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Estimation of Physicochemical properties of Acetonitrile and Formamide from 293.15-313.15K

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Abstract

Density, viscosity and refractive indices for a binary system of acetonitrile and formamide at 293.15, 298.15, 303.15, 308.15, 313.15K were experimentally determined over the mole fraction range (0.1225-0.9187) and atmospheric pressure. Theoretical results were computed from Jouyban Acree model, based on least square method and compared with experimental findings. Relative standard deviation (RSD) for density, viscosity and refractive indices was treated as a criterion of success. Corresponding RSD at 293.15, 298.15, 303.15, 308.15, 313.15K are $(1.0 \pm 0.5\% , 0.98 \pm 0.8\% , 0.98 \pm 0.8\% , 0.95 \pm 0.4\% , 0.94 \pm 0.7\%)$,$(2.30 \pm 5.8\% , 2.28 \pm 7.5\% , 2.26 \pm 7.9 , 2.21 \pm 10.8\% , 2.28 \pm 13.4\%)$ *and* $(1.39 \pm 0.2\% , 1.39 \pm 0.3\% , 1.39 \pm 0.3\% , 1.38 \pm 0.3\% , 1.38 \pm 0.2\%)$ *respectively.* R^2 *values for density, viscosity and refractive index were also calculated to determine the accuracy of the mathematical model. This study shows that model deals fair agreement with experimental findings for all the physico-chemical properties of binary system at different temperatures with acceptable deviations in calculation.*

Keywords: Acetonitrile, formamide, viscosity, correlation, theoretical.

Introduction

Physicochemical properties of liquids are important data used various thermodynamic applications[1-3]. These properties were utilized to understand the transport phenomenon and liquid - liquid interaction. Data of these physicochemical properties are used in the development of various theoretical calculations. Continuing our work[4], experimental values of binary system from 293.15-313.15K temperature and mole fraction range of acetonitrile (0.1225-0.9187) are presented in this paper. Acetonitrile and formamide are two important liquids having wide range of applications in industry. Mahendra Nath Roy[5] measured the physicochemical properties of binary system by mixing different organic solvents with formamide at 298.15-318.15K. Jouyban Acree model[6-14] was used to estimate the physicochemical property of binary system at various temperatures:

$$\ln Y_{AB} = X_A . \ln Y_A + X_B . \ln Y_B + J_P \left[\frac{X_A . X_B}{T_0}\right] + J_Q \left[\frac{X_A . X_B . (X_A - X_B)}{T_0}\right] + J_R \left[\frac{X_A . X_B . (X_A - X_B)^2}{T_0}\right] \quad (1)$$

Rearranging the above equation

$$\ln Y_{AB} - X_A . \ln Y_A - X_B . \ln Y_B = J_P \left[\frac{X_A . X_B}{T_0}\right] + J_Q \left[\frac{X_A . X_B . (X_A - X_B)}{T_0}\right] + J_R \left[\frac{X_A . X_B . (X_A - X_B)^2}{T_0}\right] \quad (2)$$

J_P, J_Q, J_R are coefficients which could be calculated using no - intercept regression of the experimental values. Y_{AB}, Y_A and Y_B are physicochemical properties of binary system and liquid A, B respectively. The aim of this work to correlate experimentally determined physicochemical properties of acetonitrile + formamide mixture from (293.15-313.15K) with Jouyban Acree model. Various researchers[15-17] including our research[18-19] have tried to correlate the different physicochemical properties.

Materials and methods

Experiment[4] was carried out using high grade chemical of acetonitrile and formamide. Which were purchased from the German company (Merck). During experiment chemicals were purified by distillation process and middle fraction was collected. To store the chemicals dark bottles with 0.4×10^{-9}m were used. Which were degassed with vacuum pump and utilized in reduction of percentage of water. Gas chromatography was used to check the purity of chemicals and the result obtained from the purity check indicate that the purity was higher than 0.99.0 which were examined by comparing with experimental physicochemical properties with literature value as shown in Table-1.

Bicapillary pakynometer was used to measure the density of acetonitrile, formamide and their binary system. Mixtures were ShimadzuAX-200 electronic balance with uncertainty ± 0.1mg was utilized in the preparation of binary system in air tight bottle by mas. Instrument was calibrated before each set of experiments with pure water. The published value of uncertainty was found to be$\pm 6.7 Kgm^{-3}$ in density observation. For binary system average uncertainty in composition was reported below ± 0.0001.

Table-1: Experimental and literature values of physicochemical properties for acetonitrile and formamide.

T/K	ρx10^{-3}(Kg.m^{-3})		η X 10^{3}(Pa. s)		n	
	Exp	Literature[20]	Exp	Literature[20]	Exp	Literature[20]
Acetonitrile						
293.15	0.7865	0.7822	0.3699	-	1.3409	1.3441
298.15	0.7811	0.7765	0.3426	0.3410	1.3402	1.3416
303.15	0.7733	0.7713	0.3201	0.3240	1.3392	-
308.15	0.7665	-	0.3408	-	1.3283	-
313.15	0.7605	-	0.3348	-	1.3260	-
Formamide						
293.15	1.1320	1.1339	3.7542	3.7640	1.4409	1.4448
298.15	1.1290	1.1292	3.3220	3.302	1.4370	1.4468
303.15	1.1250	-	2.9663	-	1.4359	-
308.15	1.1210	-	2.6531	-	1.4280	-
313.15	1.1117	-	2.4039	-	1.4250	-

Abbe thermostatically controlled refractometer (Atago-3T) was used in the experimentation of refractive index of pure and binary system. During experimentation the measurement of refractive index for each sample was carried out 3 times and mean of these observations was used in calculation. Uncertainty was fond to be ± 0.0001.

The viscosities of acetonitrile, formamide and mixtures of different composition were determined by Ubbelohde suspended-level viscometer at different temperature and atmospheric pressure. Instrument was calibrated by highly pure water and organic solvent (benzene). Digital stop watch was used to record the flow time of liquids with uncertainty ± 0.01sec. during viscosity determination the viscometer was put in ± 0.01K temperature-controlled water bath.

Results and discussion

Table-1 represents the comparison between experimental and literature values of all the three physicochemical properties for acetonitrile and formamide from temperature 293.15 - 313.15 K. Table-2 to 4 presents the calculated values of J_P, J_Q, J_R for density, viscosity and refractive index and their respective standard deviation respectively. Calculations of Jouyban Acree model were performed using no intercept regression method. R^2 values for density. Viscosity and refractive index for binary system at temperatures 293.15, 298.15, 303.15, 308.15, 313.15K are presented in Table-5. R^2 values calculated for density and refractive index for all five temperatures are 0.9999 whereas R^2 values calculated for viscosity are 0.9975, 0.9960, 0.9956, 0.9918 and 0.9882 at 293.15, 298.15, 303.15, 308.15, 313.15K respectively. Which confirm an excellent correlation between experimental and calculated values. Standard deviation calculated for density lies in the range $0.0040 < \delta\rho < 0.0080$. The highest value of standard deviation was found to be at 298.15K. The values of standard deviation for viscosity increase with increase in temperature and lies in the range $0.1343 < \delta\eta < 0.2398$. The highest value of standard deviation was found to 313.15K. The value for standard deviation calculated for refractive index firstly increases with increase in temperature than decreases. For binary mixture lies in the range $0.0027 < \delta n < 0.0046$. The highest value of standard deviation for refractive index was found to be at 308. 15K. Standard deviation calculated from Equation (6) for all three physicochemical properties are very small which confirm the accuracy between calculated data and experimental data.

$$\ln\rho_{AB} = X_A.\ln\rho_A + X_B.\ln\rho_B + J_P\left[\frac{X_A.X_B}{T_0}\right] + J_Q\left[\frac{X_A.X_B.(X_A-X_B)}{T_0}\right] + J_R\left[\frac{X_A.X_B.(X_A-X_B)^2}{T_0}\right] \quad (3)$$

Where: $\rho_{A,}$, $\rho_{B,}$ and $\rho_{AB,}$ are density of pure liquid A, B and binary mixture AB at absolute temperature T_0.

$$\ln\eta_{AB} = X_A.\ln\eta_A + X_B.\ln\eta_B + J_P\left[\frac{X_A.X_B}{T_0}\right] + J_Q\left[\frac{X_A.X_B.(X_A-X_B)}{T_0}\right] + J_R\left[\frac{X_A.X_B.(X_A-X_B)^2}{T_0}\right] \quad (4)$$

Where: $\eta_{A,}$, $\eta_{B,}$ and $\eta_{AB,}$ are viscosity of pure liquid A, B and binary mixture at absolute temperature T_0.

$$\ln n_{AB} = X_A.\ln n_A + X_B.\ln n_B + J_P\left[\frac{X_A.X_B}{T_0}\right] + J_Q\left[\frac{X_A.X_B.(X_A-X_B)}{T_0}\right] + J_R\left[\frac{X_A.X_B.(X_A-X_B)^2}{T_0}\right] \quad (5)$$

Where: $n_{A,}$, $n_{B,}$ and $n_{AB,}$ are refractive index of pure liquid A, B and associate AB at absolute temperature T_0.

Table-2: Coefficient of density (ρ) calculated from Equation (3) and standard deviation (δρ) at various temperatures.

T/K	J_P	J_Q	J_R	S.D. (δρ)
293.15	100.0168	35.0234	69.1154	0.0057
298.15	97.2023	50.9447	24.6988	0.0080
303.15	92.8621	54.5535	40.8852	0.0077
308.15	61.1534	18.7274	-7.3719	0.0040
313.15	49.6377	0.2055	45.9659	0.0068

Table-3: Coefficient of viscosity (η) calculated from Equation (4) and standard deviation (δη) at various temperatures.

T/K	J_P	J_Q	J_R	S.D.(δη)
293.15	972.3213	826.4285	301.2898	0.1343
298.15	1117.144	750.1009	361.5461	0.1708
303.15	1223.197	719.5482	605.8906	0.1779
308.15	1298.03	452.6145	268.6483	0.2398
313.15	1385.846	145.7774	604.9682	0.3048

Table-4: Coefficient of refractive index (n) calculated from Equation (5) and standard deviation (δn) at various temperatures.

T/K	J_P	J_Q	J_R	S.D.(δn)
293.15	9.1217	-3.6908	6.0893	0.0034
298.15	10.8164	-5.8096	9.7159	0.0035
303.15	11.5750	-6.0826	10.7234	0.0035
308.15	8.5472	5.8146	22.0768	0.0046
313.15	8.0695	2.8890	10.3864	0.0027

Table-5: R^2 values for binary system at different temperatures.

T/K	R^2(ρ)	R^2(η)	R^2(n)
293.15	0.9999	0.9975	0.9999
298.15	0.9999	0.996	0.9999
303.15	0.9999	0.9956	0.9999
308.15	0.9999	0.9918	0.9999
313.15	0.9999	0.9882	0.9999

Calculation of standard deviation (δY) was carried out by equation (6) as given below

$$\delta Y = \left[\frac{\sum_{i=1}^{n}(Z_{Exp}-Z_{Cal})^2}{(D.P-A.P)}\right]^{1/2} \quad (6)$$

Where Y is physicochemical properties and A.P are no. of data points and adjusting parameters. RSD calculated for densities, viscosities and refractive indices for all five temperatures are ($1.0 \pm 0.5\%$, $0.98 \pm 0.8\%$,$0.98 \pm 0.8\%$,$0.95 \pm 0.4\%$,$0.94 \pm 0.7\%$),($2.30 \pm 5.8\%$,$2.28 \pm 7.5\%$, 2.26 ± 7.9, $2.21 \pm 10.8\%$, $2.28 \pm 13.4\%$) and ($1.39 \pm 0.2\%$,$1.39 \pm 0.3\%$, $1.39 \pm 0.3\%$, $1.38 \pm 0.3\%$,$1.38 \pm 0.2\%$) respectively. Which shows that Jouyban Acree model deals good agreement with experimental findings for all the physico-chemical properties at different temperatures with acceptable deviation in calculation. Table-6 presents the observed and theoretical values calculated for the same from Equation (3), Equation (4) and Equation (5) of Jouyban Acree model at 293.15, 298.15, 303.15, 308.15, 313. 15K. A close observation of table 6 reveals that the calculated values of respective properties from Equation (4) and Equation (5) of Jouyban Acree model at 293.15, 298.15 (3), Equation (4) and Equation (5) of Jouyban Acree model at 293.15, 298.15 (4) and Equation (4) and Equation (5) of Jouyban Acree model at 293.15, 298.15 (5) are very close to observed values. Which indicate the success of our experimental work and applicability of Jouyban Acree model.

Table-6: Experimental and Calculated values from Equation (3), (4), (5) at 293.15, 298.15, 303.15, 308.15, 313.15K.

X_1	$\rho x10^{-3}$(Kg.m^{-3})		η X 10^3(Pa. s)		n	
	EXP	Cal	EXP	Cal	EXP	Cal
T=293.15K						
0.1225	1.1258	1.1284	3.4824	3.4202	1.4387	1.4363
0.239	1.0992	1.1045	3.1358	3.1758	1.4298	1.4276
0.3499	1.0835	1.0734	2.9998	2.9893	1.4105	1.4169
0.4557	1.0405	1.0413	2.8654	2.7999	1.4058	1.4057
0.5567	1.0102	1.0096	2.4568	2.5433	1.3978	1.3946
0.6533	0.9705	0.9770	2.0265	2.1767	1.3848	1.3839
0.7456	0.9403	0.9409	1.8564	1.7055	1.3735	1.3734
0.834	0.9015	0.8986	1.3547	1.1895	1.3625	1.3630
0.9187	0.8503	0.8477	0.5852	0.7202	1.3501	1.3523
T=298.15K						
0.1225	1.1015	1.1079	3.4810	3.3041	1.4387	1.4355
0.2390	1.0825	1.0838	3.1300	3.1910	1.4290	1.4275
0.3499	1.0657	1.0583	2.9901	3.0375	1.4104	1.4168
0.4557	1.0345	1.0312	2.8644	2.8342	1.4054	1.4053
0.5567	0.9985	1.0018	2.4561	2.5468	1.3975	1.3941
0.6533	0.9624	0.9686	2.0264	2.1504	1.3846	1.3834
0.7456	0.9351	0.9307	1.8505	1.6609	1.3731	1.3732
0.8340	0.8792	0.8871	1.3540	1.1414	1.3622	1.3629
0.9187	0.8492	0.8372	0.5004	0.6799	1.3499	1.3521

T=303.15K						
0.1225	1.0998	1.1035	3.4715	3.2483	1.4380	1.4350
0.2390	1.0735	1.0763	3.1258	3.1988	1.4289	1.4272
0.3499	1.0538	1.0479	2.9002	3.0192	1.4101	1.4165
0.4557	1.0258	1.0194	2.8568	2.7879	1.4050	1.4049
0.5567	0.9802	0.9902	2.4500	2.5003	1.3970	1.3937
0.6533	0.9594	0.9585	2.0000	2.1257	1.3840	1.3830
0.7456	0.9256	0.9225	1.8222	1.6574	1.3729	1.3727
0.8340	0.8728	0.8803	1.3455	1.1412	1.3619	1.3624
0.9187	0.8402	0.8308	0.4987	0.6679	1.3489	1.3515
T=308.15K						
0.1225	1.0856	1.0861	3.4054	3.0385	1.4199	1.4237
0.2390	1.0568	1.0539	3.1025	3.1745	1.4105	1.4131
0.3499	1.0215	1.0219	2.8971	3.1063	1.4099	1.4014
0.4557	0.9856	0.9889	2.8401	2.8713	1.3904	1.3908
0.5567	0.9508	0.9543	2.4459	2.5010	1.3801	1.3821
0.6533	0.9256	0.9181	1.9982	2.0334	1.3700	1.3745
0.7456	0.8809	0.8807	1.7059	1.5240	1.3675	1.3670
0.8340	0.8405	0.8427	1.3054	1.0378	1.3599	1.3579
0.9187	0.8028	0.8044	0.4057	0.6329	1.3480	1.3455
T=313.15K						
0.1225	1.0807	1.0891	3.3901	3.2934	1.4123	1.4125
0.2390	1.0559	1.0525	3.9570	3.5339	1.4058	1.4037
0.3499	1.0158	1.0121	2.8897	3.3261	1.3945	1.3959
0.4557	0.9758	0.9728	2.8304	2.9153	1.3854	1.3875
0.5567	0.9365	0.9363	2.4358	2.4375	1.3789	1.3780
0.6533	0.8905	0.9021	1.8758	1.9446	1.3687	1.3674
0.7456	0.8726	0.8691	1.6889	1.4601	1.3555	1.3562
0.8340	0.8405	0.8355	1.2568	1.0081	1.3482	1.3451
0.9187	0.7992	0.7998	0.3944	0.6231	1.3302	1.3348

Conclusion

From the above discussion it can be concluded that Jouyban Acree model deals fair agreement with experimental values of all the three physicochemical properties at various temperatures.

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