A THERMO-ACOSTICAL INVESTIGATION ON AMINO ACETIC ACID IN AQUEOUS KCL SOLUTION

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Abstract

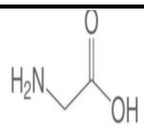
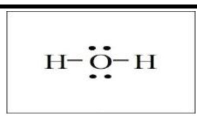
In recent years, studies on the acoustic properties of aqueous solutions of mixed electrolytes have proven useful in understanding specific ion-ion and ion-solvent interactions in solutions. [1] Ultrasonic technique to evaluate the thermodynamic properties of amino acetic acid and proteins. Using speed and density of other thermoacoustic and volumetric. also calculated l, Wada's constant(W), Rao's constant(R), adiabatic compressibility(β), acoustic impedance(Z), relative association (R_A), Relaxation strength (r), Surface tension (σ), Solvation No, Nonlinear parameter(B/A), Isothermal Compressibility (KT).

***Keywords*: -** Amino Acetic Acid, Ultrasonic velocity, Density, Thermo-acoustical parameters.

Introduction

The ultrasonic technique has been effectively employed to study the nature of molecular interaction in pure liquids, liquid mixture and ionic liquids and ionic interactions in electrolytic solution.[1] The ultrasonic method is a versatile non-destructive technique use for the understanding physicochemical properties of liquid and also behave like a powerful probe assess the acoustic properties and obtain the intermolecular interaction in the binary and ternary mixture. This mixture is use to find the various pharmaceutical, medical and technological application [2, 3]) Glycine is an amino acid that has a single hydrogen atom as a side chain. It is the easy stable amino acid with the chemical formula NH_2-CH_2-COOH. Glycine is the proteinogenic amino acids..The presented work is focused to understand the interaction of Amino Acetic Acid and KCL at different concentration 0.02- 0.2 mol /kg and different temperature 283.15K to 298.15k. Ultrasonic velocity data as such Provides limited information about the nature and the relative strengths of various types of interactions, but their derived parameters Wada's constant(W), Rao's constant(R) , adiabatic compressibility(β) , acoustic impedance(Z) , relative association(R_A), Relaxation strength (r), Surface tension (σ), Solvation No, Nonlinear parameter(B/A), Isothermal Compressibility(KT). Go in about the range of different types of interaction responsible for cleaning fluids solutions.

Material

Sr. No	Compound	Mol. Wt.	Structure	CAS No.
1	**Amino Acetic Acid**	75.07 g/mol		64-19-7
2	**H_2O**	18.01528 g/mol		7732-18-5
3	**KCL**	74.5513 g/mol		7447-40-7

Methods

The Velocity analog ultrasonic interferometer, operatingat a frequency of 2MHz, manufactured by Mittal Enterprises Pvt. was used to measure ultrasonic velocity. Ltd., New Delhi (model F-81) with an accuracy of 0.0001 m/s. The source of the ultrasonic waves was a quartz crystal excited by a high-frequency oscillator. The cell was filled with the desired solution and constant temperature water was circulated through the outer shell. The cell was allowed to equilibrate for 30 minutes. before action. The densities of the solutions.

were accurately determinedusing a 10 ml flask with a density of ± 2*10-2 kg/m3 and a digital electronic balance (Contech CA-34) with an accuracy of ± 0.0001 g. The experimental temperature was kept constant by circulating the water using an automatic thermostatic water bath supplied by lab- Hosp. A Mumbai company with a temperature accuracy of ±1K [11].

Defining Relation: -

- Acoustical Impedence (Z) = Up
- Adiabatic Compressibility(β) = $\frac{1}{U^2\rho}$
- Relaxation Strength(r) = $\left\{1-(\frac{U}{U_\infty})^2\right\}$
- Surface Tension(σ) = $\left\{(6.3 * 10^{-4})\rho U^{\frac{3}{2}}\right\}$
- Relative Association (Ra) = $\left\{\left(\frac{\rho}{\rho_o}\right)\left(\frac{U}{U_o}\right)^{\frac{1}{3}}\right\}$
- Solvation Number = M/M(1-β/β0) (100-x/x)
- Wada's constant(W) = $V_m\beta^{-1/7}$
- Rao's constant(R) = $V_mU^{1/3}$
- Isothermal Compressibility (KT1) = $\left\{1.33 * 10^{-8}/(6.4 * 10^{-4}U^{\frac{3}{2}}\rho)^{3/2}\right\}$
- Isothermal Compressibility (KT2) = $\{17.1*10^{-4}/T^{4/9}*U^2*\rho^{1/3}\}$
- Non lenear parameter(B/A1) = (2+(0.98*10^4/ U)
- Non lenear parameter(B/A2) = (-0.5+1.2*10^4/ U)

Result and Discussion: -

The experimental values of the velocity U and the density p at the temperatures283.15k, 288.15k, 293.15k and 298.15k are shown in table1. Calculated the value of acoustic impedance(Z),adiabatic compressibility(β),relaxation force(r),surface tension(σ),relative relationship(Ra),solvation index, Wada's constant(W), Rao's constant(R),the isothermal compressibility(KT), the nonlinear parameters(B/A) is shown in table 1-4.The variability of all these parameters with the concentration of distilled water and KCL with amino acetic acid is shown in fig.1-10. It is observed that the density of all the distilled water and aqueous KCL solution increase with the increase in concentration of solution as expected and decrease with increase of temperature due to the thermal energy of the system which distract the intermolecular force.[11]

It is observed that the ultrasonic velocity shows the increasing variation with increasing temperature. The ultrasonic velocity shows the increasing variation with increasing temperature. The ultrasonic velocity of water was measured at different temperatures(283.15k,288.15k,293.15k, and 293.15k) and the calculated given in Table1. It is observed that temperature and concentration affect the ultrasonic wave in the existing system(Amino Acetic Acid + Water +KCL). So, it is showing that the intermolecular interaction with association. It has been observed that the total solution density in an aqueous solution of KCL increasing KCL concentration(if the temperature remains constant) at a constant concentration, the weak electrostatic interaction of the ions does not significantly affect the surface tension. A decrease in acoustic impedance(Z)indicates weak interaction and vice versa. For a KCL solution, Z increases with increasing concentration(temperature remains constant). However, with increasing temperature(concentration remains constant),Z decreases. The Rao's and Wada's Constant remain nearly constant with increasing temperature. May be due to the increase in conductivity of the KCL solution with increasing temperature. Because of this , there is no accumulation of solute molecules in any particular region. However , the two constants above increase with increasing concentration. Relative association(Ra) is a property used to understand interactions. Two important factor influence the relative associations;(1)Degradation of associated solvent molecules in addition to the solute.(2)solvation of amino acid molecules. The first involves a decrease and the second an increase in relative association. In the present study, RA increase with amino acid concentration, suggesting a greater influence of the second factor then the first. The adiabatic compressibility decreases with increasing concentration for the four different temperatures. The decrease in adiabatic compressibility can be caused by the aggregate of a solvent molecule around a solute molecule. The tested decrease in adiabatic compressibility with concentration of amino acetic acid + KCl + H_2O indicates the formation of tightly bound systems[14].The strength of the relaxation depends entirely on the factor[1- U U ∞].Here "U" is the ultrasonic velocity of the solution and "U ∞" is a constant at 1600m/s. A decreases in the relaxation force value with increasing concentration indicates the interaction of the solution with the solvent in the system. which suggests a large link between fertilizers and salt salts. The nonlinear parameter (B/A)obtained by Hartmann-Balizer and Ballousone is related to the internal pressure ,hardness, intermolecular potential, molecular structure and molecular interaction of the liquid. Non-linearity parameters for both systems as a function of concentration at 288.15k.(Joshi et al, 2017). The decreasing trends of both parameters indicate that the interaction between the solute and solvent components is stronger at higher concentrations. General trends in isothermal compressibility (Kt1 and KT2). It was found that as the concentration af acetic acid increases, Aminp decreasing fertilizer concentration appears to be the results of a corresponding decrease in free volume.(Millero , 1969). As the weight fraction of fertilizers in electrolyte solutions increases, most of the water molecules are electro filtered, and therefore the water decreases, resulting in a decrease in compressibility.

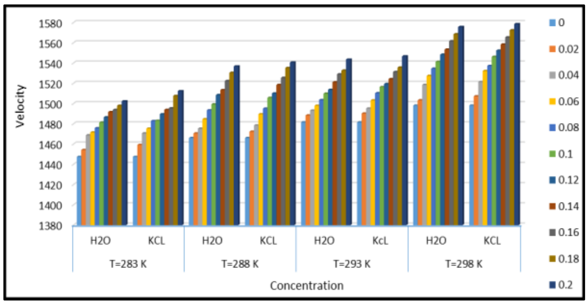


Fig.1. Ultrasonic velocity at different temperature and concentration

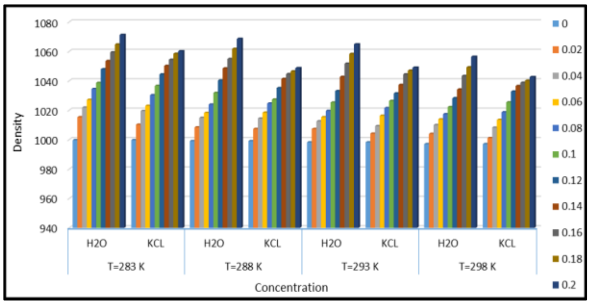


Fig.2. Ultrasonic Density at different temperature and concentration.

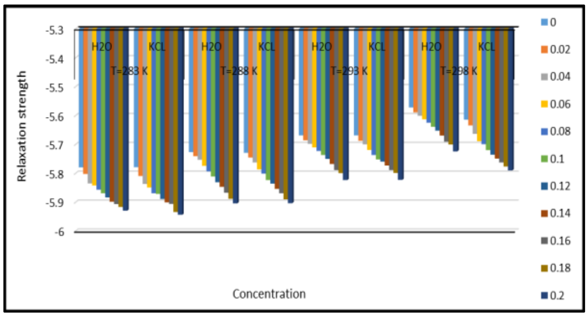


Fig.3. Relaxation strength at different temperature and concentration

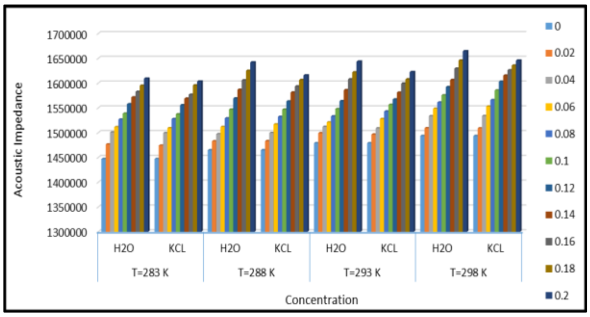


Fig.4. Acoustic Impedance at different temperature and concentration

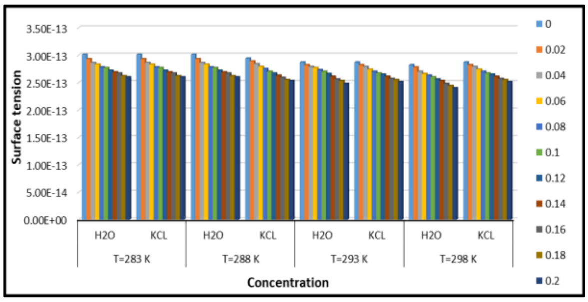


Fig.5. Surface tension at different temperature and concentration

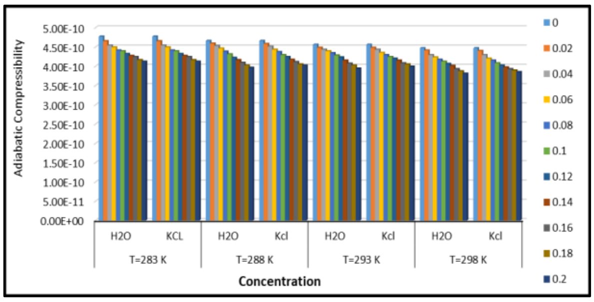


Fig. 6. Adiabatic compressibility at different temperature and concentration

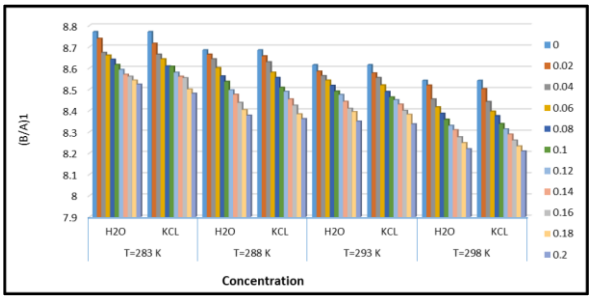


Fig. 7 Nonlinear parameter(B/A)1 at different temperature and concentration

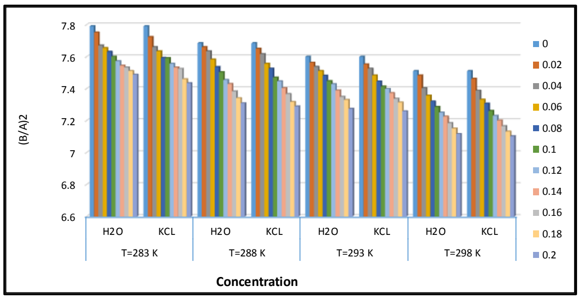


Fig. 8. Nonlinear parameter(B/A)2 at different temperature and concentration

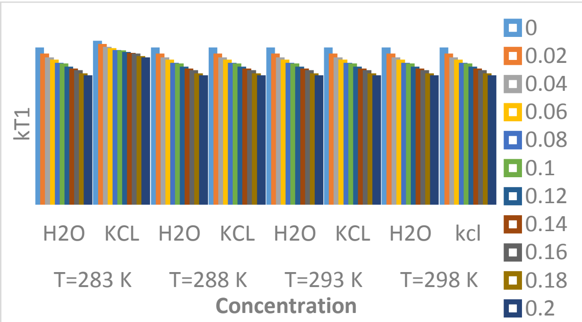


Fig. 9 Isothermal Compressibility (kT1) at different temperature and concentration

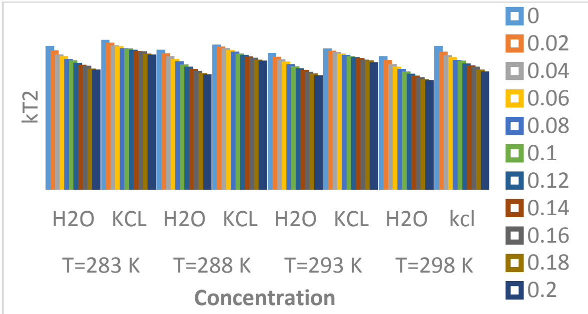


Fig. 10 Isothermal Compressibility (kT2) at different temperature and concentration

Conclusion:

Ultrasound velocity and density were measured for both systems with different concentrations of amino acetic acid as solute, at different temperatures (283.15–298.15K). The solvent-solvent interaction present indicates that it results in an attractive force due to the structure's tendency to form, and the solute interaction indicates that it results in an electrostatic force due to the structure's tendency to be inhibited. According to concentration the value of Velocity, Density, Acoustic impedance are showing the increasing trends and the values of surface tension, adiabatic compressibility, isothermal compressibility, isothermal compressibility, non-linear parameters are showing the decreasing trends, which exhibits a good association in the System II instead of System I.

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Table 1. The Values of Ultransonic Velocity, Density, Acoustic impedance, Adiabatic Compressibility at different temperature and concentration.

Conc.	Velocity		Density		Acoustic Impedance		Adiabatic Compressibility	
	H_2O	KCL	H_2O	KCL	H_2O	KCL	H_2O	KCL
				283 K				
0	1447.427	1447.428	999.7	999.7	1446992.77	1446993.77	4.77E-10	4.77E-10
0.02	1454.25	1459.27	1015.264	1010.2	1476447.67	1474154.55	4.65E-10	4.65E-10
0.04	1468.689	1470.56	1021.803	1019.5	1500710.83	1499235.92	4.54E-10	4.54E-10
0.06	1471.531	1475.34	1027.014	1023.023	1511282.94	1509306.75	4.49E-10	4.49E-10
0.08	1475.804	1482.815	1034.468	1030.263	1526672.01	1527689.43	4.41E-10	4.41E-10
0.1	1481.304	1483.12	1038.653	1036.532	1538560.84	1537301.34	4.39E-10	4.39E-10
0.12	1486.512	1489.55	1047.892	1044.362	1557704.03	1555629.42	4.32E-10	4.32E-10
0.14	1491.739	1493.9	1053.423	1050.123	1571432.17	1568778.75	4.27E-10	4.27E-10
0.16	1493.812	1495.4	1059.361	1054.325	1582486.17	1576637.61	4.24E-10	4.24E-10
0.18	1497.963	1507.63	1064.701	1058.422	1594882.7	1595708.76	4.16E-10	4.16E-10
0.2	1502.304	1512.32	1071.192	1060.137	1609256.03	1603266.39	4.12E-10	4.12E-10
				288K				
0	1466.032	1466.032	999.1	999.1	1464713	1464713	4.66E-10	4.66E-10
0.02	1470.612	1472.33	1008.314	1007.32	1482839	1483107	4.59E-10	4.58E-10

0.04	1475.307	1478.47	1014.836	1014.36	1497195	1499701	4.53E-10	4.51E-10
0.06	1484.667	1489.52	1018.192	1018.354	1511676	1516859	4.46E-10	4.43E-10
0.08	1493.447	1495.13	1023.849	1024.63	1529064	1531955	4.38E-10	4.37E-10
0.1	1499.309	1505.74	1031.734	1027.237	1546888	1546751	4.31E-10	4.29E-10
0.12	1508.438	1510.12	1040.235	1035.123	1569130	1563160	4.22E-10	4.24E-10
0.14	1513.392	1518.46	1048.497	1041.241	1586787	1581083	4.16E-10	4.17E-10
0.16	1522.348	1525.44	1054.823	1044.559	1605808	1593412	4.09E-10	4.11E-10
0.18	1530.436	1535.19	1061.734	1046.468	1624916	1606527	4.02E-10	4.05E-10
0.2	1536.783	1540.66	1068.496	1048.654	1642046	1615619	3.96E-10	4.02E-10
				293 K				
0	1481.496	1481.496	998.2	998.2	1478829	1478829	4.56E-10	4.56E-10
0.02	1488.361	1490.263	1007.287	1004.123	1499207	1496407	4.48E-10	4.48E-10
0.04	1493.132	1495.137	1012.499	1009.165	1511795	1508840	4.43E-10	4.43E-10
0.06	1497.934	1503.205	1015.301	1016.25	1520854	1527632	4.39E-10	4.35E-10
0.08	1503.589	1510.33	1019.63	1021.56	1533104	1542893	4.34E-10	4.29E-10
0.1	1509.838	1516.338	1025.213	1026.32	1547906	1556248	4.28E-10	4.24E-10
0.12	1513.612	1519.345	1033.099	1031.45	1563711	1567128	4.23E-10	4.20E-10
0.14	1521.122	1524.258	1042.649	1037.254	1585996	1581043	4.15E-10	4.15E-10
0.16	1528.904	1531.265	1051.643	1044.38	1607861	1599223	4.07E-10	4.08E-10
0.18	1532.634	1535.695	1058.29	1046.929	1621971	1607764	4.02E-10	4.05E-10
0.2	1543.496	1546.65	1064.83	1048.966	1643561	1622383	3.94E-10	3.99E-10
				298 K				
0	1498.101	1498.101	997	997	1493607	1493607	4.47E-10	4.47E-10
0.02	1503.304	1507.235	1003.936	1001.12	1509221	1508923	4.41E-10	4.40E-10
0.04	1518.44	1521.342	1009.938	1008.19	1533530	1533802	4.29E-10	4.29E-10
0.06	1527.347	1532.214	1013.832	1013.45	1548473	1552822	4.23E-10	4.20E-10
0.08	1534.463	1537.234	1017.36	1018.632	1561101	1565876	4.17E-10	4.15E-10
0.1	1541.321	1546.253	1022.154	1025.32	1575467	1585404	4.12E-10	4.08E-10
0.12	1548.361	1552.342	1028.23	1032.72	1592071	1603135	4.06E-10	4.02E-10
0.14	1553.401	1558.412	1034.117	1036.511	1606398	1615311	4.01E-10	3.97E-10
0.16	1561.63	1565.426	1043.368	1038.697	1629355	1626003	3.93E-10	3.93E-10
0.18	1568.53	1572.426	1049.239	1040.146	1645763	1635553	3.87E-10	3.89E-10
0.2	1575.632	1578.455	1056.345	1042.579	1664411	1645664	3.81E-10	3.85E-10

Table 2. The values of relaxation strength, surface tension, relative association, solvation no at different temperature and concentration.

Conc.	**Relaxation Strength**		**Surface tension**		**Relative association**		**Solvation Number**	
	H_2O	**KCL**	**H_2O**	**KCL**	**H_2O**	**KCL**	**H_2O**	**KCL**
				283 K				
0	-5.77903	-5.77864	3.01E-13	3.01E-13	0.33333	0.33333	9.18E-09	1.26E-10
0.02	-5.80224	-5.80902	2.93E-13	2.93E-13	0.33693	0.33410	9.16E-09	1.26E-10
0.04	-5.83476	-5.83661	2.86E-13	2.86E-13	0.33577	0.33458	9.13E-09	1.25E-10
0.06	-5.84201	-5.84893	2.83E-13	2.83E-13	0.33683	0.33465	9.12E-09	1.25E-10
0.08	-5.85651	-5.86859	2.78E-13	2.78E-13	0.33829	0.33532	9.11E-09	1.25E-10
0.1	-5.86863	-5.87092	2.77E-13	2.77E-13	0.33840	0.33729	9.10E-09	1.25E-10
0.12	-5.88351	-5.88869	2.72E-	2.72E-	0.34021	0.33837	9.09E-	1.25E-10

			13	13			09	
0.14	-5.89840	-5.90027	2.69E-13	2.69E-13	0.34081	0.33925	9.08E-09	1.24E-10
0.16	-5.90605	-5.90562	2.67E-13	2.67E-13	0.34225	0.34026	9.07E-09	1.24E-10
0.18	-5.91621	-5.93383	2.62E-13	2.62E-13	0.34303	0.33882	9.07E-09	1.24E-10
0.2	-5.92902	-5.94331	2.60E-13	2.60E-13	0.34309	0.33831	9.06E-09	1.24E-10
				288K				
0	-5.72659	-5.72887	3.01E-13	2.94E-13	0.33333	0.33333	1.26E-10	1.26E-10
0.02	-5.74079	-5.74538	2.93E-13	2.89E-13	0.33536	0.33463	1.26E-10	1.26E-10
0.04	-5.7527	-5.76205	2.86E-13	2.84E-13	0.33645	0.33557	1.26E-10	1.26E-10
0.06	-5.77404	-5.78599	2.83E-13	2.79E-13	0.33543	0.33440	1.25E-10	1.25E-10
0.08	-5.79345	-5.80075	2.78E-13	2.75E-13	0.33532	0.33519	1.25E-10	1.25E-10
0.1	-5.81082	-5.82294	2.77E-13	2.70E-13	0.33658	0.33368	1.25E-10	1.25E-10
0.12	-5.83096	-5.83573	2.72E-13	2.67E-13	0.33730	0.33526	1.25E-10	1.25E-10
0.14	-5.84635	-5.85363	2.69E-13	2.63E-13	0.33886	0.33539	1.25E-10	1.25E-10
0.16	-5.86697	-5.8691	2.67E-13	2.59E-13	0.33890	0.33492	1.25E-10	1.25E-10
0.18	-5.88797	-5.88993	2.62E-13	2.55E-13	0.33932	0.33340	1.25E-10	1.25E-10
0.2	-5.90402	-5.90317	2.60E-13	2.53E-13	0.34007	0.33291	1.25E-10	1.25E-10
				293 K				
0	-5.66833	-5.66833	2.87E-13	2.87E-13	0.333333	0.333333	1.26E-10	1.26E-10
0.02	-5.68559	-5.68743	2.82E-13	2.82E-13	0.334816	0.333339	1.26E-10	1.26E-10
0.04	-5.69777	-5.69962	2.79E-13	2.79E-13	0.335473	0.33392	1.26E-10	1.26E-10
0.06	-5.7099	-5.71897	2.77E-13	2.74E-13	0.335323	0.33446	1.26E-10	1.26E-10
0.08	-5.72214	-5.73634	2.73E-13	2.70E-13	0.335487	0.334621	1.25E-10	1.25E-10
0.1	-5.7365	-5.75176	2.70E-13	2.67E-13	0.335927	0.334849	1.25E-10	1.25E-10
0.12	-5.75002	-5.7591	2.66E-13	2.65E-13	0.337667	0.335856	1.25E-10	1.25E-10
0.14	-5.76775	-5.77263	2.61E-13	2.61E-13	0.339106	0.336658	1.25E-10	1.25E-10
0.16	-5.78864	-5.78832	2.56E-13	2.57E-13	0.34029	0.337419	1.25E-10	1.25E-10
0.18	-5.79922	-5.79874	2.53E-13	2.55E-13	0.341608	0.337267	1.25E-10	1.25E-10
0.2	-5.82333	-5.82266	2.48E-13	2.51E-13	0.3413	0.33553	1.25E-10	1.25E-10
				298 K				
0	-5.57195	-5.61403	2.82E-	2.87E-13	0.33333	0.33333	1.26E-	1.26E-10

			13		3	3	10	
0.02	-5.58882	-5.63399	2.78E-13	2.82E-13	0.334491	0.332682	1.26E-10	1.26E-10
0.04	-5.60084	-5.66324	2.70E-13	2.79E-13	0.333136	0.331925	1.26E-10	1.26E-10
0.06	-5.61281	-5.68866	2.66E-13	2.74E-13	0.33247	0.331289	1.26E-10	1.26E-10
0.08	-5.62482	-5.69902	2.63E-13	2.70E-13	0.33208	0.331896	1.26E-10	1.26E-10
0.1	-5.63891	-5.71967	2.60E-13	2.67E-13	0.33216	0.332127	1.26E-10	1.26E-10
0.12	-5.65213	-5.73536	2.56E-13	2.65E-13	0.332616	0.333211	1.26E-10	1.26E-10
0.14	-5.6694	-5.74892	2.53E-13	2.61E-13	0.333435	0.333132	1.26E-10	1.26E-10
0.16	-5.68996	-5.76245	2.48E-13	2.57E-13	0.334645	0.332339	1.26E-10	1.26E-10
0.18	-5.70034	-5.77602	2.44E-13	2.55E-13	0.335047	0.331321	1.24E-10	1.26E-10
0.2	-5.72407	-5.7897	2.40E-13	2.51E-13	0.335796	0.330827	1.24E-10	1.26E-10

Table 3. The values of Isothermal Compressibility, nonlinear parameter at different temperature and Concentration

Conc.	**KT1**		**KT2**		**B/A1**		**B/A2**	
	H_2O	**KCL**	**H_2O**	**KCL**	**H_2O**	**KCL**	**H_2O**	**KCL**
				283 K				
0	6.36E-11	6.64E-11	6.36E-11	6.64E-11	8.770635	8.770630	7.79057	7.79056
0.02	6.1E-11	6.5E-11	6.15E-11	6.51E-11	8.738868	8.715686	7.75167	7.72328
0.04	5.94E-11	6.38E-11	5.96E-11	6.39E-11	8.672617	8.664128	7.67055	7.66015
0.06	5.85E-11	6.33E-11	5.88E-11	6.34E-11	8.659730	8.642536	7.65477	7.63371
0.08	5.72E-11	6.25E-11	5.76E-11	6.26E-11	8.640448	8.609051	7.63116	7.59271
0.1	5.68E-11	6.24E-11	5.7E-11	6.25E-11	8.615792	8.607691	7.60097	7.59105
0.12	5.56E-11	6.17E-11	5.58E-11	6.18E-11	8.592614	8.579168	7.57258	7.55612
0.14	5.48E-11	6.12E-11	5.5E-11	6.13E-11	8.569513	8.560010	7.54430	7.53266
0.16	5.42E-11	6.1E-11	5.46E-11	6.11E-11	8.560397	8.553430	7.53313	7.52460
0.18	5.28E-11	5.99E-11	5.33E-11	6E-11	8.542217	8.500268	7.51087	7.45951
0.2	5.19E-11	5.94E-11	5.28E-11	5.96E-11	8.523313	8.480110	7.48773	7.43482
				288K				
0	6.36E-11	6.3597E-11	6.18E-11	6.4109E-11	8.684711	8.684711	7.68536	7.68536
0.02	6.1E-11	6.1011E-11	6.03E-11	6.3341E-11	8.663892	8.656116	7.65986	7.65034
0.04	5.94E-11	5.9387E-11	5.89E-11	6.2624E-11	8.642685	8.628474	7.63390	7.61649
0.06	5.85E-11	5.8507E-11	5.76E-11	6.1628E-11	8.600807	8.579301	7.58262	7.55628
0.08	5.72E-11	5.7222E-11	5.65E-11	6.1022E-11	8.562001	8.554614	7.53510	7.52605
0.1	5.68E-11	5.685E-11	5.51E-11	6.0044E-11	8.536344	8.508428	7.50368	7.46950
0.12	5.56E-11	5.5556E-11	5.41E-11	5.9547E-11	8.496787	8.48955	7.45524	7.44638
0.14	5.48E-11	5.4759E-11	5.3E-11	5.8786E-11	8.47552	8.453907	7.42920	7.40274
0.16	5.42E-11	5.4177E-11	5.22E-11	5.8172E-11	8.437424	8.424376	7.38256	7.36658
0.18	5.28E-11	5.2793E-11	5.11E-11	5.7361E-11	8.403404	8.383575	7.34090	7.31662
0.2	5.19E-11	5.195E-11	5.06E-11	5.6924E-11	8.376958	8.360910	7.30851	7.28887

				293 K				
0	6.36E-11	6.36E-11	6.04E-11	6.24E-11	8.614935	8.614935	7.599921	7.599921
0.02	6.1E-11	6.1E-11	5.86E-11	6.14E-11	8.584424	8.576021	7.56256	7.552270
0.04	5.94E-11	5.94E-11	5.74E-11	6.09E-11	8.563385	8.554583	7.536798	7.526020
0.06	5.85E-11	5.85E-11	5.64E-11	6.01E-11	8.542344	8.519404	7.511034	7.482943
0.08	5.72E-11	5.72E-11	5.52E-11	5.94E-11	8.517739	8.488648	7.480904	7.445284
0.1	5.68E-11	5.68E-11	5.43E-11	5.88E-11	8.490763	8.462939	7.447873	7.413803
0.12	5.56E-11	5.56E-11	5.34E-11	5.85E-11	8.474579	8.450148	7.428056	7.398141
0.14	5.48E-11	5.48E-11	5.26E-11	5.8E-11	8.442613	8.429358	7.388914	7.372683
0.16	5.42E-11	5.42E-11	5.17E-11	5.74E-11	8.40982	8.399937	7.34876	7.336658
0.18	5.28E-11	5.28E-11	5.11E-11	5.7E-11	8.394221	8.381476	7.329658	7.314052
0.2	5.19E-11	5.19E-11	5.02E-11	5.61E-11	8.349223	8.336275	7.274559	7.258704
				298 K				
0	6.36E-11	6.3597E-11	5.89E-11	6.3597E-11	8.541615	8.541615	7.510141	7.510141
0.02	6.1E-11	6.1011E-11	5.72E-11	6.1011E-11	8.518974	8.501972	7.482417	7.461599
0.04	5.94E-11	5.9387E-11	5.52E-11	5.9387E-11	8.453992	8.441681	7.402848	7.387773
0.06	5.85E-11	5.8507E-11	5.4E-11	5.8507E-11	8.416355	8.395973	7.356761	7.331804
0.08	5.72E-11	5.7222E-11	5.31E-11	5.7222E-11	8.386599	8.375087	7.320325	7.306229
0.1	5.68E-11	5.685E-11	5.19E-11	5.685E-11	8.358182	8.337902	7.285529	7.260696
0.12	5.56E-11	5.5556E-11	5.09E-11	5.5556E-11	8.329273	8.313042	7.250131	7.230255
0.14	5.48E-11	5.4759E-11	5E-11	5.4759E-11	8.308738	8.288453	7.224985	7.200146
0.16	5.42E-11	5.4177E-11	4.92E-11	5.4177E-11	8.275494	8.260277	7.184279	7.165645
0.18	5.28E-11	5.2793E-11	4.85E-11	5.2793E-11	8.247888	8.232408	7.150475	7.131520
0.2	5.19E-11	5.195E-11	4.79E-11	5.195E-11	8.219726	8.208603	7.115992	7.102371