977) [5]. The overall sign of V^E are due to the net effect of +ve and –ve contributions because of the dissociation of bonds or creation of new bonds between like components, and also because of the chance of new bond creation e.g. hydrogen bonds between the unlike molecules. The sign of negativity in V^E increase in the order:

C_4H_3O-CHO + C_2H_5OH > C_4H_3O-CHO + $CH_3(CH_2)_3OH$ > C_4H_3O-CHO+ $CH_3CHOHCH_2CH_3$

These values are clue of the existence of powerful contrasting interaction. The +ve trend in V^E values of C_4H_3O-CHO + $CH_3CHOHCH_2CH_3$ are because of the rupture of the H-bonding in CH3CHOHCH2CH3 (self association) being greater than intermolecular bond formation between C_4H_3O-CHO + $CH_3CHOHCH_2CH_3$. These results indicate that the C_4H_3O-CHO forms strong complex with ethanol than with butan-1-ol. The complexation of C_4H_3O-CHO with $CH_3CHOHCH_2CH_3$ is lowest; this may be due to extra CH_3 group and its place on the butanol. The negativity in the values of V^E show stronger contrasting interaction compensating higher to the +ve contribution to V^E.

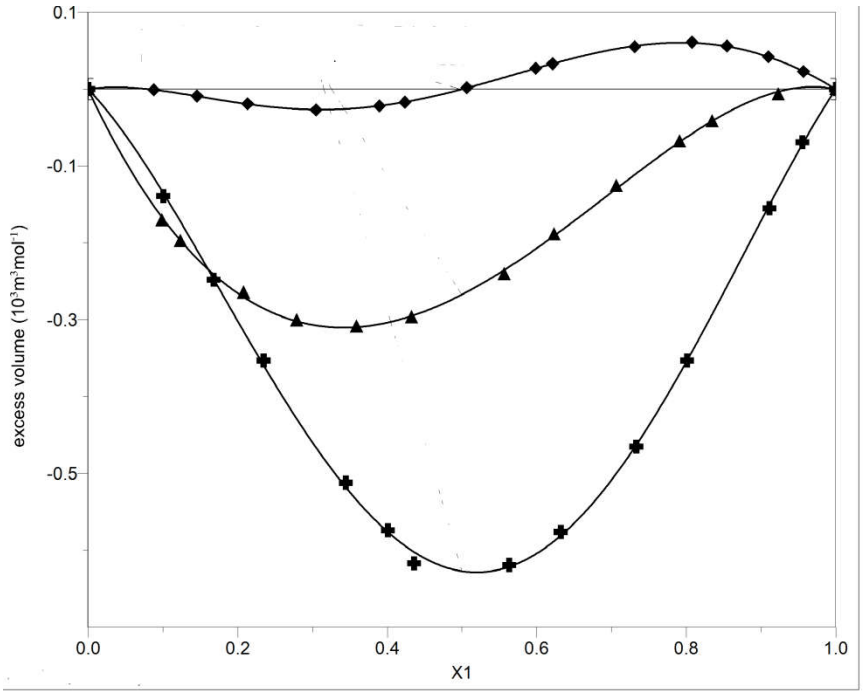

Figure 1: Excess volumes for various mixtures at 303.15K. C_4H_3O-CHO(1)+ethanol(2)(●)(C_4H_3O-CHO + $CH_3(CH_2)_3OH$ (▲) C_4H_3O-CHO + $CH_3CHOHCH_2CH_3$ (◆)

Table1: Experimental values of excess molar volumes at 303.15K for systems of C_4H_3O-CHO(x1) + ethanol (x2), C_4H_3O-CHO(x1) + butan-1-ol(x2) and C_4H_3O-CHO(x1) + butan-2-ol (x2)

X1	**$V^E/10^3m^3mol^{-1}$**	**X1**	**$V^E/10^3m^3mol^{-1}$**	**X1**	**$V^E/10^3m^3mol^{-1}$**
C_4H_3O-CHO + ethanol		**C_4H_3O-CHO**+ butan-1-ol		**C_4H_3O-CHO** + butan-2-ol	
0.1003	-0.139	0.0987	-0.171	0.0876	-0.001
0.1676	-0.248	0.1234	-0.198	0.1456	-0.009
0.2345	-0.353	0.2076	-0.265	0.2132	-0.019
0.3444	-0.512	0.2786	-0.301	0.3045	-0.027
0.4008	-0.574	0.3588	-0.309	0.3892	-0.022
0.4356	-0.617	0.4322	-0.297	0.4233	-0.017
0.5631	-0.619	0.5567	-0.241	0.5067	0.002
0.6321	-0.576	0.6233	-0.189	0.5987	0.027
0.7332	-0.465	0.7066	-0.126	0.6212	0.033
0.8009	-0.353	0.7909	-0.068	0.7311	0.055
0.9112	-0.155	0.8345	-0.042	0.8077	0.061
0.9551	-0.069	0.9231	-0.007	0.8542	0.056
				0.9097	0.042
				0.9567	0.023

Table 2: Parameters of Eq 1 for the Excess Molar Volumes, and the standard deviations ,σ,of C_4H_3O-CHO(1)+ethanol(2); (C_4H_3O-CHO (1) + butan-1-ol(2); and (C_4H_3O-CHO (1) + butan-2-ol (2), at the temperature 303.15 K.

System	A_0	A_1	A_2	A_3	$\sigma/(10^3 m^3 mol^{-1})$
C_4H_3O-CHO(1)+ethanol(2)	-2.508	-0.3037	1.265	0.0672	0.006
C_4H_3O-CHO (1) + butan-1-ol(2)	-1.070	0.9996	0.1201	0.1501	0.003
C_4H_3O-CHO (1) + butan-2-ol (2)	-0.00099	0.5067	0.3742	0.277	0.0005

CONCLUSION

The present investigation reveals existence of donor-acceptor interaction in the liquid state. Positivity in excess volume occurs when there is dipolar, dispersive and induction forces are believed to be present. Negative values of excess volume are an indication of specific interaction between individual components. In the present case, hydrogen bonding may be due to presence of interaction of nonbonding electrons of oxygen present on 2-furaldehyde and H atom of methyl or ethyl group of alcohol. The positive excess volume for the system of furfural and 2-butanol is an indication of the dissociation or rupture of the hydrogen bonding in 2-butanol being greater than intermolecular bond formation. We concluded that the 2-furaldehyde molecules are employed in the creation of H-bonding with the above-mentioned alcohols, for instance C_2H_5OH, $CH_3(CH_2)_3OH$ or $CH_3CHOHCH_2CH_3$, thus changing the values of excess volume as shown in Fig. 1.

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REFERENCES

1. Bozell JJ, Petersen GR. (2010). Technology development for the production of biobased products from biorefinery carbohydrates—the US department of energy's top 10 revisited, Green Chem. 12, 539–554.
2. Yan K, Wu G, Lafleur T, Jarvis C. (2014). Production, properties and catalytic hydrogenation of furfural to fuel additives and value-added chemicals, Renewable Sustainable Energy Rev. 38, 663–676.
3. Singh VK, Tripathi AD, Yadav P, Chahal N. Sehgal A. (2020). Excess Molar Volumes of Binary Liquid Mixtures of Cyclohexanone +Dichloromethane, + Trichloromethane, + 1,1,1-Trichloroethane and 1,2 Dichloroethane at 308.15 K. Bull. of Pure & Appl. Sci. Volume 39C(1), 32-37.
4. Tripathi AD, Singh VK, Purohit M, Bisht K, Rajput M. (2021). Excess Molar Volumes of Binary Liquid Mixtures of Ketocyclohexane (C6H10O), +CH2Cl2, +CHCl3, +CH2ClCH2Cl, +CHClCCl2, and +CCl 3CH3 at 303.15 K. Bull. of Pure & Appl. Sci. Volume 40C(1), 1-6.
5. Radojkovic N, Tasic A, Grojdanic D, Djordjevic B, Malic D. (1977). Excess volumes of acetone+benzene acetone + cyclohexane, and acetone + benzene + cyclohexane at 298.15 K, J. Chem. Thermodyn. 9, 349–356.

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