PROJECT REPORT SUMMARY

THERMOPHYSICAL PROPERTIES OF TERNARY MIXTURES CONTAINING ACRYLIC ESTERS + ALCOHOLS + HYDROCARBONS –MEASUREMENTS AND CALCULATIONS.

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INTRODUCTION

Origin of the research problem:

Studies on the thermodynamic and thermophysical behavior of binary liquid mixtures of acrylic esters + aliphatic and aromatic organic solvents and acrylic esters + alkanols are of great utility from the practical as well as theoretical point of view. The production of higher homologues of acrylic esters is done by by the trans-esterification reaction in which a methyl ester is reacted with an alkanol of the desired chain characteristics in an inert medium consisting of an aliphatic or aromatic solvent. The knowledge of various excess thermodynamic and thermophysical functions for such mixtures thus is of great help in optimizing the process parameters needed for an efficient design of the trans-esterification process at the industrial scale. Acrylic esters differ from aliphatic esters by the fact that , in the former there is an unsaturation alongside the esteric function group in the same molecule., the acrylic esters are best candidates for studying the proximity effects due to unsaturation on ester linkages or vice versa. The binary systems of methyl methaacrylate with methanol and ethanol exhibited positive excess molar and isobaric heat capacities. The studies dealing with the thermophysical behavior of acrylic esters + 1- alkanols + organic solvents (aliphatic as well as aromatic) are scarce in the literature. Therefore, as a continuation of my previous work Ireported densities,speeds of sounds and viscosities of ternary mixtures of methyl acrylate +1- alkanols (1-pentanol,1- hexanol, 1-heptanol,1- octanol, 1- decanol, 1- dodecanol) + n- heptane have been measured across the compositions at 298.15 and 308.15 K. Excess properties were calculated across the mole fraction range.

OBJECTIVES

- To measure densities, speed of sound and viscosities of the ternary mixtures across the compositions at 298.15 and 308.15 K.
- To calculate excess molar volumes, excess isoentropic compressibilities and viscosity deviations and establish mathematical relations for the excess quantities.

EXPERIMENTAL METHODOLOGY

Materials:

MMA of pure grade (> 99.5 %) was used without any further purification.

1-pentanol,1- hexanol, 1- octanol, 1- decanol, 1- dodecanol and n- heptane,of analytical reagent quality (> 99 %) chemical were purchased from local suppliers.These chemicals were purified by standard procedures.

Methods:

The ternary mixtures were prepared by mass in hermetically sealed glass vials of about 15 cm^3. The solutions of each composition were prepared fresh, and the primary properties were measured on the same day to avoid any error in the measurement due to evaporation loss. The uncertainty in the mole fraction was estimated to be less than +/- 0.0001.

Densities and speed of sounds of pure liquids and their mixtures were measured with a high precision vibrating tube digital densimeter (Anton Paar, DMA 5000) and an ultrasonic interferometer (Mittal Enterprises, New Delhi) operating at a fixed frequency of 2 MHz at department of chemistry, Sardar Patel University, VallabhVidyanagar, Gujarat. The densimeter was calibrated with air and degassed, for times distilled water at measuring temperatures. The instrument has a built in temperature adjustment unit and the temperature around the tube was maintained toa precision of 0.001 K , but the accuracy in the temperature was 0.001 K as Pt 100 sensors were employed. The temperature within the measuring cell of interferometer was maintained within 0.001K. The repeatability in the measured densities and speed of sound were 3x 10^{-6}g.$cm^{-3}$and 1.1 m.s^{-}.

Viscosities of pure and mixture components were obtained from the measure flow times using two suspended Ubbelohde viscometer to cover all the mixtures. The calibration of viscometers was done with triple distilled water and double distilled cyclohexane.

RESULTS AND CONCLUSIONS

Table-1 Densities of pure components at T =(298.15 and 308.15) K.

	298.15 K	308.15 K
Methyl acrylate	0.947567g.cm^{-3}	0.935617g.cm^{-3}
1-pentanol	0.810792	0.802796
1- hexanol	0.815326	0.808479
1-heptanol	0.818814	0.811733
1- octanol	0.821797	0.814678
1- decanol	0.826644	0.819678
1- dodecanol	0.830684	0.822836
n- heptane	0.679787	0.671283

Table-2Densities and speeds of sound for Methyl Acrylate + 1-pentanol + n-heptane at 298.15 and 308.15 K.

Mole fraction			Density g.cm^{-3}		speed of sound m .s^{-}	
x_1	x_2	x_3	298.15 K	308.15 K	298.15 K	308.15 K
0.0587	0.1788	0.7625	0.706976	0.698233	1134.99	1093.44
0.2024	0.1858	0.6118	0.734606	0.725439	1129.97	1088.85
0.5926	0.0872	0.3202	0.815590	0.805004	1128.34	1086.82
0.4946	0.1114	0.3940	0.791819	0.781616	1125.91	1084.61
0.7660	0.0467	0.1873	0.864256	0.852957	1138.61	1096.78
0.2074	0.3173	0.4753	0.753894	0.744848	1147.37	1107.24
0.3754	0.2849	0.3397	0.789846	0.780241	1147.15	1107.27
0.7061	0.1226	0.1713	0.859491	0.848513	1147.67	1106.78
0.1133	0.5397	0.3470	0.765496	0.756980	1181.53	1143.09
0.4818	0.3163	0.2019	0.835726	0.815807	1161.76	1122.47
0.3126	0.4448	0.2426	0.800272	0.791067	1173.09	1134.51
0.1959	0.6623	0.1418	0.806334	0.797804	1211.69	1174.91
0.5993	0.3234	0.0773	0.865651	0.855340	1178.74	1139.80
0.2793	0.2887	0.4320	0.766498	0.757195	1143.93	1103.85
0.4495	0.1953	0.3552	0.784433	0.794400	1095.88	1036.36

Table-3 Densities and speeds of sound for Methyl Acrylate + 1- hexanol + n-heptane at 298.15 and 308.15 K.

Mole fraction			Density g.cm^{-3}		speed of sound m .s^{-}	
x_1	x_2	x_3	298.15 K	308.15 K	298.15 K	308.15 K
0.0534	0.1948	0.7518	0.711507	0.702890	1144.64	1103.48
0.1977	0.1881	0.6142	0.736507	0.727498	1139.26	1098.51
0.5984	0.0833	0.3183	0.816974	0.806460	1132.66	1091.31
0.4969	0.1086	0.3945	0.792687	0.782575	1030.52	1089.44
0.7693	0.0447	0.1860	0.864582	0.853320	1140.49	1098.65
0.2078	0.3136	0.4786	0.757509	0.748630	1159.26	1119.60
0.4099	0.2337	0.3564	0.791169	0.781554	1149.90	1110.0
0.7091	0.1206	0.1703	0.860007	0.849125	1152.41	1111.56
0.1176	0.5308	0.3516	0.770990	0.762674	1200.54	1162.51
0.4946	0.3040	0.2014	0.827850	0.818109	1173.10	1134.04
0.3112	0.4443	0.2445	0.802701	0.793763	1191.13	1153.02
0.2105	0.6694	0.1201	0.814324	0.806063	1238.50	1202.66
0.6109	0.3087	0.0804	0.864668	0.854583	1188.94	1150.28
0.2803	0.2949	0.4248	0.771085	0.761974	1157.24	1117.64
0.4556	0.1919	0.3525	0.796729	0.786897	1144.67	1104.46

Table-4Densities and speeds of sound for Methyl Acrylate + 1- heptanol + n-heptane at 298.15 and 308.15 K.

Mole fraction			**Density g.cm^{-3}**		**speed of sound m .s^{-}**	
x_1	x_2	x_3	298.15 K	308.15 K	298.15 K	308.15 K
0.0506	0.1950	0.7544	0.714261	0.705734	1151.79	1110.85
0.2082	0.1833	0.6085	0.740976	0.732024	1145.19	1104.74
0.5954	0.0869	0.3177	0.816402	0.805986	1136.26	1095.12
0.4977	0.1103	0.3920	0.793965	0.783939	1135.82	1094.84
0.7652	0.0487	0.1860	0.864028	0.852856	1143.74	1102.14
0.2123	0.3142	0.4736	0.762165	0.753437	1172.20	1132.93
0.4069	0.2322	0.3609	0.793146	0.783705	1160.27	1220.70
0.7088	0.1176	0.1736	0.858640	0.847910	1157.80	1117.35
0.1203	0.5347	0.3450	0.778344	0.770254	1221.50	1184.13
0.4941	0.3054	0.2005	0.828873	0.819349	1185.75	1147.05
0.3071	0.4489	0.2440	0.805269	0.796587	1209.04	1171.49
0.1984	0.6834	0.1182	0.816648	0.808672	1262.47	1226.67
0.6072	0.3133	0.0795	0.863391	0.853570	1201.23	1163.02
0.2776	0.2993	0.4231	0.773798	0.764888	1171.59	1132.39
0.4533	0.1931	03536	0.797767	0.788098	1153.19	1113.25

Table-5Densities and speeds of sound for Methyl Acrylate + 1- octanol + n-heptane at 298.15 and 308.15 K.

Mole fraction			Density g.cm^{-3}		Speed of sound m .s^{-}	
x_1	x_2	x_3	298.15 K	308.15 K	298.15 K	308.15 K
0.0565	0.1891	0.7544	0.717585	0.709117	1157.99	1117.26
0.2070	0.1829	0.6101	0.743921	0.735130	1153.20	1112.94
0.5992	0.0850	0.3158	0.818014	0.807672	1140.32	1099.29
0.4981	0.1069	0.3950	0.794733	0.784835	1139.94	1099.19
0.7708	0.0456	0.1836	0.864929	0.853782	1145.15	1103.50
0.2078	0.3177	0.4745	0.766374	0.757749	1182.55	1143.54
0.4134	0.2279	0.3587	0.795914	0.786638	1169.23	1130.01
0.7118	0.1163	0.1718	0.858906	0.848277	1162.02	1121.56
0.1185	0.5294	0.3531	0.780707	0.772758	1237.04	1199.74
0.4983	0.3012	0.2006	0.829788	0.820462	1198.37	1160.45
0.3174	0.4387	0.2439	0.808458	0.799937	1223.46	1186.41
0.2099	0.6681	0.1220	0.819184	0.811338	1278.17	1243.17
0.6113	0.3078	0.0809	0.862483	0.852868	1211.93	1173.96
0.2872	0.2872	0.4256	0.777728	0.768942	1180.85	1141.92
0.4542	0.1867	0.3591	0.797956	0.788377	1159.13	1119.26

Table-6 Densities and speeds of sound for Methyl Acrylate + 1- decanol + n-heptane at 298.15 and 308.15 K.

Mole fraction			Density g.cm^{-3}		Speed of sound m .s^{-}	
x_1	x_2	x_3	298.15 K	308.15 K	298.15 K	308.15 K
0.0559	0.1874	0.7567	0.723035	0.714703	1171.58	1131.20
0.2051	0.1846	0.610.	0.749036	0.740458	1168.53	1128.79
0.6009	0.0862	0.3129	0.819874	0.809684	1148.73	1108.04
0.4941	0.1106	0.3953	0.796381	0.785549	1150.37	1109.99
0.7691	0.0447	0.1862	0.863563	0.852558	1149.35	1107.84
0.2071	0.3118	0.4811	0.771212	0.762889	1206.21	1167.78
0.4073	0.2303	0.3624	0.798175	0.789167	1188.02	1149.41
0.7078	0.1162	0.1760	0.856799	0.846418	1171.66	1131.65
0.1205	0.5443	0.3352	0.787744	0.780103	1271.88	1235.18
0.4902	0.3037	0.2061	0.829673	0.820668	1218.20	1180.18
0.3086	0.4352	0.2562	0.809275	0.802754	1250.38	1213.37
0.2069	0.6718	0.1213	0.822973	0.815413	1310.77	1275.40
0.6050	0.3159	0.0791	0.861016	0.851755	1232.80	1195.06
0.2800	0.2921	0.4279	0.781454	0.772901	1201.99	1163.43
0.4528	0.1904	0.3568	0.801462	0.792195	1176.30	1137.12

Table-7Densities and speeds of sound for Methyl Acrylate + 1- dodecanol + n-heptane at 298.15 and 308.15 K.

Mole fraction			Density g.cm^{-3}		Speed of sound m .s^{-}	
x_1	x_2	x_3	298.15 K	308.15 K	298.15 K	308.15 K
0.0522	0.1896	0.7582	0.728706	0.720526	1186.68	1146.75
0.2042	0.1833	0.6125	0.753791	0.745766	1182.35	1143.04
0.5920	0.0857	0.3223	0.817918	0.807919	1155.83	1116.02
0.4913	0.1062	0.4025	0.796390	0.786806	1158.19	1118.22
0.7671	0.0438	0.1891	0.862353	0.851434	1152.98	1111.84
0.2114	0.3088	0.4798	0.777772	0.769759	1227.99	1190.32
0.4076	0.2314	0.3610	0.800917	0.792096	1204.94	1166.35
0.7105	0.1188	0.1707	0.856935	0.846736	1181.50	1142.01
0.1196	0.5246	0.3558	0.794485	0.786977	1292.23	1256.17
0.4916	0.3009	0.2075	0.830787	0.822035	1236.77	1199.10
0.3086	0.4446	0.2468	0.814734	0.806763	1274.85	1238.23
0.2030	0.6756	0.1214	0.825798	0.818477	1341.97	1306.84
0.6088	0.3118	0.0794	0.859809	0.850849	1251.77	1214.38
0.2779	0.2934	0.4287	0.785913	0.777607	1224.14	1186.10
0.4572	0.1894	0.3534	0.803500	0.794383	1191.05	1151.76

Table-8Excess volumes for Methyl Acrylate + 1-pentanol + n-heptane at 298.15 and 308.15 K.

Mole fraction			Excess volume V_m^E	
x_1	x_2	x_3	298.15 K	308.15 K
0.0587	0.1788	0.7625	0.3470	0.3833
0.2024	0.1858	0.6118	0.6962	0.7537
0.5926	0.0872	0.3202	0.7976	0.8813
0.4946	0.1114	0.3940	0.9120	0.9963
0.7660	0.0467	0.1873	0.5017	0.5741
0.2074	0.3173	0.4753	0.5573	0.5910
0.3754	0.2849	0.3397	0.6548	0.7019
0.7061	0.1226	0.1713	0.5394	0.6035
0.1133	0.5397	0.3470	0.1935	0.1931
0.4818	0.3163	0.2019	0.5747	0.6152
0.3126	0.4448	0.2426	0.4793	0.4966
0.1959	0.6623	0.1418	0.2351	0.2120
0.5993	0.3234	0.0773	0.4777	0.5111
0.2793	0.2887	0.4320	0.6046	0.6483
0.4495	0.1953	0.3552	2.2218	-0.6382

Table-9 Excess volumes for Methyl Acrylate + 1-hexanol + n-heptane at 298.15 and 308.15 K.

Mole fraction			Excess volume V_m^E	
x_1	x_2	x_3	298.15 K	308.15 K
0.0534	0.1948	0.7518	0.2313	0.2789
0.1977	0.1881	0.6142	0.6976	0.7658
0.5984	0.0833	0.3183	0.7909	0.8806
0.4969	0.1086	0.3945	0.9272	1.0212
0.7693	0.0447	0.1860	0.5294	0.6071
0.2078	0.3136	0.4786	0.4981	0.5631
0.4099	0.2337	0.3564	0.8601	0.9462
0.7091	0.1206	0.1703	0.5136	0.5923
0.1176	0.5308	0.3516	0.1414	0.1935
0.4946	0.3040	0.2014	0.6124	0.6891
0.3112	0.4443	0.2445	0.4597	0.5268
0.2105	0.6694	0.1201	0.3077	0.3690
0.6109	0.3087	0.0804	0.5796	0.6512
0.2803	0.2949	0.4248	0.5350	0.6050
0.4556	0.1919	0.3525	0.7714	0.8573

Table-10Densities and speeds of sound for Methyl Acrylate + 1- heptanol + n-heptane at 298.15 and 308.15 K.

Mole fraction			**Excess volume V_m^E**	
x_1	x_2	x_3	298.15 K	308.15 K
0.0506	0.1950	0.7544	0.1853	0.2122
0.2082	0.1833	0.6085	0.5996	0.6485
0.5954	0.0869	0.3177	0.8909	0.9743
0.4977	0.1103	0.3920	0.9284	1.0116
0.7652	0.0487	0.1860	0.5138	0.5853
0.2123	0.3142	0.4736	0.4608	0.4951
0.4069	0.2322	0.3609	0.6607	0.7183
0.7088	0.1176	0.1736	0.5652	0.6300
0.1203	0.5347	0.3450	-0.1176	-0.1187
0.4941	0.3054	0.2005	0.5865	0.6366
0.3071	0.4489	0.2440	0.3974	0.4245
0.1984	0.6834	0.1182	0.2270	0.2385
0.6072	0.3133	0.0795	0.5908	0.6379
0.2776	0.2993	0.4231	0.5577	0.5966
0.4533	0.1931	03536	0.7481	0.8129

Table-11 Densities and speeds of sound for Methyl Acrylate + 1- octanol + n-heptane at 298.15 and 308.15 K.

Mole fraction			**Excess volume V_m^E**	
x_1	x_2	x_3	298.15 K	308.15 K
0.0565	0.1891	0.7544	0.1397	0.1523
0.2070	0.1829	0.6101	0.4294	0.4487
0.5992	0.0850	0.3158	0.8182	0.8916
0.4981	0.1069	0.3950	0.8584	0.9243
0.7708	0.0456	0.1836	0.5375	0.6061
0.2078	0.3177	0.4745	0.2022	0.2214
0.4134	0.2279	0.3587	0.6164	0.6508
0.7118	0.1163	0.1718	0.5982	0.6564
0.1185	0.5294	0.3531	-0.0200	-0.0413
0.4983	0.3012	0.2006	0.3210	0.6514
0.3174	0.4387	0.2439	0.3870	0.3905
0.2099	0.6681	0.1220	0.2663	0.2545
0.6113	0.3078	0.0809	0.6520	0.6831
0.2872	0.2872	0.4256	0.3767	0.3903
0.4542	0.1867	0.3591	0.7822	0.8396

Table-12Densities and speeds of sound for Methyl Acrylate + 1- decanol + n-heptane at 298.15 and 308.15 K.

Molefraction			Excess volume V_m^E	
x_1	x_2	x_3	298.15 K	308.15 K
0.0559	0.1874	0.7567	0.0473	0.0429
0.2051	0.1846	0.610.	0.2843	0.2771
0.6009	0.0862	0.3129	0.7585	0.8214
0.4941	0.1106	0.3953	0.7961	0.8527
0.7691	0.0447	0.1862	0.5904	0.6518
0.2071	0.3118	0.4811	0.1870	0.1732
0.4073	0.2303	0.3624	0.5756	0.5936
0.7078	0.1162	0.1760	0.6697	0.7186
0.1205	0.5443	0.3352	0.5964	0.5627
0.4902	0.3037	0.2061	0.6279	0.6470
0.3086	0.4352	0.2562	0.5371	0.2082
0.2069	0.6718	0.1213	0.3088	0.2845
0.6050	0.3159	0.0791	0.6565	0.6819
0.2800	0.2921	0.4279	0.4360	0.4400
0.4528	0.1904	0.3568	0.6604	0.6895

Table-13Densities and speeds of sound for Methyl Acrylate + 1- dodecanol + n-heptane at 298.15 and 308.15 K.

Molefraction			**Excess volume V_m^E**	
x_1	x_2	x_3	298.15 K	308.15 K
0.0522	0.1896	0.7582	-0.1264	0.2044
0.2042	0.1833	0.6125	0.0998	-0.0584
0.5920	0.0857	0.3223	0.8024	0.8317
0.4913	0.1062	0.4025	0.8123	0.8299
0.7671	0.0438	0.1891	0.6249	0.6732
0.2114	0.3088	0.4798	-0.0046	-0.1494
0.4076	0.2314	0.3610	0.6620	0.6102
0.7105	0.1188	0.1707	0.8093	0.8232
0.1196	0.5246	0.3558	-0.1162	-0.3161
0.4916	0.3009	0.2075	0.7106	0.6363
0.3086	0.4446	0.2468	0.4980	0.3546
0.2030	0.6756	0.1214	0.4522	0.2292
0.6088	0.3118	0.0794	0.8258	0.7549
0.2779	0.2934	0.4287	0.4094	0.3107
0.4572	0.1894	0.3534	0.8646	0.8411

Experimentally measured densities, speed of sounds of mixtures were listed in above tables.The deviations in excess molar volumes of ternary mixtures as calculated from Redlich-Kister(RK), Tsao and Smith(TS)and Kohler (K)were found tovary from 0 to 0.008, 0.006 to 0.15 and 0.001 to 0.093 cm^3 mol^{-}respectively. Therefore it is concluded that the experimental ternary excess molar volumes are the best reproduced by the RK equation. There exist a large difference in positive excess molar volumes for mixtures containing n- heptane as compared to other organic solvents.

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Esters in general are of the best candidates that are available in wide structural variations namely aliphatic, aromatic or even acrylic types. The lone pairs of electrons in carbonyl groups offer sites for interaction with other electrophilic groups. Ester species also exist as polar associates in the pure liquid state. In view of these feature, the binary systems of esters + hydrocarbons namely methyl ester (acetate to decanoate) + (heptane or nonane)[1], alkyl benzoate + n- heptane [2] , alkyl formats + benzene [3], aliphatic esters + toluene, + ethyl benzene , and +benzene [4] ,ethyl acetate + cyclohexane have been received much attention for the thermophysical property evaluation. Similarly, the thermophysical properties such as density, speed of sound, enthalpy of mixing and dynamic viscosities for 1- alcohol + n-alkane systems [5-18] have been reported and the measured properties for the binary mixtures across the compositions were converted into respective excess or deviation functions. A qualitative analysis of these functions was given in terms of type interactions in the bulk state.

As compared to extensive data available on mixtures consisting of aliphatic esters, 1-alcohols, n- alkanes and aromatic solvents, there exist only few studies that deal with binary or ternary systems involving acrylic esters as one of the components.

The systematic measurements of volumetric, transport, acoustic and dielectric properties of MMA + 1- alkanols (methanol to 1-hexanol)[19,20]and alkyl (methyl-, ethyl- and butyl-)acrylates + 1- alkanols (1- heptanol to 1- dodecanol)[21-23]and ternary mixtures of methyl acrylate + 1- propanol (or butanol) + organic solvents (n-hexane, n- heptane, cyclohexane, benzene and toluene)[24] have been reported. The analysis of the excess and deviation functions revealed that even though the thermophysical behavior of acrylic esters +1- alkanol mixtures is similar to that of their counterpart alkylalkanoate + 1- alkanol systems, the presence of unsaturation in the acrylic esters seems to produces additional specific interactions between the ester and -OH groups. Packing effects in terms of n-π interactions between the lone pair electrons of oxygen of alcoholic –OH group and π electron clouds of ester molecules are also possible. More precious studies on acrylic ester + 1- alkanols and alkyl alkanoate + same 1- alkanols under identical experimental conditions are needed so that one can make direct quantitative comparison to ascertain the role of unsaturation in the interactions between acrylic esters and 1- alkanols.

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Annexure –VII

UNIVERSITY GRANTS COMMISSION
BAHADUR SHAH ZAFAR MARG
NEW DELHI – 110 002.

PROFORMA FOR SUBMISSION OF INORMATION AT THE TIME OF SENDING THE FINAL REPORT OF THE WORK DONE ON THE PROJECT.

1.	TITLE OF THE PROJECT	Thermophysical properties of Ternary Mixtures Containing Acrylic esters + Alcohols + Hydrocarbons – Measurements and calculations.
2.	NAME AND ADDRSS OF THE PRINCIPAL INVESTIGATOR	Dr. M.K.VALAND Chemistry Department, Viththalbhai Patel & Rajratna P. T. Patel Science College, Vallabh Vidyanagar-388120. Dist. Anand, Gujarat.
3.	NAME AND ADDRSS OF THE INSTITUTION	Viththalbhai Patel & Rajratna P. T. Patel Science College, Vallabh Vidyanagar-388120. Dist. Anand, Gujarat.
4.	UGC APPROVAL LETTER NO. AND DATE	47-154/12(WRO) 21-02-2013.
5.	DATE OF IMPLIMEMTATION	26-07-2013.
6.	TENURE OF THE PROJECT	From 26-07-2013 to 25-07-2015..
7.	TOTAL GRANT ALLOCATED	Rs. 1,05,000/-
8.	TOTAL GRANT RECEIVED	Rs. 72500/-
9.	FINAL EXPENDITURE	Rs.67,038
10.	TITLE OF THE PROJECT	Thermophysical properties of Ternary Mixtures Containing Acrylic esters + Alcohols + Hydrocarbons – Measurements and calculations.
11.	OBJECTIVES OF THE PROJECT	• To measure densities, speed of sound and viscosities of the ternary mixtures across the compositions at 298.15 and 308.15 K. • To calculate excess molar volumes, excess isoentropic compressibilities and viscosity deviations and establish a mathematical relations for the excess quantities.
12.	WHETHER OBJECTIVES WERE ACHIEVED (GIVE DETAILS)	YES • Studies on thermodynamic and thermophysical behavior of binary liquid mixtures of acrylic esters + aliphatic and aromatic organic solvents and acrylic

esters + alkanols are of great utility from the practical as well as theoretical point of view. The production of higher homologues of acrylic esters is done by by the trans-esterification reaction in which a methyl ester is reacted with an alkanol of the desired chain characteristics in an inert medium consisting of an aliphatic or aromatic solvent. The knowledge of various excess thermodynamic and thermophysical functions for such mixtures thus is of great help in optimizing the process parameters needed for an efficient design of the trans-esterification process at the industrial scale.

13.	ACHIEVEMENTS FROM THE PROJECT	The densities, speed of sound and viscosities of the ternary mixtures of methyl acrylate +1- alkanols (1-pentanol,1- hexanol, 1- octanol, 1- decanol, 1-dodecanol) + n- heptane have been measured across the compositions at 298.15 and 308.15 K. Excess properties were calculated across the mole fraction range.
14.	SUMMARY OF THE FINDINGS (IN 500 WORS)	Acrylic esters are important industrial chemicals and are widely used as precursors in the production of technically important high polymeric and latex systems. The production of higher homologues of acrylic esters on an industrial scale is done by trans-esterification reactions in which an acrylic ester is reacted with a 1-alcohol having a longer alkyl chain length. Acrylic esters are also most interesting theoretically because they have unsaturation alongside of a carbonyl group in the same molecule. Despite the above mentioned industrial and theoretical interests, the thermophysical behavior of binary and ternary liquid mixtures consisting of acrylic esters as one of the components in general and acrylic ester + 1- alcohols in particular were not thoroughly investigated earlier. The densities, speed of sound and viscosities (thermophysical properties) of a total six ternary mixtures consisting of Methyl acrylate(MA) + 1- Pentanol + n- Heptane, Methyl Acrylate(MA) +1- Hexanol +n-Heptane, Methyl Acrylate(MA) + 1-Heptanol +n-Heptane, Methyl Acrylate(MA) + 1-Octanol +n-Heptane, Methyl Acrylate(MA) + 1-Decanol +n-Heptane, Methyl Acrylate(MA) + 1-Dodecanol +n-Heptane has been measured. The speeds of sound are calculate

by using free length and collision factor theories. The mixture viscosities are correlated by the Grunbrg and Nissan. McAllister, and Auslander equations. Excess molar volumes, excess isoentropic compressibilities and viscosity deviations were calculated. Different excess properties such as excess molar volumes, excess isoentropic compressibilities and viscosity deviations were also estimated from the data of respective binary pairs. Validity of different empirical equations and models for simultaneous ternary data of respective binary pairs.

Compositions can be identified based on predominant interactions between given two components in a ternary system. The measured excess thermodynamic and thermophysical functions for ternary mixtures is useful in optimizing the process parameters needed for an efficient design of the trans- esterification process at the industrial scale. Acrylic esters differ from aliphatic esters by the fact that, in the former there is an unsaturation alongside the esteric function group in the same molecule. Therefore, the acrylic esters are best candidates for studying the proximity effects due to unsaturation on ester linkage or vice versa. The binary systems of methyl methaacrylate(MMA) with methanol and ethanol exhibited positive excess molar and isobaric heat capacities. The systematic measurements of volumetric, acoustic and transport properties of MMA + 1- alkanols (methanol to 1- hexanol) and alkyl (methyl-, ethyl-, and butyl-) acrylates + 1- alkanols (1- heptanols to 1- dodecanol) and ternary mixtures of methyl acrylate + 1- propane +organic solvents (n- hexane, n- heptane, cyclohexane, benzene and toluene) and excess and deviation functions of these systems revealed that even though the thermophysical behavior of acrylic ester + 1-alkanol mixtures is similar to that of their counterpart alkylalkanoate + 1- alkanol systems, the presence of unsaturation in the acrylic esters seems to produces additional specific interactions between the ester and -OH group and π- interactions between the ester and –OH groups. Packing effect in terms of n- π interactions between the lone pair electrons of oxygen of alcoholic –OH group and π- electron clouds of ester molecules are also possible.

15.	CONTRIBUTION TO THE SOCIETY (GIVE DETAILS)	The measurements of densities, speed of sound and viscosities of the ternary mixtures of methyl acrylate +1-alkanols (1-pentanol,1- hexanol, 1- octanol, 1- decanol, 1- dodecanol) + n- heptane covered the gap that exist due to the lack of data on these ternary systems.
16.	WHETHER ANY PH.D. ENROLLED/PRODUCED OUT OF THE PROJECT	**NO (IT'S A MINOR RESEARCH PROJECT)**
17.	NO. OF PUBLICATIONS OUT OF THE PROJECT (PLEASE ATTACH)	**NIL**

mvaland

Dr. M.K.VALAND
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