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MOLECULAR INTERACTION STUDY OF 18-CROWN-6 WITH ONE MILLIMOLE SALT SOLUTION AT 298.15 K AND 308.15 K BY ULTRASONIC VELOCITY MEASUREMENT.

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Abstract: -

The presentresearch work gives investigation on the effect of temperature variation on the thermodynamic and transport properties of binary system involving 18-crown-6 ether and alkali metal salts. The binary liquid system (18-crown-6 + one millimole of alkali metal salts) were investigated at 298.15 K and 308.15K. Thermodynamic parameters such as adiabatic compressibility (Ks), free length (L_f) and acoustic impedance (Z)were calculated and used to understand the complexation and the interaction in between 18-crown-6 and alkali metal ions.In this binary systems of 18-crown-6 ether formed a strong complexation with alkali metal ions as the following order - KBr > KCl > NaBr > NaCl> LiBr > LiCl.

Keywords:-

18-crown-6, alkali metal salts, binary system, interaction, and complexation.

1. Introduction:-

The experimental importance of the binary mixture rather than single liquid component has achieved much more greatness during the last 20 years in assessing the complexationinteraction in between 18-crown-6 and alkali metal ions and studying the physico-chemical behavior of such systems.[1-2]

The reported study of the 18-crown-6 and their interactions with an alkali metal salts has been a main focus in supramolecular chemistry due to their capacity to form highly selective interaction and stable complexation as host-guest nature.[3]. In this present research work, 18-crown-6 specific interest as proper as its cavity size which is proper to accommodated alkali metals cations such as Li^+, Na^+& K^+. The interaction in between 18-crown-6 and alkali metal ions (Li^+, Na^+& K^+) that is complexation depend on thermodynamic factors, salvation energy, environment of metal ions, temperature etc.[4-5].Thermodynamics and its transports properties of such systems are plays vital role for applications in extraction process, catalysis and delivery of drugs[6-7].

The another important factor temperature that direct effect on the interaction of alkali metal cations and 18-crown-6, enthalpy of and entropy of the systems, complex stability, viscosity and ionic mobility [8]. Therefore for better understanding the stability of complexes, conductivityand interaction of alkali metal ion with 18-crown-6 ethers. That is thermodynamic properties controlling the temperature is most important even small variation in temperature it effects thermodynamics and transport properties of binary liquid mixture system. Therefore for systematic study of binary system (18-crown-6 + alkali metal ion) at temperature variation gives the dipper knowledge of molecular interaction of mechanism of complexation [9-10].

The main aim of this investigation to find out the effect of temperature on the thermodynamics and transport properties of binary systems at 298.15K and 308.15K. It is carried out by studying theadiabatic compressibility (Ks), free length (L_f), acoustic impedance (Z)etc. can established the modified role of temperature in modulating the interactions in between the 18-crown-6 ether and alkali metal salts.

In this research paper we investigate the interaction and complexation in between 18-crown-6 and alkali metal ions and also studied of variation of temperature on the interaction at 298.15K and 308.15K.

Binary system:-Various concentrations of 18-crown-6 + 1 millimole aqueous solution of alkali metal salt (LiCl/ LiBr/ NaCl/ NaBr/KCl/ KBr) solution.

Experimental details:-

All the chemicals were used in this present research work of an analytical reagent (AR) grades with minimum assay of 99.9% purity, which were obtained from Spectrochem. The various concentrations of the binary liquid mixtures were prepared in terms of mole fraction. The mole fractions of 18-crown-6 were varied from 0.0 to 0.01 with 1 millimolesaqueous solution of alkali metal salts (LiCl/LiBr/ NaCl / NaBr/ KCl / KBr) solution.

i) Ultrasonic velocity measurement:-

An ultrasonic velocity in binary liquid mixtures of all concentration has been measured at 2 MHz frequency by using "ASICO" made ultrasonic interferometer supplied by Ambala electronics, Hariyana, with a high degree of accuracy. The measuring cell of interferometer is a specially designed double walled vessel with arrangement for constant temperature. A digital constant temperaturewater bath with accuracy of ± 0.1K has been used to circulate water through the outer jacket of the double walled measuring cell containing measuring cell containing the experimental liquid [11].

ii) Density measurement:-

The density was determined using bicapillary pycnometer of bulb capacity 8×10^{-6} m^3 with graduated stem. The pycnometer was calibrated with tripled distilled water, toluene and benzene. [12].

iii) Viscosity measurement:-

An ubbelohde viscometer (20 ml)was used for the viscosity measurement and flow time determined using digital clock having an accuracy of ± 0.1S.

The calibrated values of densities and viscosities were close agreement with literature values [13].

Table:-1 Calibration of bicapillary pycnometer and Ubbelohde viscometer literature values and experimental values.

Chemicals	Temp.	Density (ρ)		Ultrasonic velocity (U)	
		Literature	Calculated	Literature	Calculated
Water	298.15K	0.9970	0.9970	1497	1488
	308.15K	0.9940	0.9941	1522	1513.6
Carbon tetrachloride	298.15K	1.5867	1.5861	930	928
	308.15K	1.5989	1.5654	902	899.2
Toluene	298.15K	0.8623	0.8619	1308	1296.8
	308.15K	0.8550	0.8531	1288	1284

Theory:-

The following thermodynamic parameters were calculated from Jacobson's relation. [14-16**]**

Adiabatic compressibility $Ks = \frac{1}{U^2 d_1}$ --- (1)

Intermolecular free length (L_f) = $k\sqrt{Ks}$ --- (2)

Ultrasonic velocity $U = \lambda f$ ---- (3)

Specific acoustic impedance $Z = U\ d_1$ ---- (4)

Where, λ - is wavelength, f - is frequency (2MH$_Z$), d_1 and d_0 measured densities of solution and pure solvent.U and $U_0$are the experimental ultrasonic velocities of the solution and pure solvent respectively, Ks is the adiabatic compressibility of solution.

Result and discussion:-

The calculated physical and acoustic parameters of binarysystem are listed in table 2, 3, 4, 5, 6 & 7

Table:-2 Ultrasonic velocity data for various concentration of 18C6 + 1 millimole aqueous solution of LiCl.

Temp K	Conc.	U (m/s)	P (kg/m^3)	Ks ×10^{-7} (N/m^2)	Z	L_f ×10^{-10}
298.15	0	1421.6	0.9957	4.96	1415.4	6.56
	0.00125	1380.1	0.9960	5.27	1374.5	6.75
	0.0025	1389.7	0.9962	5.19	1384.4	6.70
	0.005	1398.2	0.9964	5.13	1393.1	6.66
	0.01	1410.3	0.9966	5.04	1405.5	6.61
308.15	0	1470.4	0.9933	4.65	1460.5	6.35
	0.00125	1401.2	0.9935	5.12	1392.0	6.66
	0.0025	1413.3	0.9937	5.03	1404.3	6.60
	0.005	1423.2	0.9939	4.96	1414.5	6.55
	0.01	1435.4	0.9941	4.88	1426.9	6.50

Table:-3 Ultrasonic velocity data for various concentration of 18C6 + 1 millimole aqueous solution of LiBr.

Temp K	Conc.	U (m/s)	P (kg/m^3)	Ks ×10^{-7} (N/m^2)	Z	L_f ×10^{-10}
298.15K	0	1420.8	0.9958	4.97	1414.8	6.56
	0.00125	1392.1	0.9962	5.17	1386.8	6.69
	0.0025	1399.3	0.9964	5.12	1394.2	6.66
	0.005	1409.4	0.9966	5.05	1404.6	6.61
	0.01	1421.2	0.9968	4.96	1416.6	6.55
308.15K	0	1464	0.9934	4.69	1454.3	6.37
	0.00125	1412.2	0.9937	5.04	1403.3	6.61
	0.0025	1425.1	0.9939	4.95	1416.4	6.55
	0.005	1438.8	0.9941	4.85	1430.3	6.48
	0.01	1452.6	0.9943	4.76	1444.3	6.42

Table:-4 Ultrasonic velocity data for various concentration of 18C6 + 1 millimole aqueous solution of NaCl.

Temp K	Conc.	U (m/s)	P (kg/m^3)	Ks ×10^{-7} (N/m^2)	Z	L_f ×10^{-10}
298.15	0	1428	0.9959	4.92	1422.1	6.53
	0.00125	1402.1	0.9964	5.10	1397.0	6.64
	0.0025	1412.3	0.9966	5.03	1407.4	6.60
	0.005	1418.6	0.9968	4.98	1414.0	6.57
	0.01	1427.2	0.9970	4.92	1422.9	6.53
308.15	0	1460.8	0.9935	4.71	1451.3	6.39

	0.00125	1417.1	0.9939	5.01	1408.4	6.58
	0.0025	1429.2	0.9941	4.92	1420.7	6.53
	0.005	1442.3	0.9943	4.83	1434.0	6.47
	0.01	1456.4	0.9945	4.74	1448.3	6.40

Table:-5 Ultrasonic velocity data for various concentration of 18C6 + 1 millimole aqueous solution of NaBr.

Temp K	Conc.	U (m/s)	P (kg/m^3)	Ks $\times 10^{-7}$ (N/m^2)	Z	L_f $\times 10^{-10}$
298.15	0	1438.4	0.9960	4.85	1432.6	6.48
	0.00125	1411.1	0.9966	5.03	1406.3	6.60
	0.0025	1422.2	0.9968	4.95	1417.6	6.55
	0.005	1435.4	0.9970	4.86	1431.0	6.49
	0.01	1447.6	0.9972	4.78	1443.5	6.43
308.15	0	1465.6	0.9936	4.68	1456.2	6.37
	0.00125	1436.2	0.9941	4.87	1427.7	6.49
	0.0025	1444.3	0.9943	4.82	1436.0	6.46
	0.005	1456.4	0.9945	4.74	1448.3	6.40
	0.01	1470.1	0.9947	4.65	1462.3	6.34

Table:-5 Ultrasonic velocity data for various concentration of 18C6 + 1 millimole aqueous solution of KCl.

Temp K	Conc.	U (m/s)	P (kg/m^3)	Ks $\times 10^{-7}$ (N/m^2)	Z	$L_f \times 10^{-10}$
298.15	0	1441.6	0.9961	4.83	1435.9	6.46
	0.00125	1432.4	0.9968	4.88	1427.8	6.50
	0.0025	1441.3	0.9970	4.82	1436.9	6.46
	0.005	1453.1	0.9972	4.74	1449.0	6.41
	0.01	1465.2	0.9974	4.67	1461.3	6.36
308.15	0	1468	0.9937	4.66	1458.7	6.36
	0.00125	1454.4	0.9943	4.75	1446.1	6.41
	0.0025	1463.1	0.9945	4.69	1455.0	6.37
	0.005	1475.3	0.9947	4.61	1467.4	6.32
	0.01	1486.6	0.9949	4.54	1479.0	6.27

Table:-6 Ultrasonic velocity data for various concentration of 18C6 + 1 millimole aqueous solution of KBr.

Temp K	Conc.	U (m/s)	P (kg/m^3)	Ks $\times 10^{-7}$ (N/m^2)	Z	L_f $\times 10^{-10}$
298.15	0	1396	0.9962	5.15	1390.6	6.67
	0.00125	1452.7	0.9970	4.75	1448.3	6.41
	0.0025	1460.2	0.9972	4.70	1456.1	6.38
	0.005	1473.4	0.9974	4.61	1469.5	6.32
	0.01	1485.1	0.9976	4.54	1481.5	6.27
308.15	0	1445.6	0.9938	4.81	1436.6	6.45
	0.00125	1473.1	0.9945	4.63	1464.9	6.33
	0.0025	1481.2	0.9947	4.58	1473.3	6.30
	0.005	1494.2	0.9949	4.50	1486.5	6.24
	0.01	1507.5	0.9951	4.42	1500.1	6.18

1) Density:-

In this investigation, densities of binary mixture were increases with increase in concentration of 18-crown-6, indicating stronger interaction. Experimental data also shows that, density decreases with increase in temperature, reflecting weaker complexation KCl salt showed higher density than NaCl and NaCl shows higher density than LiCl. So, K^+ formed more stable complex and strong interaction with 18-crown-6 than Na^+ and Li^+ ion.[17].

Thus order of complexation and interaction of 18-crown-6 with alkali metal ions as

KBr > KCl > NaBr > NaCl>LiCl > LiBr.

2) Ultrasonic velocity:-

An ultrasonic velocity of binary system increases with increase the concentration of 18-crown-6 this reveals that due to structural modification in the solution there is complexation and interaction in between alkali metal ion and 18-crown-6. At higher temperature enhanced the molecular movement and weakening the interaction and complexation. [18].

3) Adiabatic Compressibility (Ks):-

In the present research work, the adiabatic compressibility decreases with increase in concentration of 18-crown-6 ether that reveals, increase in the interaction and complexation in the binary liquid system.

4) Free length (L_f):-

Intermolecular free length decreases with increase the concentration of 18-crown-6. This indicates that, stronger interaction in between alkali metal cations and 18-crown-6.

5) Acoustic impedance: - (z)

Acoustic impedance (z) to be almost reciprocal of adiabatic compressibility (βad). In this present workacoustic impedance increases with increases the concentration of 18-crown-6, it indicating stronger interaction and complexation in alkali metal ions and 18-crown-6 [19-20].

Conclusion:-

This research work reports experimental data for density and ultrasonic velocity for the binary system,over the entire range of mole fraction at 298.15K and 308.15K, from these experimental data the related parameters were calculated. It is observed that there is strong interaction with K+ ion rather than Na+ and Li+ due to optimal cavity size of 18-crown-6 ether. The existence of complexation and interaction in between 18-crown-6 and alkali metal ions more favored at lower temperature and heavy alkali metal cation; it confirmed from the experimental and calculated data of ρ, U, L_f, Z, and Ks. The existenceof strong complexation and interaction in the both systems as-

KBr > KCl > NaBr > NaCl> LiBr > LiCl

The graphical presentation of adiabatic compressibility (Ks), intermolecular free length (L_f) and acoustic impendence (Z) of binary systems at 298.25K and 308.15K

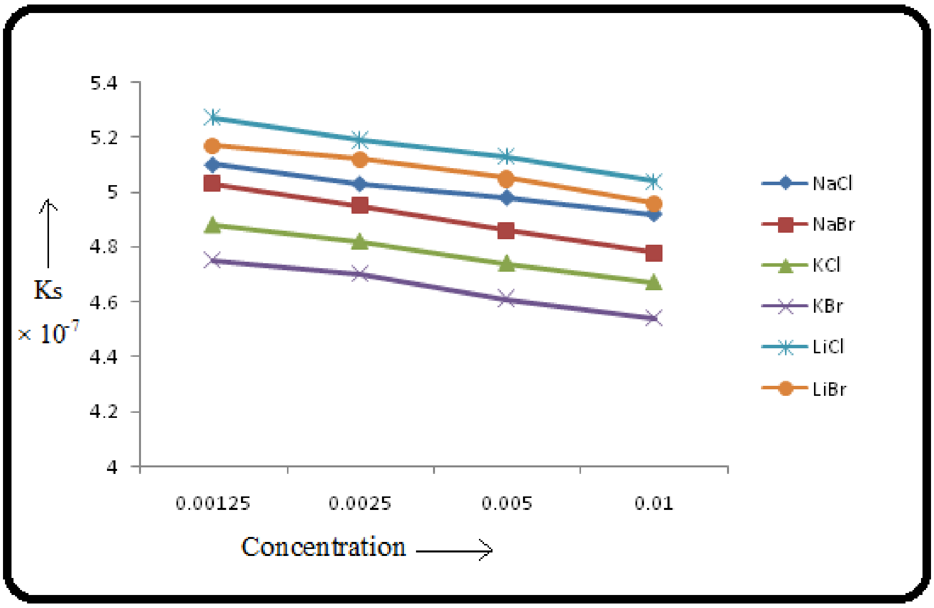

Fig:-1 Adiabatic compressibility (Ks) for the Binary System at 298.15K

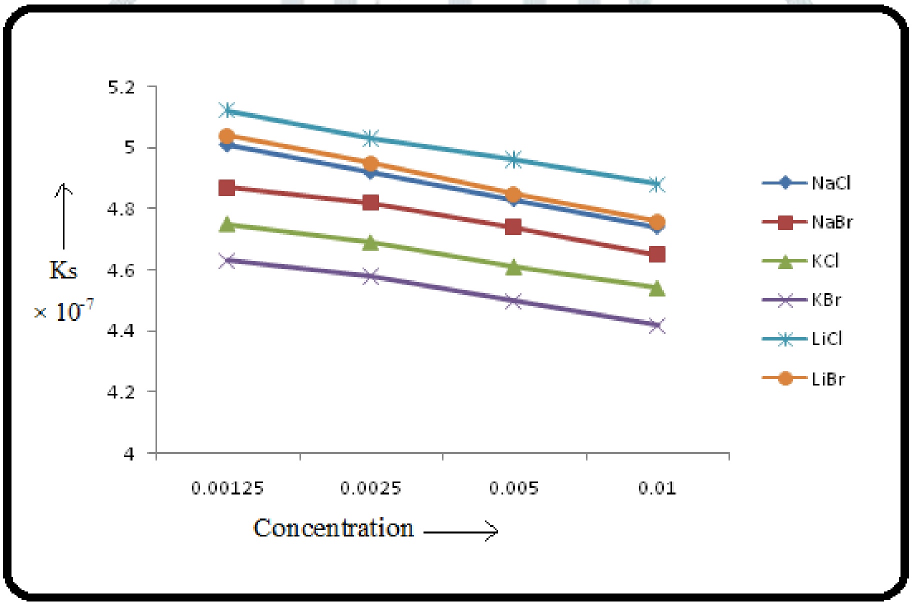

Fig:-2 Adiabatic compressibility (Ks) for the Binary System at 308.15K

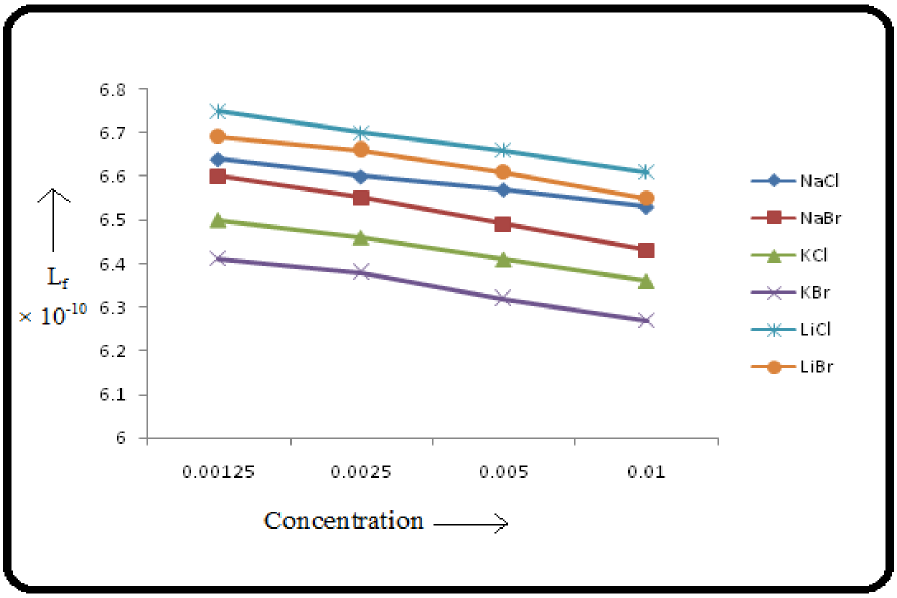

Fig:-3 Intermolecular free length (L_f) for the Binary System at 298.15K

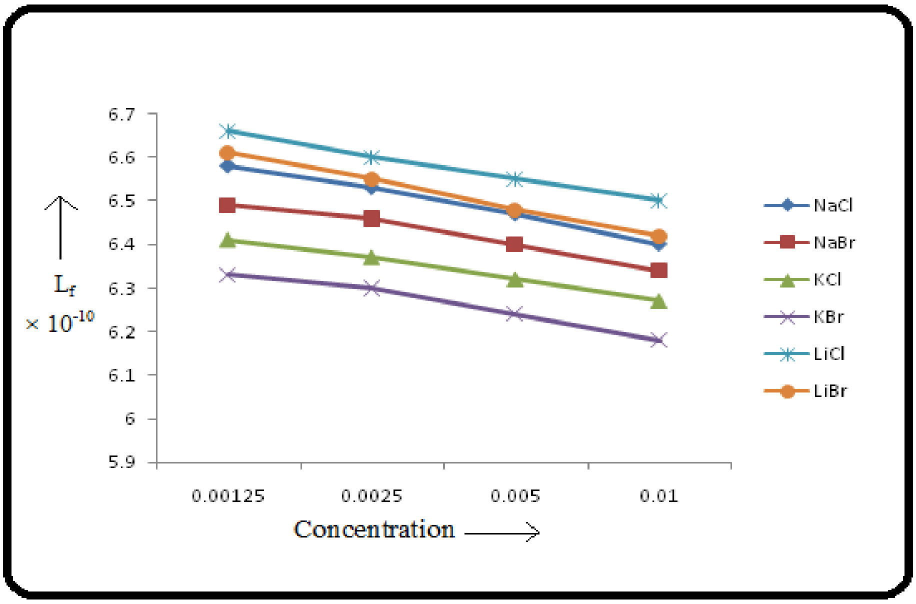

Fig:-4 Intermolecular free length (L_f) for the Binary System at 308.15K

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