iJRASET
International Journal For Research in Applied Science and Engineering Technology

INTERNATIONAL JOURNAL FOR RESEARCH

IN APPLIED SCIENCE & ENGINEERING TECHNOLOGY

Volume: 8 **Issue:** XI **Month of publication:** November 2020

DOI: https://doi.org/10.22214/ijraset.2020.32051

www.ijraset.com

Call: 08813907089 | E-mail ID: ijraset@gmail.com

International Journal for Research in Applied Science & Engineering Technology (IJRASET)
ISSN: 2321-9653; IC Value: 45.98; SJ Impact Factor: 7.429
Volume 8 Issue XI Nov 2020- Available at www.ijraset.com

Acoustic and Thermodynamic Investigation of Caffeine at Different Temperature

Vikas D. Umare
Janata Mahavidyalaya Chandrapur-442401 (M. S.) India

Abstract: ***The ultrasonic velocity, adiabatic compressibility, free length, apparent molar compressibility and apparent molar volume determination is important tools for investigation of structure of compound and nature of intermolecular force of attraction between components in homogeneous solution. The attractive and repulsive force between components of solution shows remarkable effect on physical and chemical properties of solution and subsequently affects density, viscosity and ultrasonic velocity of solution. In the present work, ultrasonic velocity, density and viscosity of caffeine have been measured at different concentration and at different temperature. From experimental data different thermo acoustic parameters like adiabatic compressibility, free length and acoustic impendence have been evaluated. These parameters have been studied in term of intermolecular interactions between components of this system.***

Keywords: Caffeine, ultrasonic velocity, intermolecular interactions, adiabatic compressibility, free length, apparent molar compressibility

I. INTRODUCTION

Caffeine (1, 3, 7-trimethylxanthine) is a purine alkaloid. It is white crystalline solid with bitter taste and widely used in beverages, chocolate and in some medicines. It is central nervous system stimulator, diuretics, increases metabolic rate and found to active against Parkinson's disease[1-5]. Recently, ultrasonic velocity measurements have been extensively used to detect molecular interactions in binary mixtures. It is non-destructive investigation and applicable to the different field like medicinal, agricultural, industrial, polymer chemistry[6-10]. The ultrasonic velocity is used to derive acoustic parameters and predict the intermolecular interaction between solute and the solvent. Thus variation of ultrasonic velocity and related acoustic parameters with concentration at different temperature offers lot of knowledge like structural, physiochemical behaviour solute, inter and intra-molecular interactions in the solution. In the present investigation, different concentration of caffeine solution was prepared. The density and viscosity of all solution was measured using pyknometer and Ostwald viscometer respectively at different temperature. The ultrasonic velocity of all solution is measured using ultrasonic interferometer at 2 MHz frequency. We evaluated different parameters viz., adiabatic compressibility, intermolecular free length, relaxation time, classical absorption, apparent molar compressibility and apparent molar volume from measured density and viscosity and ultrasonic velocity values.

II. EXPERIMENTAL

The analytical grade caffeine was purchased from SD fine chemicals. The double distilled water was used as a solvent to prepare 0.01M to 0.1M solution. All the weighing were made on digital balance with an accuracy of ± 0.0001g. The density (ρs) of solutions was performed with recalibrated pyknometer with accuracy ± 0.0001 g/cm^3. The viscosity (η) of solution was measured by recalibrated Oswald's viscometer. All the measurements were carried out at 301.15, 306.15 and 310.15 K. The ultrasonic velocity of solution was measured with multi-frequency (1-10MHz) ultrasonic interferometer at 2MHz with ±2 m/s accuracy. The interferometer was filled with test solution and water was circulated around the cell. Accuracy in temperature measurement was maintained by thermostatic water bath**.**

III. THEORY

The following acoustic parameters have been calculated from measured value of ultrasonic velocity, density, viscosity using following standard expression.

1) *Ultrasonic velocity (U_s):* Ultrasonic velocity is the speed in which sound travels through a given material and it is given by $U_s = f \times \lambda$ (ms^{-1}) where λ and f is wavelength and frequency of the ultrasonic wave respectively.
2) *Adiabatic Compressibility (β_s):* The adiabatic compressibility was be calculated by from ultrasonic velocity and density of solution by equation 1.

$$\beta s = 1/ U_s^2 \rho s \ (m^2N^{-1}) \qquad \text{……..}\mathbf{1}$$

Where- Us and ρs is ultrasonic velocity and density of solution.

3) *Intermolecular Free Length (L_f):* The intermolecular free length is temperature dependent, measures distance between the surfaces of the molecules in the liquid medium. It is given by **equation 2**

$$L_f = K\sqrt{\beta_s}(A^0) \quad \text{.....2}$$

Where K and β_s are Jacobson's constant and adiabatic compressibility

4) *Relaxation Time (τ):* It is the characteristic time in which a system relaxes under certain conditions. It is calculated by equation 3.

$$\tau = 4/3\ \beta_s \times \eta_s \quad \text{.....3}$$

Where β_s and η_s are adiabatic compressibility and viscosity of the solution respectively

5) *Classical Absorption (α/f^2):* It is given by equation 4.

$$(\alpha/f^2)=8\eta\pi^2/\ 3\rho_s U_s^3\ (m^3mol) \quad \text{.....4}$$

Where η_s, ρs and U_s is viscosity, density and ultrasonic velocity of solution respectively.

6) *Apparent Molal Compressibility (Φ_K):* It is calculated by using the equation 5.

$$\Phi_K= [10^3\ x(\beta_s\rho_0-\beta_0\rho_s)/m\rho_s\rho_0] + [\beta_s M/\rho_s]\ (m^3N^{-1}) \text{.....5}$$

Where β_s andβ_0 is adiabatic compressibility of solution and solvent ρ_0 and ρ_s is density of solution and solvent, m is molar concentration and M is molecular weight of solute.

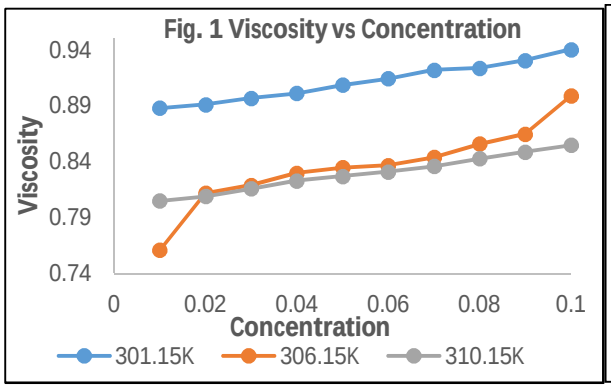
7) *Apparent Molal Volume (Φ_v):* It is calculated by using the **equation 6.**

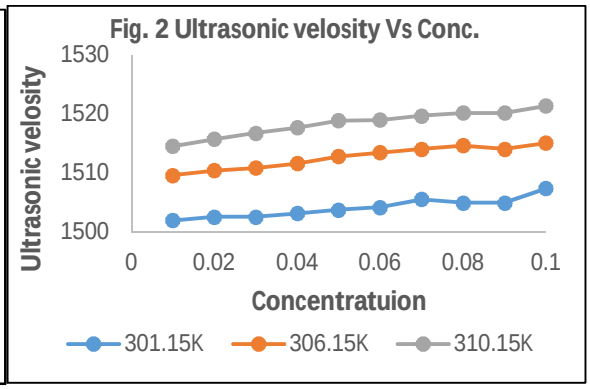
$$\Phi v = [10^3\ x\ (\rho_0-\rho_s)/m\rho_s\rho_0] + [M/\rho_s]\ (m^3mol^{-1}) \text{.....6}$$

Where ρ_0 and ρ_s is density of solution and solvent, m is molar concentration and M is molecular weight of solute.

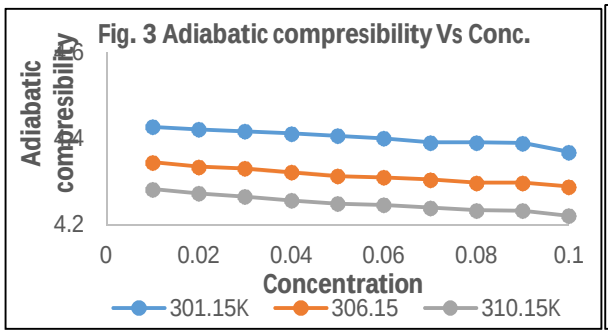
IV. RESULT AND DISCUSSION

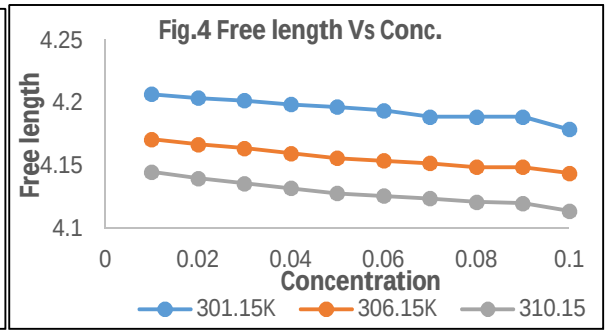
The experimentally measured values of ultrasonic velocity, density and viscosity of aqueous solution of caffeine at 301.15K, 306.15K, and 310.15K temperature were presented in table 1. The acoustic parameters like adiabatic compressibility, intermolecular free length, relaxation time, classical absorption, apparent molar volume and apparent molar compressibility were tabulated in table 1.The variation of derived acoustic parameters with composition were presented in fig 3-8. The density of caffeine solution increases with increasing in concentration and decreases density with rise in temperature for same concentration of the solution at different temperature (Table 1). Increase concentration of caffeine in solution makes the medium denser due to its aggregation in the solution [11-12]. The decreasing trends of density with temperature might be due to weakening of intermolecular cohesive forces between solute and solvent[13]. The perusal table 1 and fig. 1 clearly shows that viscosity of solution increases with increases in concentration of solution and decreases with increase in temperature. As concentration of caffeine in solution increases, cohesion between layers of medium increases which indicates strong cohesive forces between solute and solvent. The rise of temperature weakens cohesive forces between solute and solvents and subsequently lowers viscosity of solution[14-15]. The ultrasonic velocity shows almost same trends with composition (fig. 2) confirmed intermolecular interaction and molecular association in the system[16-18].



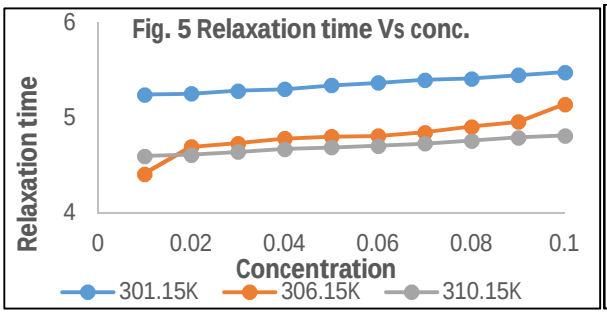


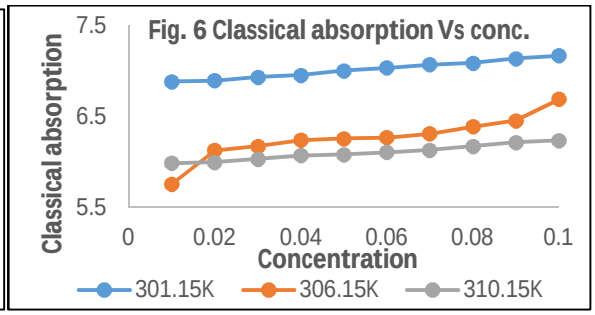
The variation of adiabatic compressibility with composition of solution is given in fig. 3. It shows decreasing trends with increase in concentration. When caffeine is added to water, it gets associated with water molecules by pulling the water molecule from the bulk due to force of attraction. Due to this volume available in solvent molecule for the next incoming ions gets decreases[19]. The variation in intermolecular free length with concentration is shown in fig. 4. Increase in concentration leads to decreases the gap between two solutes which is explained by intermolecular free length. As concentration of solute increases intermolecular free length goes on decreasing[20-21].In the present study intermolecular free length decreases linearly with increasing concentration. This trend indicates that there is a significant interaction between caffeine and water molecule and subsequently shows structure forming behaviour between them.



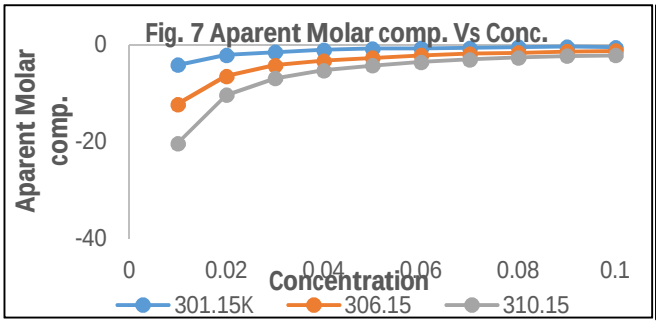


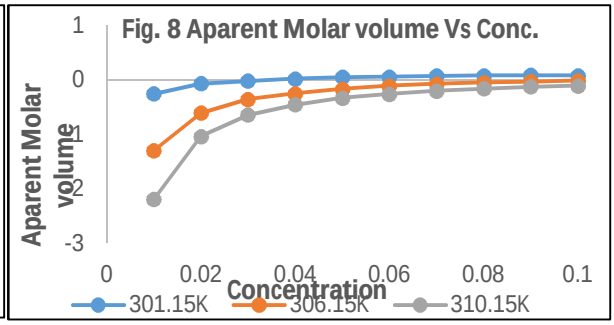
The variation of relaxation time (τ) with composition of solution is given in fig. 5. It increases with increases with concentration in the system but decreases with increase in temperature. This trend suggest solute solvent interaction in the system[22-25].The decrease value of τ with rise in temperature supports weakening of hydrogen bonding in the system. The variation of classical absorption with composition is explained in fig. 6. It is observed that classical absorption is increases with increase in composition of solution indicating more stability of molecules which supports strong intermolecular interactions through hydrogen bonding[26].





The variation of apparent molal compressibility (Φk) is described in fig. 7.The value of Φk are found to increase with increasing composition indicating significant intermolecular interaction in the system and decreases with increase with temperature indicating weak intermolecular interaction in the system. The negative value of Φk supported that caffeine have structural influence on solvent and indicated ionic and hydrophilic interaction in the system[27-28]. The variation of apparent molal volume (Φv) is defined in fig. 8. The variation of apparent molal volume is observed at lower concentration of solution and remains constant at higher concentration. It is found that the value of Φv is decreases as concentration increases at all the temperature. The decrease value of Φv with increasing composition of solution suggests strong ionic interaction in the solution[29]. The high Φv suggests that strong solute solvent interaction occurring in the system and low Φv value supports strong ion-ion interaction in the system[30-31].





V. CONCLUSION

In the present investigation, the observed trends and variation of density, viscosity and ultrasonic velocity and some thermo-acoustical parameters of aqueous solution of caffeine with molar composition at 2MHz frequency at different temperature was studied. The measured and derived thermo-acoustic parameters are helpful for understanding nature of caffeine and solvent and type and strength of interaction between them.

VI. ACKNOWLEDGEMENT

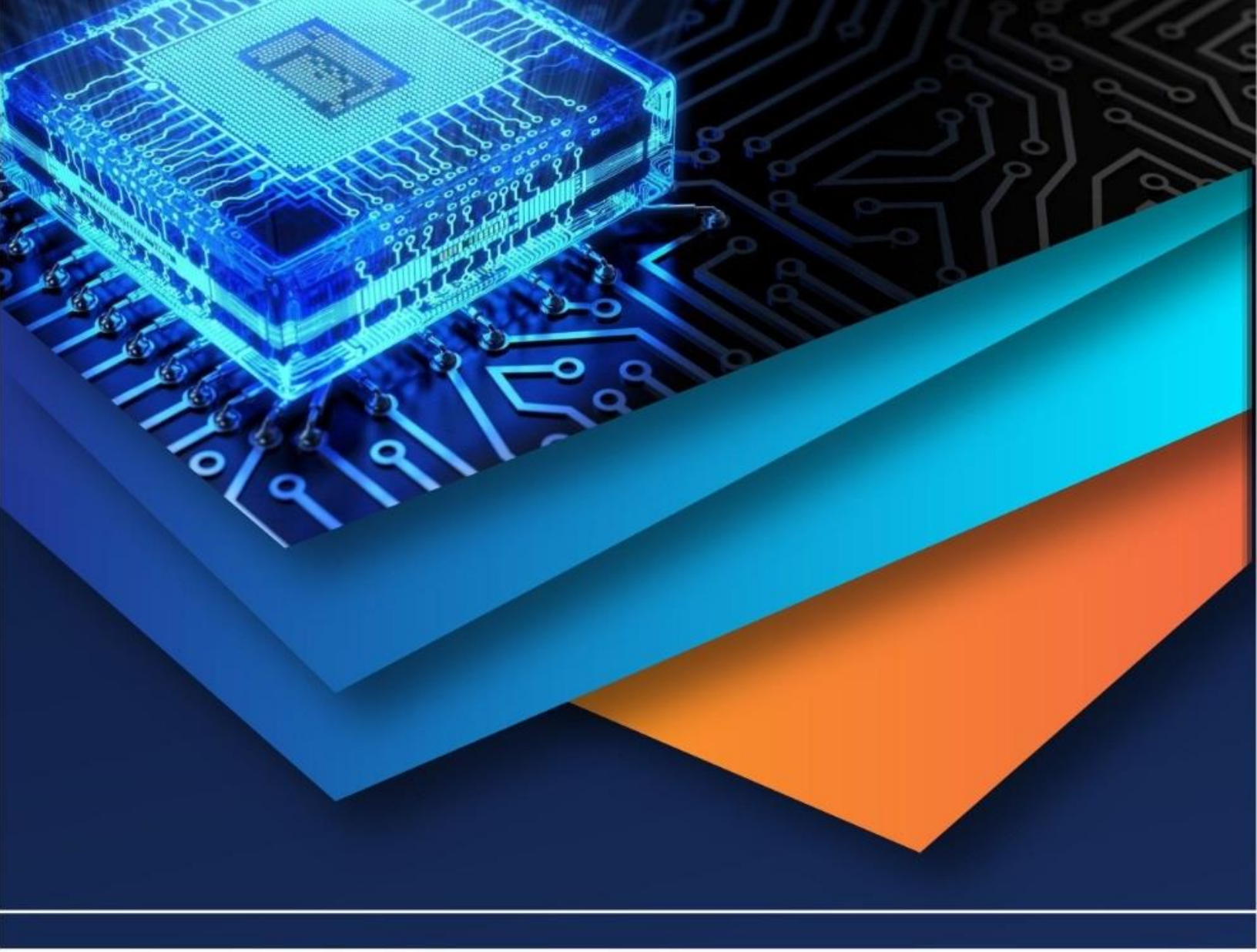
The author is thankful to M. Subhas, Principal, Janata Mahavidyalaya, Chandrapur (M. S.) for providing necessary facility during work.

Table 1. Measured value of ultrasonic velocity (Us), density (ρs), viscosity (η) and some derived acoustic parameters like adiabatic compressibility (β_S), free length (Lf), relaxation time (τ), classical absorption (α/f), apparent molar compressibility (Φk) and apparent molar volume (Φv)

Temp.	conc.	ρs	η ×10^{-3}	Us	β_sx 10^{-10}	Lf x 10^{-11}	τ x 10^{-10}	α/f^2x10^{-12}	Φk x10^{-10}	Φv
301.15	0.01	1001.03	0.8881	1501.94	4.428	4.207	5.244	6.885	-4.166	-0.251
	0.02	1001.7	0.8912	1502.54	4.422	4.204	5.254	6.896	-2.129	-0.062
	0.03	1002.87	0.8972	1502.54	4.417	4.202	5.284	6.934	-1.48	-0.016
	0.04	1003.24	0.9013	1503.14	4.412	4.199	5.302	6.955	-1.067	0.027
	0.05	1003.48	0.9088	1503.75	4.407	4.197	5.34	7.003	-0.796	0.056
	0.06	1004.35	0.9146	1504.19	4.401	4.194	5.366	7.035	-0.693	0.064
	0.07	1004.72	0.9222	1505.56	4.391	4.189	5.399	7.072	-0.634	0.077
	0.08	1005.46	0.9241	1504.96	4.391	4.189	5.411	7.089	-0.485	0.083
	0.09	1005.83	0.9309	1504.96	4.39	4.189	5.448	7.139	-0.373	0.091
	0.1	1007.3	0.9406	1507.39	4.369	4.179	5.479	7.168	-0.524	0.086
306.15	0.01	1009.98	0.761	1509.64	4.345	4.171	4.408	5.758	-12.29	-1.29
	0.02	1011.1	0.812	1510.43	4.335	4.167	4.694	6.128	-6.428	-0.604
	0.03	1011.47	0.819	1510.91	4.331	4.164	4.729	6.172	-4.206	-0.351
	0.04	1012.59	0.83	1511.65	4.322	4.16	4.783	6.239	-3.289	-0.242
	0.05	1012.96	0.835	1512.87	4.313	4.156	4.802	6.259	-2.668	-0.163
	0.06	1012.96	0.837	1513.5	4.31	4.154	4.81	6.266	-2.145	-0.104
	0.07	1013.34	0.844	1514.1	4.305	4.152	4.844	6.309	-1.815	-0.067
	0.08	1014.08	0.856	1514.71	4.298	4.149	4.906	6.386	-1.608	-0.044
	0.09	1014.83	0.865	1514.1	4.298	4.149	4.957	6.456	-1.369	-0.026
	0.1	1015.57	0.899	1515.14	4.289	4.144	5.141	6.691	-1.273	-0.011
310.15	0.01	1017.75	0.805	1514.61	4.283	4.145	4.597	5.985	-20.3	-2.184
	0.02	1018.5	0.809	1515.78	4.273	4.14	4.61	5.997	-10.38	-1.033
	0.03	1018.88	0.816	1516.81	4.266	4.136	4.641	6.034	-6.942	-0.637
	0.04	1019.63	0.823	1517.78	4.257	4.132	4.672	6.07	-5.293	-0.449
	0.05	1020	0.827	1518.96	4.249	4.128	4.685	6.083	-4.265	-0.328
	0.06	1020.76	0.831	1519.07	4.246	4.126	4.704	6.106	-3.533	-0.254
	0.07	1021.13	0.836	1519.78	4.24	4.124	4.726	6.132	-3.013	-0.196
	0.08	1021.88	0.843	1520.25	4.234	4.121	4.759	6.173	-2.646	-0.157
	0.09	1022.26	0.849	1520.25	4.233	4.12	4.791	6.215	-2.297	-0.122
	0.1	1023.39	0.855	1521.49	4.221	4.114	4.812	6.237	-2.148	-0.102

REFERENCES

[1] Caballero B, Finglas P and Toldra F; 2015, Encyclopedia of Food and Health, Elsevier Science
[2] Ascherio, A., Zhang, S.M., and Hernan, M.A. 2001, 50: 56–63.
[3] La Vecchia, C. 2005, 42:444–446.
[4] Salazar-Martinez, E., Willett and W.C., Ascherio, A. et al. 2004, 140: 1–8
[5] Carrillo, J.A. and Benitez, J. 2000, 39:127–153
[6] Jahagirdar D. V., Indian J. of Pure and Applied Physics, 2000, 38, 645-650
[7] Shekar D. M. and Dhanlaxmi Ramkumar; J. of Pure and Applied Ultrason. 2002, 24,6-67
[8] Riyazuddeen and Islam, J. of Pure and Applied Ultrason. 1997; 19, 16-25
[9] PatilK.C.Inter.J.Applicable.Chem.,2018, 7(5),1434-1441.
[10] PatilK.C.;Der.PharmaChemical,2017,9(13),46-54,0975- 413X
[11] S. Punitha, A. Panneerselam; Int. J. Chem. Tech. Research. 2015, 7(2), 629-638
[12] K. C. Patil and C. M. Dudhe; 2016, 8, (20), 227-233.
[13] R. C. Devi, R. Mutthamal, R. Kesavasami; 2017, 7 (11), 20288-20395
[14] K. C. Patil, V. S. Singh; Int.J. of Research in Advent tech., 2018, 6 (7), 1451-1455
[15] A. S. Aswar and D. S. Chaudhari; J of Pure. Applied Ultrason. 2014, 6, 46-50
[16] S. Nathiyanatham, L. Palaniappan; Arabian J. of Chemistry, 2012, 5 (1), 25-30.
[17] V. A. Giratkar; J. of Chem., Biology. and Physical Sci., 2017, 7 (3), 661-676
[18] R. S. Shriwas, O. P. Chimankar; Journal Pure Applied Ultrason. 2014, 36, 65-68
[19] R. J. Fort, W. R. Moore; Trans. Faraday. Soc., 1965, 61, 2102–2110
[20] S. Nathiyanatham, S. Palaniappan L., Acta Cienc. Indica, 2006, 37, 392
[21] S. Nathiyanatham, S. Palaniappan L., Acta Cienc. Indica, 2005, 31, 533
[22] S. A. Shah and S. M. Gadegone, Int. J. of Resch. In Bioscience, Agri. and Tech., 2014, l.1(2), 1160-1168.
[23] N. Sawhney and M. Sharma, J. of Chemical and Pharma. Research.2014, 6(4), 1232-1242.
[24] Kumar D. and Shravan Rao; Indian J. of pure and applied physics , 2007,45 (3), 210-220
[25] O. P. Chimankar, N. R. Pawar, Int. J. of research in Engg. and Tech., 2014, 3 (6), 315-323.
[26] Patil K. J. and Ali S. T., Indian Journal of Chemistry; 1983, 22A, 410
[27] R. Palani, S. Balkrishnan and B. G. Lakshmi, J. of Physical Science, 2011, 22 (1), 131-141
[28] Sathyavathi A. V., Acoustica, 1973, 28, 17
[29] Balachandran , Nature, 1961, 191, 164
[30] R. Palani and S. Balkrishnan; Int. J. of Chem Tech Research, 2011, 3 (1), 284-289
[31] Dhanlakshmi A; Journal of Acoustic society India, 2000, 23, 1-4, 385-388.



10.22214/IJRASET

45.98

IMPACT FACTOR: 7.129

IMPACT FACTOR: 7.429

INTERNATIONAL JOURNAL FOR RESEARCH

IN APPLIED SCIENCE & ENGINEERING TECHNOLOGY