THERMODYNAMIC INTERACTIONS IN BINARY AND TERNARY SYSTEMS CONTAINING SULFOLANE, DIMETHYLSULFOXIDE, TOLUENE AND WATER AT 303.15K

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Abstract

This paper reports experimental densities and refractive indices of binary and ternary systems containing sulfolane, or dimethylsulfoxide, toluene and water over the whole composition range of mixtures at 303.15 K and atmospheric pressure. From these data, excess molar volumes, V^E and molar refraction changes of mixing, δR were calculated. The obtained values of V^E and ΔR for the binary mixtures were fitted to the Redlich – Kister equation and the binary parameters were used in the correlation of the ternary results with Redlich – Kister and Cibulka polynomial equations. The significance of these results is discussed in terms of the structural changes in the mixtures.

Introduction

Dipolar a protic solvents sulfolane, dimethylsulfoxide (DMSO), and their mixtures with water and polar solvents are particularly important solvents with a high relative permittivity(1). They have versatile applications: (i) as an efficient extracting agents for low molar mass aromatic hydrocarbons (benzene, toluene, xylenes) from petroleum products such as naphtha, hydrogenated pyrrolysis gasoline and reformat, (ii) good solvents for special polymers, (iii) good solvents media for some electroanalytical studies, (iv) electrolyte medium of lithium batteries and others.

This work forms part of a program to determine excess thermodynamic properties for a number of binary and ternary mixtures which include sulfolane or dimethylsulfoxide as the common component and n– alkanes as a non common component.

In a previous investigation the excess molar volumes of binary mixtures of sulfolane or dimethylsulfoxide + benzene at the temperature 303.15 K and normal atmospheric pressure were measured (2). The purpose of the present study was to investigate the effect of the variation of solvents on the excess properties for this kind of ternary mixtures, sulfolane or dimethylsulfoxide + toluene + water at the same temperature and pressure conditions.

The excess molar volumes V^E and molar refraction changes of mixing δR for binary mixtures sulfolane (1) + toluene (2), sulfolane (1) + water (3), dimethylsulfoxide (1) + toluene (2), and dimethylsulfoxide (1) + water (3) were reported. This excess property was fitted to the Redlich – Kister equation (3).The binary parameters were used in the correlation of the ternary results with the Cibulka equation(4).

Smooth representations of the results are described and used to construct the curves of constant excess volumes and molar refraction changes of mixing for both ternary mixtures. The possibilities of predicting excess properties of the ternary mixtures using those for the binary mixtures have been analyzed.

Experimental Section

Chemicals. Sulfolane, dimethyl-sulfoxide, toluene (Fluka AG, Puriss.P.a) were of 99.5 moles percent minimum purity. All liquids were stored over freshly activated molecular sieves of type 4A (Union Carbide) and filtered before use. The purity of the pure component liquids was confirmed by g.l.c analysis; doubly distilled water was used as the standard liquid with conductivity less than 0.05μs cm^{-1}.

Mixtures were prepared by mass using Mettler AE 200 balance with an accuracy of ± 10^{-4} covering the whole composition range. Precautions were taken such as using samples recently prepared and reducing to a minimum the vapor space in the vessels, to avoid preferential evaporation during manipulation and the subsequent composition errors. The possible error in the mole fraction is less than ± 2 × 10^{-4}. The purities of the compounds were checked by determining their densities and refractive indices at 303.15 K, which were reasonably in accordance with values found in the literature Table (1).

Table (1)
Densities (ρ) and Refractive Indices (n_D) of Pure Components at 303.15 K.

Component	**ρ/ g.cm^{-3}**		**n_D**	
	exptl.	**Lit.**	**exptl.**	**Lit.**
Sulfolane	1.26140	1.26139(3) 1.26138(4)	1.4818	1.4820(3)
Dimethylsulfoxide	1.09118	1.09115(5) 1.09119(6) 1.09110(7)	1.4748	1.4748(5)
Toluene	0.85791	0.85789(8) 0.85785(9)	1.4905	1.4904 8)
Water	0.99564	0.99565(10)	1.3317	1.3319(10)

Measurements. Densities ρ were measured with a digital Anton Paar DMA 60 / 602 densimeter with a resolution of ±2×10^{-6}. The experimental technique has been described previously (11). The refractive indices were measured with an Abbe refractometer (type 3T) with an accuracy of ±2×10^{-4}. Both apparatuses were connected to Haake F_3 circulating water bath with proportional temperature control and an automatic drift correction system that kept the samples at the desired temperature (303.15 K) with an accuracy of ±10^{-2} K. The error in the determination of V^E and ΔR were estimated to be better than ±2×10^{-4} cm3.mol^{-1}.

Results

The experimental data of densities, ρ, refractive indices, n_D, excess molar volumes, V^E, and the deviations in molar refractivity, ΔR, of binary and ternary mixtures are shown in Tables (2– 4) and illustrated in Figs. (1–6). In these tables, x_i is the mole fraction of component i in the mixture. The excess molar volumes for binary and ternary mixtures were calculated from the relation:-

$$V^E = \sum_{i=1}^{N} x_i \, M_i \, (\rho^{-1} - \rho_i^{-1}) \, \ldots\ldots\ldots\ldots\ \ldots(1)$$

where M_i is the molecular weight of component I in the mixture, ρ_i are the densities of the pure components, and N is the number of components in the mixture.

Deviations in molar refractivity, ΔR, were calculated from the following equation:

$$\Delta R / \mathrm{cm}^3.\mathrm{mol}^{-1} = R_m - \sum_i \phi_i \, R_i \ \ldots\ldots\ \ldots(2)$$

$$R_m = \left(\frac{n_D^2 - 1}{n_D^2 + 1} \right) \times \left(\sum_i x_i \, M_i / \rho \right) \ \ldots\ldots\ldots\ \ldots(3)$$

$$R_i = \left(\frac{n_D^2 - 1}{n_D^2 + 1} \right) \left(\frac{M_i}{\rho_i} \right) \ \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ \ldots(4)$$

and

$$\phi_i = \frac{x_i \, V_i}{\sum\limits_{i=1}^{m} x_i V_i} \ \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ \ldots(5)$$

where ρ is the densities, n_D and n_{Di} are the measured refractive indices of the binary or ternary mixtures and the pure component liquids, respectively. V_i and φ_i are the molar volume and volume fraction of the i-th component liquids respectively.

Table (2)
Densities ρ, Refractive Indices n_D, Excess Volumes, V^E and ΔR changes of Mixing for Binary Mixtures at 303.15 K.

x_1	ρ/ g.cm^{-3}	n_D	V^E/cm^3.mol^{-1}	ΔR/cm^3.mol^{-1}
Sulfolane (1) + Toluene (2)				
0.04987	0.90195	1.4900	-0.3205	-0.9203
0.10584	0.92242	1.4894	-0.5154	-1.1779
0.17814	0.96071	1.4882	-0.6813	-1.2987
0.25853	1.00816	1.4876	-0.8396	-2.0989
0.30193	1.01378	1.4868	-0.9814	-1.4580
0.40058	1.04846	1.4860	-1.0522	-1.3104
0.50357	1.08644	1.4852	-1.0718	-1.3049
0.60615	1.12247	1.4849	-0.9811	-0.9514
0.71089	1.15799	1.4836	-0.8347	-0.7168
0.80971	1.19295	1.4830	-0.6359	-0.4809
0.90502	1.22640	1.4824	-0.2770	-0.2207
0.95025	1.24376	1.4820	-0.1296	-0.1437
Sulfolane (1) + water (2)				
0.04874	1.05741	1.3726	-0.1090	-3.7395
0.10758	1.09800	1.3872	-0.1368	-6.5884
0.20525	1.14994	1.4165	-0.1486	-8.7005
0.30072	1.18082	1.4341	-0.1220	-9.2186
0.40429	1.20365	1.4480	-0.0913	-8.8321
0.50805	1.21979	1.4575	-0.0486	-7.8837
0.55109	1.22652	1.4613	-0.0342	-7.3747
0.60674	1.23167	1.4646	-0.0257	-6.6386
0.70888	1.24119	1.4703	0.0063	-5.1153
0.80594	1.24852	1.4748	0.0284	-3.5048
0.90844	1.25525	1.4783	0.0312	-1.7065
0.94998	1.25862	1.4800	0.0232	-0.9481

Table (2) continued:

x_1	ρ/ g.cm^{-3}	n_D	V^E/cm^3.mol^{-1}	ΔR/cm^3.mol^{-1}
Dimetheylsulfoxide (1) + Toluene (2)				
0.05694	0.87915	1.4902	-0.1641	-0.6247
0.10253	0.89164	1.4900	-0.2305	-0.7041
0.20291	0.90318	1.4897	-0.2708	-0.9443
0.27544	0.91988	1.4885	-0.3047	-1.3186
0.36433	0.93704	1.4870	-0.3192	-1.4753
0.45581	0.95098	1.4862	-0.3188	-1.5497
0.50408	0.96718	1.4858	-0.3101	-1.6312
0.60357	0.98174	1.4842	-0.2951	-1.6423
0.65452	1.00050	1.4826	-0.2691	-1.5332
0.70490	1.01457	1.4816	-0.2411	-1.0324
0.80997	1.03551	1.4803	-0.1923	-0.7016
0.90174	1.05038	1.4781	-0.1521	-0.4494
Dimetheylsulfoxide (1) + water (2)				
0.05498	1.02119	1.3620	-0.1574	-2.1553
0.10157	1.03925	1.3721	-0.3180	-3.5150
0.20923	1.06484	1.3873	-0.6084	-5.3511
0.30356	1.08170	1.4164	-0.8322	-5.6978
0.35041	1.08620	1.4304	-0.8637	-5.6049
0.40389	1.08928	1.4416	-0.9012	-5.4199
0.50602	1.09292	1.4572	-0.8745	-4.8244
0.60652	1.09349	1.4663	-0.7485	-4.0307
0.70471	1.09272	1.4708	-0.5635	-3.1387
0.80304	1.09158	1.4718	-0.3546	-2.1932
0.90542	1.08996	1.4721	-0.0945	-1.1139
0.94925	1.08982	1.4730	-0.0536	-0.6066

Table (3)
Densities, ρ, Refractive Indices, n_D, Excess Molar Volumes, V^E and ΔR Values for Sulfolane (1) + Toluene (2) + Water (3) at 303.15 K.

x_1	x_2	ρ/ g.cm^{-3}	n_D	V^E/cm^3.mol^{-1}	ΔR/cm^3.mol^{-1}
0.35425	0.57117	1.01929	1.4768	-1.7286	-2.2196
0.37125	0.52812	1.03078	1.4923	-1.6628	-2.3784
0.41473	0.48139	1.04932	1.4911	-1.5422	-2.5110
0.43069	0.48068	1.05300	1.4914	-1.5324	-2.5662
0.45375	0.49771	1.05565	1.4931	-1.6388	-2.7276
0.47028	0.46681	1.06474	1.4924	-1.5383	-2.9059
0.49142	0.35365	1.09115	1.4858	-1.0597	-3.5484
0.53672	0.30994	1.11043	1.4843	-0.9057	-3.6154
0.55021	0.27134	1.12260	1.4820	-0.7560	-4.0603
0.57895	0.29652	1.12161	1.4849	-0.8673	-2.0017
0.59318	0.30681	1.12155	1.4859	-0.9031	-1.6088
0.60809	0.32803	1.12398	1.4901	-1.0078	-1.5926
0.63148	0.28461	1.13404	1.4862	-0.8723	-1.3111
0.65382	0.30740	1.13187	1.4882	-0.9481	-1.1328
0.68625	0.28850	1.14148	14871	-0.8878	-1.0129
0.71171	0.24252	1.15718	1.4864	-0.7457	-0.7525
0.74435	0.23051	1.16507	1.4868	-0.7303	-0.6754
0.76329	0.21893	1.17141	1.4872	-0.7557	-0.5564
0.79082	0.18846	1.18240	1.4858	-0.7256	-0.5283
0.81241	0.16956	1.19295	1.4866	-0.7276	-0.5029
0.83308	0.14640	1.19498	1.4826	-0.7168	-0.5001
0.85843	0.12481	1.20486	1.4828	-0.7258	-0.4896
0.87178	0.10518	1.21286	1.4821	-0.6904	-0.4209
0.90050	0.08923	1.22093	1.4823	-0.7124	-0.2735
0.95318	0.03851	1.24392	1.4819	-0.4779	-0.2184
0.97021	0.02046	1.24816	1.4800	-0.4248	-0.2058
0.98952	0.01032	1.25712	1.4820	-0.3817	-0.1247

Table (4)
Densities, ρ, Refractive Indices, n_D, Excess Molar Volumes, V^E and ΔR Values for Dimethylsulfoxide (1) + Toluene (2) + Water (3) at 303.15 K.

x_1	x_2	ρ/ g.cm^{-3}	n_D	V^E/cm^3.mol^{-1}	ΔR/cm^3.mol^{-1}
0.50616	0.40683	0.96861	1.4809	-0.3638	-4.7594
0.52248	0.34161	0.98134	1.4780	-0.3921	-4.7176
0.54948	0.42580	0.96944	1.4829	-0.3091	-4.2901
0.56021	0.40052	0.97427	1.4820	-0.3094	-4.2455
0.58768	0.31056	0.99252	1.4782	-0.3356	-4.3907
0.61725	0.26266	1.00267	1.4764	-0.3346	-4.1810
0.63342	0.24408	1.00995	1.4758	-0.3301	-3.9953
0.65147	0.22901	1.01458	1.4754	-0.3167	-3.7992
0.66278	0.27302	1.00539	1.4783	-0.2640	-3.6353
0.68618	0.24632	1.01258	1.4775	-0.2484	-3.1841
0.70806	0.22833	1.01792	1.4771	-0.2311	-2.9959
0.72513	0.21254	1.02253	1.4770	-0.2189	-2.6334
0.75682	0.20399	1.02621	1.4772	-0.1836	-2.5512
0.77165	0.18146	1.03239	1.4763	-0.1782	-2.2693
0.79082	0.16251	1.03805	1.4768	-0.1654	-1.8481
0.80164	0.14756	1.04239	1.4749	-0.1601	-1.6753
0.82241	0.12242	1.04999	1.4740	-0.1474	-1.4558
0.85565	0.08185	1.06269	1.4726	-0.1230	-1.3198
0.87325	0.06432	1.06842	1.4720	-0.1063	-1.0528
0.89082	0.05326	1.07220	1.4719	-0.0864	-0.7575
0.90118	0.04927	1.07365	1.4724	-0.0752	-0.6802
0.92156	0.04462	1.07556	1.4733	-0.0573	-0.3959
0.94431	0.03461	1.07919	1.4738	-0.0408	-0.3453
0.95424	0.03208	1.08025	1.442	-0.0375	-0.2842
0.97130	0.03004	1.08333	1.4745	-0.0406	-0.2531
0.99241	0.00842	1.09102	1.4748	-0.0318	-0.1753

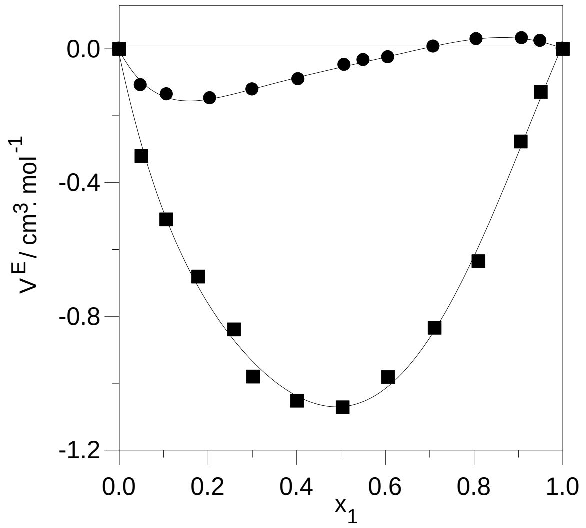

Fig. (1) : Excess molar volumes, V^E, as a function of composition at: 303.15 303.15 K: (■) x_1 sulfolane +x_2 K, (●) x_1 sulfolane + x_2 water. DMSO + x_2 water.

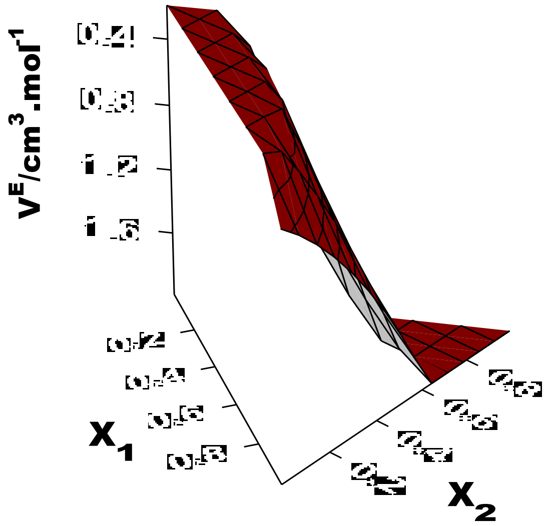

Fig. (3) : Excess molar volume for ternary system x_1 sulfolane + x_2 toluene + x_3 water at 303.15 K.

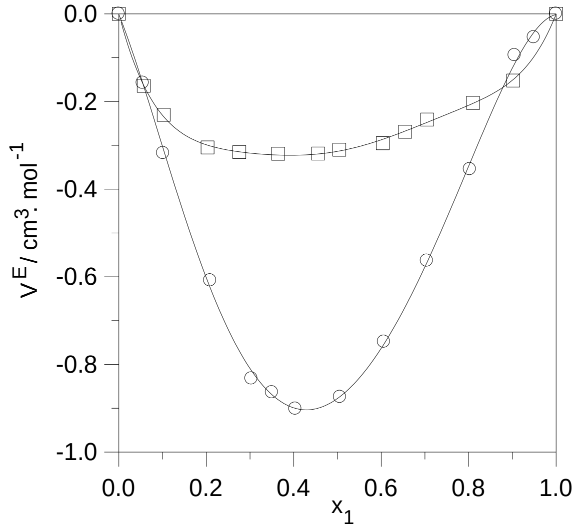

Fig. (2) : Excess molar volumes, V^E, as a function of composition at as a function of composition at 303.15 303.15 K: (□) x_1 DMSO + x_2 toluene, (○) x_1 toluene.

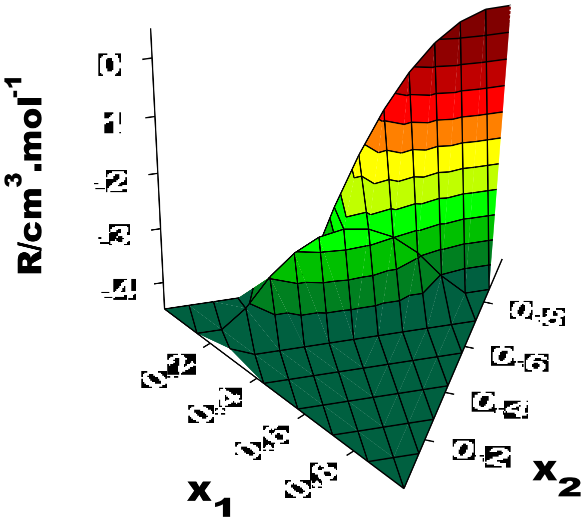

Fig.(4) : Molar refraction changes of mixing for ternary system x_1 sulfolane + x_2 toluene + x_3 water at 303.15 K.

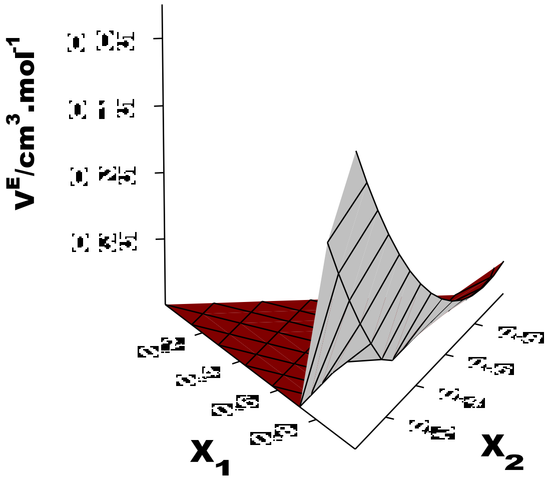

Fig. (5) : Excess molar volume for ternary system x_1 dimethylsulfoxide + x_2 toluene + x_3 water at 303.15 K.

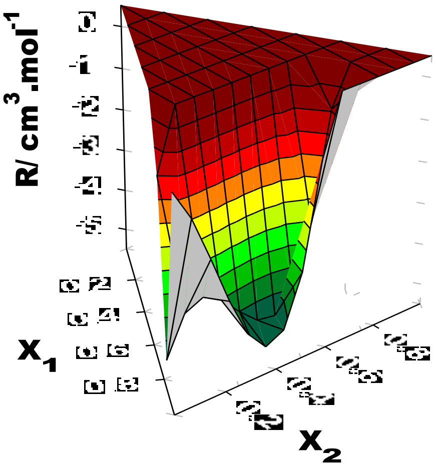

Fig. (6) : Excess molar volume for ternary system x_1 dimethylsulfoxide +x_2 toluene + x_3 water at 303.15 K.

The calculated values of V^E and ΔR for binary mixtures were correlated with the Redlich – Kister equation(12):

$$Y^E = x(1-x) \sum_{k=0}^{k} A_k (2x-1)^k, \; k=0,1,... \qquad \text{...........................} \; ...(6)$$

where Y^E is V^E or ΔR and x is the mole fraction of the first component of the mixture.

For the ternary system the Redlich–Kister equation is:

$$Q_{123} = Q_{12} + Q_{23} + Q_{13} + x_1x_2x_3(A + B(x_1 - x_2) + C(x_2 - x_3) + D(x_1 - x_3) + E(x_1 - x_2)^2) + F(x_2 - x_3)^2 + G(x_1 - x_3)^2 + \cdots) \qquad \text{...........................} \; ...(7)$$

where Q_{123} represents V^E or ΔR for the ternary mixtures sulfolane (1) + toluene (2) + water (3) and DMSO(1) + toluene (2) + water (3) and Q_{ij} is the binary contribution expressed by Redlich – Kister polynomial, with, in this case, Q_{23} equal to zero(14) because of the immiscibility of toluene and water..

On the other hand, The V^E and ΔR values were correlated with the composition by means of the Cibulka (13) equation:

$$Q_{123} = Q_{12} + Q_{13} + Q_{23} + x_1 x_2 x_3 (A + Bx_1 + C x_2 + D x_1^2) \qquad \text{...........................} \; ...(8)$$

The A_k values for Q_{12} (sulfolane + toluene) or (DMSO + toluene) and Q_{13} (sulfolane + water) or (DMSO + water) are summarized in Table 5 together with the corresponding standard deviations

The unweighted least – squares method was used to fit the polynomial to the data. The parameters for fitting eqs.6 – 8 and the corresponding standard deviations obtained is given in Table 5 for binary mixtures and Table 6 for ternary mixtures, respectively. The standard deviations were calculated using the following equation(15):

$$\sigma = \left(\frac{\sum_{1}^{n_{DAT}} (Z_{exp} - Z_{pred})^2}{n_{DAT} - n_{PAR}} \right)^{1/2} \qquad \text{.....} \; ...(9)$$

In this equation Z is the value of the property, n_{DAT} is the number of experimental data, and n_{PAR} is the number of parameters.

Table (5)

Polynomial coefficients (A_j) and Standard deviation, σ obtained for Fits of Eq 6 to the V^E and ΔR composition Data for the Binary Systems.

property	A_O	A_1	A_2	A_3	A_4	σ
Sulfolane (1) + Toluene (2)						
$V^E/cm^3.mol^{-1}$	-4.3497	-0.2381	1.5502	3.3282	-4.0314	0.0035
$\Delta R/cm^3.mol^{-1}$	-5.3222	4.2308	1.4531	5.6403	-12.0956	0.0043
Sulfolane (1) + water (2)						
$V^E/cm^3.mol^{-1}$	-0.2121	0.5816	-0.2534	0.9749	-0.5980	0.0056
$\Delta R/cm^3.mol^{-1}$	-31.8919	21.1664	-13.9868	14.8341	-10.8997	0.0023
Dimetheylsulfoxide (1) + Toluene (2)						
$V^E/cm^3.mol^{-1}$	-1.2745	0.2867	0.1986	0.3566	-2.2997	0.0010
$\Delta R/cm^3.mol^{-1}$	-6.7421	-0.2669	7.0636	4.1292	-10.4762	0.0018
Dimetheylsulfoxide (1) + water (2)						
$V^E/cm^3.mol^{-1}$	-3.4600	1.6018	0.8359	-0.1136	1.9438	0.0033
$\Delta R/cm^3.mol^{-1}$	-19.3667	14.4795	-11.7329	2.6240	2.4335	0.0043

Table (6)

Polynomial coefficients and standard deviations (σ) for Eqs. (7) and (8) fitted from experimental **data of the ternary systems at 303.15 K.**

property	A	B	C	D	E	F	G	σ
Sulfolane (1) + Toluene (2) + water (3)								
Redlich–Kister Eq.(7)								
$V^E/cm^3.mol^{-1}$	1.8442	7.0457	-10.8648	-3.9207	-11.0403	0.5044	-0.0015	0.0003
$\Delta R/cm^3.mol^{-1}$	4.0428	9.1922	-6.8570	-3.0099	-3.0015	5.9377	0.0668	0.0006
Cibulka Eq.(8)								
$V^E/cm^3.mol^{-1}$	-0.1382	0.2104	0.1529	-0.0797	–	–	–	0.0072
$\Delta R/cm^3.mol^{-1}$	-0.2774	-0.5722	0.8546	0.8322				0.0031
Dimetheylsulfoxide (1) + Toluene (2) + water (3)								
Redlich–Kister Eq.(7)								
$V^E/cm^3.mol^{-1}$	0.4396	-0.1156	-0.5173	-0.7329	0.4939	0.0065	-0.0004	0.0002
$\Delta R/cm^3.mol^{-1}$	0.7154	-2.1869	0.5974	-1.6928	6.6989	0.0126	-0.0049	0.0004
Cibulka Eq.(8)								
$V^E/cm^3.mol^{-1}$	0.0154	0.0262	-0.0111	0.0109	–	–	–	0.0022
$\Delta R/cm^3.mol^{-1}$	-3.9489	2.4951	5.3291	1.5508				0.0090

Discussion

Excess molar volumes, V^E at 303.15 K for binary mixtures of, sulfolane + toluene and DMSO + toluene, are negative over the whole mole fraction range, reaching a minimum around -0.1220, and -1.8500 $cm^3.mol^{-1}$ respectively. Figs. (1 and 2). The reasonable explanation for this fact is as follows. Sulfolane and dimethyl sulfoxide are polar molecules and toluene is a non-polar molecule. The mixtures formed by sulfolane or dimethyl sulfoxide and toluene not only have dipolar–dipolar interaction between sulfolane or dimethyl sulfoxide molecules, but also have the interaction of dipolar- induced forces between sulfolane or dimethyl sulfoxide molecules and toluene molecules. It is shown that sulfolane is the most favorable one to form close packing with toluene comparison with dimethyl sulfoxide.

The interaction between unlike molecules seems to be stronger than the intramolecular interactions, leading to negative values of excess molar volumes(16). In addition, the relatively higher polarity of sulfolane molecules as compared with DMSO molecules may be another factor contributing to the volume contraction of the mixtures. So this explained the higher negative values of the excess molar volumes, V^E for binary mixture of sulfolane + toluene as compared with V^E data for binary mixture of DMSO + toluene

For binary mixture DMSO + water there is a minimum in V^E in the water rich region, Fig. (2), which is related to the composition of dimethylsulfoxide + water. Such behavior is similar to that obtained by Markarian and co workers (7) Such behavior is a result of destroying the self – associated water molecules (breaking hydrogen bonds in water) and a new complex is formed through hydrogen bonding between sulfoxide group of DMSO and the hydroxyl group of water. This indicates that the new hydrogen bonding in DMSO – water mixtures are stronger than that between pairs of water and dipolar association in DMSO.

For the binary mixture of sulfolane + water the excess molar volumes is sigmoidal with an initial negative region followed by a positive lobe at high sulfolane mole fraction. Values of molar refraction changes of mixing, ΔR are negative for all binary mixtures under study.

The ternary systems of sulfolane (1) + toluene (2) + water (3) and DMSO (1) + toluene (2)+ water (3)show negative values of excess molar volumes. Figures 3 and 5. In the same manner, the mixture sulfolane (1) + toluene (2) + water (3) exhibits relatively large negative V^E values for the entire range of homogenous mixtures, Fig. (3). For both systems the deviations are not zero. This suggests that the ternary mixtures are not ideal in terms of constituent binaries, indicating that the third component modifies both the nature and degree of molecular interactions between the two other component liquids.

The molar refraction changes of mixing (ΔR) are also negative for both ternary systems under study, Figures 4 and 6.The ΔR data follow the same general pattern as described above for V^E.

The Redlich–Kister polynomial equation provided a satisfactory correlation of the binary data, Table (5). In the case of the ternary systems, the Redlich–Kister equation gives a better correlation than those obtained by the Cibulka equation, which can be inferred by the lower value of the mean standard deviation, Table (6).

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الخلاصة

يتضمن هذا البحث قياس الكثافة و معامل الانكسار بطريقة عملية للمخاليط ثنائية و ثلاثية المكون المحتوية على السلفولان او ثنائي مثيل سلفوكسايد مع التلوين و الماء على المدى الكلي من الكسور المولية في درجة حرارة 303،١٥ كلفن و الضغط الجوي. من القياسات العملية تم حساب الحجوم المولارية الفائضة V^E و التغييرات في معامل الانكسار المولاري ΔR للامزجة الثنائية و الثلاثية المكون.تم معايرة قيم الـ V^E و δR المحسوبة بأستخدام علاقة ردلخ – كستر و استخراج معاملات المخاليط ثنائية المكون و التي استخدمت لتعيير النتائج المحسوبة للانظمة ثلاثية المكون بأستخدام معادلة ردلخ – كستر و معادلة كابولكا متعددة الحدود. نوقشت النتائج المستحصلة و التأثيرات المتبادلة لجميع المخاليط بالاعتماد على التراكيب الكيميائية للمركبات المستخدمة في هذه الدراسة.