Molecular Interaction for the binary system of o-chloro phenol with methanol,ethanol, 1-propanol and 2-propanol at 298.15K by measuring the densities and viscosities

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Abstract

this project are studied the molecular interaction for the binary system that is contained o-chlorophenol with methanol, ethanol, 1-propanol,and 2-propanol by measuring the densities ,and viscosities than conferred this to excess molar quantities by get the excess molar volume and deviation from viscosities and explain this by two figure Than get the standared divation and parameters to the eqution of polynomial by using Redlick –Kister form.

Interdiction

There is many studies that is taken methanol,ethanol,1-propanol,2-propanol, with polar and non polar solvents like water,alcholes,ethers,but there is less then studied With the cyclic supestitution compound so we get the cyclic aromatic compound that is contained two conditions the first are it contained hydroxyl group that is forming phenol. and the second are chloride ion in para regin and that is get stability for the o-chlorophenol one of the [(1)] studied molecular interaction for the painary system of 2-propoxyethanol and 2-isopropoxyethanol with methanol, 1-propanol, 2-propanol and 1-pentanol at298.15K by excess molar volumes and viscosities and that is show negative deviation for this system except 1-pentanol

in anather project that[(2)] studied the molecular interaction for the project of γ-butyrolactone with methanol,ethanol,1-butanol,and 1-octanol in 298.15K by measured the relative permittivity (έ),densities(ρ),refractive indices ($n_{D)}$ and ultrasonic velocities (u),that is show molecular interaction was vary clear and litereture.[(3)] were measured Densities and viscosities

For the binary mixtures (methanol, ethanol, 1-propanol, and 2-propanol with Nitromethane) at temperatures from 293.15K to 313.15K by the excess molar quantities that is show two kind of dilation from ideality

At last project were[(4)] studied the same alcohols with synthetics C_6 +Mixture from 298.15K to 318.15K by densities and viscosities properties and they gat the same result

Materials

In table (1) the compound that is used in project and the purity and the sours of the compound

Compound	Company	Purity
o-chlorophenol	RDSH*	99%
Methanol	Merck	99.8%
Ethanol	Merck	99.8%
1-propanol	S.R.L**.	99.5%
2-propanol	S.R.L.	99.8%

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** Scientific Resserch Labritory Bombay

O-chlorophenol was fractionally distilled over Zn powder the middle fraction redistilled over BaO and the middle colorless fraction collected all the alcohol were partially degassed at low pressure and dried over 0.4 nm molecular sives (Fluka,AG)the results of the measurements of their densities and viscosities at (298.15)K and atmospheric pressure are given in table (2) with some values taken from the literature which agreed with it

Table (2) experimental value of densities and viscosities for the component in this studies and in the reference at (298.15) K.

Compound	Exp.densities	Ref.densities	Exp.viscosities	Ref.viscosities
o-chlorophenol	1.25861	1.25854[5]	3.38117	3.3813[5]
Methanol	0.78639	0.78637[6]	0.55134	0.5513[6]
Ethanol	0.78670	0.78628[7]	1.08965	1.087[4]
1-propanol	0.79931	0.79958[8]	1.93148	1.927[10]
2-propanol	0.78032	0.78090[9]	2.04434	2.0436[10]

The uncertainly in the mole fraction is $\pm 5X10^{-5}$.all the solutions of different composition were prepared by mass in a $25cm^3$Erlenmeyer Flask provided with ajoint stopper using amattle AB20A balance with an uncertainty of ±0.1mg

For the densities used water bath model (mgw LAUDAM3) for KRUSS company with thermometer to get a high accuracy in (±0.0l°), and using pecnometar constant volume($5cm^3$)with stopper contained capillary tube

To measured the viscosities used viscometer from (Schott-Gerate) model (Avs-300) with computerizes system to calculate the (flow time) (t) .that is joined with two photo cells by climb and this climb were fixed inside the bath water from (Schott-Gerate CT 1150) with thermostat and thermometer to get (298.15K) the precision in the temperature was (±0.01°)

Results

The excess molar volumes[11] ($V^{\acute{\varepsilon}}$) for o-chlorophenol+methanol, ethanol, 1-propanol and 2-propanol, at 298.15K were get by used the following question

$$V_m^{\varepsilon} = \frac{X_1M_1 + X_2M_2}{\rho_m} - \frac{X_1M_1}{\rho_1} - \frac{X_2M_2}{\rho_2} \quad (1)$$

Where X_1,$X_2$are the mole fractions for o-chlorophenol (X_1),and another alcohols (X_2) ,M_1,M_2, are the molar masses for o-chlorophenol and alcohols respectively ,ρ_m,ρ_1,ρ_2 is the densities for mixture ,and for the pure o-chlorophenol and alcohols

The result of measurements of $V^{\acute{\epsilon}}$ excess molar volumes are listed in table (3) and graphically represented in figure (1)

From viscosities found the deviation of the viscosities ($\Delta\eta$)[12] by using the following equation

$\Delta\eta=\eta_m-\eta_1X_1-\eta_2X_2$

(2) Where η_m,η_1,η_2 are the dynamic viscosity of the mixture, o-chlorophenol, and alchohol for the pure component respectively the results of ($\Delta\eta$) deviation of the viscosities are listed in table (3) and graphically represented in figure (2)

Table (3):-density ,viscosity ,excess molar volume ,and deviation of viscosity for the binary system of o-chlorophenol (X_1)+methanol,ethanol,1-propanol,and 2-propanol (X_2) at 298.15 K

Methanol (X_2)

X_1	ρ / g.cm^3	cpη /	$V^{\acute{\epsilon}}$	$\Delta\eta$
0.1034	0.87805	0.93844	-0.106	0.0945
0.2132	0.95762	1.32266	-0.188	0.168
0.3269	1.02517	1.70341	-0.229	0.227
0.4008	1.06252	1.92653	-0.225	0.241
0.5398	1.12293	2.33188	-0.223	0.253
0.6187	1.15213	2.53815	-0.201	0.236
0.7041	1.18053	2.74182	-0.172	0.198
0.7634	1.19797	2.90063	-0.115	0.188
0.8129	1.21217	3.01071	-0.101	0.159
0.8740	1.22872	3.13761	-0.089	0.113
0.9461	1.24673	3.29664	-0.065	0.068

Ethanol (X_2)

X_1	ρ /g.cm^3	η /cp	$V^{\acute{\epsilon}}$	$\Delta\eta$
0.0958	0.85014	1.36021	-0.0763	0.051
0.2109	0.92013	1.69293	-0.147	0.12
0.3208	0.98055	1.99177	-0.1742	0.167
0.4016	1.02110	2.21163	-0.179	0.204
0.5185	1.07633	2.50581	-0.161	0.228
0.6122	1.11662	2.71351	-0.125	0.221

0.6819	1.14478	2.87313	-0.091	0.22
0.7485	1.17032	3.01285	-0.0504	0.208
0.8056	1.19155	3.12069	-0.032	0.185
0.8561	1.20976	3.19992	-0.0218	0.148
0.9311	1.23566	3.31048	-0.003	0.087

1-propanol (X_2)

X_1	ρ/g.cm^3	η /cp	V^{ε}	$\Delta\eta$
0.1066	0.83758	2.16301	-0.059	0.077
0.1911	0.88052	2.33351	-0.108	0.125
0.2802	0.92485	2.48268	-0.125	0.145
0.3286	0.94860	2.56384	-0.127	0.156
0.4689	1.01608	2.76024	-0.103	0.149
0.5631	1.06050	2.87081	-0.081	0.123
0.6391	1.09553	2.94597	-0.039	0.088
0.7173	1.13148	3.02534	-0.021	0.054
0.8253	1.18013	3.12610	0.024	-0.0018
0.9107	1.21857	3.23881	0.0239	-0.0129
0.9514	1.23679	3.29721	0.019	-0.0135

2-propanol (X_2)

X_1	ρ/g.cm^3	η/cp	V^{ε}	$\Delta\eta$
0.0894	0.82805	2.23259	-0.048	0.0687
0.1606	0.86488	2.35743	-0.0763	0.0984
0.2346	0.90246	2.47196	-0.0878	0.114
0.3198	0.94495	2.59885	-0.0918	0.127
0.4092	0.98853	2.70437	-0.0756	0.113
0.4918	1.02806	2.78259	-0.0564	0.0808
0.5734	1.06638	2.85987	-0.031	0.049
0.6598	1.10622	2.92468	0.0027	-0.0017
0.7393	1.14231	2.98263	0.031	-0.05
0.8175	1.17743	3.06069	0.046	-0.0764
0.9231	1.22445	3.20596	0.038	-0.0724

V^e

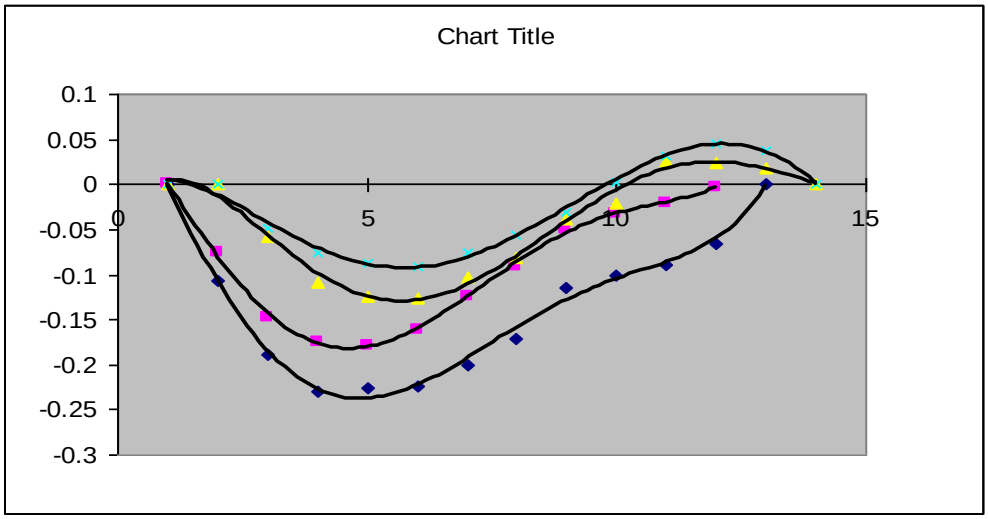

Figure (1) Excess molar Valium V^e with mole fraction for o-chlorophenol (X_1) with (♦)methanol, (■)ethanol, (▲)1-propanol, (×)2-propanol at 298.15K .

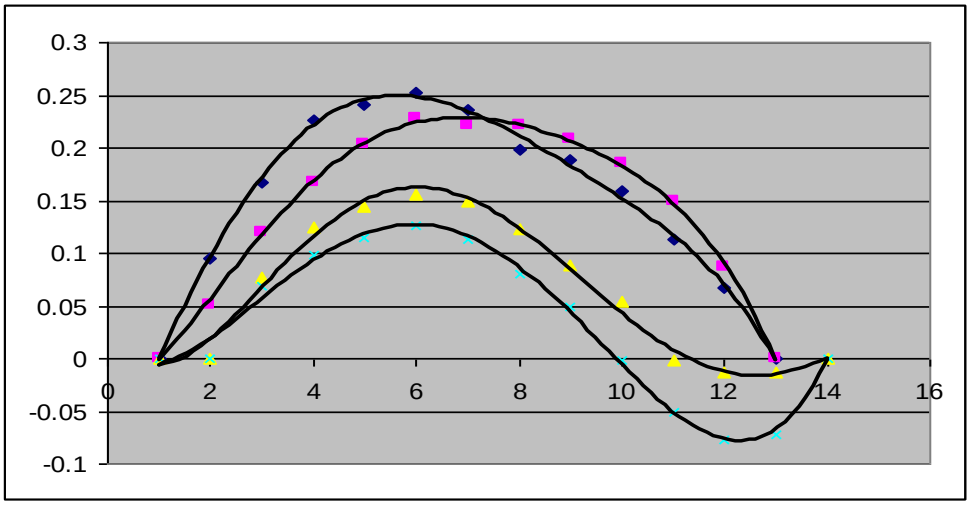

Figure (2) Divation in viscosity for o-chlorophenol (X_1) with (♦) methanol, (■)ethanol, (▲)1-propanol, (×) 2-propanol at 298.15K

The excess molar volumes and deviations in viscosity were represented mathematically by the Redlich –Kister equation [13]

$$Y_{(x)}=X_1(1-X_1)\sum A_i(X_1-X_2)^I \qquad (3)$$

Where $Y^{\acute{\varepsilon}}$is $V^{\acute{\varepsilon}}$, or Δη, X_1 is the mole fraction of alcohol,and (A_i) are the coefficients of the polynomial equation .the values of coefficients (A_i) were determined by a multiple regression analysis based on the least –squares method and were summarized along with the standard deviations between the experimental and fitted values of the respective functions in table(4) the corresponding standard

Deviation was defined by equation.

$$\delta=[\ (Y_{ex}-Y_{cal})^2 / m-n\ ]^{1/2} \qquad (4)$$

Where m is the number of experimental points

Table (5): standard deviation and parameter of equation of polynomial

Methanol

system	A_0	A_1	A_2	A_3	δ
$V^{\acute{\varepsilon}}$	-0.88	0.35	-0.15	-0.015	0.014
Δη	0.9	0.5	0.25	0.0564	0.0093
Ethanol					
$V^{\acute{\varepsilon}}$	-0.64	0.55	0.29	-0.1	0.005
Δη	0.88	0.4	0.2	0.056	0.007
1-propanol					
$V^{\acute{\varepsilon}}$	-0.384	0.6	0.27	-0.03	0.0065
Δη	0.56	-0.538	-0.38	-0.05	0.0041
2-propanol					
$V^{\acute{\varepsilon}}$	-0.212	0.61	0.247	0.05	0.003
Δη	0.32	-0.75	-0.46	-0.55	0.0066

Discussion

The choice of o-chlorophenol has been based on its limited polymerization through

Intermolecular hydrogen bonding in the pure state for molecules of (o-chlorophenol) the addition of alcohols causes anther effecte of interaction ((intramolecul))

The rupture of intramolecular and intermolecular wase hydrogen bonding in o-chlorophenol and this will be followed by association of unlike molecules through inter- Molecular hydrogen bonding

TO the deviation from ideal mixing are attributed to the desperation forces [14-15] In most theories of the behavior of non-electrolyte solutions the major contribution

In such theories the deviations are expected to be positive .

Negative deviation from ideal behavior in mixtures of molecules deferent in size can be accounted for by geometric considerations.

Attempts have been made to explain the behavior of liquid mixtures on the basis of sign and magnitude of the excess volumes $V^{\acute{\epsilon}}$.

A negative value of $V^{\acute{\epsilon}}$ indicates strong interaction between the components of the mixtures while positive ualue are indicative of weaker interaction then strength of interaction between the unlike molecules increases,so $V^{\acute{\epsilon}}$ become increasingly negative .

Figures (1) show negative $V^{\acute{\epsilon}}$ with well marked maxima at (0.3)and (0.4) mole fractions of o-chlorophenol respectively .the negative values of $V^{\acute{\epsilon}}$ for the liquid systems are well explained the terms of the dipole-dipole interaction between them.

A cording to fort and moore[16] the values of $\Delta\eta$ are positive for the systems in which desperation forces are dominate ,becoming less positive and then increasingly negative in (1-propanol),(2-propanol) as the strength of interaction decreases .

Figure (2) shows that the value of $\Delta\eta$ are positive at the firest in all the systems and it is only positive in (methanol), and (ethanol)

So the resolet[17] of the excess molar volume and divation from viscosities can be explaind as (i) specific interaction between the unlike molecules ,and(ii) geometric effect

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التداخلات الجزيئية للنظام ثنائي المكون من اورثوا –كلوروفينول مع الميثانول والايثانول ١-بروبانول و٢-بروبانول عند درجة حرارة ٢٩٨,١٥ وذلك بقياس الكثافة واللزوجة

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الخلاصة

في هذه الدراسة درست التداخلات الجزيئية للنظام الثنائي المكون من الاورثو –كلوروفينول مع كحولات الميثانول،الايثانول،١-بروبانول، و ٢-بروبانول حيث قيست الكثافة واللزوجة ولمدى كامل من الكسور المولية

والتي حولت إلى الكميات المولية الفائضة فوجد الحجم المولي الفائض وانحراف اللزوجة عن المثالية والتي وضحت باستخدام الرسوم البيانية كما استخدمت معادلة – Redlik Kister لحساب الانحراف المعياري ومعاملات المعادلة متعددة الحدود