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Studies on excess molar volumes for binary mixtures of Propylene carbonate with secondary alcohols

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ABSTRACT

Densities (r) for binary mixtures of propylene carbonate (PC) with secondary alcohols viz. 3-methyl-1-butanol (3-Me-1-buOH), 2-butanol (2-BuOH), 2-methyl-1-propanol (2-Me-1-PrOH) and 2-propanol (2-PrOH) have been measured at 288.15-308.15 K over the entire range of composition. Experimental values of density are used to calculate excess molar volumes (V^E) for all the binary mixtures at 288.15-308.15 K. The results obtained have been fitted to Redlich-Kister equation and discussed in terms of molecular interactions present amongst the mixing components.

Introduction:

Molecular interactions existing between any two components have been the subject of numerous studies in solution chemistry. To study the possible interactions between the components, various techniques, such as volumetric, viscometric, and ultrasonic, are widely used. These techniques are fundamentally related to the binding forces between the atoms or the molecules. Increasing interests have been shown by several workers for the study of molecular interactions in binary1-4 liquid mixtures in recent past using these techniques.

PC is a highly polar aprotic solvent with a large dipole moment. It shows dipole–dipole interactions with little or no specific association. It is used in the production of polycarbonates and polyester elastomers, for separation of carbon dioxide and hydrogen

sulûde and reûnery aromatics in the oil industry, and as a component of electrolytes in lithium ion rechargeable batteries. Alcohols exist in associated form and are having various applications. 2-Me-1-Propanol is used in the synthesis of flotation agents, flavours, perfumes, dyestuffs, wetting agents. In industrial cleaners, paint removers, solvent for many natural resins, linseed and castor oils.

3-Me-1-Butanol is used as solvent for fats, resins, alkoxides etc. for manufacturing isoamyl (amyl) compounds, isovaleric acid, mercury fulminate, pyroxylin, artificial silk, lacquers, smokeless powders in microscopy; for determining fat in milk.

2-propanol is used in antifreeze compositions, as solvent for gums, shellac, essential oils; in the extraction of alkoxides; in quick drying oils; in quick drying inks, in denaturing ethanol; in body rubs, hand lotions, after shave lotions and similar cosmetics. Also as solvent for cresote, resins, gums, in manufacture of acetone, glycerol, isopropyl acetate. Isobutyl alcohol or 2-butanol is used for manufacturing esters for fruit flavoring, essential solvent in paints, varnish removers.

This paper is a continuation of our research on thermodynamic properties of liquid-liquid systems containing PC as one of the binaries.5-8 I report here densities for binary mixtures of PC with secondary alcohols viz. 3-methyl-1-butanol, 2-butanol, 2-methyl-1-propanol and 2-propanol at 288.15-308.15 K respectively over the entire range of composition. From the experimental values of densities (r) excess molar volumes ($V\!E$) have been calculated. The results obtained have been fitted to Redlich-Kister equation. The obtained results are discussed in terms of intermolecular interactions present amongst the mixing components.

Experimental:

PC (supplied by Merck) was refluxed over anhydrous calcium carbonate and distilled at atmospheric pressure.9,10 3-Methyl-1-butanol (Sarabhai M. Chemicals), 2-butanol (Merck), 2-methyl-1-propanol (Sarabhai M. Chemicals), and 2-propanol (S. D. Fine Chem) were distilled at atmospheric pressure. The middle fraction collected, of all the liquids were stored over 4 Å type molecular sieves to reduce water content. Double distilled liquids were used. The binary liquid mixtures were prepared by mixing known masses of pure liquids in airtight-stoppered bottles in order to minimize the

evaporation losses. All measurements of mass were performed on a Mettler one pan balance which can be read up to the fifth decimal place with an accuracy of ±0.05 mg. The densities of the pure liquids and their binary mixtures were measured using the single arm capillary pyknometer. The accuracy in the density measurements was found to be of ±5x10-5 g cm-3. The details of the density measurements are same as reported in our previous paper5. For all the measurements, the temperature was controlled by circulating the water through an ultra thermostat Julabo F-25 (made in Germany) which has an accuracy of ±0.020C.

Results and Discussion:

The experimental values of densities (r) for pure PC and secondary alcohols along with their binary mixtures over the whole composition range at 288.15-308.15 K are listed in Table 1 as a function of mole fraction x1 of PC. From table 1, the values of densities are increasing with increasing mole fraction of the first component i.e. PC and decreasing with increasing temperature for all the systems studied.

The measured values of densities (r) are utilised to calculate11,12 excess molar volumes (VE) for the binary mixtures of PC (1) with secondary alcohols (2) at 288.15-308.15 K by using equation (1) as follows:

$$VE = [(x1M1+x2M2)/r12] - (x1M1/r1) - (x2M2/r2) \quad (1)$$

Where r12 is the density of the mixture and M1, x1, r1, M2, x2 and r2 are molar masses, mole fractions and densities of pure component PC (1) and secondary alcohols (2) respectively.

Table 1: Densities (r) for the binary mixtures of PC (1) with secondary alcohols (2) at 288.15-308.15 K

Propylene carbonate (1) + 3-me-1-butnaol (2)						Propylene carbonate (1) + 2-butnaol					
x1	288.15	293.15	298.15	303.15	308.15	x1	288.15	293.15	298.15	303.15	308.15
0.0000	0.81312	0.81030	0.80686	0.80309	0.79918	0.0000	0.81106	0.80648	0.80235	0.79896	0.79065
0.0236	0.82097	0.81796	0.81436	0.81055	0.80656	0.0184	0.81594	0.81148	0.80727	0.80418	0.79602
0.0383	0.82692	0.82379	0.82006	0.81622	0.81218	0.0404	0.82185	0.81763	0.81365	0.81057	0.80258
0.0641	0.83591	0.83260	0.82872	0.82484	0.82074	0.0653	0.82885	0.82487	0.82103	0.81804	0.81024
0.0925	0.84556	0.84209	0.83807	0.83415	0.82998	0.0809	0.83345	0.82953	0.82585	0.82284	0.81515
0.1976	0.87941	0.87556	0.87126	0.86724	0.86297	0.0948	0.83788	0.83381	0.83025	0.82722	0.81961
0.3024	0.91163	0.90767	0.90338	0.89929	0.89508	0.2072	0.87476	0.87093	0.86765	0.86486	0.85782
0.3984	0.94108	0.93719	0.93307	0.92893	0.92484	0.3013	0.90924	0.90539	0.90198	0.89934	0.89260
0.5039	0.97493	0.97116	0.96730	0.96310	0.95915	0.4036	0.94967	0.94564	0.94185	0.93926	0.93272
0.6016	1.00904	1.00537	1.00171	0.99743	0.99356	0.5089	0.99345	0.98942	0.98545	0.98245	0.97601
0.7057	1.04977	1.04609	1.04248	1.03806	1.03418	0.6014	1.03325	1.02928	1.02469	1.02162	1.01525
0.7978	1.09086	1.08698	1.08322	1.07861	1.07456	0.7068	1.08015	1.07563	1.07101	1.06710	1.06081
0.9046	1.14589	1.14145	1.13716	1.13222	1.12776	0.8102	1.12615	1.12137	1.11642	1.11201	1.10585
1.0000	1.20867	1.20338	1.19758	1.19253	1.18716	0.9106	1.17035	1.16537	1.15995	1.15529	1.14965
						1.0000	1.20867	1.20338	1.19758	1.19253	1.18716

Propylene carbonate (1) + 2-me-1-propanol (2)						Propylene carbonate (1) + 2-propanol					
x1	288.15	293.15	298.15	303.15	308.15	x1	288.15	293.15	298.15	303.15	308.15
0.0000	0.80954	0.80202	0.79797	0.79416	0.79006	0.0000	0.79102	0.78540	0.78118	0.77635	0.77204
0.0247	0.81729	0.81012	0.80629	0.80271	0.79883	0.0204	0.79772	0.79228	0.78802	0.78338	0.77954
0.0425	0.82302	0.81615	0.81240	0.80896	0.80512	0.0406	0.80457	0.79929	0.79499	0.79047	0.78654
0.0638	0.82994	0.82340	0.81973	0.81643	0.81264	0.0606	0.81145	0.80633	0.80202	0.79758	0.79312
0.0836	0.83651	0.83025	0.82665	0.82346	0.81965	0.0821	0.81907	0.81408	0.80979	0.80539	0.80135
0.1075	0.84456	0.83855	0.83507	0.83198	0.82820	0.0968	0.82434	0.81945	0.81518	0.81079	0.80692
0.2111	0.88114	0.87525	0.87275	0.86978	0.86598	0.2180	0.87073	0.86630	0.86259	0.86024	0.85765
0.2997	0.91432	0.90865	0.90630	0.90310	0.89924	0.3076	0.90769	0.90336	0.90032	0.89825	0.89585
0.3979	0.95281	0.94725	0.94473	0.94125	0.93712	0.4117	0.95277	0.94854	0.94617	0.94345	0.94165
0.5090	0.99812	0.99254	0.98955	0.98585	0.98154	0.5053	0.99470	0.99124	0.98856	0.98625	0.98435
0.6007	1.03662	1.03115	1.02745	1.02354	1.01924	0.5994	1.03755	1.03425	1.03152	1.02965	1.02745
0.7009	1.07946	1.07398	1.06962	1.06538	1.06103	0.7058	1.08613	1.08235	1.07966	1.07658	1.07468
0.8156	1.12907	1.12353	1.11860	1.11412	1.10954	0.8148	1.13530	1.13168	1.12762	1.12436	1.12168
0.9004	1.16583	1.16053	1.15515	1.15038	1.14535	0.9040	1.17445	1.16962	1.16505	1.16185	1.15845
1.0000	1.20867	1.20338	1.19758	1.19253	1.18716	1.0000	1.20867	1.20338	1.19758	1.19253	1.18716

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The uncertainty in the measured values of VE were found to be +0.003 cm3mol-1. The calculated excess molar volumes VE for all the binary mixtures over the entire composition range at 288.15-308.15 K as a function of mole fraction of x1 of propylene carbonate are reported in Table 2.

The calculated values of V^E were correlated with the Redlich-Kister polynomial[13] at 298.15 K only as expressed in equation (2)

$$Y^E = x_1x_2 \sum a_i (x_1-x_2)^i \quad (2)$$

The coefficients in equation (2) were estimated by least square fitting and standard deviations were calculated by equation (3)

$$\sigma = \sum(Y^E_{Experimental} - Y^E_{calculated})^2/ (D-N)^{0.5} \quad (3)$$

where D and N are the number of data points and number of parameters respectively. The regression results for the excess molar volumes (V^E) for binary mixtures of PC (1) with secondary alcohols (2) at 298.15 K are reported in Table 3.

Figures 1.1-1.4 show the graphical variation of VE for binary mixtures of PC with secondary alcohols at 288.15, 293.15, 298.15, 303.15 and 308.15 K. In case of 3-me-1-butnaol mixtures the VE values are found to be negative up to 0.2 mole fraction and then positive from mole fraction 0.3 onwards. Thus showing a sigmoidal shape. The positive as well as negative values are found to be decreasing with increasing temperatures. The maximum positive value is found to be at 0.7 mole fraction of propylene carbonate. For rest of the alcohol mixtures the VE values are found to be completely positive but becoming very slight negative towards the end. These values are found to be decreasing with increasing temperatures. The maximum positive values are found at 0.3 mole fraction of PC for all the studied temperatures.

Table 2: Excess molar volumes (VE) for the binary mixtures of PC (1) with secondary alcohols (2) at 288.15-308.15 K

Propylene carbonate (1) + 3-me-1-butnaol (2)						Propylene carbonate (1) + 2-butnaol					
x1	288.15	293.15	298.15	303.15	308.15	x1	288.15	293.15	298.15	303.15	308.15
0.0000	0.000	0.000	0.000	0.000	0.000	0.0000	0.000	0.000	0.000	0.000	0.000
0.0216	-0.153	-0.134	-0.119	-0.118	-0.112	0.0184	0.213	0.200	0.207	0.171	0.158
0.0383	-0.247	-0.217	-0.189	-0.187	-0.178	0.0404	0.454	0.413	0.393	0.353	0.326
0.0641	-0.352	-0.305	-0.265	-0.262	-0.251	0.0653	0.693	0.626	0.587	0.535	0.492
0.0925	-0.418	-0.359	-0.308	-0.305	-0.290	0.0809	0.818	0.744	0.686	0.635	0.583
0.1976	-0.310	-0.232	-0.173	-0.172	-0.161	0.0948	0.896	0.839	0.766	0.716	0.658
0.3024	0.152	0.218	0.254	0.252	0.243	0.2072	1.403	1.317	1.203	1.115	1.020
0.3984	0.701	0.740	0.738	0.734	0.702	0.3013	1.487	1.398	1.288	1.175	1.070
0.5039	1.278	1.283	1.236	1.229	1.175	0.4036	1.341	1.265	1.181	1.051	0.951
0.6016	1.668	1.643	1.562	1.554	1.484	0.5089	1.071	0.990	0.908	0.806	0.723
0.7057	1.829	1.784	1.682	1.677	1.600	0.6014	0.790	0.699	0.659	0.553	0.490
0.7978	1.696	1.649	1.544	1.544	1.473	0.7068	0.427	0.378	0.325	0.276	0.238
0.9046	1.182	1.152	1.069	1.080	1.031	0.8102	0.161	0.128	0.088	0.065	0.051
1.0000	0.000	0.000	0.000	0.000	0.000	0.9106	0.011	-0.009	-0.027	-0.044	-0.061
						1.0000	0.000	0.000	0.000	0.000	0.000

Propylene carbonate (1) + 2-me-1-propanol (2)						Propylene carbonate (1) + 2-propanol					
x1	288.15	293.15	298.15	303.15	308.15	x1	288.15	293.15	298.15	303.15	308.15
0.0000	0.000	0.000	0.000	0.000	0.000	0.0000	0.000	0.000	0.000	0.000	0.000
0.0247	0.151	0.114	0.085	0.056	0.026	0.0204	0.260	0.245	0.247	0.229	0.181
0.0425	0.248	0.180	0.140	0.092	0.056	0.0406	0.497	0.467	0.472	0.443	0.403
0.0638	0.351	0.250	0.198	0.132	0.087	0.0606	0.708	0.665	0.669	0.632	0.645
0.0836	0.436	0.308	0.245	0.164	0.120	0.0821	0.911	0.857	0.857	0.817	0.787
0.1075	0.525	0.374	0.294	0.201	0.150	0.0968	1.037	0.975	0.972	0.931	0.883
0.2111	0.758	0.614	0.419	0.305	0.244	0.2180	1.707	1.607	1.538	1.305	1.125
0.2997	0.802	0.653	0.436	0.339	0.276	0.3076	1.852	1.747	1.607	1.351	1.151
0.3979	0.736	0.597	0.391	0.313	0.266	0.4117	1.750	1.639	1.431	1.237	0.980
0.5090	0.575	0.462	0.292	0.224	0.183	0.5053	1.485	1.314	1.124	0.897	0.647
0.6007	0.412	0.311	0.195	0.138	0.087	0.5994	1.119	0.940	0.747	0.489	0.261
0.7009	0.238	0.164	0.091	0.054	-0.002	0.7058	0.651	0.518	0.313	0.155	-0.098
0.8156	0.078	0.040	-0.001	-0.029	-0.075	0.8148	0.181	0.043	-0.068	-0.208	-0.404
0.9004	0.008	-0.023	-0.041	-0.054	-0.072	0.9040	-0.156	-0.199	-0.281	-0.422	-0.566
1.0000	0.000	0.000	0.000	0.000	0.000	1.0000	0.000	0.000	0.000	0.000	0.000

Table 3: Adjustable parameters *ai*, of the Redlich-Kister (Eq. (2)) and standard deviations s, (Eq. (3)) of excess molar volumes (VE) for the binary mixtures of PC (1) + secondary alcohols (2) at 298.15 K.

System studied	Coefficients			
	a_1	a_2	a_3	σ
PC (1) + 3-Me-1-Butanol	4.8362	8.9908	-1.3097	0.0382
PC (1) + 2-Butanol	3.7643	-5.6605	0.9354	0.0127
PC (1) + 2-Me-1-Propanol	1.2076	-2.1141	0.2663	0.0050
PC (1) + 2-propanol (2)	4.6213	-8.0432	-0.3454	0.0370

Figure 2.5 shows graphical variation of VE for binary mixtures of PC with 3-methyl-1-butanol, 2-butanol, 2-methyl-1-propanol and 2-propanol at 298.15 K.

References :-

1) C. Shanmuga Priya, S. Nithya, G. Velraj, A. N. Kanappan. International Journal of Advanced Science and Technology, 18, 59, 2010.
2) S. Sharma, P. B. Patel, R. S. Patel, J. J. Vora. E-Journal of Chemistry, 4(3), 343, 2007.
3) Oana Ciocirlan, Olga Iulian. J. Serb. Chem. Soc. 73 (1), 73, 2008.
4) R. Uvarani, J. Sivapragasam. E-Journal of Chemistry, 6(4), 1150, 2009.
5) D. S. Wankhede, M. K. Lande, B. R. Arbad. J. Chem. Eng. Data, 50, 261, 2005.
6) D. S. Wankhede, N. N. Wankhede, M. K. Lande, B. R. Arbad. J. Sol. Chem., 34, 233, 2005.
7) *D. S. Wankhede, N. N. Wankhede, M. K. Lande, B. R. Arbad. Ind. J. Pure & Appl. Phys., 44, 919, 2006.*
8) D. S. Wankhede, N. N. Wankhede. Phys. Chem. Liq ,46, (3), 319, 2008.
9) J. A. Riddick, W. B. Bunger, T. K. Sakano. Organic solvents, 4th ed; Techniques of Chemistry series; Wiley: New York, 1986; Vol. 2. PP. 74, 434, 990.