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Excess Refractive Index, Polarizability, Polarization and Solution Volumes of Saturated Phthalic Acid in Mixed ($MeOH-H_2O$) at Different Temperatures

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Keywords

Phthalic Acid, Refractive Index, Excess Refractive Index, Polarization, Solution Volume

The refractive indexes and the densities of saturated solution of saturated phthalic acid in mixed ($MeOH-H_2O$) solvents were measured at four different temperatures, 298.15K, 303.15K, 308.15K And 313.15K. From the values of the measured refractive indices and the densities, the excess refractive indices, the atomic, electronic polarizations, the molar volumes, polarizabilities and the induced dipole moment were calculated and discussed. On the other hand, the molar volumes and solvated diameters were also evaluated. Measuring the refractive index properties are necessary for manufacturing industries especially in that using optical devices.

Introduction

Phthalic acid is an organic compound derived from benzene and used in the manufacture of dyes, perfumes, pharmacetucal and synthetic fibers. Refractive index and density measurements were expected to explain solute – solvent interactions [1-2]. Detection of liquid concentration by optical refractive index was already known in old time [3]. The first laboratory instrument to accurate measure the refractive index of liquids was developed by Ernst Abbe in 1874. Many authors used both refractive index and density to study the ion –solvent and solvent –solvent interactions [3-4], with water [5-7] and other organic solvents [8-10]. All phthalates are miscible with PVC (polyvinyl chloride) when added to plastics and resins, they improve the workability during fabrication, modify the properties and give rise to new phthalates are used for manufacturing flexibile PVC, which is consumed for manufacturing of some goods like films and sheeting. Optical measurement technique such as refractive indexes is used in experimental fluid mechanics to investigate pure fluids or dilute suspensions. Phthalic acid can be used in manufacturing of wires, cables, conducting sheets with high electrical resistivity [10-12]. Refractive index plays an important role in many areas of material science with reference to thin film technology and fiber optics.

Similarly, measurement of refractive index is widely used in analytical chemistry to determine the concentration of pollutions [13-16]. The present work includes the estimation of excess refractive indexes, molar volumes, polarizabilities and induced dipole moments for saturated phthalic acid solutions at 298.15K, 303.15K, 308.15K, and 313.15K. The evaluated physical parameters for phthalic acid are important in studying the solvation processes and facilitate its need in optical, manufacturing of film and sheeting materials [17-20]. The aim of this work is giving valuable refraction data for phthalic acid that can be used in industry and environment.

Experimental

Phthalic acid and methanol pure chemicals were supplied from EL. Nasr Pharmaceutical Chemicals CO. The Refractive indexes of saturated solutions of adipic acid were measured using a refractometer of the type ATAGO 3T. NO 52507 and circulating water was circulated around the prism of refractometer to keep the temperature constant through ultra-Thermostat of the type Kottermann.

The saturated solutions were prepared by adding the excess amount of the solid acid in 10 ml. of the corresponding solvent mixtures, using closed test tubes. The solutions were vigorously shaken in ultra-thermostat of the type (SIBATA-SU-20) with an output of 30 W of 50 KHZ Frequency.

Results and Discussion

From the values measured refractive indexes (n), the excess refractive indexes (n_E) can be evaluated by applying equation (1) in mixed solvents, (MeOH-H_2O).

$$n_E = n_{mixture} – (x_{s1}.n_1 + x_{s2}.n_2) \quad (1)$$

Where, X_{S1}, X_S, n_1 and n_2 are the mole fractions by weight and the refractive indexes of the organic solvent MeOH and water, respectively.

The values of X_{S1} and X_{S2} were calculated by applying equation (2):

$$\frac{\frac{vol\%(1)xd1}{M1}}{\frac{vol\%(1)xd1}{M1} + \frac{vol\%(2)xd2}{M2}} = X_{s1} \quad (2)$$

where d_1, d_2, M_1, M_2, vol %(1) and vol %(2) are the densities, the molecular weights and the volume percentages of the organic solvents methanol (MeOH) and water, respectively. The values of X_{s2} in equation 2 is equal to (1-X_{s1}).

From measured refractive indexes values for phthalic acid, the molar refraction (R) was calculated using equation (3).

$$R = \frac{n^2-1}{n^2+2} V = P_A + P_E = P_D = P_T \quad (3)$$

Where V is the molar volume of saturated phthalic acid solutions which equal ($\frac{M}{d}$), where M and d are the molecular weight and the measure density of saturated phthalic acid solutions at different used temperatures

The right hand side of equation (3) is equal to the total molar polarization or distortion polarization which equal to the summation of both the electronic polarization (P_E) and atomic polarization (P_A). The atomic (P_E) polarization (P_A) was calculated [22-30].

From equation 4, the values for saturated phthalic acid solutions are sited in Tables1, 2, 3, and 4 at different temperatures.

$$P_A = 1.05\ n^2 \quad (4)$$

The value for molecular polarizability (α) can be calculated from optical refractive index (n) of the saturated phthalic acid solutions containing N molecules per unit volume. The refractive index is related to the polarizability of saturated molecules by Lorenz-Lorenz formula [31-40] as explained in equation (5).

$$\frac{n^2-1}{n^2+2} = \frac{4\ \bar{n}\ \alpha\ \pi}{3} \quad (5)$$

Where $\bar{n} = \frac{N}{V}$, N is Avogadro‘s number and V is the molar volume of saturated phthalic acid solutions. Applying equation (5), the polarizabilities of saturated phthalic acid solutions were calculated at different temperatures and presented in Tables 1, 2, 3, and 4.

The electronic polarization (P_E) can be calculated by using equation (3) on subtracting the atomic polarization values (P_A) from the total polarization (P_T). The dipole moments for saturated phthalic acid solutions induced by the solvent and mixed (MeOH-H_2O) solvents were calculated using equation (6) after applying the dielectric constant values with those values of mixed (MeOH-H_2O) solvents.

$$\frac{(\varepsilon-n^2)(2\varepsilon-n^2)}{\varepsilon(n^2+2)^2} = \frac{4\ \pi\ N g\ \mu^2}{4\ K\ T\ V} \quad (6)$$

In using Onsager solution g=1, which is Onsager cavity field [40-44]. The evaluated induced dipole moments for saturated solutions of phthalic acid in mixed (MeOH_H_2O) solvents were presented in Tables 1, 2, 3, and 4 at different temperatures.

The solvated diameters of the saturated phthalic acid solutions in mixed (MeOH-H_2O) solvents were calculated using equation (7) considering spherical form of the solvated phthalic acid solutions [45-51].

$$V=\frac{1}{6} N \pi \sigma^3 \tag{7}$$

Where σ the solvated diameters and N is Avogadro's number

The measured refractive indices (n), the excess refractive indices (n_E), the molar refraction (R), the atomic polarization (P_A), electronic polarization (P_E), polarizability (α), and the molar volumes (V), and the solvated diameters are listed in Tables 1, 2, 3, and 4 at different temperatures. The relation between mole fraction (X_s), (α) and (μ) for phthalic acid in mixed methanol-water solvents at 308.15K temperature as example in three and two dimensions are shown in Fig. 1 and 2.

Table (1). *Refraction parameters for saturated phthalic acid in mixed methanol-water solvents at 298.15K.*

n_d^E	μ x10^{22}	ϵ	α x10^{23}	Nx 10^{-21}	P_E	P_T	P_A	R	n_d	X_s
0	2.276	78.3	1.322	3.783	-1.664	0.207	1.871	33.342	1.335	0
1.404	2.261	73.744	1.407	3.549	-1.869	0.209	1.892	35.501	1.339	0.0999
3.517	2.383	67.884	1.433	3.541	-1.798	0.2127	1.901	36.152	1.345	0.2284
7.104	1.964	60.169	1.562	3.324	-1.702	0.2174	1.926	39.364	1.354	0.3976
5.665	1.764	49.129	1.609	3.271	-1.722	0.22	1.943	40.583	1.36	0.6397
0	1.425	32.7	1.652	3.234	-1.735	0.223	1.959	41.674	1.366	1

Table (2). *Refraction parameters for saturated phthalic acid in mixed methanol-water solvents at 303.15K.*

n_d^E	μ x10^{22}	ϵ	α x10^{23}	n x10^{-21}	P_E	P_T	P_A	R	n_d	Xs
0	2.251	76.75	1.355	3.783	-1.667	0.207	1.875	35.185	1.336	0
1.004	20223	72.25	1.414	3.549	-1.657	0.209	1.886	35.659	1.3405	0.0999
3.145	2.094	66.46	1.416	3.541	-1.69	0.213	1.909	36.536	1.3465	0.2284
7.003	1.954	58.84	1.575	3.324	-1.711	0.218	1.929	39.725	1.3555	0.3976
5.304	1.755	47.93	1.614	3.271	-1.723	0.221	1.944	40.723	1.3612	0.6397
0	1.904	31.71	1.66	3.234	-1.736	0.224	1.96	41.871	1.3665	1

Table (3). *Refraction parameters for saturated phthalic acid in mixed methanol-water solvents at 308.15K.*

n_d^E	μ x10^{22}	ϵ	α x10^{23}	n x10^{-21}	P_E	P_T	P_A	R	n_d	Xs
0	2.26	75	1.392	3.563	-1.669	0.2079	1.876	35.12	1.337	0
0.954	2.188	70.72	1.436	3.491	-1.678	0.2101	1.888	36.229	1.341	0.0999
3.031	2.044	65.22	1.459	3.49	-1.691	0.2135	1.905	36.815	1.347	0.2284
7.803	1.708	57.98	1.595	3.277	-1.714	0.2194	1.933	40.228	1.357	0.3976
5.484	1.673	47.65	1.62	3.266	-1.726	0.2217	1.947	40.852	1.362	0.6397
0	1.436	32.21	1.756	3.054	-1.738	0.2248	1.963	43.025	1.367	1

Table (4). *Refraction parameters for saturated phthalic acid in mixed methanol-water solvents at 313.15K.*

n_d^E	μ x10^{22}	ϵ	α x10^{23}	n x10^{-21}	PE	PT	PA	R	n_d	Xs
0	2.5413	73.2	1.412	3.527	-1.6723	0.2087	1.888	35.618	1.337	0
0.404	2.3169	68.88	1.427	3.523	-1.2107	0.2107	1.891	35.999	1.342	0.0999
2.417	2.2107	63.32	1.479	3.455	-1.693	0.214	1.905	37.297	1.348	0.2284
7.104	2.0621	56.01	1.641	3.194	-1.7167	0.2195	1.936	41.381	1.358	0.3976
4.665	1.849	45.55	1.696	3.129	-1.7283	0.2234	1.95	42.975	1.363	0.6397
0	1.4845	29.98	1.772	3.042	-1.743	0.2259	1.969	44.698	1.369	1

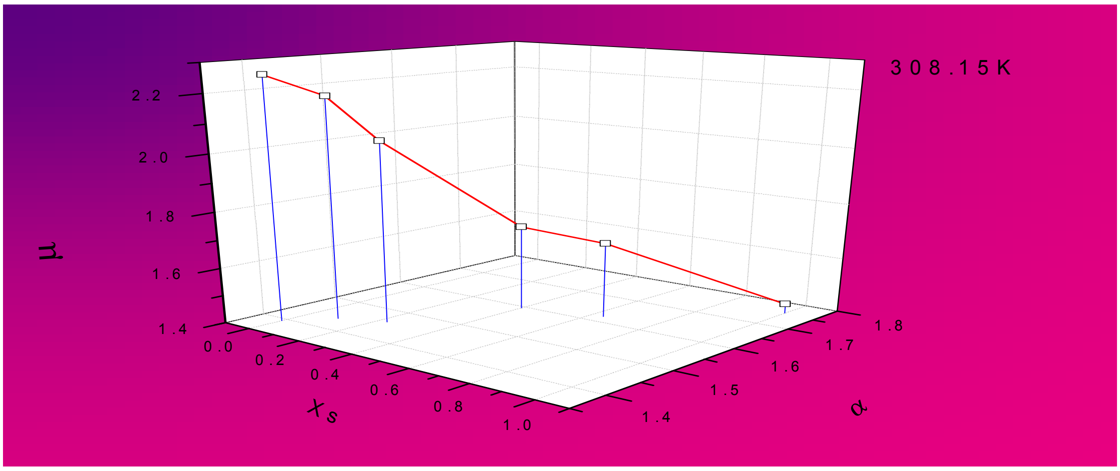

Fig. (1). *The relation between mole fraction (X_s), (α) and (μ) for phthalic acid in mixed methanol-water solvents at 308.15K.*

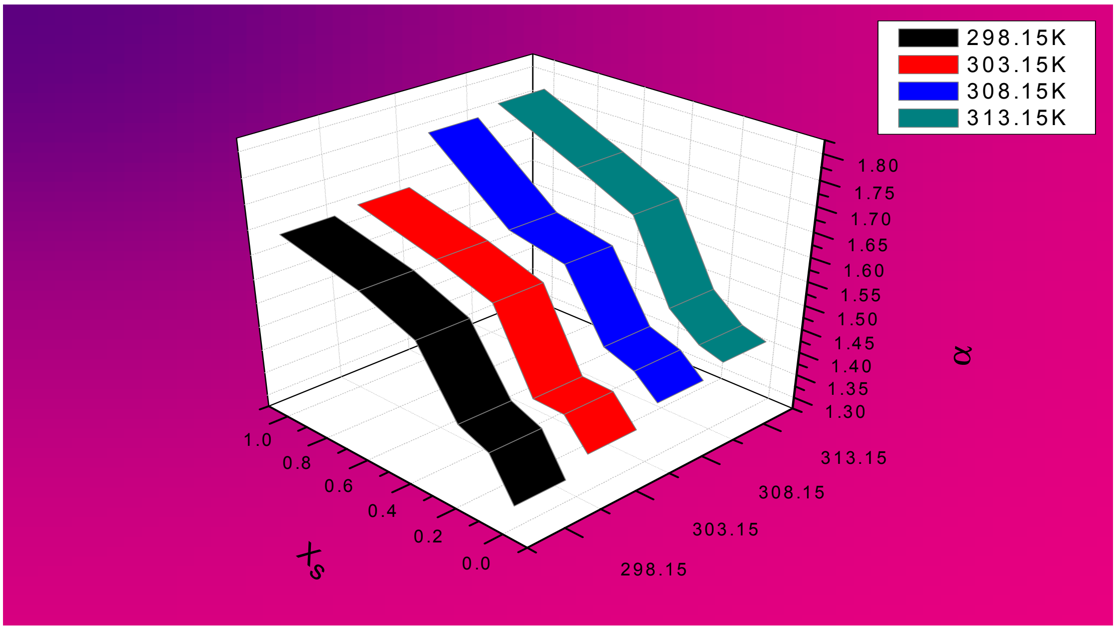

Fig. (2). *The relation between mole fraction (X_s) and (α) for phthalic acid in mixed methanol-water solvents at different temperatures.*

Conclusion

Valuable data for saturated phthalic acid were obtained like induced dipole moments and polarizabilities in the discussed mixed solvents and at different temperatures indicating the ion solvent interactions. Maximum excess n_E refractive index for saturated phthalic acid solutions were increased in mixed (MeOH-H_2O) solvents show maxima at x_s (mole fraction) MeOH equal 0.3976 indicating maximum interaction at this point. All polarization parameters for phthalic acid solutions were increased by increasing both methanol and temperature due to more mobility and velocity of ionic species in the used solvents. The data given here in this work can be used for analytical determination of saturated phthalic acid solution in the mixed solvents used. ■

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