Special Issue Published in International Journal of Trend in Research and Development (IJTRD), ISSN: 2394-9333, www.ijtrd.com

Theoretical Prediction of Refractive Index of Isovaleric Acid with Isopropyl Myristate, Bromoform and n-Butyl Iodide at Five Different Temperatures

[1]K. Umamakeshvari, [2]U. Sankar and [3]A.Mozes Ezhil Raj
[1] Assistant Professor, Department of Physics, St. Johns College, Palayamkottai, TamilNadu, India
[2]Associate Professor, Department of Physics, Sri KGS Arts College, Srivaikuntam, Tamilnadu, India
[3]Professor, Department of Physics, Scott Christian College, Nagercoil, Tamilnadu, India

***Abstract*--** Refractive index of Isovaleric acid with Isopropyl myristate, Bromoform, and n-Butyl iodide have been measured at 298K, 303K, 308K, 313K and 318K over the whole mole fraction range were measured. The theoretical refractive index of binary mixtures was predicted using Gladstone-Dale, Heller, Newton and Eyring-John relations. The validity of these relations has been analyzed by comparing the experimental and theoretical refractive index. Comparison of various mixing rules has been expressed in terms of Root Mean Square deviation (RMSD).

Keywords *- Refractive index, Abbe's refractometer, Isovaleric acid, Bromoform,n-butyl iodide Binary Mixtures,Mixing Rules.*

I. INTRODUCTION

This work is continue of our research on thermodynamic properties of system withphenol and xylenes and it presents the experimental data containing density and refractiveindices of binary mixtures at 303K and excess parameters have been computed [1]. Manyresearchers have been studied the theoretical refractive index measurements by the refractiveindex mixing rules [2-5]. The generally used theoretical rules are Gladstone-Dale, Heller, Newton and Eyring-John. The validity of the mixingrules has been tested by several researchers pointed out the important of mixing rules [6-10].In the present study, we report the experimental and theoretical refractive index of binarymixtures, from these the validity of the mixing rules have been analyzed

II. EXPERIMENTAL DETAILS

Isovaleric acid (AR grade), Bromoform (AR grade)and Isopropyl myristate (AR grade) and n-btyl iodide (AR grade) were commercially obtained from S D fine- Chem Limited (India) and used without further purification. Binary mixtures of bromoform, Isopropyl myristateand n-butyl iodide with Isovaleric acid were prepared at 11 different concentrations by volume. Assuming ideal mixing behaviour the concentration was converted into the mol fraction..The values of refractive indices of pure liquids, and of the binary mixtures have been determined by using Abbe's refractometer at wavelength of sodium D-light. The maximum measurement error in n value is ±0.02%..The measurement accuracy in refractive index is 0.3%.

III. THEORY

Theoretical refractive index of binary mixtures of Isopropyl myristate, Bromoform and n-Butyl iodide with Isovaleric acid has been predicted by using the various theoretical relations.

Eyring-John (E-J)[11]

$$n = n_A\phi^2{}_A + n_B\phi^2{}_B + 2(\mathrm{n_A n_B})^{1/2}$$

Gladstone- Dale (G-D)[12]

$$n-1 = (\mathrm{n_A}-1)\phi_\mathrm{A} + (\mathrm{n_B}-1)\phi_\mathrm{B}$$

Newton (Nw)[13]

$$n^2-1 = (\mathrm{n^2{}_A}-1)\phi_\mathrm{A} + (\mathrm{n^2{}_B}-1)\phi_\mathrm{B}$$

Heller (H)[14]

$$\frac{(n-n_A)}{n_A} = \frac{3}{2}\times\frac{\left(\left(\frac{n_B}{n_A}\right)^2-1\right)}{\left(\left(\frac{n_B}{n_A}\right)^2+2\right)}\phi_B$$

where n, $\mathrm{n_{A,}n_B}$, ϕ_A , ϕ_B represent refractive index of mixture, Isovaleric acid and Isopropyl myristate, Isovaleric acid and Bromoform, and Isovaleric acid and n-Butyl iodide and mole fraction of these three mixtures respectively.

$$R.M.S.D = \left(\frac{1}{m\sum(\mathrm{n_{exp}}-\mathrm{n_{cal}})^2}\right)^{1/2} \quad [15]$$

where m is the number of data points.

IV. RESULTS AND DISCUSSION

Measured values of refractive index of Isopropyl myristate, Bromoform and n-butyl iodide with Isovaleric acid mixtures are presented in Table 1.

Table 1: Variation of refractive indices (n) at different molefractions of Isopropyl myristate (X2)+ Isovaleric acid (X1), Bromoform + Isovaleric acid and n-butyl iodide+ Isovaleric acid at different temperatures

Temp (K)	Isopropyl myristate + Isovalericacid		Bromoform + Isovaleric acid		n-butyl iodide+ Isovaleric acid	
	X2	n	X2	n	X2	n
	0	1.432	0	1.592	0	1.494
	0.1	1.431	0.1	1.572	0.1	1.473
	0.2	1.43	0.2	1.55	0.2	1.465
	0.3	1.428	0.3	1.52	0.3	1.457
	0.4	1.426	0.4	1.495	0.4	1.45
	0.5	1.423	0.5	1.476	0.5	1.443
	0.6	1.421	0.6	1.455	0.6	1.431
	0.7	1.419	0.7	1.438	0.7	1.419
	0.8	1.414	0.8	1.423	0.8	1.413
	0.9	1.41	0.9	1.408	0.9	1.405
298	1	1.401	1	1.401	1	1.401

	0	1.431	0	1.59	0	1.493
	0.1	1.43	0.1	1.569	0.1	1.47
	0.2	1.428	0.2	1.546	0.2	1.462
	0.3	1.425	0.3	1.517	0.3	1.454
	0.4	1.424	0.4	1.491	0.4	1.447
	0.5	1.422	0.5	1.473	0.5	1.441
	0.6	1.419	0.6	1.451	0.6	1.428
	0.7	1.416	0.7	1.435	0.7	1.417
	0.8	1.411	0.8	1.42	0.8	1.41
	0.9	1.406	0.9	1.404	0.9	1.403
303	1	1.399	1	1.399	1	1.399
	0	1.431	0	1.588	0	1.491
	0.1	1.427	0.1	1.567	0.1	1.467
	0.2	1.426	0.2	1.54	0.2	1.459
	0.3	1.424	0.3	1.516	0.3	1.451
	0.4	1.422	0.4	1.49	0.4	1.445
	0.5	1.42	0.5	1.47	0.5	1.438
	0.6	1.417	0.6	1.448	0.6	1.426
	0.7	1.414	0.7	1.432	0.7	1.414
	0.8	1.409	0.8	1.416	0.8	1.408
	0.9	1.405	0.9	1.396	0.9	1.4
308	1	1.395	1	1.395	1	1.395
	0	1.426	0	1.584	0	1.489
	0.1	1.424	0.1	1.563	0.1	1.464
	0.2	1.423	0.2	1.536	0.2	1.455
	0.3	1.419	0.3	1.516	0.3	1.448
313	0.4	1.418	0.4	1.492	0.4	1.442
	0.5	1.417	0.5	1.472	0.5	1.436
	0.6	1.414	0.6	1.446	0.6	1.424
	0.7	1.411	0.7	1.428	0.7	1.411
	0.8	1.409	0.8	1.414	0.8	1.406
	0.9	1.403	0.9	1.398	0.9	1.398
	1	1.394	1	1.394	1	1.394
	0	1.421	0	1.581	0	1.487
	0.1	1.42	0.1	1.561	0.1	1.461
	0.2	1.419	0.2	1.532	0.2	1.452
	0.3	1.416	0.3	1.513	0.3	1.445
	0.4	1.415	0.4	1.49	0.4	1.439
	0.5	1.414	0.5	1.472	0.5	1.434
	0.6	1.409	0.6	1.444	0.6	1.422
	0.7	1.406	0.7	1.426	0.7	1.409
	0.8	1.401	0.8	1.412	0.8	1.404
	0.9	1.4	0.9	1.396	0.9	1.396
318	1	1.391	1	1.391	1	1.391

Table 2: Comparison Of Exp Ref Index Data With Theoretical Values Of The Binary Mixtures Of Isovaleric Acid+ Isopropyl Myristate

Mole Fraction	Eyring-John (EJ)				
	298K	303K	308K	313K	318K
0	1.432	1.43	1.427	1.415	1.401
0.1	1.429	1.45	1.457	1.419	1.647
0.2	1.51	1.462	1.462	1.437	1.837
0.3	1.51	1.49	1.5	1.455	1.972
0.4	1.524	1.5	1.511	1.511	2.052
0.5	1.61	1.512	1.518	1.523	2.076
0.6	1.5	1.568	1.577	1.509	2.045
0.7	1.419	1.448	1.438	1.444	1.959
0.8	1.406	1.411	1.41	1.4	1.817
0.9	1.4	1.401	1.398	1.389	1.620
1	1.398	1.396	1.394	1.385	1.367

Mole Fraction	Gladstone-Dale (G-D)				
	298K	303K	308K	313K	318K
0	1.399	1.396	1.394	1.367	1.368
0.1	1.402	1.4	1.397	1.37	1.371
0.2	1.405	1.403	1.401	1.374	1.374
0.3	1.409	1.406	1.404	1.377	1.378
0.4	1.412	1.41	1.407	1.381	1.381
0.5	1.415	1.413	1.411	1.384	1.384
0.6	1.419	1.416	1.414	1.387	1.388
0.7	1.422	1.42	1.417	1.391	1.391
0.8	1.425	1.426	1.421	1.394	1.394
0.9	1.429	1.428	1.424	1.397	1.398
1	1.432	1.43	1.427	1.401	1.401

Mole Fraction	Newton (NW)				
	298K	303K	308K	313K	318K
0	1.399	1.396	1.394	1.367	1.368
0.1	1.402	1.4	1.397	1.37	1.371
0.2	1.405	1.403	1.401	1.374	1.374
0.3	1.409	1.406	1.404	1.377	1.378
0.4	1.412	1.41	1.407	1.381	1.381
0.5	1.415	1.413	1.411	1.384	1.384
0.6	1.419	1.416	1.414	1.387	1.388
0.7	1.422	1.42	1.417	1.391	1.391
0.8	1.425	1.423	1.421	1.394	1.394
0.9	1.429	1.426	1.424	1.397	1.398
1	1.432	1.43	1.427	1.401	1.401

Mole Fraction	Heller(H)				
	298K	303K	308K	313K	318K
0	1.399	1.396	1.394	1.367	1.368
0.1	1.402	1.4	1.397	1.37	1.371
0.2	1.405	1.403	1.401	1.374	1.374
0.3	1.409	1.406	1.404	1.377	1.378
0.4	1.412	1.41	1.407	1.381	1.381
0.5	1.415	1.413	1.411	1.384	1.384
0.6	1.419	1.416	1.414	1.387	1.388
0.7	1.422	1.42	1.417	1.391	1.391
0.8	1.425	1.423	1.421	1.394	1.394
0.9	1.429	1.426	1.424	1.397	1.398
1	1.432	1.43	1.427	1.401	1.401

Table 3: Comparison Of Exp Ref Index Data With Theoretical Values Of The Binary Mixtures Of Isovaleric Acid+ Bromoform

Mole Fraction	Eyring-John (EJ)				
	298K	303K	308K	313K	318K
0	1.588	1.582	1.575	1.564	1.555
0.1	1.59	1.591	1.581	1.575	1.799
0.2	1.596	1.599	1.588	1.586	1.985
0.3	1.599	1.604	1.592	1.596	2.111
0.4	1.6	1.609	1.599	1.599	2.180
0.5	1.546	1.615	1.605	1.6	2.189
0.6	1.492	1.588	1.546	1.611	2.140
0.7	1.433	1.566	1.524	1.564	2.033
0.8	1.4	1.492	1.452	1.482	1.867
0.9	1.399	1.402	1.4	1.402	1.643
1	1.392	1.386	1.379	1.368	1.359

Mole Fraction	Gladstone-Dale (G-D)				
	298K	303K	308K	313K	318K
0	1.399	1.399	1.385	1.375	1.376
0.1	1.418	1.412	1.405	1.395	1.395
0.2	1.438	1.432	1.424	1.414	1.415
0.3	1.457	1.452	1.444	1.434	1.434
0.4	1.477	1.471	1.464	1.453	1.454
0.5	1.496	1.491	1.483	1.473	1.473
0.6	1.516	1.51	1.503	1.492	1.493
0.7	1.536	1.53	1.522	1.512	1.513
0.8	1.555	1.549	1.542	1.532	1.532
0.9	1.575	1.569	1.561	1.551	1.552
1	1.594	1.589	1.581	1.571	1.571

Mole Fraction	Newton (NW)				
	298K	303K	308K	313K	318K
0	1.399	1.393	1.385	1.375	1.376
0.1	1.419	1.414	1.406	1.396	1.396
0.2	1.44	1.434	1.427	1.416	1.417
0.3	1.46	1.454	1.447	1.437	1.437
0.4	1.48	1.474	1.467	1.456	1.457
0.5	1.5	1.494	1.486	1.476	1.477
0.6	1.519	1.513	1.506	1.496	1.496
0.7	1.538	1.532	1.525	1.515	1.515
0.8	1.557	1.551	1.544	1.534	1.534
0.9	1.576	1.57	1.563	1.552	1.553
1	1.594	1.589	1.581	1.571	1.571

Mole Fraction	Heller(H)				
	298K	303K	308K	313K	318K
0	1.399	1.393	1.385	1.375	1.376
0.1	1.418	1.412	1.404	1.394	1.395
0.2	1.437	1.431	1.423	1.413	1.414
0.3	1.456	1.45	1.442	1.432	1.433
0.4	1.475	1.469	1.461	1.451	1.452
0.5	1.494	1.488	1.48	1.47	1.471
0.6	1.513	1.507	1.499	1.489	1.490
0.7	1.532	1.526	1.518	1.508	1.509
0.8	1.551	1.545	1.538	1.527	1.528
0.9	1.57	1.564	1.557	1.546	1.547
1	1.589	1.583	1.576	1.565	1.566

Table 4: Comparison Of Exp Ref Index Data With Theoretical Values Of The Binary Mixtures Of Isovaleric Acid+ N-Butyl Iodide

Mole Fraction	Eyring-John (EJ)				
	298K	303K	308K	313K	318K
0	1.495	1.49	1.484	1.478	1.474
0.1	1.514	1.499	1.494	1.488	1.721
0.2	1.538	1.509	1.504	1.498	1.910
0.3	1.544	1.529	1.514	1.508	2.043
0.4	1.555	1.539	1.524	1.508	2.119
0.5	1.575	1.549	1.554	1.528	2.138
0.6	1.569	1.459	1.454	1.458	2.099
0.7	1.485	1.449	1.434	1.448	2.004
0.8	1.445	1.429	1.424	1.418	1.852
0.9	1.405	1.419	1.414	1.408	1.642
1	1.397	1.392	1.386	1.38	1.376

Mole Fraction	Gladstone-Dale (G-D)				
	298K	303K	308K	313K	318K
0	1.399	1.393	1.388	1.382	1.377
0.1	1.408	1.403	1.397	1.392	1.387
0.2	1.418	1.413	1.407	1.402	1.397
0.3	1.428	1.423	1.417	1.412	1.407
0.4	1.438	1.433	1.427	1.422	1.417
0.5	1.448	1.443	1.437	1.432	1.426
0.6	1.457	1.453	1.447	1.441	1.436
0.7	1.467	1.462	1.457	1.451	1.446
0.8	1.477	1.472	1.466	1.461	1.456
0.9	1.487	1.482	1.476	1.471	1.466
1	1.497	1.491	1.486	1.481	1.475

Mole Fraction	Newton (NW)				
	298K	303K	308K	313K	318K
0	1.399	1.393	1.388	1.382	1.377
0.1	1.409	1.403	1.397	1.392	1.387
0.2	1.419	1.413	1.407	1.402	1.397
0.3	1.429	1.423	1.417	1.412	1.407
0.4	1.439	1.433	1.427	1.422	1.417
0.5	1.449	1.443	1.437	1.432	1.427
0.6	1.459	1.453	1.447	1.441	1.437
0.7	1.469	1.462	1.457	1.451	1.447
0.8	1.479	1.472	1.466	1.461	1.456
0.9	1.489	1.482	1.476	1.471	1.466
1	1.497	1.491	1.486	1.481	1.475

Mole Fraction	Heller(H)				
	298K	303K	308K	313K	318K
0	1.399	1.393	1.388	1.382	1.377
0.1	1.408	1.403	1.397	1.392	1.387
0.2	1.418	1.413	1.407	1.402	1.397
0.3	1.428	1.423	1.417	1.412	1.406

0.4	1.438	1.433	1.427	1.421	1.416
0.5	1.448	1.443	1.437	1.431	1.426
0.6	1.458	1.453	1.447	1.441	1.435
0.7	1.468	1.462	1.457	1.45	1.445
0.8	1.476	1.472	1.466	1.459	1.455
0.9	1.486	1.482	1.476	1.469	1.464
1	1.495	1.491	1.486	1.479	1.474

A close perusal from the tables shows that all theoretical mixing rules shows good agreement with the experimental values. The average percentage deviation obtained for the binary liquid systems Isovaleric acid with bromoform shows good agreement than the another liquid systems. All the binary mixtures show better agreement in the lower concentration. This study shows that all the theoretical mixing rules are inter related well within the limits of the experimental error.[16-19].

Table 5: Values Of Rmsd Against Various Mixing Rules Of Isovaleric Acid-Isopropyl Myristate Mixture

Mixing rules	RMSD				
	298	303	308	313	318
	Refractive index				
Eyring - John	0.027	0.028	0.029	0.029	0.029
Gladstone-Dale	4.401	4.259	4.259	3.256	2.731
Newton	4.406	4.264	4.264	3.261	2.735
Heller	4.406	4.264	4.264	3.254	2.728

Table 6: Values Of Rmsd Against Various Mixing Rules Of Isovaleric Acid-Bromoform Mixture

Mixing rules	RMSD				
	298	303	308	313	318
	Refractive index				
Eyring - John	0.026	0.026	0.026	0.026	0.026
Gladstone-Dale	0.721	0.722	0.72	0.724	0.725
Newton	0.72	0.721	0.719	0.724	0.725
Heller	0.732	0.733	0.73	0.733	0.734

Table 7: Values Of Rmsd Against Various Mixing Rules Of Isovaleric Acid-N-Butyl Iodide Mixture

Mixing rules	RMSD				
	298	303	308	313	318
	Refractive index				
Eyring - John	0.027	0.027	0.027	0.027	0.027
Gladstone-Dale	1.516	1.525	1.526	1.532	1.531
Newton	1.515	1.524	1.525	1.533	1.532
Heller	1.528	1.536	1.536	1.542	1.54

The Root Mean Square Deviation (RMSD) values for the Eyring-Johns (E-J), Gladstone-Dale (G-D), Newton (Nw), and Heller (H) are presented in table 3. As RMSD values indicate, refractive index for mixtures under consideration. A close similarity is observed between the E-J and G-D relations. The RMSD values for E-J and G-D relations are found to be identical when volume additivity is assumed. The best predictions are observed for the E-J followed by G-D while the RMSD values predicted by Nw and Heller relations are relatively higher. Since the liquid mixtures of different nature and significantly different molecular sizes are considered, a particular relation provides good agreement at one place and deviates at others. This study indicates that all the theoretical mixing rules are interrelated in a simple quantitative manner and perform well within the limits of experimental error. The applicability of these semi-empirical relations for predicting refractive indices has also been emphasized by others

CONCLUSION

The refractive indices were reported for the liquid mixtures of Isovaleric acid with Isopropyl myristate, Bromoform and n-Butyl iodide at 298K, 303K, 308K, 313K and 318K.the variation in refractive index on mixing is calculated shows better agreement with the theoretical mixing rules. For the mixture of Isovaleric acid and bromoform shows better than other two liquid systems. Eyring-John shows good results than the other theoretical relations and Heller shows maximum deviation. These deviations can be minimized to some extent by considering the change in volume of the liquid with refractivity during the mixing.

References

[1] R.J.Sengwa, S. Sankhla, V.Khatri, S.Choudhary, Static permittivity and molecular interactions in binary mixtures ofethanolamine with alcohols and amides, Fluid Phase Equilib, 293 ,2010, 137-140.

[2] Sangita Sharma, Jasmin Bhalodia, Jayesh Ramani & Rignesh Patel (2011). Density,excess molar volumes and refractive indices of β-pinene with o,m,p-xylene and tolueneat 303.15, 308.15 and 313.15K. Physics and Chemistry of liquids,49(6), 765-776

[3] Manapragada V Rathinam, Sudir Mohite and Manapragada S. Kumar (2010). Densities,Viscosities and Refractive Indices of Binary mixtures of Diethyl oxalate with someKetones at (303.15, 308.15 and 313.15)K. Journal of Chemical and EngineeringData, 55, 5946-5952

[4] Dyaneshwar S. Wankhede, (2011). Refractive indices for binary mixtures of propyleneCarbonate. International Journal of Chemistry research, 2, 23-26

[5] Aleksandar Z Tasic., Bojan D Djordjevic., & Dusan K. Grozdanic (1992). Use ofmixing rules in predicting refractive Indices and Specific refractivities for some Binaryliquid mixtures. Journal of Chemical and Engineering Data, No. 3, 37.

[6] Rita Mehra., (2003). Application of Refractive index mixing rules in binary systems ofHexadecane and hepta decane with n-alkanols at different temperatures. Proc. IndianAcad. Sci.(Chem. Sci) 115,147-154

[7] Mohammed Taghi Zafarani-Moattar and Roghayeh Majdan-Cegincara (2007). Viscosity,Density, speed of sound and refractive index of binary mixtures of organic solvent +ionic liquid, 1-Butyl-3-methylimidazolium Hexafluorophosphate at 298.15K. Journal ofChemical and Engineering Data, 52, 2359-2364

[8] Kumar, S., and Jeevanandhan, P., (2012). Density, Refractive index and Excess molarvolume of binary mixtures of 2-Chloroaniline in DMSO and DMF at 308.15K, 313.15Kand 318.15K. International Journal of Recent Sciences and Research, 3, 192-196.
[9] Dnyaneshwar Shamrao Wankhede (2012). Refractive index, molar refraction andcomparative refractive index study of propylene carbonate binary liquid mixtures. ActaChim. Slov, 59, 258-263.
[10] Dubey, G.P., Tripathi N., & Bhatia, S.C. (2005). Refractive index of ternary liquid systems of squalane cyclohexane+benzene and +Hexane+cyclohexane). Indian Journal of Pure and Applied Physics, 43, 175-179.
[11] Eyring H & John M S, Significant liquid structures,(John Wiley, New York), 1969.
[12] Gladstone F & Dale D, Philos Trans R Soc, 148 ,1858, 887.
[13] Kurtz S S & Ward A L J, Franklin Inst, 222 ,1936, 563.
[14] Heller W, Phys Rev, 5,1945, 68.
[15] Bottcher C F J & Bordewijk P, Theory of Electrical Polarisation, Vol2.Elseiver, Amsterdam, 1978.
[16] Sangita Sharma, Pragnesh B Patel, Rignesh S, Patel & Vora, J J. Density a comparative refractive indexstudy on mixing properties of binary liquid mixtures of Eucalyptol with Hydro carbons at 303.15, 308.15 and 313.15K,E-Journal of Chemistry, 4, 2007,343-349.
[17] Narendra, K., Krishnamoorthy, P.,& Srinivasu, Ch. Refractive indices of binary liquid mixtures at different temperatures, Asian Journal of applied sciences, 4, 2011, 535-541.
[18] Anwar Ali, Anil Kumar Nain, Dinesh Chand & Rizwan Ahamed, Viscosities and Refractive Indices of binary mixtures at different temperatures: An Experimental and Theoretical Study, Indian Journal of Chemistry, 44, 2005, 511-515.
[19] M. Meenachiand P. Krishnamoorthy, Theoretical prediction of refractive index of Phenol with hydrocarbons at 303K, Mechanica Confab, 2, 2013, 2320-2491.