# Acoustic Studies in the Binary Mixtures of Dimethyl Carbonate with Salicylates at Different Temperatures

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#### **Abstract**

For the binary mixtures of Di Methyl Carbonate (DMC)+Methyl Salicylate (MS), + Ethyl Salicylate (ES) and +Benzyl Salicylate (BS), ultrasonic velocity(U), density( $\rho$ ) and viscosity ( $\eta$ ) were measured over the entire composition range at four different temperatures 303.15, 308.15, 313.15 and 318.15K. From the experimental data, excess values of molar volume and inter molecular free length and deviation in adiabatic compressibility and viscosity were computed. The values of  $V^E$ ,  $\Delta\beta_{ad}$  and  $L_f^E$  have been fitted to Redlich – Kister polynomial equation to estimate binary coefficients and standard deviationbetween the experimental and computed values.

**Keywords**: Di methyl carbonate, densities, speed of sound, viscosity, adiabatic compressibilities, molar volumes, inter molecular free lengths.

## 1. Introduction

The molecular interactions and physico-chemical behavior of mixes of binary liquids are best understood through an appreciation of their acoustic properties. The study of molecular structure requires knowledge of how molecules interact in solutions. The form and internal structure of molecules can be altered by their interactions with one another. A variety of size-dependent connections, molecule packing, mobility, physicochemical behavior, and the types and intensities of intermolecular interactions can be gleaned from measurements of acoustical parameters<sup>1-5</sup>.

Ubangara Mary and P. Neeraja6 examined and studied the ultrasonic speed (U), density ( $\rho$ ), and viscosity ( $\eta$ ) of binary liquid solutions of isobutyl methyl ketone, cyclohexanone, and methyl salicylate.

They were able to extrapolate some acoustical properties from these readings. The full concentration range, including the extremes, is considered in the analysis of these parameters. data. Over the whole concentration range, with the excess values of these parameters are also examined.

The acoustic characteristics of a binary liquid mixture of methyl salicylate and benzene were determined by Chandra Bhan Singh et al.<sup>7</sup> at three distinct temperatures. The obtained ultrasonic velocity, density, and viscosity measurements are used to derive the acoustic parameters.

Volumetric and viscometric data have been employed in various cresol binary combination studies<sup>8-10</sup>. These researchers discovered not only hydrogen bonding, but also robust intermolecular interactions. The combination of dimethyl carbonate and salicylates is a binary system that has not been studied extensively.

# 2. Experimental Techniques

# a) Velocity Measurements

The formula U=f can be used to calculate the ultrasonic velocity. The research makes use of a generator with a frequency of 2 MHz. Adjusting the high frequency generator's anode current meter to its highest reading was a painstaking process that required a micrometer screw.

While adjusting the micrometer screw for n peaks, we should keep track of how many times the anode current was at its maximum.

 $d = n\lambda/2$ 

The speed in meters per second can be easily determined by multiplying the distance the reflector is moved by 20 peaks by 100. Since the distance 'd' may be measured to an accuracy of 0.01 mm or better using a micrometer, the precision of the velocity is mostly dependent on the precision of the distance measurement. The precision of the acceleration measurement was +0.02%.

## b) Density Measurements

In the current study, a specific gravity bottle of 5ml volume sutilised to determine of pure liquids' density ( $\rho$ ) and all mixtures of the liquids at various temperatures from 303.15K, to 318.15K with an interval of 5K. One of the standards for the liquids' purity was their density. For achieving thermal equilibrium, the specific gravity bottle was kept for 15

minutes in the thermostat. Once they reach room temperature, they are taken out of the thermostat and weighed. There is a 0.5mg margin of error in the density measurements.

# c)Viscosity Measurements

Using an Ubbelohde capillary viscometer with a 0.55mm diameter and calibrated with double-distilled water, the viscosity was determined at temperatures of 303.15, 308.15, 313.15, and 318.15K. Calibration of the viscometer is accomplished using pure water, and the liquid is then allowed to stand for roughly 30 minutes in a thermostatic water bath in order to minimize temperature changes. The precision of the viscosity measurements is 0.005 mPas.

#### 3. Theoretical Considerations

## i) Molar volume

$$V = M / \rho$$
 3.1

# ii). Excess Volume (VE)

$$V^{E} = V - (V_{1}X_{1} + V_{2}X_{2})$$
 3.2

where  $X_1$  &  $X_2$  are the mole fractions of pure liquids and  $V_1$ &  $V_2$  are the mean molar volumes respectively.

## iii. Adiabatic Compressibility (βad)

$$\beta_{ad} = 1/\rho U^2$$
 3.3

## iv. Deviation in Adiabatic compressibility (Δβad)

$$\Delta \beta_{ad} = \beta_{ad} - (\beta_{ad1} X_1 + \beta_{ad2} X_2)$$
 3.4

where pure liquids' adiabatic compressibilities are indicated as  $\beta_{ad1}$  and  $\beta_{ad2}$ .

# v). Intermolecular free length (L<sub>f</sub>)

$$L_{\rm f} = K (\beta_{\rm ad})^{1/2}$$
 3.5

Jacobson constant is indicated as K.

# vi). Excess Intermolecular free length (L<sub>f</sub><sup>E</sup>)

$$L_f^E = L_f - (L_{f1}X_1 + L_{f2}X_2)$$
 3.6

pure liquids' intermolecular free length are L<sub>f1</sub> and L<sub>f2</sub>respevtively

## vii). Deviation in Viscosity (Δη)

The equation for deviation in viscosity is

$$\Delta \eta = \eta_{\text{mix}} - (X_1 \eta_1 + X_2 \eta_2)$$
 3.7

The the liquid mixture and the pure liquids' viscosities are indicated as  $\eta_{mix}$ ,  $\eta_1$  and  $\eta_2$  are respectively.

#### 4. Purification of solvents

The purity of the substance used in an experiment directly affects the accuracy and precision of the results. As a result, ensuring the highest possible purity of the compounds employed is crucial. Different purification procedures, detailed in full in the literature <sup>12-14</sup>, were devised with the type and functional groups of the compounds in mind.

Table-1: Literature Data in comparision with experimental data<sup>10-13</sup> at 308.15K

Liquid	Density(ρ	o) Kg/m <sup>3</sup>	Velocity of Ultrasonic Sound(U)m/s		
	Exptl	Lit	Exptl	Lit	
Dimethyl Carbonate	1.0562	1.0567115	1175.3	1177 <sup>15</sup>	
Methyl Salicylate	1.1752	$1.1750^{16}$	1389.7	1390.4 <sup>16</sup>	
Ethyl Salicylate	1.1181	$1.1180^{16}$	1348.4	1354.4 <sup>16</sup>	
Benzyl Salicylate	1.1063	1.1065 <sup>16</sup>	1497.2	1498.4 <sup>16</sup>	

The organic liquids available are all of the best possible quality. After being distilled, combined with a burette, and utilized in an experiment, the liquids need around 5-6 hours to reach temperature equilibrium.

Table 1 displays the results of a comparison between the experimental values and data from the literature.

## Results

The experimental data for density, viscosity, and ultrasonic velocity (U) at temperatures of 303.15, 308.15, 313.15, and 318.15 K for the three binary mixtures (Di Methyl Carbonate + Salicylates) are shown in Table 2. Over a large temperature range, we examined the ultrasonic velocity, viscosity, and density of binary mixes containing different concentrations of dimethyl carbonate (X1). This particular interaction between distinct molecules is indicated by the fact that the experimentally recorded values fluctuate nonlinearly with mole fraction of di methyl carbonate.

Table-2: Ultrasonic velocity (U), density ( $\rho$ ), deviations in adiabatic compressibility ( $\Delta\beta_{ad}$ ) and viscosity( $\Delta\eta$ ), excess values of molar volume ( $V^E$ ) and intermolecular free length ( $L_f^E$ ) binary mixtures of Di Methyl Carbonate with three salicylates under study.

	T		I				
			Density		$\Delta \beta_{ad} \times 1$		
Molefraction	Velocity	Viscosit	ρ , ,	V <sup>E</sup> cm <sup>3</sup> mol <sup>-1</sup>	0 <sup>-12</sup> m <sup>2</sup> N <sup>-1</sup>	L <sub>f</sub> EAo	4 B
X <sub>1</sub>	U m/s	yηcP	gm/cm <sup>3</sup>	· Methyl Sal		L <sub>f</sub> A	Δη cP
	DIMI	tilyi Carb	303.15		icylate(2)		
0.0000	1389.70	2.9660	1.1752	0.0000	0.0000	0.0000	0.000
0.1476	1379.65	2.8546	1.1660	-0.2864	-2.6115	-0.0332	0.000
0.2803	1367.20	2.7967	1.1563	-0.4941	-4.6474	-0.0586	0.508
0.4004	1355.59	2.6916	1.1461	-0.6419	-6.3698	-0.0801	0.693
0.5095	1342.33	2.5653	1.1360	-0.7860	-7.6647	-0.0960	0.831
0.6091	1327.21	2.4014	1.1250	-0.8382	-8.4922	-0.1057	0.907
0.7003	1296.50	2.0825	1.1128	-0.7814	-7.7251	-0.0941	0.809
0.7843	1263.62	1.7519	1.0996	-0.6425	-6.2839	-0.0748	0.681
0.8617	1233.78	1.3290	1.0865	-0.5204	-4.6689	-0.0545	0.446
0.9334	1205.00	0.9547	1.0721	-0.2955	-2.6468	-0.0304	0.245
1.0000	1175.30	0.5490	1.0566	0.0000	0.0000	0.0000	0.000
	I		308.15				
0.0000	1374.40	2.6540	1.1685	0.0000	0.0000	0.0000	0.000
0.1476	1366.50	2.5620	1.1596	-0.3138	-2.9890	-0.0377	0.223
0.2803	1355.00	2.5068	1.1501	-0.5383	-5.2918	-0.0661	0.452
0.4004	1342.00	2.3900	1.1401	-0.6905	-7.0897	-0.0879	0.591
0.5095	1328.10	2.2872	1.1300	-0.8319	-8.4812	-0.1045	0.721
0.6091	1311.00	2.1614	1.1192	-0.8951	-9.2764	-0.1134	0.808
0.7003	1279.00	1.8740	1.1071	-0.8379	-8.4364	-0.1009	0.716
0.7843	1247.00	1.5669	1.0941	-0.7066	-7.0751	-0.0828	0.588
0.8617	1214.97	1.2081	1.0811	-0.5835	-5.2198	-0.0598	0.395
0.9334	1187.00	0.8547	1.0669	-0.3680	-3.2372	-0.0367	0.195
1.0000	1153.70	0.5180	1.0507	0.0000	0.0000	0.0000	0.000
			313.15	K			
0.0000	1358.5000	2.4040	1.1678	0.0000	0.0000	0.0000	0.000
0.1476	1354.8887	2.2790	1.1589	-0.3955	-3.5265	-0.0377	0.158
0.2803	1344.5138	2.2299	1.1487	-0.6206	-6.0920	-0.0661	0.364
0.4004	1332.5930	2.1310	1.1381	-0.7879	-8.1326	-0.0879	0.495
0.5095	1318.7529	2.0396	1.1275	-0.9406	-9.6688	-0.1045	0.613
0.6001	1202 4005	1.0500	1 11/0	0.0004	10 (275	0.1124	0.722
0.6091	1302.4895	1.9580	1.1160	-0.9994	10.6375	-0.1134	0.722
0.7003	1273.1050	1.6808	1.1031	-0.9258	10.0793	-0.1009	0.620
0.7843	1235.6060	1.4016	1.0895	-0.7982	-8.2435	-0.0828	0.502
0.8617	1203.5266	1.0810	1.0760	-0.6836	-6.3702	-0.0598	0.330
0.9334	1175.6114	0.7570	1.0610	-0.4485	-4.3444	-0.0367	0.143
1.0000	1135.0000	0.4860	1.0433	0.0000	0.0000	0.0000	0.000
			318.15	l .			
0.0000	1343.00	2.2180	1.1645	0.0000	0.0000	0.0000	0.000
0.1476	1344.22	2.1020	1.1560	-0.4830	-4.2016	-0.0443	0.141
0.2803	1336.34	2.0363	1.1456	-0.7236	-7.2122	-0.0755	0.307
0.4004	1323.86	1.9501	1.1350	-0.9187	-9.4516	-0.1000	0.431
				:	-		
0.5095	1307.25	1.8740	1.1241	-1.0744	10.9678	-0.1180	0.545
0.6091	1289.09	1.7954	1.1121	-1.1191	-	-0.1288	0.640

		1	1		11.0202				
					11.9283				
0.7003	1257.63	1.5341	1.0988	-1.0330	11.2581	-0.1197	0.538		
0.7843	1222.83	1.2930	1.0850	-0.9152	-9.7049	-0.1157	0.338		
0.8617	1188.15	0.9807	1.0710	-0.7807	-7.5439	-0.0724	0.266		
0.9334	1159.19	0.6950	1.0558	-0.5498	-5.3676	-0.0490	0.106		
1.0000	1113.00	0.4730	1.0367	0.0000	0.0000	0.0000	0.000		
Di Methyl Carbonate + Ethyl Salicylate									
		Tivicingi	303.151		yiuce				
0.0000	1355.50	3.1770	1.1181	0.0000	0.0000	0.0000	0.000		
0.1622	1348.40	2.9712	1.1136	-0.2100	-2.5096	-0.0318	0.220		
0.3034	1339.00	2.8398	1.1190	-0.4641	-4.4434	-0.0518	0.220		
0.4275	1329.00	2.7023	1.1057	-0.6235	-5.9414	-0.0747	0.649		
0.5374	1319.30	2.5389	1.1007	-0.7662	-7.1555	-0.0897	0.774		
0.6354	1311.00	2.3605	1.0955	-0.8261	-8.1879	-0.1025	0.853		
0.7233	1286.00	2.0546	1.0890	-0.7590	-7.5197	-0.0927	0.778		
0.8026	1256.50	1.7046	1.0814	-0.5995	-6.0488	-0.0727	0.637		
0.8745	1229.00	1.2720	1.0738	-0.4532	-4.3939	-0.0523	0.393		
0.9401	1201.10	0.9180	1.0649	-0.2100	-2.2584	-0.0264	0.211		
1.0000	1175.30	0.5490	1.0562	0.0000	0.0000	0.0000	0.000		
			308.151						
0.0000	1338.60	2.2530	1.1153	0.0000	0.0000	0.0000	0.000		
0.1622	1330.80	2.1570	1.1110	-0.2704	-2.6974	-0.0335	0.185		
0.3034	1325.60	2.1290	1.1068	-0.5216	-5.1357	-0.0640	0.402		
0.4275	1315.70	2.0560	1.1019	-0.6681	-6.7915	-0.0842	0.545		
0.5374	1306.50	1.9906	1.0972	-0.8156	-8.1804	-0.1011	0.670		
0.6354	1295.00	1.8931	1.0917	-0.8714	-9.0572	-0.1114	0.742		
0.7233	1268.20	1.6570	1.0849	-0.7995	-8.2543	-0.0999	0.659		
0.8026	1239.20	1.3941	1.0772	-0.6526	-6.8141	-0.0810	0.534		
0.8745	1210.10	1.0730	1.0695	-0.5174	-4.9593	-0.0579	0.337		
0.9401	1184.00	0.7816	1.0606	-0.2916	-2.9599	-0.0342	0.160		
1.0000	1153.70	0.5180	1.0507	0.0000	0.0000	0.0000	0.000		
	'		313.151	K					
0.0000	1324.00	2.2530	1.1080	0.0000	0.0000	0.0000	0.000		
0.1622	1321.00	2.0860	1.1042	-0.3388	-3.3052	-0.0335	0.120		
0.3034	1314.50	2.0286	1.1000	-0.5920	-5.8285	-0.0640	0.312		
0.4275	1306.30	1.9488	1.0953	-0.7559	-7.7801	-0.0842	0.451		
0.5374	1299.00	1.8674	1.0905	-0.8960	-9.4582	-0.1011	0.564		
0.6251	1006.50	1.7051	1.0050	0.0400	10.2611	0.1114	0.665		
0.6354	1286.50	1.7951	1.0850	-0.9492	10.3611	-0.1114	0.665		
0.7233	1262.04	1.5607	1.0780	-0.8543	-9.8205	-0.0999	0.586		
0.8026	1226.22	1.3004	1.0708	-0.7520	-7.7722 5.0052	-0.0810	0.466		
0.8745 0.9401	1198.18 1170.68	1.0005 0.6871	1.0629	-0.5940	-5.9952 -3.7760	-0.0579	0.293		
1.0000	1170.68	0.6871	1.0536	-0.3287 0.0000	0.0000	-0.0342 0.0000	0.095		
1.0000	1133.00	0.4800	318.151		0.0000	0.0000	0.000		
0.0000	1306.80	2.0060	1.1057	0.0000	0.0000	0.0000	0.000		
0.1622	1304.40	1.8893	1.1021	-0.4254	-3.6719	-0.0410	0.132		
0.3034	1301.30	1.8176	1.0975	-0.4234	-6.7111	-0.0719	0.132		
0.4275	1297.40	1.7460	1.0928	-0.8956	-9.2466	-0.0954	0.395		
0.5374	1285.70	1.6956	1.0877	-1.0399	7.2 100	-0.0754	0.513		
0.5574	1203.70	1.0730	1.00//	-1.03/7		-0.113/	0.213		

	I	1	1		10.7205	1				
					10.7285					
0.6354	1273.07	1.6400	1.0819	-1.1021	11.7559	-0.1259	0.608			
0.7233	1245.95	1.3919	1.0745	-1.0046	11.0259	-0.1176	0.495			
0.8026	1215.00	1.1820	1.0668	-0.8873	-9.4534	-0.0910	0.406			
0.8745	1182.00	0.8909	1.0582	-0.6945	-7.1015	-0.0692	0.226			
0.9401	1153.93	0.6481	1.0486	-0.4380	-4.7571	-0.0431	0.083			
1.0000	1113.00	0.4730	1.0367	0.0000	0.0000	0.0000	0.000			
210000				Benzyl Salic		******				
			303.151	-						
0.0000										
0.2118	1461.00	5.6055	1.1023	-0.1655	-3.8283	-0.0479	0.183			
0.3769	1430.80	4.7998	1.0990	-0.3977	-6.5556	-0.0821	0.398			
0.5090	1410.70	4.1920	1.0957	-0.5851	-8.8688	-0.1117	0.607			
0.5070	1110.70	1.1720	1.0757	0.3031	-	0.1117	0.007			
0.6172	1390.36	3.6419	1.0923	-0.7280	10.4344	-0.1315	0.726			
0.7075	1372.00	3.1505	1.0885	-0.8038	11.5287	-0.1453	0.793			
0.7839	1333.89	2.6155	1.0830	-0.6956	10.6218	-0.1317	0.731			
0.8495	1288.82	2.0660	1.0771	-0.5641	-8.4636	-0.1025	0.586			
0.9063	1250.64	1.4900	1.0708	-0.4142	-6.2709	-0.0747	0.362			
0.9561	1210.37	1.0046	1.0630	-0.1560	-3.1914	-0.0372	0.184			
1.0000	1175.30	0.5490	1.0562	0.0000	0.0000	0.0000	0.000			
			308.151	K						
0.0000	1485.90	6.0800	1.1030	0.0000	0.0000	0.0000	0.000			
0.2118	1452.10	5.0389	1.0990	-0.2046	-4.3586	-0.0541	0.137			
0.3769	1425.50	4.3350	1.0958	-0.4810	-7.6252	-0.0949	0.351			
0.5090	1411.10	3.7298	1.0921	-0.6337	10.5703	-0.1328	0.481			
0.6172	1397.70	3.2783	1.0884	-0.7706	12.8221	-0.1616	0.631			
0.7075	1370.50	2.8571	1.0844	-0.8476	13.5045	-0.1687	0.712			
0.7839	1328.60	2.3209	1.0789	-0.7581	12.4191	-0.1523	0.601			
0.8495	1280.70	1.8490	1.0724	-0.5851	10.0708	-0.1206	0.494			
0.9063	1238.50	1.3299	1.0660	-0.4425	-7.4957	-0.0881	0.291			
0.9561	1197.80	0.8750	1.0589	-0.2572	-4.3458	-0.0502	0.113			
1.0000	1153.70	0.5180	1.0507	0.0000	0.0000	0.0000	0.000			
			313.151	K		<u> </u>				
0.0000	1471.80	6.0800	1.0995	0.0000	0.0000	0.0000	0.000			
0.2118	1435.70	4.9780	1.0955	-0.2741	-4.5684	-0.0541	0.083			
0.3769	1409.20	4.2100	1.0918	-0.5331	-8.0807	-0.0949	0.238			
0.5090	1393.50	3.6409	1.0879	-0.7159	11.1513	-0.1328	0.408			
0.6172	1375.40	3.1540	1.0838	-0.8406	13.2219	-0.1616	0.527			
0.7075	1352.00	2.7270	1.0794	-0.9096	14.2383	-0.1687	0.605			
0.7839	1315.50	2.2303	1.0735	-0.8180	13.5715	-0.1523	0.536			

					-		
0.8495	1262.85	1.7578	1.0673	-0.7068	10.7752	-0.1206	0.430
0.9063	1219.43	1.2609	1.0603	-0.5338	-7.9425	-0.0881	0.251
0.9561	1180.47	0.7906	1.0521	-0.2760	-4.7699	-0.0502	0.059
1.0000	1135.00	0.4860	1.0433	0.0000	0.0000	0.0000	0.000
			318.15	K			
0.0000	1457.00	5.4540	1.0950	0.0000	0.0000	0.0000	0.000
0.2118	1422.20	4.4807	1.0914	-0.3810	-5.1025	-0.0555	0.082
0.3769	1402.00	3.8086	1.0875	-0.6345	-9.3711	-0.0987	0.232
					-		
0.5090	1387.50	3.2887	1.0837	-0.8519	12.8265	-0.1373	0.370
					-		
0.6172	1363.40	2.8360	1.0796	-0.9942	14.7005	-0.1628	0.456
0.7075	1241.50	2.4070	1.0740	1.0460	15 0010	0.1744	0.550
0.7075	1341.50	2.4879	1.0749	-1.0460	15.9810	-0.1744	0.558
0.7839	1299.20	2.0152	1.0689	-0.9537	14.9141	-0.1638	0.466
0.7639	1299.20	2.0132	1.0009	-0.9337	14.9141	-0.1036	0.400
0.8495	1254.40	1.5700	1.0626	-0.8431	12.8157	-0.1266	0.347
0.9063	1204.70	1.1350	1.0551	-0.6366	-9.2995	-0.0914	0.195
0.9561	1162.40	0.7479	1.0465	-0.3554	-5.6175	-0.0541	0.155
1.0000	1113.00	0.4730	1.0367	0.0000	0.0000	0.0000	0.000

Table 2 shows that as the temperature of a binary liquid rises, its ultrasonic wave velocity falls. The bonds between molecules may become more easily broken at higher temperatures. When heat is applied to a binary mixture, the distance between molecules grows, allowing sound waves to travel further than they would in their pure solvents. As the temperature of a binary mixture rises, so does the rate at which ultrasonic waves travel through it.

According to Table 2, the binary liquid combination loses density and viscosity as its temperature rises. Particularly sensitive to inter-molecular interactions in liquid mixtures are excess characteristics such molar volume excess values( $V^E$ ) and viscosity deviations( $\Delta\eta$ ), which can be used to characterize the effect of interaction<sup>17</sup>.

When an excess parameter has a value other than zero, it indicates non-linearity and component interaction<sup>18</sup>. The estimated excess/deviations of parameters were shown in Figures 1(a)–3(d).

# **Figure Captions**

Fig 1(a): Excess molar volumevariations with the molefraction of DMC for the system DMC

+ Methyl Salycilate

Fig 1(b): Adiabatic compressibility deviations with DMCs molefraction for the system DMC

+ Methyl Salycilate

Fig 1(c): Variation of excessinter molecular free length with DMC mole fraction for the system DMC + Methyl Salycilate

Fig 1(d): Deviation in viscosity variations with the molefraction of DMC for DMC + Methyl Salycilate system

Fig 2(a): Variation of excess molar volume for DMC + Ethyl Salycilate system with the molefraction of DMC

Fig 2(b): Changein deviation in adiabatic compressibility with the molefraction of common compound for the system DMC + Ethyl Salycilate

Fig 2(c): Variation of excessintermolecular free length for the system DMC + Ethyl Salycilate with DMC's molefraction

Fig 2(d): Viscositydeviations with the common compound's molefraction for the system DMC + Ethyl Salycilate

Fig 3(a): Variation of excess molar volume with the molefraction of DMC for the system DMC + Benzyl Salycilate

Fig 3(b): Variation of deviation in adiabatic compressibility with the mole fraction of DMC for the system DMC + Benzyl Salycilate

Fig 3(c): Variation of excess inter molecular free length for DMC + Methyl Salycilate system with the mole fraction of DMC

Fig 3(d): Deviation in viscosity variation with the mole fraction of DMC for the system DMC + Methyl Salycilate

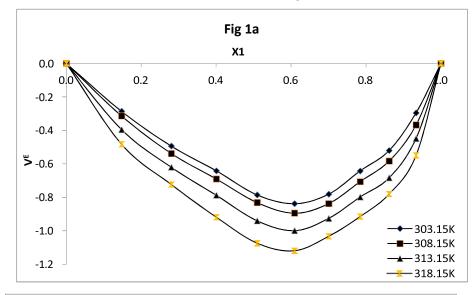
#### 6. Discussion

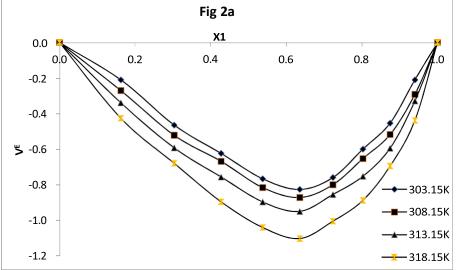
# 6.1 Excess Molar Volume(V<sup>E</sup>)

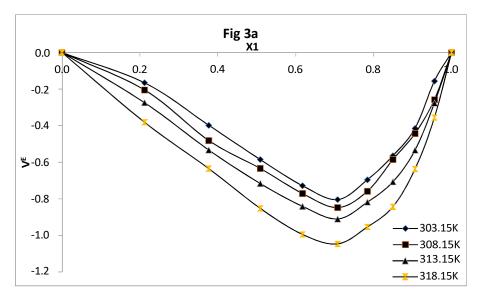
There is a potential for considerable H-bonding between the components of binary mixes of di methyl carbonate and salicylates due to the presence of the hetero element oxygen (C=O) in DMC and the aromaticity of salicylates. Di methyl carbonate is an aprotic, polar solvent with a tiny dipole moment of 0.90 D. Di methyl carbonate is polar because of the electronegative difference between the carbon and oxygen in the carbonyl group, which results in a partial negative charge on the O2 atom (O-) and a partial positive charge on the carbon atom (C+). It is therefore argued that dimethyl carbonate, when in liquid form, exhibits dipole-dipole interaction. The di methyl carbonate's two OCH3 (strong electron donating) groups connected to (C=O) have a potent positive inductive effect, stabilizing C's partial positive charge.

The OH group of a salicylate, which contains oxygen, can generate hydrogen bonds between molecules if the salicylate is arranged in an orthogonal fashion. Hydrogen bonding was studied by Boule19 to determine its effect on the molar ratios of polar liquid solutions. He discovered that the volume of complexes formed with hydrogen bonds decreases as their bonding strength increases.

When salicylates are mixed with solvents like di methyl carbonate, the volume of the solution may change due to two processes: (1) the depolymerization of the hydrogen-bonded salicylates that are self-associating with the solvent, and (2) the creation of new hydrogen bonds between the salicylates and the solvent. Salicylate and dimethyl carbonate (3) have unusual solute-solvent interactions. The first factor contributes to positive excess volumes, whereas the second and third factors contribute to negative excess volumes. The overall







variables.change in volume depends on the relative importance of these factors.

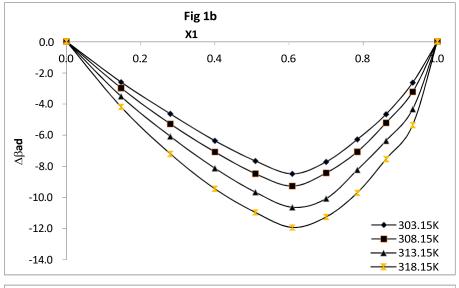
The actual variation in the volume of the binary systems is attributable to the predominance of the second and third elements mentioned previously, as well as the variation in the shape and size of the component molecules. Hydrogen bonds are utilized by each system to particularly interact with dissimilar molecules, as evidenced by the negative deviations of each system. The V<sup>E</sup> values are included in the order shown below.

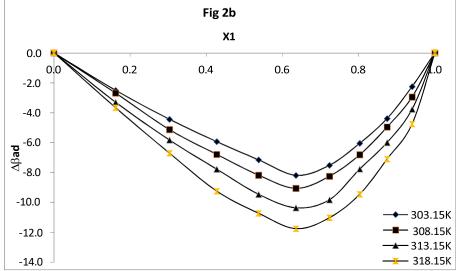
Methyl Salicylate > Ethyl Salicylate > Benzyle Salicylate

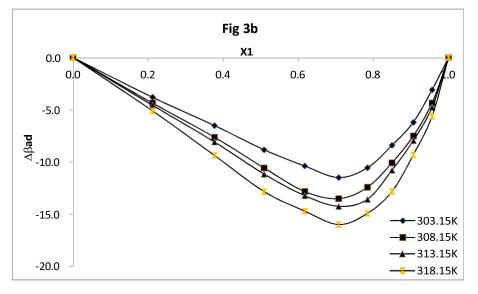
## **6.2** Adiabatic Compressibility Variations (Δβ<sub>ad</sub>):

Adiabatic compressibility is connected to the internal arrangement of molecules, just like excess molar volume. Equation (3.2) is used to calculate a mixture's adiabatic compressibility  $\beta$ ad.

Figure 2 shows the variations in adiabatic compressibility as a function of the mole fraction of DMC at 303.15, 308.15, 313.15, and 318.15 K. For all binary mixes of DMC+salicylate over the whole range of composition, ad values are negative. A negative excess compressibility is a sign of strong heteromolecular interaction in liquid mixtures, according to Fort and Moore<sup>11</sup>, and is attributed to interactions between dipole-dipole, dipole-induced dipoles, charge transferand hydrogen bonding between dissimilar components. A positive sign denotes weak interaction.







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A negative sign in the adiabatic compressibility of a mixture indicates that pure liquids compress more than it, which suggests the combination's molecules bind together more strongly than they would in their pure state. In general, the following elements determine the sign and size of an advertisement:

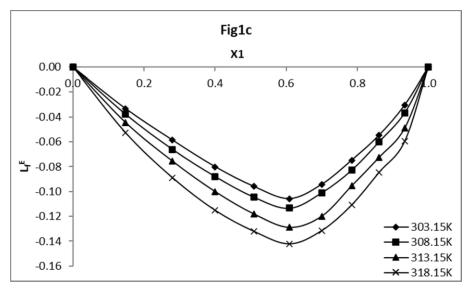
- 1. The different molecules' shapes and sizes at the molecular level
- 2. Destroying the H-bonding
- 3. The connection of H-bonds
- 4. The molecule-to-molecule creation of complexes.

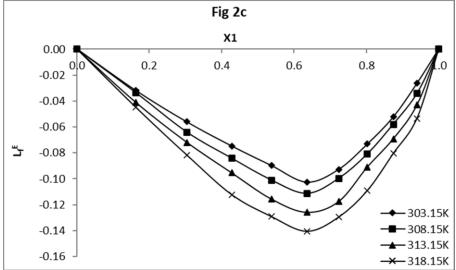
The first two factors contribute positively to the ad, whereas the next two factors contribute negatively.

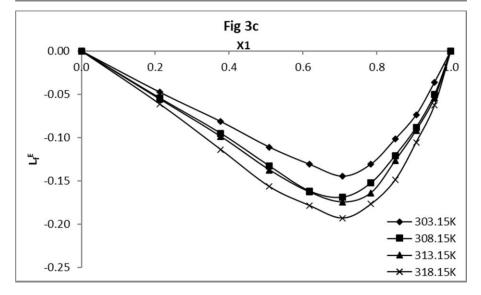
It can be seen from Figure 2 that the fluctuation is non-linear and that, for any given concentration, adiabatic compressibility diminishes as temperature rises. The mole fraction of dimethyl carbonate at which the negative deviation in adiabatic compressibility peaks is 0.6 (in the methyl Salicylate binary system). These numbers imply that there is a specific interaction between the mixture's constituent parts.

# 6.3 Inter Molecular Free Length (L<sub>f</sub><sup>E</sup>)

The distance between the surfaces of adjacent molecules is known as the intermolecular free length. It was discovered that a number of contributions, some of which are of a physical or chemical character, affect the sign and size of the estimated values of  $L_f^E$ . While the chemical contributions entail the dissolution of hydrogen bound complexes, which produces positive  $L_f^E$  values, the physical contributions include dispersion forces or weak Vanderwaal forces. The system becomes more ordered as a result of enhanced intermolecular interactions when specific interactions, result in negative  $L_f^E$  values. The ultrasonic sound transmission in liquid systems is determined by both adiabatic compressibility ad and free length  $L_f$ .





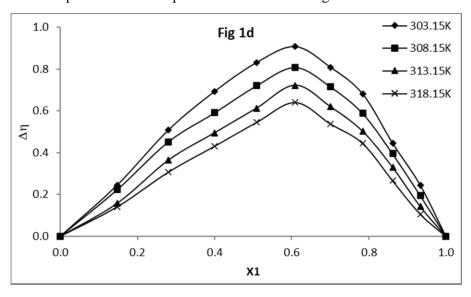


Inter molecule free length is another intriguing measure that depicts structural adjustment in solution.  $L_f$  is calculated as a function of molefraction and temperature for all systems, and the results show that  $L_f$  declines as di methyl carbonate mole fractions rise. The extremely slight decrease in  $L_f$  is attributable to the salicylates' inter hydrogen bonding breaking, which was followed by the required interactions between the molecules, despite the fact that significant interactions between dissimilar molecules are involved. All of the systems' excess  $L_f$  values exhibit negative deviations, showing that the components are strongly interdependent.

## 6.4 Deviation in Viscosity (Δη)

At all temperatures, the deviations are positive for all of these systems. The combined influences of elements including component molecule and shape, as well as intermolecular forces, determine the volume and magnitude of  $\Delta\eta$ . The dominating effect will dictate the values of  $\Delta\eta$  in systems where all possible interactions are present. The present case's deviations in viscosities are all positive across the whole spectrum of composition and at all temperatures, indicating that distinct interactions between dissimilar molecules predominate.

This finding is consistent with the findings from data on velocity and other pertinent parameters. For many binary solvent systems, there is a link between the sign of and the sign of V<sup>E</sup> 25,26, i.e., is negative when V<sup>E</sup> is positive and vice versa. This association is also supported by our findings. The structure becomes more compact and has positive values as a result of certain interactions and accommodating small size molecules into the spaces between larger molecules. The values of V<sup>E</sup>, Δβ<sub>ad</sub>, L<sub>f</sub>Eand Δηhave been fitted to equation of Redlich – Kister polynomial to estimate coefficients of binary systems and standard deviation from the experimental to computed values. The data is given in Table 3.



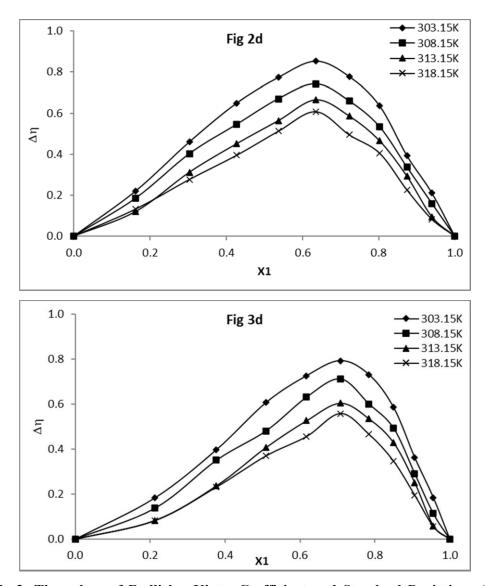


Table 3: The values of Redlich - Kister Coefficient and Standard Deviations ( $\sigma$ ) of Di Methyl Carbonate (1)+ Methyl/Ethyl/Benzyl Salicylate(2).

T/K	$A_0$	$A_1$	$A_2$	A <sub>3</sub>	A4	σ				
	Di Methyl Carbonate (1)+ Methyl Salicylate(2)									
	Deviation in Adiabtic Compressibility (Δβad)									
303.15K	-31.9905	23.2692	26.7623	-21.8283	-43.8518	0.3032				
308.15K	-35.1356	23.8189	27.2667	-18.2964	-50.8615	0.3313				
313.15K	-40.6241	27.2404	39.9505	-17.0967	-82.9397	0.4996				
318.15K	-45.8358	26.5147	34.5396	-6.9209	-85.0437	0.4988				
Excess Molar Volume (V <sup>E</sup> )										
303.15K	-3.1718	2.1422	2.3319	-1.7749	-4.6667	0.0322				
308.15K	-3.4087	2.2176	2.8053	-1.3590	-6.3476	0.0380				

313.15K	-3.8469	2.3014	3.2872	-1.3723	-8.3938	0.0399	
318.15K	-4.3752	2.1714	3.4510	-0.6988	-9.9859	0.0352	
		<b>Excess Inter</b>	molecular Fr	ee Length (Lf <sup>l</sup>	E)		
303.15K	-0.4027	0.2847	0.3973	-0.3130	-0.6062	0.0042	
308.15K	-0.4348	0.2824	0.3947	-0.2659	-0.6750	0.0044	
313.15K	-0.4980	0.3179	0.5497	-0.2589	-1.0571	0.0064	
318.15K	-0.5539	0.2937	0.4653	-0.1310	-1.0386	0.0061	
		Devia	ition in Visco	sity (Δη)			
303.15K	3.3984	-2.3156	-1.6794	1.7383	1.6495	0.0291	
308.15K	2.9870	-2.3758	-1.8931	2.5410	2.0708	0.0353	
313.15K	2.6251	-2.4945	-2.3353	2.9439	2.1009	0.0423	
318.15K	2.2961	-2.2974	-1.7107	2.9306	1.0849	0.0336	
		Di Methyl Car	bonate (1)+ l	Ethyl Salicylat	e(2)		
		<b>Deviation in A</b>	diabtic Comp	pressibility (Δβ	Bad)		
303.15K	-28.8731	30.1455	16.4588	-33.6974	-33.9944	0.3953	
308.15K	-32.7521	31.5416	25.9388	-29.4296	-53.6201	0.4729	
313.15K	-37.9132	37.3371	41.3451	-37.9612	-90.2373	0.6288	
318.15K	-43.4581	35.2196	31.5257	-17.9908	-77.7524	0.4921	
		Exces	s Molar Volu	ume (V <sup>E</sup> )			
303.15K	-2.9751	2.7680	1.6574	-2.4506	-2.1168	0.0371	
308.15K	-3.1962	2.9013	2.6894	-2.6740	-5.5524	0.0488	
313.15K	-3.4840	2.6194	1.0862	-1.7743	-3.4915	0.0328	
318.15K	-4.1189	2.9271	2.0874	-1.8459	-6.5888	0.0307	
		Excess Inte	rmolecular fi	ree length (L <sub>f</sub> E	)		
303.15K	-0.3643	0.3831	0.2556	-0.4726	-0.4782	0.0054	
308.15K	-0.4068	0.3901	0.3689	-0.4085	-0.7006	0.0063	
313.15K	-0.4654	0.4550	0.5569	-0.5200	-1.1400	0.0080	
318.15K	-0.5261	0.4127	0.4214	-0.2592	-0.9343	0.0060	
			tion in Visco				
303.15K	3.0475	-2.6716	-0.7057	1.9867	0.4113	0.0254	
308.15K	2.6145	-2.5967	-0.9231	2.5494	0.6545	0.0281	
313.15K	2.2317	-2.6877	-0.3610	2.8355	-1.1642	0.0281	
318.15K	2.0256	-2.7657	-1.0780	3.7671	0.6941	0.0372	
310.13K						0.0372	
Di Methyl Carbonate (1)+ Benzyl Salicylate(2)  Deviation in Adiabtic Compressibility (Δβad)							
303.15K -34.4536 57.2316 -5.2584 -70.7706 -55.8845 0.6670							
308.15K	-40.9091	77.3165	21.8577	-113.2676	-138.9864	0.9726	
313.15K	-43.1554	81.7124	25.4095	-118.5172	-154.5633	1.1285	
318.15K	-50.0434	71.0867	5.1176	-62.4098	-101.8777	0.7365	
	1		s Molar Volu		, ,		
303.15K	-2.7698	5.4230	1.9151	-8.0899	-10.2454	0.0899	
308.15K	-2.4200	6.4815	3.4598	-11.4702	-13.5458	0.1227	
300.13IX	-2.7200	0.7013	J.7J/0	-11.7/02	-13.3730	0.122/	

313.15K	-2.7968	3.7406	-0.9178	-2.4310	-2.0888	0.0343			
318.15K	-3.3380	3.9090	-0.9024	-2.4585	-3.8654	0.0253			
	Excess Intermolecular free length (L <sub>f</sub> <sup>E</sup> )								
303.15K	-0.4332	0.7708	-0.0114	-1.0753	-0.8029	0.0096			
308.15K	-0.5132	1.0115	0.3311	-1.5951	-1.8002	0.0129			
313.15K	-0.5308	1.0450	0.3655	-1.6262	-1.9394	0.0147			
318.15K	-0.6106	0.8780	0.0943	-0.8586	-1.1684	0.0092			
		Devia	ition in Visco	sity (Δη)					
303.15K	2.3753	-2.9327	2.0610	0.3398	-3.0695	0.0162			
308.15K	1.8679	-3.0925	3.1352	1.3688	-5.1526	0.0287			
313.15K	1.6081	-1.2613	5.1337	-3.8189	-12.3115	0.0508			
318.15K	1.4267	-2.9484	1.9562	2.6143	-3.5040	0.0297			

## 5. Conclusions:

Experimental measurements of density, viscosity, and ultrasonic speed for the binary mixture of Di Methyl Carbonate (1)+ Methyl Salicylate/Ethyl Salicylate/Benzyl Salicylate) have been made at four different temperatures from 303.15 to 318.15K with 5K variation over the full composition range. The experimental data were utilized to construct the parameters, ad, V<sup>E</sup>, and L<sub>f</sub><sup>E</sup>, in order to investigate the nature of interaction in the current binary systems. Redlich - Kister type polynomial equations are used to suit the deviations and excess properties. The observed negative values of,  $\beta_{ad}$ ,  $V^E$ , and  $L_f^E$  in the analyzed binary mixtures amply demonstrate the dominance of a particular interaction in the binary liquids. The relationship between adiabatic compressibility ( $\beta_{ad}$ ) and intermolecular free length ( $L_f^E$ ) and ultrasonic velocity (U) is inverse. The observed positive/negative values of excess/deviations properties are attributed to the dipole-dipole interactions, specific acid-base interactions, geometrical fitting of small molecules into the bigger molecules's voids and Hbonding interactions among the components of hetero-molecules. The ordering of strong interaction among the component molecules is as follows: (Di Methyl Carbonate+Methyl Salicylate) > (Di Methyl Carbonate +Ethyl Salicylate) > (Di Methyl Carbonate+Methyl Salicylate).

#### References

- 1. Archna Saxena and Chandra Mohan Saxena, *I Jof Recent Scientific Research* **13(08)**, 2159 (2022).
- 2. S.K.Bindhani, G.K.Roy and Y.K.Mohanty, Russian J of Physical Chemistry A. 94, 1827, (2020).
- 3. D. Chinnarao, Ch. V Padmarao, K. Raja, Srilatha and M, B. Venkateswara Rao, *I J Of Engineering Research & Technology*, **9(4)**, DOI: 10.17577/IJERTV9IS040093 (2020).
- 4. Dr. Jayant Balwant Patwardhan, *J of Emerging Technologies and Innovative Research*, **9(10)**, 337 (2022).
- 5. Dhirendra Kumar Sharma, Suneel Kumar and Chander Pal Prajapati, *I J of Chemistry Studies*, **6(2)**, 47, (2022).
- 6. D. Ubangara Mary and P. Neeraja, *International Refereed Journal of Engineering and Science*, **1(4)**,54 (2012).
- 7. Chandra Bhan Singh, Avanesh Kumar and Soran Singh, *Rasayan J of chem.*, **5** (3), 420 (2012).
- 8. R. Ahluwalia, Ritu Gupta, J. L. Vashisht and R. K. Wanchoo; *J Solution Chem* 42, 945 (2013).
- 9. Sk. Fakruddin, Ch.Srinivasu and K.Narendra; 2 I(3) 164, (2012).
- 10. S.C.Bhatia, R.Rani, R.Bhatia and H.Anand; *J. Chem. Thermodynamics*, **43**, 479 (2011).
- 11. R.J. Fort, W.R. Moore, Transactions of the Faraday Society 61, 2012 (1965).
- 12. C. Raghupathi Rao , I *J Pure Appl Phys*, **29**, 12 (1991).
- J.A. Reddick, W.B.Bunger and T.K. Sankano, Organic Solvents, Vol II 4<sup>th</sup> Ed,
   A. Weissberger Ed, Wiley Interscience, New York, (1986).
- 14. A. Weissberger, E.S. Proskaner, J.A. Riddick and E.E. Toops Jr, Organic Solvents, Vol II 2<sup>nd</sup> Ed, A. Weissberger Ed, Wiley Interscience, New York, (1955).
- 15. R. Ren, Y.Zuo, Q.Zhou, H.Zhang and S.Zhang,; J. Chem. Eng. Data56, 27 (2011).
- 16. D.V.M.Kriahna Reddy, P.B.Sandhya Sri, K.A.K.Raj Kumar and L.Vykuntha Rao, *Oriental J of Chemistry*, **39(2)**, 340, (2023).
- 17. G.V. Rama Rao, A.V. Sarma and C. Rambabu, *I J of Pure and Applied Physics*, **42**, 820 (2004)
- 18. Ch.kavita, A.Ratnakar, M.Durga Bhavani and K.Narendra *International Research Journal of Pure & Applied Chemistry*, **4(2)**, 213 (2014).

- 19. P. Boule., Acid. Sci. Ser., 5, 268 (1969).
- C. Jaya Prakash Raju.; K. Rambabu.; D. Ramachandran and C. Ramababu, *Phy. Chem of Liquids*, 34, 51 (1997).
- G. V. Gangadhara Rao, S. Suriya Shihab, D. Das, Shaik Babu and K. W. Chu.,
   13(4), 2123 (2020).
- 22. S. S. Yadava, Y. Singh and Neetu Kushwaha, *Global Journal of Molecular Sciences.*, **4(2)**, 118 (2009).
- 23. Ch. Udayalakshmi, Shaik Beebi, P. B. Sandhya Sri, V. N. S. R. Venkateswararao, G. Lakshmana Rao and C. Rambabu, *Rasayan J of Chemistry*, **13(7)**, 202 (2020).
- 24. A. Nagarjuna.; K. V. Yamini Kanth.; G. Balaji Prakash and Debashis Das., *Rasayan J of Chemistry*, **12(4)**, 1774 (2019).
- 25. G.V. Rama Rao, A. Viswanatha Sharma, C. Rambabu, *Indian Journal of Pure and Applied Physics*, **42**, 820 (2004).
- 26. Y. Marcus and Ion Solvation, chapter. 6, Wiley, New York, (1985).