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Intermolecular Interactions and Refractive Indices: Experimental Data and Prediction of Oxygenated Fuel Additives with Hydrocarbons

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Oxygen containing compounds specifically alkanol and ether are being used as oxygenate fuel additives. The refractive indices (n_D) of oxygenated fuel additive, aliphatic and aromatic hydrocarbon and their mixtures were measured at 298.15 K to 318.15 K. The mixtures selected were diisopropyl ether (DIPE) + benzene, toluene, *n*-alkane (C_6-C_8) or benzene, toluene (1) + alkane (2) and all possible combinations of alkanes at 298.15 K to 318.15 K. Various mixing rules like Gladstone-Dale, Arago-Biot, Heller, Weiner, Newton and Erying–John were applied for the theoretical estimation of refractive index and compared with experimental refractive indices of binary mixtures. Polynomial equation was applied to the measured data to calculate standard deviation. The Δn were further interpreted in terms of intermolecular interactions between the oxygenated fuel additive, aliphatic and aromatic hydrocarbons.

Keywords: Oxygenate, Refractive index, Diisopropyl ether, Hydrocarbons, Intermolecular interactions.

INTRODUCTION

Increase in global warming and extinction of fossil fuels is a great issue now a day. So the researchers have much interest in the alternative bio-fuels [1-3], which include biodiesel, bioalcohol, vegetable oil, propane and other biomass sources. Bio-fuels are used as oxygenated compounds in motor fuel [4]. The oxygenates are the oxygen containing compounds such as ethers, alkanol and ester used as fuel additives. The oxygen present in these oxygenates help in complete combustion of fuel. These are also good antiknocking agent with high octane number [5,6]. Now days due to carcinogenic nature of benzene it needs to be replaced [7,8] and toluene is a good candidate as it has similar property as benzene but much less carcinogenic [9]. In this sense, it is an interesting research object to study the thermophysical of the oxygenate with hydrocarbons.

The dependency of volume, acoustic or optical properties of multi-component mixtures on concentration or temperature is a useful indicator for reality of significant effects resulting due to intermolecular interactions. Thus, these mixing properties have significance in design and simulation process. In previous work [10-28], the thermophysical properties like excess volume, excess enthalpy, deviation in viscosity and ultrasonic speed of the binary systems of oxygenate with hydrocarbons have been studied. In this paper, the refractive indices (n_D) of diisopropyl ether (DIPE) + benzene, toluene, *n*-alkane (C_6-C_8) or benzene, toluene (1) + alkane (2) and all possible combinations of alkanes at 298.15 to 318.15 K are reported. Redlich–Kister equation have been used to correlate experimental values of refractive indices of binary mixtures. These deviations in n_D have been used to understand the nature of interaction between unlike molecules. Various mixing rules were applied for the theoretical estimation of n_D and these estimated values have been compared quantitatively with experimental n_D of binary mixtures.

EXPERIMENTAL

Diisopropyl ether was purified by standard procedure [29] and other chemicals *e.g.*, *n*-octane, *n*-heptane, *n*-hexane, toluene and benzene (Merck, > 99 %) were doubly distilled and kept in amber coloured bottles over molecular sieves (4A). For the measurement of density of the purified samples, Anton Paar DSA-5000 was used with an uncertainty of ± 10^{-3} kg m^{-3}.

n_D data were measured with a refractometer (Abbemat-200) with temperature controlled within ± 0.01 K having accuracy up to ± 1×10^{-4}. The binary mixtures were made using a balance of precision ± 0.1 mg (OHAUS, AR224CN).

The densities (ρ) and n_D for pure compounds and their binary systems are given in Tables 1 and 2, respectively.

RESULTS AND DISCUSSION

Deviation in refractive index (Δn) have been calculated as:

$$\Delta n = n_D - \sum_{i=1}^{2} x_i n_{Di} \quad (1)$$

TABLE-1
PURITIES, MEASURED DENSITIES (ρ) AND REFRACTIVE INDICES (n_D) OF PURE COMPOUNDS

Compound	GC results (wt. %)	Temp. (K)	ρ (kg m^{-3})		n_D	
			This work	Literature	This work	Literature
DIPE	99.7	298.15	718.522	718.207 [30]	1.3654	1.3655 [31]
		308.15	707.966	707.664 [30]	1.3598	1.3605 [31]
		318.15	697.220	696.931 [30]	1.3541	
Benzene	99.8	298.15	873.612	873.550 [32]	1.4972	1.4977 [32]
		308.15	862.894	862.930 [32]	1.4899	1.4910 [33]
		318.15	852.103		1.4821	
Toluene	99.8	298.15	862.058	862.220 [32]	1.4937	1.4944 [32]
		308.15	852.715	852.880 [32]	1.4877	1.4887 [32]
		318.15	843.303		1.4815	
n-Hexane	99.6	298.15	655.296	654.800 [34]	1.3733	1.3736 [34]
		308.15	646.128	645.780 [35]	1.3679	1.3670 [36]
		318.15	636.779	636.390 [35]	1.3624	
n-Heptane	99.7	298.15	679.575	679.750 [37]	1.3846	1.3850 [34]
		308.15	671.018	671.190 [37]	1.3793	1.3803 [38]
		318.15	662.341	662.500 [37]	1.3740	
n-Octane	99.8	298.15	698.718	698.570 [37]	1.3953	1.3960 [34]
		308.15	690.596	690.440 [37]	1.3902	1.3908 [38]
		318.15	682.380	682.230 [37]	1.3853	

TABLE-2
REFRACTIVE INDEX (n_D) AND DEVIATION IN REFRACTIVE INDEX (Δn)
FOR BINARY SYSTEMS AT DIFFERENT TEMPERATURES

x_1	298.15 K		308.15 K		318.15 K	
	n_D	Δn	n_D	Δn	n_D	Δn
DIPE (1) + Benzene (2)						
0.0491	1.4881	-0.0026	1.4815	-0.0020	1.4743	-0.0015
0.1058	1.4772	-0.0061	1.4709	-0.0052	1.4647	-0.0039
0.1745	1.4653	-0.0089	1.4589	-0.0083	1.4523	-0.0075
0.2149	1.4587	-0.0102	1.4525	-0.0094	1.4465	-0.0081
0.3064	1.4442	-0.0126	1.4389	-0.0111	1.4333	-0.0096
0.4302	1.4272	-0.0133	1.4218	-0.0121	1.4175	-0.0095
0.5168	1.4154	-0.0137	1.4098	-0.0129	1.4052	-0.0108
0.6222	1.4034	-0.0118	1.3976	-0.0114	1.3918	-0.0107
0.7258	1.3919	-0.0097	1.3863	-0.0092	1.381	-0.0082
0.8105	1.3832	-0.0072	1.3777	-0.0068	1.3743	-0.0041
0.9334	1.3708	-0.0034	1.3657	-0.0028	1.3603	-0.0023
DIPE (1) + Toluene (2)						
0.0400	1.4877	-0.0009	1.4819	-0.0007	1.4762	-0.0002
0.0875	1.4808	-0.0017	1.4754	-0.0011	1.4701	-0.0002
0.1530	1.4705	-0.0036	1.4658	-0.0023	1.4605	-0.0015
0.2243	1.4599	-0.0050	1.4556	-0.0034	1.4501	-0.0028
0.3022	1.4485	-0.0064	1.4446	-0.0044	1.4377	-0.0053
0.3797	1.4385	-0.0065	1.4327	-0.0064	1.4268	-0.0063
0.4600	1.4279	-0.0068	1.4219	-0.0070	1.4159	-0.0070
0.5473	1.4168	-0.0067	1.4113	-0.0064	1.4053	-0.0065
0.6867	1.4001	-0.0055	1.3968	-0.0031	1.3905	-0.0035
0.7940	1.3878	-0.0040	1.3834	-0.0028	1.3786	-0.0017
0.9072	1.3755	-0.0018	1.3709	-0.0008	1.3649	-0.0010

DIPE (1) + *n*-Hexane (2)						
0.0399	1.3722	-0.0008	1.3669	-0.0007	1.3614	-0.0007
0.1031	1.3714	-0.0011	1.3663	-0.0008	1.3608	-0.0007
0.1832	1.3707	-0.0012	1.3656	-0.0008	1.3601	-0.0008
0.2459	1.3701	-0.0013	1.3648	-0.0011	1.3591	-0.0013
0.3603	1.3692	-0.0013	1.3637	-0.0013	1.358	-0.0014
0.4834	1.3681	-0.0014	1.3625	-0.0015	1.3568	-0.0016
0.5624	1.3676	-0.0013	1.3621	-0.0012	1.3564	-0.0013
0.6891	1.367	-0.0009	1.3615	-0.0008	1.3556	-0.0011
0.7958	1.3668	-0.0002	1.3609	-0.0006	1.3551	-0.0007
0.9091	1.366	-0.0001	1.3604	-0.0001	1.3547	-0.0002
0.9577	1.3657	0.0000	1.3601	0.0000	1.3544	-0.0001
DIPE (1) + *n*-Heptane (2)						
0.0398	1.3843	0.0005	1.3791	0.0006	1.3738	0.0006
0.1061	1.3832	0.0006	1.3779	0.0007	1.3727	0.0008
0.2002	1.3818	0.0010	1.3765	0.0011	1.3714	0.0014
0.2830	1.3806	0.0014	1.3754	0.0016	1.3703	0.0019
0.3965	1.3788	0.0018	1.3736	0.0020	1.3683	0.0022
0.5073	1.3769	0.0020	1.3717	0.0023	1.3663	0.0024
0.6051	1.3749	0.0019	1.3695	0.0020	1.3642	0.0022
0.7157	1.3722	0.0013	1.3671	0.0018	1.3617	0.0019
0.8200	1.3699	0.0010	1.3648	0.0015	1.3591	0.0014
0.9189	1.3678	0.0008	1.3624	0.0010	1.357	0.0013
0.9711	1.3664	0.0004	1.3608	0.0004	1.3553	0.0006
DIPE (1) + *n*-Octane (2)						
0.0475	1.3944	0.0005	1.3891	0.0003	1.3844	0.0006
0.1172	1.3926	0.0008	1.3873	0.0007	1.3825	0.0009
0.2036	1.3903	0.0011	1.3852	0.0012	1.3802	0.0013
0.2917	1.3881	0.0015	1.3831	0.0018	1.3781	0.0019
0.3958	1.3852	0.0017	1.3801	0.0019	1.3751	0.0021
0.5047	1.3821	0.0019	1.3769	0.0020	1.3718	0.0022
0.6067	1.3789	0.0017	1.3737	0.0019	1.3685	0.0021
0.7233	1.3752	0.0015	1.3699	0.0017	1.3647	0.0020
0.8296	1.3718	0.0013	1.3662	0.0012	1.3612	0.0018
0.9241	1.3686	0.0009	1.3633	0.0012	1.3579	0.0014
0.9619	1.3672	0.0007	1.3618	0.0008	1.3561	0.0008
Benzene (1) + *n*-Hexane (2)						
0.0578	1.3769	-0.0037	1.3713	-0.0039	1.3657	-0.0038
0.1429	1.3841	-0.0071	1.378	-0.0076	1.3722	-0.0075
0.2477	1.3936	-0.0105	1.3874	-0.0109	1.3812	-0.0110
0.3224	1.401	-0.0124	1.3948	-0.0126	1.389	-0.0121
0.4592	1.4158	-0.0145	1.4103	-0.0138	1.4059	-0.0116
0.5648	1.4283	-0.0151	1.4216	-0.0153	1.4158	-0.0143
0.6742	1.4437	-0.0132	1.4373	-0.0130	1.4316	-0.0116
0.7527	1.4546	-0.0120	1.4479	-0.0119	1.4419	-0.0106
0.8199	1.4642	-0.0107	1.458	-0.0100	1.452	-0.0086
0.8860	1.4752	-0.0079	1.4687	-0.0073	1.4629	-0.0056
0.9470	1.4929	0.0023	1.4864	0.0029	1.4796	0.0038
Benzene (1) + *n*-Heptane (2)						
0.0756	1.3896	-0.0046	1.3877	-0.0016	1.3822	-0.0020
0.1647	1.3962	-0.0079	1.3919	-0.0071	1.3873	-0.0063
0.2800	1.4047	-0.0123	1.3978	-0.0138	1.3919	-0.0139
0.3631	1.4099	-0.0164	1.4026	-0.0180	1.3951	-0.0196
0.4848	1.4223	-0.0175	1.4156	-0.0182	1.4089	-0.0186
0.6328	1.4382	-0.0181	1.4317	-0.0183	1.4249	-0.0183
0.7026	1.4471	-0.0170	1.4415	-0.0160	1.4337	-0.0169
0.7737	1.4572	-0.0148	1.4478	-0.0175	1.4416	-0.0165
0.8402	1.4648	-0.0146	1.4579	-0.0146	1.4501	-0.0151
0.8936	1.4736	-0.0118	1.4672	-0.0111	1.4597	-0.0111
0.9494	1.4886	-0.0030	1.4808	-0.0036	1.472	-0.0047

Benzene (1) + *n*-Octane (2)						
0.0647	1.3982	-0.004	1.3922	-0.0046	1.3868	-0.0050
0.1477	1.4028	-0.007	1.3966	-0.0085	1.3914	-0.0084
0.2713	1.4097	-0.013	1.4013	-0.0161	1.3954	-0.0163
0.3634	1.4163	-0.016	1.4096	-0.0170	1.4035	-0.0171
0.4416	1.4226	-0.018	1.4138	-0.0205	1.4078	-0.0204
0.5695	1.4342	-0.019	1.4276	-0.0195	1.4179	-0.0226
0.6790	1.4458	-0.019	1.4388	-0.0192	1.429	-0.0221
0.7369	1.4533	-0.017	1.4466	-0.0171	1.4392	-0.0175
0.8240	1.4663	-0.013	1.4585	-0.0139	1.4508	-0.0143
0.9109	1.4794	-0.009	1.4725	-0.0085	1.4653	-0.0082
0.9567	1.4885	-0.004	1.4812	-0.0044	1.4732	-0.0047
Toluene (1) + *n*-Hexane (2)						
0.0513	1.3778	-0.0017	1.3731	-0.0009	1.3674	-0.0011
0.1268	1.3853	-0.0033	1.3806	-0.0025	1.3761	-0.0014
0.2149	1.3942	-0.0050	1.3889	-0.0047	1.3844	-0.0036
0.2875	1.4021	-0.0058	1.3969	-0.0054	1.3924	-0.0042
0.4089	1.4161	-0.0064	1.4107	-0.0062	1.4057	-0.0054
0.5180	1.4289	-0.0068	1.4235	-0.0065	1.4182	-0.0059
0.6311	1.4432	-0.0061	1.4375	-0.0060	1.432	-0.0056
0.7134	1.4539	-0.0053	1.4478	-0.0056	1.4429	-0.0045
0.8078	1.4669	-0.0037	1.4615	-0.0032	1.4561	-0.0025
0.9093	1.4806	-0.0022	1.4749	-0.0019	1.4691	-0.0016
0.9520	1.4865	-0.0014	1.4805	-0.0015	1.4744	-0.0014
Toluene (1) + *n*-Heptane (2)						
0.0557	1.3894	-0.0013	1.3841	-0.0012	1.3786	-0.0014
0.1150	1.394	-0.0032	1.3887	-0.0031	1.3833	-0.0031
0.2130	1.4021	-0.0057	1.3966	-0.0058	1.391	-0.0059
0.3099	1.4107	-0.0077	1.4049	-0.0080	1.3992	-0.0081
0.4294	1.4218	-0.0096	1.416	-0.0098	1.4105	-0.0097
0.5055	1.4293	-0.0105	1.4238	-0.0103	1.4183	-0.0100
0.6126	1.4419	-0.0095	1.4362	-0.0095	1.4306	-0.0093
0.7040	1.4523	-0.0091	1.4467	-0.0089	1.4407	-0.0090
0.8255	1.4676	-0.0071	1.4616	-0.0072	1.4556	-0.0071
0.9190	1.4812	-0.0037	1.475	-0.0039	1.4687	-0.0041
0.9556	1.4858	-0.0031	1.4797	-0.0032	1.4738	-0.0029
Toluene (1) + *n*-Octane (2)						
0.0587	1.3999	-0.0012	1.3951	-0.0008	1.3902	-0.0007
0.1550	1.4046	-0.0060	1.3996	-0.0057	1.3946	-0.0056
0.2536	1.4121	-0.0082	1.4069	-0.0080	1.4015	-0.0082
0.3542	1.4196	-0.0106	1.4141	-0.0106	1.4084	-0.0110
0.4731	1.4298	-0.0121	1.4243	-0.0120	1.4186	-0.0122
0.5751	1.4394	-0.0125	1.4337	-0.0126	1.4279	-0.0127
0.6441	1.4467	-0.0120	1.4411	-0.0119	1.4349	-0.0124
0.7281	1.4561	-0.0108	1.4503	-0.0109	1.4439	-0.0114
0.8221	1.4679	-0.0083	1.4618	-0.0086	1.4558	-0.0086
0.8824	1.4753	-0.0068	1.4699	-0.0063	1.4639	-0.0063
0.9593	1.4884	-0.0013	1.4819	-0.0018	1.4758	-0.0018
n-Hexane + *n*-Heptane (2)						
0.0413	1.3851	-0.0002	1.3804	-0.0002	1.3754	-0.0002
0.1134	1.3842	-0.0002	1.3794	-0.0002	1.3744	-0.0002
0.1963	1.3831	-0.0002	1.3783	-0.0002	1.3732	-0.0003
0.2827	1.382	-0.0003	1.3771	-0.0003	1.372	-0.0003
0.4067	1.3804	-0.0003	1.3754	-0.0003	1.3702	-0.0004
0.5276	1.3789	-0.0003	1.3738	-0.0003	1.3685	-0.0004
0.6030	1.378	-0.0003	1.3729	-0.0002	1.3675	-0.0004
0.7246	1.3765	-0.0002	1.3713	-0.0002	1.3659	-0.0003
0.8268	1.3753	-0.0002	1.37	-0.0002	1.3645	-0.0003
0.8874	1.3745	-0.0002	1.3692	-0.0002	1.3639	-0.0001
0.9496	1.3738	-0.0001	1.3684	-0.0002	1.3631	0.0000

n-Hexane + *n*-Octane (2)						
0.0513	1.3944	0.0003	1.3896	0.0004	1.3847	0.0004
0.1233	1.3933	0.0008	1.3883	0.0007	1.3834	0.0007
0.2153	1.3914	0.0009	1.3865	0.0009	1.3818	0.0013
0.3073	1.3897	0.0012	1.3849	0.0014	1.3801	0.0017
0.4324	1.3877	0.0020	1.3835	0.0028	1.3783	0.0028
0.5524	1.3857	0.0026	1.3812	0.0032	1.3764	0.0037
0.6357	1.3834	0.0021	1.3789	0.0028	1.3743	0.0035
0.7478	1.3808	0.0020	1.3761	0.0025	1.3712	0.0030
0.8384	1.3781	0.0013	1.3728	0.0013	1.3679	0.0018
0.8975	1.3765	0.0010	1.3711	0.0009	1.3657	0.0009
0.9498	1.3746	0.0002	1.3693	0.0003	1.3639	0.0003
n-Heptane + *n*-Octane (2)						
0.0509	1.3949	0.0001	1.3899	0.0003	1.385	0.0003
0.1208	1.3942	0.0002	1.3893	0.0004	1.3843	0.0004
0.2109	1.3936	0.0006	1.3885	0.0006	1.3835	0.0006
0.2993	1.3927	0.0006	1.3877	0.0008	1.3826	0.0007
0.4122	1.3915	0.0006	1.3865	0.0008	1.3814	0.0008
0.5249	1.3905	0.0008	1.3853	0.0008	1.3803	0.0009
0.6104	1.3895	0.0007	1.3843	0.0008	1.3792	0.0008
0.7427	1.388	0.0006	1.3828	0.0007	1.3776	0.0007
0.8315	1.3869	0.0005	1.3818	0.0007	1.3765	0.0006
0.9190	1.3859	0.0004	1.3807	0.0005	1.3753	0.0004
0.9639	1.3851	0.0001	1.3799	0.0002	1.3746	0.0002

where x_i and n_{Di} represent the mole fraction and the refractive index of the i^{th} component, respectively and n_D is the refractive index of binary liquid mixture. Experimental n_D and Δn data of binary systems are given in Table-2. The Δn values were also fitted to polynomial equation (Figs. 1 and 2).

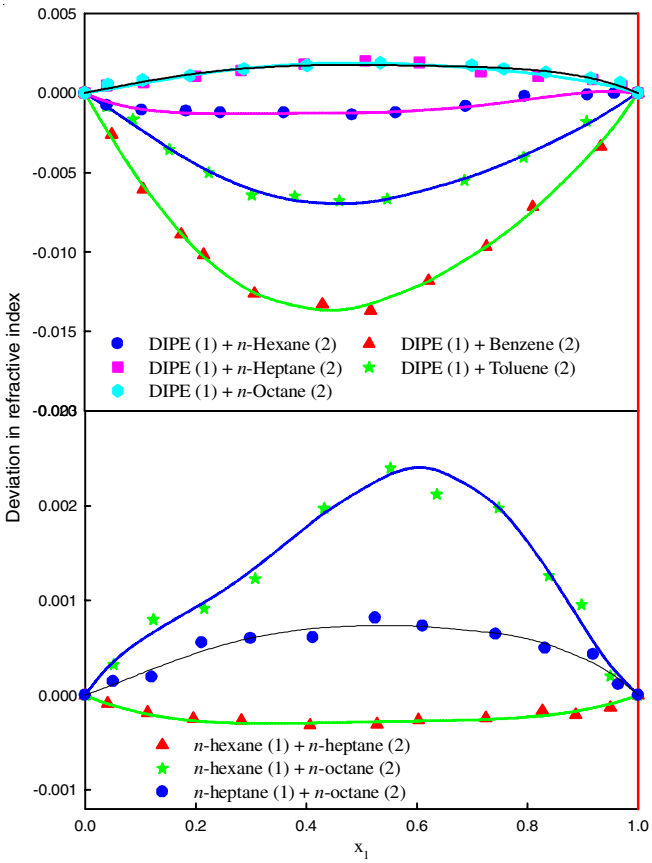

Fig. 1. Deviation in refractive index for the binary (1 + 2) mixtures as a function of mole fraction of x_1 at 298.15 K. Symbols represent experimental values and lines represent values calculated from Redlich-Kister equation

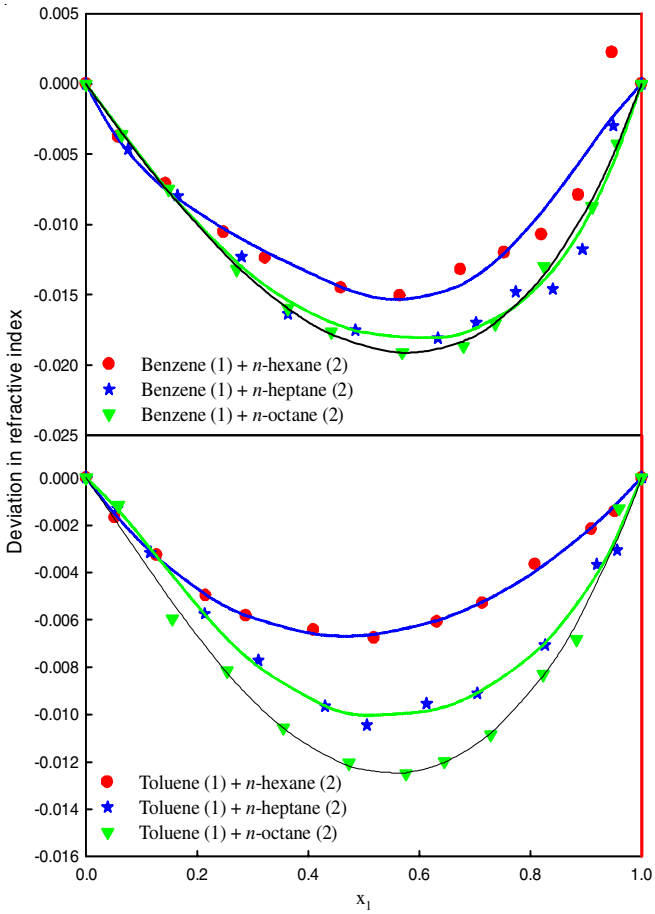

Fig. 2. Deviation in refractive index for the binary (1 + 2) mixtures as a function of mole fraction of x_1 at 298.15 K. Symbols represent experimental values and lines represent values calculated from Redlich-Kister equation

$$\Delta n = x_1(1-x_1)\left(\sum_{n=1}^{4} A^{(j)}(2x_1-1)^{(j-1)}\right) \quad (2)$$

where $A^{(j)}$ are the adjustable parameters and calculated by fitting Δn data in eqn. 2 respective standard deviations σ(Δn) were recorded in Table-3.

For quantitative determination of n_D following mixing relations were used:

Arago-Biot (A-B):

TABLE-3
ADJUSTABLE PARAMETERS OF REDLICH–KISTER EQUATION ($A^{(j)}$) AND STANDARD DEVIATION (σ)

Temperature (K)	$A^{(1)}$	$A^{(2)}$	$A^{(3)}$	$A^{(4)}$	σ
DIPE (1) + Benzene (2)					
298.15	-0.0536	0.0148	-0.0029	-0.0111	0.0000
308.15	-0.0502	0.0089	0.0010	-0.0021	0.0004
318.15	-0.0432	0.0045	0.0079	0.0111	0.0010
DIPE (1) + Toluene (2)					
298.15	-0.0276	0.0063	0.0047	-0.0083	0.0002
308.15	-0.0253	0.0087	0.0236	-0.0092	0.0006
318.15	-0.0263	0.0129	0.0329	-0.0238	0.0004
DIPE (1) + *n*-Hexane (2)					
298.15	-0.0050	0.0013	-0.0010	0.0092	0.0001
308.15	-0.0052	0.0008	0.0009	0.0053	0.0002
318.15	-0.0059	0.0003	0.0012	0.0055	0.0002
DIPE (1) + *n*-Heptane (2)					
298.15	0.0076	-0.0005	-0.0001	0.0031	0.0002
308.15	0.0084	0.0004	0.0016	0.0038	0.0002
318.15	0.0091	-0.0009	0.0032	0.0061	0.0002
DIPE (1) + *n*-Octane (2)					
298.15	0.0071	-0.0002	0.0038	0.0043	0.0001
308.15	0.0079	-0.0021	0.0026	0.0105	0.0002
318.15	0.0086	-0.0006	0.0057	0.0094	0.0002
Benzene (1) + *n*-Hexane (2)					
298.15	-0.0598	-0.0204	-0.0007	0.0428	0.0014
308.15	-0.0595	-0.0209	-0.0004	0.0568	0.0022
318.15	-0.0544	-0.0185	0.0004	0.0694	0.0023
Benzene (1) + *n*-Heptane (2)					
298.15	-0.0708	-0.0195	-0.0193	-0.0184	0.0002
308.15	-0.0764	-0.0048	0.0000	-0.0702	0.0014
318.15	-0.0788	0.0019	0.0047	-0.0891	0.0012
Benzene (1) + *n*-Octane (2)					
298.15	-0.0748	-0.0226	-0.0074	-0.0049	0.0000
308.15	-0.0804	-0.0095	-0.0105	-0.0165	0.0008
318.15	-0.0865	-0.0281	0.0000	0.0183	0.0011
Toluene (1) + *n*-Hexane (2)					
298.15	-0.0266	0.0032	-0.0024	0.0001	0.0002
308.15	-0.0263	0.0027	0.0040	-0.0044	0.0004
318.15	-0.0233	0.0002	0.0100	-0.0033	0.0004
Toluene (1) + *n*-Heptane (2)					
298.15	-0.0401	-0.0054	-0.0012	-0.0159	0.0004
308.15	-0.0401	-0.0020	-0.0023	-0.0246	0.0003
318.15	-0.0394	-0.0015	-0.0048	-0.0242	0.0002
Toluene (1) + *n*-Octane (2)					
298.15	-0.0494	-0.0104	0.0006	-0.0050	0.0006
308.15	-0.0497	-0.0094	0.0032	-0.0108	0.0005
318.15	-0.0511	-0.0109	0.0056	-0.0090	0.0006
n-Hexane (1) + *n*-Heptane (2)					
298.15	-1.12×10^{-3}	2.23×10^{-4}	-1.22×10^{-3}	-4.60×10^{-5}	4.90×10^{-5}
308.15	-1.15×10^{-3}	3.60×10^{-4}	-1.09×10^{-3}	-5.47×10^{-4}	5.31×10^{-5}
318.15	4.24×10^{-4}	1.24×10^{-3}	-3.31×10^{-3}	9.01×10^{-4}	3.27×10^{-4}
n-Hexane (1) + *n*-Octane (2)					
298.15	8.765×10^{-3}	6.783×10^{-3}	-2.216×10^{-3}	-8.802×10^{-3}	1.791×10^{-4}
308.15	1.170×10^{-2}	8.881×10^{-3}	-8.077×10^{-3}	-1.120×10^{-2}	2.134×10^{-4}
318.15	1.310×10^{-2}	1.210×10^{-2}	-6.856×10^{-3}	-1.620×10^{-2}	8.508×10^{-5}
n-Heptane (1) + *n*-Octane (2)					
298.15	2.95×10^{-3}	2.69×10^{-4}	8.21×10^{-4}	1.43×10^{-3}	8.12×10^{-5}
308.15	3.14×10^{-3}	-4.39×10^{-4}	2.74×10^{-3}	2.42×10^{-3}	4.50×10^{-5}
318.15	3.31×10^{-3}	5.00×10^{-4}	1.43×10^{-3}	-4.00×10^{-5}	5.83×10^{-5}

$$n_D = n_{D1}\phi_1 + n_{D2}\phi_2 \quad (3)$$

Gladstone-Dale (G-D):

$$n_D - 1 = (n_{D1} - 1)\phi_1 + (n_{D2} - 1)\phi_2 \quad (4)$$

Lorentz-Lorenz (L-L):

$$\frac{n_D^2 - 1}{n_D^2 + 2} = \left(\frac{n_{D1}^2 - 1}{n_D^2 + 2}\right)\phi_1 + \left(\frac{n_{D2}^2 - 1}{n_D^2 + 2}\right)\phi_2 \quad (5)$$

Heller (H):

$$\frac{n_D - 1}{n_D} = \frac{3}{2}\left(\frac{(n_{D2}/n_{D1})^2 - 1}{(n_{D2}/n_{D1})^2 + 2}\right)\phi_2 \quad (6)$$

Weiner (W):

$$\frac{n_D^2 - n_{D1}^2}{n_D^2 + 2n_{D2}^2} = \left(\frac{n_{D2}^2 - n_{D1}^2}{n_{D2}^2 + 2n_{D2}^2}\right)\phi_2 \quad (7)$$

Newton (Nw):

$$n_D^2 - 1 = (n_{D1}^2 - 1)\phi_1 + (n_{D2}^2 - 1)\phi_2 \quad (8)$$

Eyring and John (E-J):

$$n_D = n_{D1}\phi_1^2 + 2(n_{D1}n_{D2})^{1/2}\phi_1\phi_2 + n_{D2}\phi_2^2 \quad (9)$$

In all above equations, n_D, n_{D1} and n_{D2} are the refractive index of mixture and its pure component, respectively. ϕ_1 and ϕ_2 represent the volume fraction of pure components and given by

$$\phi_1 = \frac{x_1 V_1}{\sum x_i V_i} \text{ and } \phi_2 = \frac{x_2 V_2}{\sum x_i V_i} \quad (10)$$

From these mixing rules standard deviation were also calculated which are reported in Table-4. From Table-4 it can be seen that for all the binary mixtures all mixing rules have good results.

TABLE-4
STANDARD DEVIATION OF CALCULATED VALUES OF REFRACTIVE INDEX USING VARIOUS CORRELATIONS

Binary system	Temp. (K)	AB	GD	LL	Weiner	Heller	Newton	Eyring
DIPE (1) + Benzene (2)	298.15	0.0260	0.0260	0.0247	0.0391	0.0243	0.0273	0.0254
	308.15	0.0010	0.0010	0.0010	0.0011	0.0010	0.0010	0.0010
	318.15	0.0041	0.0041	0.0053	0.0100	0.0055	0.0028	0.0047
DIPE (1) + Toluene (2)	298.15	0.0816	0.0816	0.0816	0.0807	0.0817	0.0815	0.0816
	308.15	0.0035	0.0035	0.0048	0.0110	0.0051	0.0023	0.0042
	318.15	0.0039	0.0039	0.0052	0.0106	0.0055	0.0028	0.6551
DIPE (1) + *n*-Hexane (2)	298.15	0.0020	0.0020	0.0020	0.0020	0.0020	0.0020	0.0020
	308.15	0.0017	0.0017	0.0017	0.0015	0.0017	0.0017	0.0017
	318.15	0.0011	0.0011	0.0011	0.0012	0.0011	0.0011	0.0011
DIPE (1) + *n*-Heptane (2)	298.15	0.0013	0.0013	0.0013	0.0016	0.0013	0.0013	0.0013
	308.15	0.0009	0.0009	0.0010	0.0008	0.0010	0.0009	0.0010
	318.15	0.0019	0.0019	0.0020	0.0017	0.0020	0.0019	0.0019
DIPE (1) + *n*-Octane (2)	298.15	0.0018	0.0018	0.0018	0.0024	0.0018	0.0019	0.0018
	308.15	0.0010	0.0010	0.0010	0.0011	0.0010	0.0010	0.0010
	318.15	0.0012	0.0012	0.0013	0.0009	0.0013	0.0011	0.0012
Benzene (1) + *n*-Hexane (2)	298.15	0.0037	0.0037	0.0029	0.0138	0.0031	0.0047	0.0033
	308.15	0.0037	0.0037	0.0030	0.0136	0.0031	0.0046	0.0033
	318.15	0.0034	0.0034	0.0031	0.0127	0.0030	0.0040	0.0032
Benzene (1) + *n*-Heptane (2)	298.15	0.0127	0.0127	0.0117	0.0192	0.0121	0.0137	0.0122
	308.15	0.0057	0.0057	0.0048	0.0127	0.0052	0.0066	0.0053
	318.15	0.0064	0.0064	0.0055	0.0130	0.0059	0.0072	0.0060
Benzene (1) + *n*-Octane (2)	298.15	0.0092	0.0092	0.0084	0.0153	0.0087	0.0100	0.0088
	308.15	0.0052	0.0052	0.0045	0.0120	0.0046	0.0059	0.0048
	318.15	0.0066	0.0066	0.0059	0.0129	0.0060	0.0074	0.0063
Toluene (1) + *n*-Hexane (2)	298.15	0.0061	0.0061	0.0072	0.0087	0.0070	0.0050	0.0067
	308.15	0.0005	0.0005	0.0012	0.0107	0.0012	0.0013	0.0007
	318.15	0.0010	0.0010	0.0020	0.0100	0.0020	0.0007	0.0015
Toluene (1) + *n*-Heptane (2)	298.15	0.0017	0.0017	0.0026	0.0082	0.0024	0.0009	0.0021
	308.15	0.0014	0.0014	0.0007	0.0096	0.0013	0.0022	0.0010
	318.15	0.0013	0.0013	0.0007	0.0095	0.0012	0.0022	0.0010
Toluene (1) + *n*-Octane (2)	298.15	0.0009	0.0009	0.0007	0.0076	0.0010	0.0015	0.0007
	308.15	0.0020	0.0020	0.0013	0.0083	0.0016	0.0027	0.0016
	318.15	0.0023	0.0023	0.0016	0.0084	0.0020	0.0030	0.0020
n-Hexane (1) + *n*-Heptane (2)	298.15	0.0012	0.0012	0.0012	0.0013	0.0012	0.0012	0.0012
	308.15	0.0010	0.0010	0.0010	0.0011	0.0010	0.0010	0.0010
	318.15	0.0011	0.0011	0.0011	0.0012	0.0011	0.0011	0.0011
n-Hexane (1) + *n*-Octane (2)	298.15	0.0012	0.0012	0.0012	0.0010	0.0012	0.0012	0.0012
	308.15	0.0014	0.0014	0.0014	0.0012	0.0014	0.0013	0.0014
	318.15	0.0017	0.0017	0.0017	0.0015	0.0017	0.0017	0.0017
n-Heptane (1) + *n*-Octane (2)	298.15	0.0010	0.0010	0.0010	0.0010	0.0010	0.0010	0.0010
	308.15	0.0005	0.0005	0.0006	0.0005	0.0006	0.0005	0.0006
	318.15	0.0005	0.0005	0.0005	0.0005	0.0005	0.0005	0.0005

Figs. 1 and 2 show deviation in refractive index data *versus* x_1 for these systems. The Δn values for the DIPE (1) + *n*-heptane, *n*-octane (2) or *n*-hexane and *n*-heptane (1) + *n*-octane (2) systems are positive while negative for DIPE (1) + benzene, toluene or *n*-hexane (2), benzene or toluene (1) + C_6-C_8 (2) and *n*-hexane (1) + *n*-heptane (2) systems. The Δn values for DIPE (1) + hydrocarbon (2) at equimolar mixtures follow the sequence: *n*-octane ≈ *n*-heptane > *n*-hexane > toluene > benzene while for benzene or toluene (1) + hydrocarbon (2) the order is *n*-hexane > *n*-heptane > *n*-octane and for *n*-hexane (1) + hydrocarbon (2) the value is positive for *n*-octane and negative for *n*-heptane system.

As the refractive index is speed of light dependent property. With increase in density due to n-π intermolecular interactions between aromatic hydrocarbon and lone pair of oxygen atom in DIPE the n_D value also increase. The Δn in the DIPE + aromatic hydrocarbon mixtures for toluene are larger than benzene due to presence of one methyl group which increase the electron density on benzene ring for stronger n-π interactions [39]. While in case of aliphatic *n*-heptane or *n*-octane there is absence of π-electrons only disorder in proper orientation of hydrocarbon occur, so for DIPE (1) + alkane (2) mixtures, medium gets rarer and refractive index decreases [40]. The deviation in refractive index is also influenced with temperature. The Δn for DIPE (1) + heptane or benzene (2) mixtures is plotted against composition in Fig. 3. As shown in Fig. 3 for DIPE (1) + heptane or benzene (2) systems, with increase in temperature Δn is also increasing in both positive as well as negative deviation.

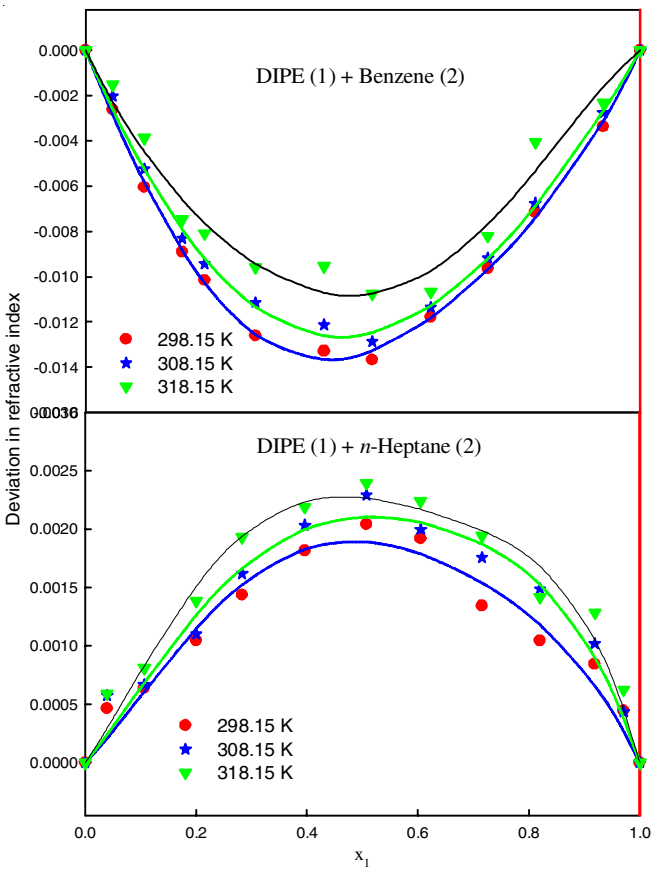

Fig. 3. Deviation in refractive index for the binary (1 + 2) mixtures as a function of mole fraction of x_1 at different temperature. Symbols represent experimental values and lines represent values calculated from Redlich-Kister equation

Conclusion

Deviations in refractive index (Δn) for DIPE and hydrocarbon systems were determined at 298.15 to 318.15 K. The Δn values for the DIPE (1) + *n*-heptane, *n*-octane (2) or *n*-hexane and *n*-heptane (1) + *n*-octane (2) systems are positive while negative for DIPE (1) + benzene, toluene or *n*-hexane (2), benzene or toluene (1) + C_6-C_8 (2) and *n*-hexane (1) + *n*-heptane (2) systems. Various mixing rules applied for the theoretical estimation of n_D have good results with experimental data for all binary systems.

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CONFLICT OF INTEREST

The authors declare that there is no conflict of interests regarding the publication of this article.

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