IJARSCT
ISSN (Online) 2581-9429
International Journal of Advanced Research in Science, Communication and Technology (IJARSCT)
Volume 2, Issue 3, June 2022
Impact Factor: 6.252

Study of Intermolecular Interaction of Allyl Bromide with Acetone Through Dielectric and Thermodynamic Properties

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Abstract: *The dielectric constant (ε_s) and Relaxation time (τ) for binary mixtures of Allyl Bromide (ALB) with Acetone (ACE) were determined for eleven concentrations at temperatures 293.15 K, 303.15 K and 313.15 K in the frequency range of 10 MHz to 10 GHz using time domain reflectometry (TDR). Density and refractive index of same mixture at same temperature are also obtained which are further used to known excess molar volume and excess molar refraction respectively. These excess parameters are compared with excess dielectric parameter. Comparison confirms that there is intermolecular interaction between AL Band Acetone ACE. The values of Kirkwood factors indicate antiparallel dipoles in ALB and parallel dipoles in ACE.*

Keywords: Static Dielectric Constant, Relaxation Time, Density, Refractive Index, etc.

I. INTRODUCTION

Dielectric study of binary mixture of liquids is very interesting subjectin chemistry, Physics, biochemistry, pharmaceutical material science and engineering. This is due to the variation of dynamic properties with concentration of solute and temperature of mixture. Now day, drug design is an important and challenging aspect for new researcher.Dielectric properties of drugs or solution is directly related to solubility of drug in solvent which are affected on its rate of dissociation in body. We know that slightly changing any one of parameter among the, concentration of solute, temperature, pressure and environmental condition there is changing physical chemical, thermodynamic, dielectric properties. The density and refractive index are fundamental properties which gives important internal information of solution.

Allyl bromide basically used as alkaline agent for many syntheses such as pharmaceutical, polymer etc. while Acetone are used from household cleaning to pharmaceutical. In Ally bromide, carbon-bromine covalent bound in which bromine has significantly greater electronegativity than carbon,that is carbon is electrophilic and bromine is nucleophilic, double bound present will have restricted to reorientation of dipole moment of molecule. Carbonyl group of acetones play an important role in their properties.

Many research groups throughout world active in this researcharea. There are many methods used to study the dielectric behavior of binary mixture of liquid. Among the all technique, Time domain reflectometry technique is one of widely used technique due to their precise,reproducibility varies with wide frequency range.

We are reported the dielectric behavior of Ally chloride with Acetone, Allyl chloride with 2-Butanone and 2-Pentanone, Allyl chloride with 2-Hexanone with different temperature in frequency range 10 MHz to 20 GHz [1-6]. As continuous study of Allyl Halide with ketone. As part of our research work, in this paper we reported study of Allyl Bromide with Acetone at temperature 293.15K, 303.15K and 313.15 K. Dielectric constant and dipole moment of acetone We are extended our work for measurement of excess molar refraction and excess molar volume for confirmation of intermolecular interaction between two solute and solvent.

Chemicals: The chemical used in this work are AR grade ALB, ACE with purity 99%. Chemical used without further purification. The solution was prepared at 11 different volume concentration by adding ACE in ALB starting from 0% to 100% in step by step 10% by micropipette with accuracy of ±0.0006ml.

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II. EXPERIMENTAL SECTION

The Hewlett Packard HP54750 A Sampling Oscilloscope with HP54754ATDR plug in module has been used for experimental measurement of complex permittivity data of sample. A fast-rising voltage pulse about 39picosecond rise time generated by tunnel diode are propagated through flexible coaxial cable with impedance 50Ω. The sample is placed at end of coaxial cable in standard military application (SMA) coaxial cell. The data acquisition of eleven concentration sample at temperature 293.15K, 303.15K and 313.15K. The detail about experimental setup, procedure and data analysis are explained as earlier [6].

The refractive index and density of same concentration and temperature are determined by Abbe's Refractometer and Pyknometer with accuracy ±0.001 and ±0.0001 respectively.

III. RESULT AND DISCUSSION

The dipole moments of Allyl Bromide and Acetones in gas phase are 1.90 D and 2.28D, respectively. Using these values of dipole moments, the values of the Kirkwood factors are 0.78 and 1.12 respectively. It indicates that the dipoles in ALB have tendency to be in antiparallel, whereas dipoles have tendency to remain parallel in pure Acetone. As these molecules are not hydrogen bonded liquids, the tendency will be due to dipole-dipole interaction. The excess properties can provide information regarding change in these opposite tendencies in mixtures.

The values of the static dielectric constant and Relaxation time of the binary mixtures are tabulated in table 1while density and refractive index are reported in table 2. From table non-linear variation of all parameter confirm the dipole-dipole complexes. ALB form dipole –dipole association through Br atom with carbonyl of Acetone. Table also show that both values of static dielectric constant and relaxation time increase with increase of ACE concentration in the mixture, whereas these values of density and refractive index have opposite trend that is decreases with concentration. The variations with respect to temperature in these parameters have also got usual trend, i.e., static permittivity, relaxation time, density and refractive index all parameters decrease with increase of temperature. The correlation among neighboring dipoles are decreases.

Table 1: Static dielectric constant and Relaxation time of Allyl Bromide +Acetone binary system

Mole fraction of ACE	293.15 K		303.15 K		313.15 K	
	ε_s	τ	ε_s	τ	ε_s	τ
0	7.14	13.20	6.74	12.24	6.54	11.39
0.1158	9.26	14.64	8.57	13.64	8.32	12.77
0.2277	10.89	16.06	10.10	15.03	9.78	14.14
0.3357	11.89	17.51	11.24	16.39	10.67	15.45
0.4401	12.70	18.81	12.06	17.68	10.96	16.62
0.5411	13.26	20.10	12.73	18.90	11.40	17.85
0.6388	13.99	21.34	13.23	20.11	12.00	19.20
0.7334	15.12	22.91	14.13	21.51	13.06	20.35
0.8251	16.61	24.83	15.45	23.22	14.70	22.08
0.9139	18.57	28.22	17.21	26.14	16.55	24.62
1	20.73	33.64	19.66	31.29	18.80	29.22

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Table 2: Density (gm/cm^3) and Refractive index of Allyl Bromide +Acetone binary system

Mole fractionof ACE	293.15 K		303.15 K		313.15 K	
	ρ	n_D	ρ	n_D	ρ	n_D
0	1.3980	1.467	1.3813	1.460	1.3645	1.455
0.1158	1.3201	1.453	1.3043	1.446	1.2888	1.440
0.2277	1.2399	1.439	1.2237	1.432	1.2093	1.426
0.3357	1.1914	1.426	1.1766	1.420	1.1623	1.414
0.4401	1.1496	1.418	1.1344	1.412	1.1201	1.406
0.5411	1.1143	1.412	1.0994	1.406	1.0853	1.400
0.6388	1.0707	1.405	1.0558	1.399	1.0426	1.393
0.7334	1.0210	1.397	1.0071	1.391	0.9940	1.386
0.8251	0.9716	1.385	0.9581	1.380	0.9453	1.374
0.9139	0.9065	1.372	0.8941	1.367	0.8817	1.361
1	0.7913	1.358	0.7799	1.353	0.7688	1.348

Table 3: a_j coefficient and standard deviation (σ) of excess parameters

	a_0	a_1	a_2	a_3	σ
		293.15 K			
ε_s^E	-3.7293	-15.3382	0.0323	6.2665	0.0319
$(1/\tau)^E$	-0.0064	0.0276	0.0120	-0.0016	0.0001
V^E	-1.1259	-29.6410	-21.1777	-15.0860	0.4752
R_m^E	-0.5921	-3.5675	-3.2040	-6.4329	0.1176
		303.15K			
ε_s^E	-3.0999	-14.1115	-5.5238	3.1480	0.0384
$(1/\tau)^E$	-0.0100	0.0281	0.0147	0.0051	0.0001
V^E	-1.0467	-29.8814	-21.7952	-15.9490	0.4933
R_m^E	-0.5594	-3.6550	-3.3502	-6.0128	0.1163
		313.15K			
ε_s^E	-5.7278	-17.3217	0.9493	9.3268	0.0589
$(1/\tau)^E$	-0.0141	0.0278	0.0119	0.0103	0.0002
V^E	-1.2531	-30.3478	-22.5073	-15.6938	0.4947
R_m^E	-0.7497	-3.4214	-3.7520	-6.2295	0.1265

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The excess parameters of binary mixture were calculated using following equation

$A^E = A_{mix} - (A_1X_1 + A_2X_2)$

Where A^E - represent excess dielectric constant, excess inverse relaxation time, excess molar volume, excess molar refraction.

A_1,A_2 and A_{mix} represent static dielectric constant, inverse relaxation time, molar volume,refractive index of liquid 1 and liquid 2 and binary mixture resp.

$X_1$and X_2 represent mole fraction of liquid 1 and liquid 2 of mixture.

The dipole moments of Allyl Bromide and Acetones in gas phase are 1.90 D and 2.28D, respectively. Using these values of dipole moments, the determined values of the Kirkwood factors are 0.78 and 1.12 respectively. It indicates that the dipoles in ALB have tendency to be in antiparallel, whereas dipoles have tendency to remain parallel in pure Acetone. As these molecules are not hydrogen bonded liquids, the tendency will be due to dipole-dipole interaction.The changeineffective Kirkwood factorwith respect totemperature not more significant instead of these agree with variation of static dielectric constant with temp. The excess properties can provide information regarding change in these opposite tendencies in mixtures. The graphical representation of excess static dielectric constant of ALB+ACE are shown in fig1. In Allyl Bromide rich region, the interaction of acetone molecule with ALB is such that the antiparallel tendency of ALB gets reduced. In ACE rich region, the interaction between ACE and ALB is such that the dipoles of ACE have tendency to be less parallel. It is interesting to see the different behavior at both end of the concentrations.

The excess inverse relaxation time as function of mole fraction of Acetone is shown in figure 2.The negative excess inverse relaxation in ALB rich region, this indicates that addition of ACE in ALB has created hindered field such that effective dipole rotates slowly. Whereas positive excess inverse relaxation time in ACE rich region, it indicates that molecular interaction produce field such that effective dipole rotates faster, i.e., the field cooperates in the rotation of dipoles. The perusal of figure 2. shows that, the negative value of excess inverse relaxation time indicates that reorientation of dipole influenced by heterogeneous interaction through dipole-dipole interaction (Carbonyl group of ACE and Br atom of ALB).

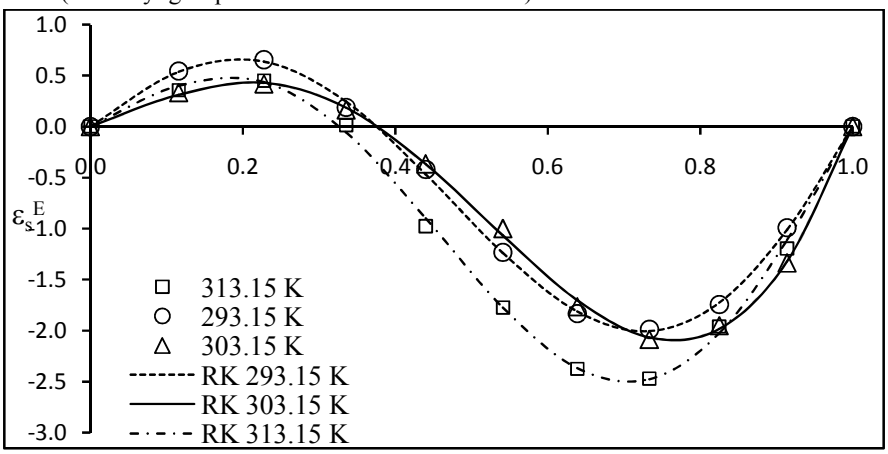

Figure 1: Excess static dielectric constant(ε_s^E) of Allyl Bromide + Acetone binary system

From figure 3, it is observed that excess molar volume is positive in nature below 0.4 mole fraction of ACE and negative above it. The positive V^E indicates that predominant effect of expansion consequent on rupture of dipole-dipole interaction between ACE molecules in ALB rich region while negative V^E in ACE rich region is nevertheless indicative of important interaction between unlike molecule and geometrical fitting on one component into another component. The maximum deviation of positive excess molar volumeat about 0.2 mole fraction of ACE while maximum negative deviation is about 0.8 mole fraction of ACE[7].

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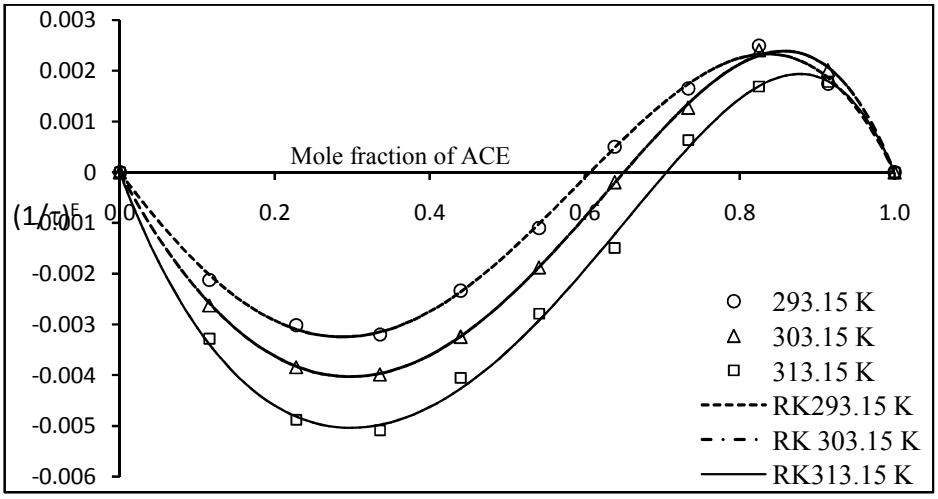

Figure 2: Excess inverse relaxation time$(1/\tau)^E$ of Allyl Bromide +Acetone binary system

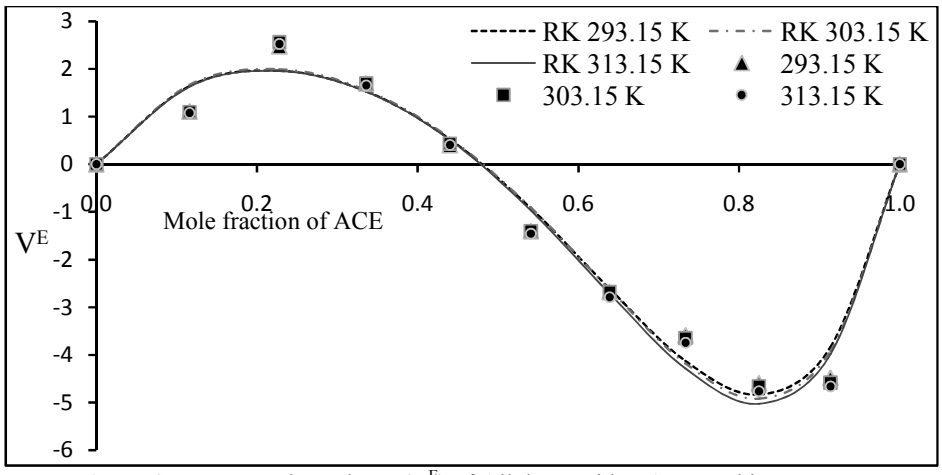

Figure 3: Excess molar volume (V^E) of Allyl Bromide +Acetone binarysystem

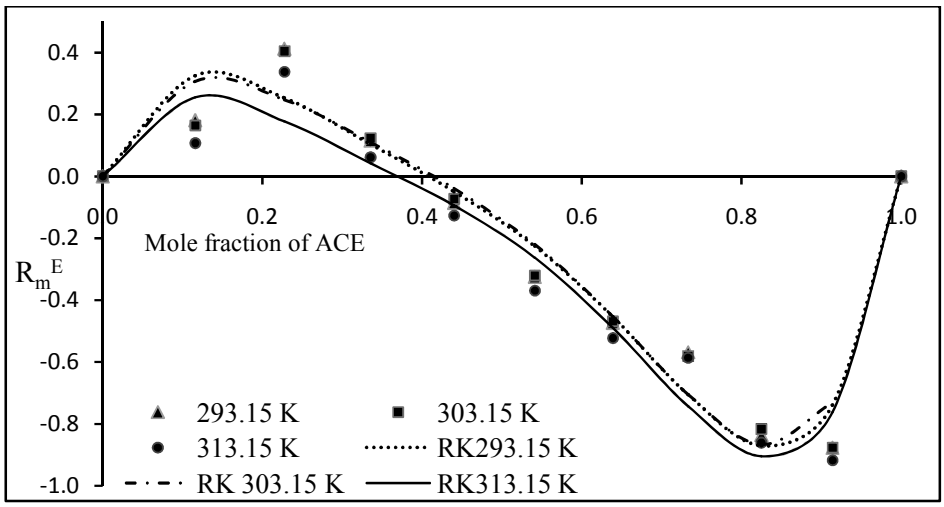

Figure 4: Excess molar refraction(R_m^E) of Allyl Bromide +Acetonebinary system

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The R_m^E values represent the electronic perturbation due to orbital mixing of the molecule. Figure 4 show R_m^E is positive in ALB rich region and negative in ACE rich region. The values of V^E and R_m^E of system supported to each other. There is slightly variation of V^E and R_m^E values with increasing temperature suggest that molecular interaction decreases with increase temperature [8].

The result of excess static dielectric constant, excess molar volume and excess molar refraction are supported to each other. They suggest that in ALB rich region hetero molecular interaction is not effective as compare to ACE rich.The excess parameters are fitted to Redlich-Kister equation to determine the values of $a_j$coefficients (RK) and standard deviation (σ) are tabulated in table 3.

The values of effective Kirkwood correlation factor are plotted in fig 5. The value of $g^{eff}$is less than one upto the 0.8 volume fraction of ACE while greater than one for 0.9 volume fraction ofACE and pure ACE. In pure ALB, the interaction is such that the dipoles have tendency to align in antiparallel direction, whereas the interaction in ACE is such that the dipoles have tendency to align in parallel direction. In mixtures, these two tendencies get mixed, i.e., in ALB rich region, ACE molecules reduces the intensity of the anti-parallism tendency resulting increase in values of g^{eff}. Similarly, in ACE rich region, ALB molecules reduces the intensity of parallelism tendency resulting decrease in values of g^{eff}[9].

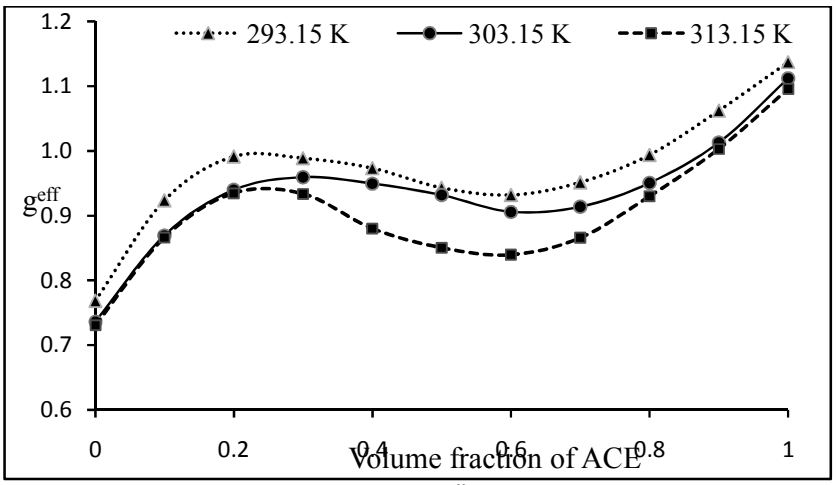

Figure 5: Effective Kirkwood correlation factor (g^{eff}) of Allyl Bromide +Acetone binary system

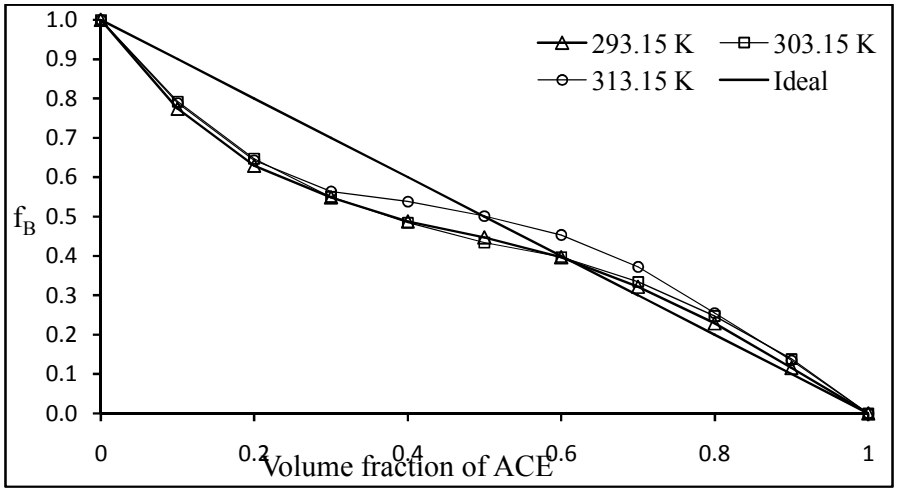

Figure 6: Bruggeman factor (f_B) of Allyl Bromide +Acetone binary system

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The information about the solute–solvent interaction is also obtained by Bruggeman factor (f_B). The effective volume of solute gets modified by solute–solvent interaction and is best illustrated by nonlinearity of Bruggeman equation.

$$f_B = \left(\frac{\varepsilon_m - \varepsilon_B}{\varepsilon_A - \varepsilon_B}\right)\left(\frac{\varepsilon_A}{\varepsilon_m}\right)^{(1/3)} = 1 - V$$

Where, V is Volume fraction of ACE, which is a qualitative measure of volume of the solute in the mixture. ε_m, ε_A and $\varepsilon_B$are the values of static dielectric constant of mixture, ALB and ACE, respectively. Bruggeman plot of system is given in figure 6. It suggests that volume of complex increases in Allyl Bromide rich region and decreases in acetone rich region. This result correlates with result of excess molar volume and excess molar refraction [10].

IV. CONCLUSION

The nonlinear behavior of static dielectric constant, Relaxation time density and refractive and their excess properties are reported. There is confirmation of intermolecular interaction through the dipole –dipole interaction between ALB and ACE.

ACKNOWLEDGEMENT

The authors are thankful to Dr. P.W. Khirade, Dept. of physics and Prof. S. C. Mehrotra, Dept. of computer science & IT, Dr. Babasaheb Ambedkar Marathwada University, Aurangabad for fruitful discussion and guidance.

REFERENCES

[1] Y. S. Sudake, S. P. Kamble, A. L. Tidar, A. P. Maharolkar, S. S. Patil and P. W.Khirade Res. J. Pharma., Bio. and Chem. Sci. 2(2), 761, (2011).
[2] Y. S. Sudake, S. P. Kamble, S. S. Patil, P. WKhirade and S. C. MehrotraJ Korean Chem. Society 56(1),20,(2012).
[3] Yuvraj Sudake, S. P. Kamble, A. P. Maharolkar, S. S. Patil and P. W. KKhirade Asian J. Chem., 24(11), 5111 (2012).
[4] Y. S. Sudake, S.P. Kamble, A. P. Maharolkar, S. S. Patil and P. W. Khirade, American Inst. Phys. 1447, 543(2012).
[5] S. P. Kamble, P. B. Undre, Y. S. Sudake, A. P. Maharolkar and P. W. Khirade, Asian J. Chem. 24(12), 5731(2012).
[6] Y. S. Sudake, S. P. Kamble, A. P. Maharolkar, S. S. Patil, P. W. Khirade and S. C. Mehrotra, Bulletin of the Korean Chemical Society, 33(10),3423(2012).
[7] J. Ortega, M. I. Paz-Andrade, E. Rodriguez-Nunez and E. Jimenez Can. J. Chem. 63, 3354,(1985).
[8] N. Hafaiedh, A. Toumi and M. Bouanz, Phys. Chem. Liq. 47(4), 399,(2009).
[9] G. Oster and J. G. Kirkwood, J. Chem. Phys. vol.11pp.175. (1943).
[10] Yuvraj Sudake, S. P. Kamble, and P. W.Khirade, J. of Applied Sci. and Computation VI(1), 875-882(2019).