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Effect of isotopy on the thermodynamic and thermoacoustical properties of solutions

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Abstract

Theoretical formulations have been developed for calculating a number of important and useful thermodynamic and thermoacoustical properties of water (or heavy water) + DMSO/DMF at 25˚C. Similar formulations have also been successfully extended for FM, AM, DMF and DMA in H_2O and D_2O at 20˚C. Thus, the effect of isotopy on the theoretically deduced properties has been studied. The results are found to be quite satisfactory, and compare well with the experimental observations.

Keywords: Thermodynamic and thermoaccoustical properties, effect of isotopy on these properties, sound speed, density, DMSO, DMF, hole theory.

Introduction

Due to great complexicity of the liquid state, the main factors which determine the physicochemical properties, namely, the intermolecular interaction and structure have been investigated very little [1]. The study of isotopic liquids which differ in the mass of the atoms, and are identical in molecular composition and structure, and they have the same types of intermolecular bonds[2]. Hence , the study of isotope effect leads to the important results on the relation of the intermolecular interaction and physicochemical properties to the mass of the nuclei and the energy of atom and molecular motion[3]. Morever, the study of

the properties of isotopic liquids is of important independent value due to then use in atomic technology, nuclear chemistry, biology and other sciences[4].

The most widely investigated stable isotopes of deuterium which is produced in the form of heavy water and used all over the world in large amounts as neutron absorb in atomic reactors and also it may become an important fuel when it is possible to control thermonuclear processes [5], Deuterium is also used widely for investigating the mechanism of chemical and biological processes.

Keeping in view the important isotopic liquids it would be worth while to study the physicochemical properties theoretically. It would be important to mention the well known monograph of Rabinovich[6]. This monograph deals with the effect of isotopy on the various equilibrium and transport properties. This compilation covers the works carried out upto 1966. The properties discussed are the vapour pressure, molal volume, critical temperature,sound velocity, compressibility, heat capacity, viscosity, surface tension etc.

Isotope effects on the thermodynamic properties of solutions have been experimentally studied by Van Hook et al[7-12] who carried out extensive studies of molar volume as a number of isotopic solutions. They have shown that molar volume isotope effects to be of critical importance in arriving at an understanding of the excess thermodynamic properties of solution. Latter on, they [13] have measured the isothernal compressibilities of C_6H_6, C_6D_6, c-C_6H_{12}, c-C_6D_{12} and then mixtures from 0.1 to 2.5 MPa at 288, 298 and 313K, to the best of our Knowledge (from literature consultation) no previous woek measurements of the ultrasonic propagation properties have been previously reported in isotopic liquids. Rabinovich[6] has reported the experimental data of sound speed, density and adiabatic compressibility of H_2O, C_6H_6, C_6H_{12}, CH_3OH,C_2H_5OH and then corresponding deuterium substituted liquids from 293.15 to 323.15K. we have sccceded in computing a number of useful and important thermodynamic properties of these isotopes from density and sound speed data[14-16]. Recently, a correlation between density-sound speed-surface tension has been employed the some isotopic liquids. Isotope effects on nonlinearity parameter, molecular radii and intermolecular free length has been theoretically studied[16].In the Marczak[17] used sound speed and density data for the study of thermodynamic properties. After an exhaustive consultation of literature we came across two papers[18-19] dealing with the effect of isotope on thermodynamics properties. In binary solutions of organic molecules. In one paper[18] excess enthalpy (H^E), excess heat Capacity(C_p^E), density(ρ) and sound

speed(u) has been accurately measured for binary systems H_2O/D_2O + DMSO/DMF at 25°C. The second paper is more uninformative as the authors have reported the experimental values of excess volume(V^E), apparent molar volume(φ_V), viscocity(η) and sound speed in H2O/D2O solutions of formamide(FM), acetamide(AM), dimethyl formamide(DMF) and dimethyl acetamide(DMA) at 20°C.

Theoretical Formulations

In the present work we have carried out the investigation of the effect of isotopy on the thermodynamic and thermoacoustical properties derived from the experimental data of density and ultrasonic speed. The following properties have been considered:-

(1) Beyer's nonlinearity acoustic parameter(B/A)
(2) Thermal expansion coefficient(α)
(3) Isothermal compressibility(β_T)
(4) Heat Capacities ratio(P_{int})
(5) Cohesive/Internal pressure(ρ_{int})
(6) Pseudo-Gruneisen Parameter (Γ)

During recent past extentive data on density and ultrasonic speed of liquids and solutions have been generated. The instruments involved for the measurements of density and ultrasonic speed are very simple, convenient, economical as well accurate are premise. In recent past [15-16] we have made correlatives between density (ρ)-ultrasonic speed (u) and the thermodynamic properties. These correlations have been found to be very successful and tested by a number of workers in the case of pure liquids, binary and higher order mixtures & very recently Marczak [17] has mentioned the applicability of these relations in his review. These correlations have been deduced on the dimensional basis. The following relations have been obtained for the various thermodynamic properties:-

Adiabatic/Isentropic Compressibility,

$$\beta_s = (u^2\rho)^{-1} \cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots(I)$$

This is the fundamental thermodynamic relation

Thermal expansion coefficient

$$\alpha = \frac{(75.6\times10^{-3})}{T^{1/9}u^{1/2}\rho^{1/3}} \qquad \text{…….(2)}$$

Isothermal compressibility

$$\beta_T = \frac{1.71\times10^{-3}}{T^{9/4}\times u^2\times\rho^{4/3}} \qquad \text{……..(3)}$$

Internal pressure

$P_{int} = 44.2T^{4/3}u^{3/2}\rho$ ……..(4) (at zero pressure)

Heat Capacities ratio

$$\Gamma = \frac{17.1}{T^{4/9}\times\rho^{1/3}} \qquad \text{……..(5)}$$

The importance, significance and theoretical formulations of Beyer's nonlinearity acoustic parameter have been discussed by a large number of workers(X), The traditional method for determining (B/A) plays a significant role in nonlinear acoustic as well as underwater acoustics.

Involves the knowledge of temperature and pressure derivatives of ultrasonic speed, α and Cp, this is the thermodynamic method developed originally by Beyer et al and extended by others. In the case the above coefficients are not available. Some alternative methods were developed.

Hartmann obtained the expression

$$\frac{B}{A} = 2 + \frac{0.98\times10^{-4}}{u} \qquad \text{…….(6)}$$

Ballow proposed the empirical rule as

$$\frac{B}{A} = -0.5 + \frac{1.2\times10^{-4}}{u} \qquad \text{…….(7)}$$

Few other methods have been developed for the determination of B/A, but these are not off general validity.

In the present works properties(1) to (6) have been calculated from ρ and u data using eqs(2) to (7) based on the theoretical considerations, the following systems have been taken for the present study:-

(I) H_2O + DMF
D_2O + DMF

(II) H_2O + DMSO
D_2O + DMSO

(III) H_2O + FM
D_2O + FM

(IV) H_2O + AM
D_2O + AM

(V) H_2O + DMA
D_2O + DMA

The experimental values of ρ and u were taken from the literature[18-19].

Results and discussion

In the present work density((ρ) and sound speed (u) data of isotopic solutions have been employed to study the isotopic effects on the basis of theoretically deduced some useful and important thermodynamic and thermoacoustical properties as mentioned earlier. The experimental of all the system (I) to (V) were taken from the literature[18-19]. Calculated values of β_s, α, β_T, P_{int},γ,σ, Γ and ν of pure liquid isotopes are presented Table 1.

In the formulation part various thermodynamic and thermoacoustic properties (1) to(6) were computed using relevant equations (1) to (7). Various systems undertaken for the study (I) to (V) are listed. Calculated values of β_s, α, β_T, P_{int},γ,σ, Γ, ν and (B/A) for the D_2O + DMSO at 298.15 K are recorded in Table 1. Columns eleven to sixteen are the values of the aforesaid

properties obtained from the hole theory[20-23]. All the properties calculated vary with the mole fractions of H_2O + DMSO at 298.15 K. Similary $P_{int,}$ V_h, γ_h,E_h and ΔE_V obtained from the applications of hole theory vary with the mole fraction of H_2O + DMSO. Similar variations in the afrosaid properties were found in the case of D_2O + DMSO, H_2O+DMF and D_2O + DMF. The increase in the mole fraction of H_2O(decrease with at of DMSO) results in a linear decrease in the values of $\beta_{s,}$ α, β_T upto x=0.750, and then start increasing, P_{int} shows a reverse trend i.e. increases linearly with x, and then starts decreasing almost near the same x.

Heat capacities ration, γ=Cp/Cv= β_T/β_s, is almost constant, as expected. The values of surface tension σ, increase linearly with x and further decreases at the same x. The pseudo-Grüneisen parameter(Γ), increases with x and then shows reverse trend near the same x as observed in other properties. The molar volume v, of isotopic liquids linearly increases at all x. Similar trend is observed in the variation on non-linearity parameter(B/A).The results of calculation from generlalized version of hole theory are depicted in columns twelve to sixteen of Table-2. Computed values include the internal pressure, P_{int}, hole volume V_h, hole radius r_h, hole creation energy E_h, and energy of vaporisation ΔE_v, V_h, r_h, E_h, are found to be constant. Again, ΔE_v increases as x increases and then shows a reverse trend at x≈0.802. The results of Table-3 show that the trend of variation of all the properties reported for D_2O(x)+ DMSO(1-x) is similar to that observed in the case of H_2O(x) + DMSO (1-X). The only difference is the magnitude. Table-4 records the values of all the properties calculate for D_2O(x)+ DMF(1-x) at 298.15K. Here, also we see that the trend of variation is some except the magnitude. Similar results were obtained for H_2O(x)+ DMF(1-x) systems as evident from Table-5.

Keeping in view the limitations and approximations made in the theoretical procedure of obtaining a number of useful and important thermodynamics and thermoacoustical properties, the trend of variations of H_2O(x) + DMSO (1-X), D_2O(x)+ DMSO(1-x), D_2O(x)+ DMF(1-x) and H_2O(x)+ DMF(1-x) is similar except the magnitude.

Conclusion

Thermodynamic and thermoacoustic properties obtained theoretically have been employed to study the effect of isotopy on the solutions. Properties of pure isotopic liquids D_2O, H_2O, DMSO and DMF have been calculated at 298.15 K. The properties calculated include $\beta_{s,}$ α,

β_T, P_{int},γ,σ, Γ, ν and (B/A). In addition generalized version of hole theory has been also been employed to obtain P_{int}, V_h, γ_h,E_h and ΔE_V.

CRediT authorship contribution statement

J.D. Panday: Supervision, Investigation, Methodology.

N.K.Soni: Writing review & editing.
S.K.Vishwakarma: Writing review & editing.
Rahul Kanaoujiya: Conceptualization, Writing - review & editing

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Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Availability of data and material

The corresponding author is willing to provide the datasets created during and/or analysed during the current work upon reasonable request.

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Glossory of Symbols

V- Molar Volume

u- Sound speed

T- Temperature ˚K

α- Thermal expansion coefficient
β_T- Isothermal Compressibility

β_s- Isentropic Compressibility

γ- Heat Capacities ratio

P_{int} - Internal Pressure

(B/A)- Nonlinearity Parameter

Γ – Pseudo-Grüneisen Parameter

P_{int}- Internal Pressure

V_h- hole volume

r_h- hole radius

E_h- hole creation energy

ΔE_V- Energy of vaporization

REFERENCES

1. S. S. de Jesus, & R. Maciel Filho, *Renewable and Sustainable Energy Reviews 157* (2022) 112039.
2. J. Chou, Y. Zhao, X. T. Li, W. P. Wang, S. J. Tan, Y. H. Wang, ... & Y. G. Guo, *Angewandte Chemie* 134 (2022) e202203137.
3. T. Udagawa, I. Hattori, Y. Kanematsu, T. Ishimoto & M. Tachikawa, *International Journal of Quantum Chemistry 122*(2022)e26962.
4. S. Abdelaal, W. Hassanin, A. M. Abdelhady, A. M. Rashad, M. F. Kassab, S. Salama, & M. H. Ibraheim, *Chemosphere* (2022)134969.
5. C. N. Taylor, *Journal of Nuclear Materials558*(2022)153396.
6. I. B. Rabinovich, Influence of isotopy on the Physicochemical Properties of liquids, Consultants Bureau, New York, P.1-269(1970) Translated from Russian.
7. M. K. Dutta-Choudhury, G. Dessauges, & W. A. Van Hook, *The Journal of Physical Chemistry86*(1982)4068-4073.
8. G. Jancso & W. A. Van Hook, *Chemical Reviews 74*(1974)689-750.
9. G. Jancsó & W. A. Van Hook, *Physica A: Statistical Mechanics and its Applications 91*(1978)619-624.
10. G. Jakli, P. Tzias & W. A. Van, *The Journal of Chemical Physics 68*(1978)3177-3190.
11. M. K. Dutta-Choudhury, & W. A. Van Hook, *The Journal of Physical Chemistry*, *84*(1980)2735-2740.

12.M. K. Dutta-Choudhury, N. Miljevic, & W. A. Van Hook, *The Journal of Physical Chemistry86*(1982), 1711-1721.

13.S. Matsuo & A. Van Hook, *Journal of Physical Chemistry 88*(1984)1032-1040.

14.J.D.Panday, A.K.Singh, R. Dey, J.Pure. Appl. Ultrason, 26(2004)100

15. J.D. Panday, V. Sanguri, Sunil, S.Kumar, J.Pure Appl.Ultrason, 38(2016)103.

16.J.D. Panday, A.K.Singh, N.K.Soni, B.S.Bhist, R.Dey, Pramana- journal of physics,67(2006)389

17. W. Marczak, *Journal of Chemical & Engineering Data*, *44*(1999)621-625.

18.K. Miyai, M. Nakamura, K. Tamura, & S. Murakami, *Journal of solution chemistry 26*(1997)973-988.

19.M. Jelinska-Kazimierczuk & J. Szydlowski, *Journal of solution chemistry30*(2001)623-640.

20.J. D. Pandey, T. Srivastava, P. Chandra, D. K. Dwivedi, & V. Sanguri, *Journal of Molecular Liquids157*(2010)158-161.

21.J. D. Pandey, V. Sanguri, & D. K. Dwivedi,. *Physics and Chemistry of Liquids 50*(2012) 69-78.

22.V. Sanguri, P. Chandra, D. K. Dwivedi, R. Sethi, & J. D. Pandey, *Proceedings of the National Academy of Sciences, India Section A: Physical Sciences 83*(2013)225-231.

23.S. C. Shrivastava, S. Srivastava, & J. D. Pandey, *Chemical Physics 549*(2021)111284.

Table-1.

Calculated values of adiabatic compressibility (βs), thermal expansivity (α), isothermal compressibility (βt), internal pressure (Pint), specific heat ratio (ϒ), surface tension (σ), Pseudo-Grüneisen Parameter(Γ),molar volume(V)of D_2O, H_2O, DMSO pure liquids 298.15 K.

Liquids	β_s T M^2N^{-1}	α kK^{-1}	β_T T M^2N^{-1}	P_{int} atm 10^8	ϒ	σ NM^{-1}	r	V CM^3M^{-1}
D_2O	41.091	1.008	54.029	55.621	1.315	42.197	1.048	88.743
H_2O	45.270	1.041	61.586	50.419	1.360	38.250	1.161	98.290
DMSO	40.971	1.008	54.020	55.628	1.318	42.202	1.060	89.476

Table-2

Calculated values of adiabatic compressibility (β_s), thermal expansivity (α), isothermal compressibility (βt), internal pressure (P_{int}), specific heat ratio (Υ), surface tension (σ), Pseudo-Grüneisen Parameter(Γ),molar volume(V) non-linearity parameter (B/A), internal pressure $(Pint)_{Hart}$, hole volume (V_h) hole radius (r_h), hole creasion energy (E_h), and energy of vaporisation (ΔE), H20+DMSO system 298.15 K.

x	β_s	α	β_T	P_{int}	Υ	σ	r	V	B/A HER	B/A Ballo	P_{int}	V_h	r_h	E_h	ΔE_v
	$T M^2N^{-1}$	kK^{-1}	$T M^2N^{-1}$	atm 10^8		NM^{-1}		CM^3M^{-1}			atm	$M^3 10^{23}$	$M10^4$	$J10^6$	$jmol^1 10^4$
0.000	41.429	1.011	54.624	55.166	1.318	41.851	1.057	87.650	8.601	7.583	251393	1.464	1.464	1.517	4.034
0.022	41.194	1.009	54.310	55.405	1.318	42.032	1.058	87.632	8.583	7.561	253305	1.464	1.464	1.517	4.051
0.050	40.898	1.007	53.916	55.709	1.318	42.263	1.060	87.610	8.560	7.533	255749	1.464	1.464	1.517	4.074
0.101	40.327	1.004	53.154	56.306	1.318	42.716	1.063	87.568	8.516	7.479	260581	1.464	1.464	1.517	4.117
0.149	39.748	1.000	52.382	56.927	1.318	43.188	1.066	87.528	8.471	7.423	265650	1.464	1.464	1.517	4.163
0.199	39.119	0.996	51.545	57.619	1.318	43.713	1.070	87.485	8.421	7.362	271350	1.464	1.464	1.517	4.213
0.257	38.344	0.991	50.516	58.498	1.317	44.379	1.074	87.439	8.359	7.286	278668	1.464	1.464	1.517	4.277
0.300	37.726	0.987	49.696	59.220	1.317	44.927	1.078	87.407	8.308	7.224	284763	1.464	1.464	1.517	4.330
0.351	36.965	0.982	48.687	60.138	1.317	45.623	1.083	87.376	8.245	7.147	292603	1.464	1.464	1.517	4.397
0.399	36.229	0.977	47.715	61.054	1.317	46.319	1.088	87.359	8.184	7.072	300558	1.464	1.464	1.517	4.464
0.450	35.401	0.971	46.625	62.122	1.317	47.129	1.095	87.361	8.112	6.985	309989	1.464	1.464	1.517	4.542
0.500	34.368	0.964	45.269	63.512	1.317	48.183	1.103	87.393	8.021	6.873	322528	1.464	1.464	1.517	4.644
0.550	33.801	0.960	44.535	64.296	1.318	48.778	1.109	87.469	7.969	6.809	329863	1.464	1.464	1.517	4.701
0.600	33.034	0.955	43.549	65.385	1.318	49.604	1.118	87.612	7.896	6.720	340283	1.464	1.464	1.517	4.781
0.650	32.378	0.950	42.722	66.332	1.319	50.322	1.127	87.849	7.829	6.638	349809	1.464	1.464	1.517	4.850
0.700	31.907	0.947	42.158	66.996	1.321	50.826	1.138	88.213	7.775	6.571	357176	1.464	1.464	1.517	4.899
0.750	31.743	0.947	42.030	67.149	1.324	50.942	1.148	88.771	7.742	6.531	360370	1.464	1.464	1.517	4.910
0.802	32.096	0.950	42.629	66.440	1.328	50.404	1.159	89.596	7.747	6.537	356192	1.464	1.464	1.517	4.858
0.847	33.064	0.958	44.075	64.798	1.333	49.159	1.166	90.585	7.801	6.603	343647	1.464	1.464	1.517	4.738
0.900	35.273	0.975	47.283	61.472	1.340	46.636	1.171	92.111	7.942	6.776	317046	1.464	1.464	1.517	4.495
0.950	38.912	1.001	52.512	56.822	1.350	43.108	1.171	93.984	8.178	7.065	279995	1.464	1.464	1.517	4.155
0.975	41.522	1.018	56.249	53.966	1.355	40.941	1.168	95.073	8.346	7.270	257704	1.464	1.464	1.517	3.946
1.000	44.774	1.039	60.912	50.837	1.360	38.567	1.164	96.284	8.548	7.518	233921	1.464	1.464	1.517	3.717

Table3 Calculated values of adiabatic compressibility (β_s), thermal expansivity (α), isothermal compressibility (βt), internal pressure (P_{int}), specific heat ratio (Υ), surface tension (σ), Pseudo-Grüneisen Parameter(Γ),molar volume(V) non-linearity parameter (B/A), internal pressure $(Pint)_{Hart}$, hole volume (V_h), hole radius (r_h), hole creasion energy (E_h), energy of vaporisation (ΔE), and thermal expansivity hole theory of D_20+DMSO system 298.15 K

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x	β_s	α	β_T	P_{int}	Υ	σ	Γ	V	B/A HER	B/A Ballo	P_{int}	V_h	r_h	E_h	ΔE_v	$\alpha_{hole\ theory}$
	$T\ M^2N^{-1}$	kK^{-1}	$T\ M^2N^{-1}$	atm 10^8		NM^{-1}		CM^3M^{-1}			atm	$M^3 10^{23}$	$M10^4$	$J10^6$	$jmol^1 10^4$	kK^{-1}
0.000	41.430	1.011	54.625	55.165	1.318	41.851	1.057	89.476	8.602	7.583	251389	1.464	1.517	4.034	49.360	1.385
0.025	41.175	1.009	54.272	55.434	1.318	42.055	1.057	89.398	8.584	7.562	253411	1.464	1.517	4.053	49.557	1.383
0.052	40.896	1.007	53.887	55.731	1.318	42.280	1.058	89.310	8.565	7.539	255647	1.464	1.517	4.075	49.773	1.380
0.103	40.338	1.004	53.117	56.336	1.317	42.739	1.059	89.134	8.526	7.492	260230	1.464	1.517	4.119	50.214	1.375
0.145	39.860	1.001	52.458	56.865	1.316	43.141	1.059	88.982	8.493	7.451	264268	1.464	1.517	4.158	50.600	1.370
0.202	39.167	0.996	51.503	57.654	1.315	43.739	1.061	88.761	8.444	7.391	270334	1.464	1.517	4.216	51.175	1.364
0.249	38.546	0.992	50.649	58.382	1.314	44.291	1.062	88.563	8.400	7.337	275975	1.464	1.517	4.269	51.705	1.357
0.300	37.853	0.987	49.697	59.219	1.313	44.926	1.063	88.343	8.350	7.276	282531	1.464	1.517	4.330	52.316	1.350
0.350	37.122	0.982	48.695	60.131	1.312	45.618	1.065	88.112	8.297	7.211	289749	1.464	1.517	4.397	52.982	1.341
0.398	36.396	0.977	47.700	61.068	1.311	46.329	1.066	87.884	8.243	7.145	297254	1.464	1.517	4.465	53.669	1.333
0.450	35.574	0.971	46.579	62.168	1.309	47.164	1.068	87.632	8.181	7.069	306179	1.464	1.517	4.546	54.479	1.322
0.500	34.780	0.966	45.498	63.272	1.308	48.001	1.071	87.397	8.120	6.994	315268	1.464	1.517	4.627	55.298	1.312
0.551	33.970	0.960	44.400	64.442	1.307	48.889	1.073	87.163	8.057	6.916	325041	1.464	1.517	4.712	56.170	1.300
0.650	32.610	0.950	42.564	66.516	1.305	50.462	1.078	86.807	7.946	6.781	342776	1.464	1.517	4.864	57.741	1.280
0.700	32.150	0.946	41.948	67.247	1.305	51.017	1.080	86.711	7.907	6.733	349197	1.464	1.517	4.917	58.311	1.272
0.750	32.006	0.945	41.761	67.472	1.305	51.188	1.082	86.718	7.894	6.717	351298	1.464	1.517	4.934	58.511	1.270
0.802	32.398	0.948	42.297	66.830	1.306	50.700	1.081	86.868	7.925	6.755	345846	1.464	1.517	4.887	58.054	1.276
0.850	33.492	0.956	43.772	65.135	1.307	49.414	1.077	87.148	8.014	6.864	331234	1.464	1.517	4.763	56.763	1.293
0.900	35.756	0.972	46.811	61.936	1.309	46.988	1.066	87.599	8.198	7.090	304055	1.464	1.517	4.529	54.255	1.325
0.950	39.666	0.999	52.043	57.205	1.312	43.399	1.048	88.168	8.507	7.468	265174	1.464	1.517	4.183	50.437	1.369
0.975	42.552	1.017	55.894	54.223	1.314	41.136	1.034	88.471	8.728	7.739	241569	1.464	1.517	3.965	47.972	1.395
1.000	46.249	1.038	60.812	50.900	1.315	38.615	1.017	88.743	9.004	8.076	216140	1.464	1.517	3.722	45.170	1.422

Table-4

Calculated values of adiabatic compressibility (β_s), thermal expansivity (α), isothermal compressibility (βt), internal pressure (P_{int}), specific heat ratio (Υ), surface tension (σ), Pseudo-Grüneisen Parameter(Γ),molar volume(V) non-linearity parameter (B/A), internal pressure $(Pint)_{Hart}$, hole volume (V_h), hole radius (r_h), hole creasion energy (E_h), and energy of vaporisation (ΔE), D_20+DMF system 298.15 K.

x	β_s T M^2N^{-1}	α kK^{-1}	β_T T M^2N^{-1}	P_{int} atm 10^8	Υ	σ NM^{-1}	Γ	V CM^3M^{-1}	B/A HER	B/A Ballo	P_{int} atm	V_h $M^3 10^{23}$	r_h $M10^4$	E_h $J10^6$	ΔE_v $jmol^1 10^4$	$\alpha_{hole\ theory}$ kK^{-1}
0.000	49.885	1.072	69.115	49.885	1.385	35.081	1.206	103.823	8.725	7.734	206135	1.464	1.517	3.381	48.009	1.36
0.024	49.515	1.07	68.558	49.515	1.385	35.294	1.206	103.623	8.706	7.712	208072	1.464	1.517	3.402	48.208	1.36
0.097	48.307	1.063	66.75	48.307	1.382	36.009	1.205	102.993	8.644	7.636	214648	1.464	1.517	3.471	48.885	1.361
0.202	46.444	1.051	63.962	46.444	1.377	37.179	1.203	101.97	8.547	7.517	225520	1.464	1.517	3.584	49.973	1.362
0.301	44.518	1.039	61.088	44.518	1.372	38.484	1.201	100.866	8.445	7.392	237824	1.464	1.517	3.709	51.167	1.364
0.399	42.473	1.026	58.044	42.473	1.367	39.988	1.198	99.639	8.334	7.256	252245	1.464	1.517	3.854	52.519	1.366
0.500	40.276	1.011	54.779	40.276	1.36	41.762	1.194	98.22	8.212	7.107	269516	1.464	1.517	4.025	54.069	1.368
0.600	38.157	0.997	51.623	38.157	1.353	43.663	1.188	96.674	8.095	6.963	288156	1.464	1.517	4.208	55.639	1.37
0.694	36.491	0.984	49.105	36.491	1.346	45.332	1.178	95.128	8.009	6.858	304198	1.464	1.517	4.369	56.842	1.373
0.899	37.331	0.987	49.58	37.331	1.328	45.005	1.116	91.451	8.198	7.09	291213	1.464	1.517	4.338	54.252	1.38
1.000	46.256	1.038	60.819	46.256	1.315	38.612	1.017	88.734	9.005	8.077	216091	1.464	1.517	3.722	45.162	1.385
0.000	49.886	1.072	69.117	49.886	1.385	35.08	1.206	103.823	8.725	7.735	206127	1.464	1.517	3.381	48.008	1.358
0.052	49.067	1.067	67.888	49.067	1.384	35.555	1.206	103.395	8.683	7.683	210473	1.464	1.517	3.427	48.458	1.359
0.152	47.352	1.057	65.319	47.352	1.379	36.599	1.204	102.473	8.595	7.575	220105	1.464	1.517	3.528	49.435	1.36
0.248	45.569	1.046	62.656	45.569	1.375	37.759	1.202	101.473	8.501	7.461	230963	1.464	1.517	3.639	50.505	1.361
0.351	43.504	1.033	59.578	43.504	1.369	39.213	1.2	100.265	8.39	7.325	244783	1.464	1.517	3.78	51.825	1.363
0.450	41.367	1.019	56.4	41.367	1.363	40.859	1.196	98.942	8.273	7.181	260692	1.464	1.517	3.938	53.287	1.365
0.549	39.213	1.004	53.199	39.213	1.357	42.689	1.191	97.479	8.153	7.034	278614	1.464	1.517	4.115	54.852	1.368
0.649	37.238	0.99	50.243	37.238	1.349	44.56	1.183	95.884	8.046	6.903	296868	1.464	1.517	4.295	56.318	1.371
0.749	35.857	0.979	48.09	35.857	1.341	46.048	1.169	94.174	7.986	6.83	310347	1.464	1.517	4.438	57.161	1.375
0.850	36.041	0.979	48.029	36.041	1.333	46.091	1.14	92.384	8.06	6.92	306262	1.464	1.517	4.442	56.128	1.379
0.948	40.112	1.003	53.064	40.112	1.323	42.771	1.079	90.375	8.463	7.414	263437	1.464	1.517	4.122	50.951	1.384
0.975	42.653	1.018	56.264	42.653	1.319	40.933	1.051	312.969	8.694	7.696	241860	1.464	1.517	3.945	168.863	1.394
1.000	46.256	1.038	60.819	46.256	1.315	38.612	1.017	309.936	9.005	8.077	216091	1.464	1.517	3.722	157.744	1.396

Table-5

Calculated values of adiabatic compressibility (β_s), thermal expansivity (α), isothermal compressibility (βt), internal pressure (P_{int}), specific heat ratio (Υ), surface tension (σ), Pseudo-Grüneisen Parameter(Γ),molar volume(V) non-linearity parameter (B/A), internal pressure $(Pint)_{Hart}$, hole volume (V_h), hole radius (r_h), hole creasion energy (E_h), and energy of vaporisation (ΔE), H_20+DMF system 298.15 K.

x	β_s	α	β_T	P_{int}	Υ	σ	Γ	V	B/A HER	B/A Ballo	P_{int}	V_h	r_h	E_h	ΔE_v	$\alpha_{hole\ theory}$
	$T\ M^2N^{-1}$	kK^{-1}	$T\ M^2N^{-1}$	$atm\ 10^8$		NM^{-1}		CM^3M^{-1}				M^310^{23}	$M10^4$	$J10^6$	$jmol^110^4$	kK^{-1}
0.000	49.884	1.072	69.113	46.242	1.385	35.081	1.206	96.407	8.725	7.734	206143	1.464	1.517	3.381	44.581	1.438
0.048	49.116	1.068	67.994	46.812	1.384	35.513	1.208	96.175	8.681	7.681	210316	1.464	1.517	3.423	45.021	1.435
0.146	47.396	1.058	65.493	48.146	1.382	36.526	1.211	95.648	8.581	7.558	220222	1.464	1.517	3.521	46.050	1.427
0.251	45.394	1.046	62.587	49.813	1.379	37.790	1.215	95.011	8.462	7.412	232824	1.464	1.517	3.642	47.328	1.417
0.348	43.399	1.033	59.701	51.609	1.376	39.153	1.219	94.360	8.340	7.263	246698	1.464	1.517	3.774	48.698	1.405
0.449	41.201	1.019	56.529	53.765	1.372	40.789	1.224	93.623	8.202	7.094	263766	1.464	1.517	3.931	50.337	1.389
0.550	38.965	1.005	53.315	56.178	1.368	42.620	1.230	92.858	8.056	6.915	283396	1.464	1.517	4.108	52.166	1.369
0.645	37.011	0.991	50.514	58.499	1.365	44.380	1.235	92.163	7.924	6.754	302762	1.464	1.517	4.278	53.914	1.349
0.749	35.535	0.981	48.397	60.408	1.362	45.828	1.238	91.573	7.824	6.631	318927	1.464	1.517	4.417	55.317	1.332
0.850	35.640	0.981	48.489	60.322	1.361	45.763	1.233	91.291	7.841	6.652	317365	1.464	1.517	4.411	55.069	1.333
0.951	39.603	1.007	53.904	55.718	1.361	42.270	1.202	91.406	8.154	7.035	275856	1.464	1.517	4.074	50.929	1.376
1.000	44.773	1.039	60.911	50.838	1.360	38.568	1.164	91.270	8.548	7.518	233925	1.464	1.517	3.717	46.399	1.417
0.000	49.877	1.072	69.105	46.246	1.385	35.085	1.206	96.407	8.724	7.734	206177	1.464	1.517	3.382	44.585	1.438
0.023	49.518	1.070	68.580	46.511	1.385	35.286	1.207	96.295	8.704	7.709	208108	1.464	1.517	3.401	44.788	1.437
0.099	48.242	1.063	66.724	47.478	1.383	36.019	1.209	95.910	8.630	7.619	215247	1.464	1.517	3.472	45.537	1.431
0.201	46.374	1.052	64.009	48.981	1.380	37.159	1.213	95.325	8.520	7.484	226501	1.464	1.517	3.582	46.691	1.422
0.298	44.445	1.040	61.212	50.650	1.377	38.425	1.217	94.700	8.404	7.342	239248	1.464	1.517	3.704	47.966	1.411
0.405	42.179	1.026	57.937	52.782	1.374	40.043	1.222	93.948	8.264	7.170	255922	1.464	1.517	3.860	49.588	1.396
0.499	40.073	1.012	54.904	54.955	1.370	41.691	1.227	93.233	8.129	7.005	273358	1.464	1.517	4.018	51.236	1.379
0.600	37.903	0.997	51.789	57.415	1.366	43.558	1.232	92.472	7.985	6.829	293633	1.464	1.517	4.198	53.093	1.359
0.692	36.238	0.986	49.405	59.481	1.363	45.125	1.236	91.857	7.872	6.690	311042	1.464	1.517	4.349	54.637	1.340
0.800	35.301	0.979	48.041	60.744	1.361	46.083	1.237	91.362	7.811	6.616	321501	1.464	1.517	4.442	55.497	1.329
0.900	36.842	0.989	50.122	58.842	1.360	44.640	1.222	91.277	7.939	6.773	303635	1.464	1.517	4.303	53.709	1.348
0.977	41.887	1.022	57.002	53.431	1.361	40.535	1.185	91.355	8.330	7.251	255874	1.464	1.517	3.907	48.811	1.396
1.000	44.773	1.039	60.911	50.838	1.360	38.568	1.164	91.270	8.548	7.518	233925	1.464	1.517	3.717	46.399	1.417