# Study of Inter Molecular Interactions in Binary Liquid Mixtures of N, N - Dimethylacetamide with Chloroform using Scaled Particle Theory (SPT)

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**Abstract:** ***Ultrasonic velocity and density have been measured in binary liquid mixture of N, N Dimethylacetamide (DMAc) with chloroform (CF) at 300K.Shape of the constituent molecules are considered as spherical, cubical, tetrahedral and six different discs with the application of scaled particle theory. To examine the intermolecular interactions in these liquid mixtures ultrasonic speeds are theoretically evaluated based on scaled particle theory. Theoretical velocities have been compared with observed velocities for each possible combination. To examine the intermolecular interactions in these liquid mixtures, ultrasonic speeds are theoretically evaluated based on scaled particle theory. An attempt has been made to predict the behavioural shape of N, N Dimethylacetamide (DMAc) and chloroform (CF).***

**Keywords:** Ultrasonic velocities, Scaled Particle Theory (SPT); Molecular interactions.

## 1. Introduction

Liquid mixtures are indispensable in almost all industries and all biological sciences. There exists an imperative need to understand these systems and to be able to predict their behavior from the molecular point of view. The use of measurable macroscopic or global quantities to probe into the microscopic, or the local properties of the system has become an essential area of research. All theories of liquids developed so far make approximations at some stages of their development. Until the theory based on distribution function reaches a form in which precise limits on the errors can be specified, there will always be role for auxiliary models of liquid state. Such models are likely to be helpful for liquid with non-simple molecules. Quite a number of such model have been proposed. The mathematics of some of these models are relatively simple as compared to that of distribution function. The study of these models assists physical insight into the liquid state. Hard convex liquid molecules model is used by many researchers [1-4]. For hard spheres, it is only necessary to determine radial distribution function g (d).Reiss[5] et al. developed a method given in Barker and Henderson[6]called the scaled particle theory (SPT)for obtaining distribution function (d) and the pressure (p) leading to an equation of state for liquid consisting hard convex molecules. Scaled particle theory[7-8]has been used my some researchers considering different shapes of liquid molecules viz. spherical, cubical and tetrahedral. Liquid molecules may be assumed to have different shapes other than spherical. Although, the chemical structure of a molecule is known, no definite shape has been attached to it in liquid state [9]. In the Barker & Henderson, it is proved that SPT works well with the equation of state for 1-D hard rods, 2-D hard discs along with 3-D hard sphere. In the present paper, using scaled particle theory, ultrasonic approach has been used for assigning a specific shape to particular liquid molecule by calculating theoretical ultrasonic velocities and comparing them with experimental velocities. If the intermolecular interactions in binary mixture are weak then molecules may retain the same shape in the mixture but for strong interactions, constituent liquid molecules may be distorted or deformed. The distortion is likely to occur in most of the cases hence the shape of liquid molecule may be called as behavioural shape in a particular mixture. The shape study of N, N Dimethylacetamide (DMAc) and chloroform (CF) liquid molecules is carried out in the present paper.

## 2. Material and Method

The liquid mixtures of various concentrations in mole fraction were prepared by taking N, N dimeyhyl acetamide and Chloroform with minimum assay (>99.9) of analytical grade (ARgrade), manufactured by Sisco Research Laboratory, Mumbai, India which were used as such without further purification. The velocity of ultrasonic waves in the liquid mixture have been measured by using a single crystal variable frequency ultrasonic interferometer supplied by Mittal Enterprises, New Delhi (M-81) working at four different frequencies (2, 4, 6 & 8MHz) with a tolerance of ± 0.005%. There is a provision of maintaining constant temperature by temperature water bath supplied by Mittal Enterprises, New Delhi.

### Scaled Particle theory (SPT)

The scaled-particle theory (SPT) offers a powerful conceptual and computational frame work within which molecular order and thermodynamic properties can be examined [10]. SPT links the microscopic parameters viz., radius, surface area and hard core volume of a molecule with the macroscopic parameters like ultrasonic speed. The ultrasonic speeds of pure liquids and their binary liquid mixtures can be estimated theoretically based on some, statistical, empirical and semi empirical models Nomoto's


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relation, Impedance dependence relation, Schaaff's collision factor theory, Jacobson's free length theory, Ideal mixing relation, Zhang-Junjie relation Danusso model and Rao's specific velocity models. However, all these models have a common drawback that, the shapes of the participating species have not been taken into consideration while estimating ultrasonic speed. On the other hand, in scaled particle theory [11] participating components are considered to have different shapes (like sphere, cube, tetrahedral, disc 1, disc 2, disc 3, disc 4, disc 5 and disc 6 ) and when the shape of the participating components match the actual shape of the species, then the theoretical ultrasonic speeds estimated based on this model will give values close to the experimental values. Although, the chemical structure of a molecule is known, no definite shape has been attached to it in liquid state. Recently, Ghosh et al.[9] have used the scaled particle theory for the binary mixtures of 1, 1, 1-trichloroethane with 1-alkanols by considering only three different shapes namely spherical, cubical and tetrahedral. However, Kalidoss et al. [12] have considered seven shapes (sphere, cube, tetrahedron, disc A, disc B, disc C and disc D) for each component while estimating the ultrasonic speeds of $CCl_4$ + benzene, $CCl_4$ + propanol using SPT. Chi-square fit determines the closeness between experimental and theoretical ultrasonic speeds when the assumed shape matches the actual shape of the components [12].

Many attempts have been made [13, 14, 15] to use Scaled Particle Theory to obtain an equation of state of hard sphere mixtures. The equation of state is described as,

$$\frac{P}{\rho kT} = \frac{1+\zeta+\zeta^2}{(1-\zeta)^3} - \frac{\pi}{2}\frac{\rho}{(1-\rho)^3}\sum_{i<j=1}^{m} X_i X_j \left(d_{ii}d_{jj}\right)^2\left[2d_{ij} + d_{ii}d_{jj}\chi\right] \quad [1]$$

Where $d_{ii}$ are the diameters of the m-components, and

$$\zeta = \frac{\pi}{6}\rho\sum_{k=1}^{m} X_k\, d_{kk}^3 \quad \chi = \frac{\pi}{6}\rho\sum_{k=1}^{m} X_k\, d_{kk}^2$$

$$d_{ij} = \frac{(d_{ii}+d_{jj})}{2}$$

$$X_i = \frac{N_i}{N}$$

Where $N_i$ is the number of hard spheres of species I and N is the total number of molecules in the mixture. Gibbons [16] and Boublik[17] applied SPT to mixtures of hard convex molecules (not necessarily spheres) and obtained an equation of state as,

$$\frac{\beta P}{\rho_N} = \frac{1}{(1-Y\rho_N)} + \frac{AB\rho_N}{(1-Y\rho_N)^2} + \frac{1}{3}\frac{B^2C\rho_N^2}{(1-Y\rho_N)^3} \quad [2]$$

Where

$$A = \sum \emptyset_i R_i, B = \sum \emptyset_i S_i, C = \sum \emptyset_i R_i^2, Y = \sum \emptyset_i V_{H,i} \quad [2.1]$$

Where, $R_i$ , $S_i$ and $V_{H,i}$ are respectively the mean radius of curvature, surface area and volume of a molecule of species i and $\varphi_i$, the volume fraction of the i$^{th}$ liquid in the mixture.

With $\gamma = \frac{C_P}{C_V}$, we have

$$\gamma\left(\frac{dP}{d\rho}\right) = U^2 \quad [3]$$

Where ρ, is the molar density and U, ultrasonic velocity in the mixture. Then the eqns.[3] and [4] yield,

$$\frac{MU^2}{\gamma RT} = \frac{1}{(1-Y\rho_N)^2}\left[1 + 2AB\left(\frac{\rho_N}{1-Y\rho_N}\right) + B^2C\left(\frac{\rho_N}{1-Y\rho_N}\right)^2\right] \quad [4]$$

The above equation for pure liquids reduces to,

$$\frac{MU^2}{\gamma RT} = \frac{1}{(1-V_H\rho_N)^2}\left[1 + RS\left(\frac{\rho_N}{1-V_H\rho_N}\right)^2\right] \quad [5]$$

Introducing the dimensionless shape parameter $X = \frac{RS}{V_H}$ and $\eta = V_H\rho_N$, eqn**[5]** is rewritten as,

$$\frac{MU^2}{\gamma RT} = \frac{[1+(X-1)\eta]^2}{(1-\eta)^4} \quad [6]$$

Solution of the above equation is obtained as,

$$\eta = K - \sqrt{K^2 + L - 1} \quad [7]$$

Where $K = 1 + L\frac{(X-1)}{2}$ and $L = \sqrt{\frac{\gamma RT}{MU^2}}$. Mean radius and surface area of a molecule can be written as,

$$R = Y\left(V_H^{\frac{1}{3}}\right) \text{ and } S = ZR^2 \quad [8]$$

Where Y and Z are the parameters related to the shape of the molecule. If the molecule is assigned different shapes (Table-1) then the corresponding values of X, Y and Z can be calculated (Table-2).Using the values of M and ϒ[18] from literature and the experimental ultrasonic velocity (U)[19], the values of η can be calculated for pure liquids for different shapes of the molecules with the help of eqn, **[7].** Table-3 contains the η values for the pure liquids.

SPT has been used to obtain an equation of state for perfectly aligned and isotropic hard spherocylinders. Many workers [20] have used above equation of state for spherical or other type of molecules to study phenomena of phase change by Monte Carlo method**.**

## Computational Aspect

Characteristics parameters while assigning different shapes to the molecules are given in the **table-1**. Using the values of molar mass (**M**), specific heat ratio (**ϒ**) from literature [18-19] and the experimental values of ultrasonic velocity (**U**), the values of **"η"** can be calculated for pure N, N Dimethyl Acetamide (DMAc) and Chloroform (CF) by considering different shapes of the molecule with the help of eqn. **(7).Table-2** contains the shape parameters for pure liquids associated with different shapes. From the relation $\boldsymbol{\eta = V_H \rho_N}$, hard core volume $V_H$ of a molecule is calculated. This volume gives molecular radius (**R**) and surface area (**S**) of the liquid molecule for different shapes. With the knowledge of **R**, **S** and $V_H$ of pure components, parameters **A**, **B**, **C** and **Y** for mixture are evaluated for different volume fractions (φ) using eqn. (2.1). From the relation $\boldsymbol{\rho_N = H / V_0}$ (where H being Avogadro's number and $V_0$ an ideal volume of the mixture).number density of the present liquid mixture is calculated. These values on substitution in eqn. **(4),** give ultrasonic velocities in binary mixtures of different compositions by assigning nine different shapes to constituent species, thus forming different possible combinations of shapes.**Table-3** gives the molecular dimensions of pure liquid molecule along with the value of **"η".** The results in terms of ultrasonic velocities in combination of shapes like Spherical-Spherical (SP-SP), Spherical-Cubical (SP-CU) etc. are presented in **tables- (5-13).** The best-fit combination of shapes of the participating component molecules is arrived at, using Chi-square test ($\chi^2$).


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## 3. Results and Discussion

When the molecule present in the liquid mixture is assigned different shapes as described in **table 1**, then the corresponding values of X, Y and Z (also known as shape parameters) can be calculated as shown in **table 2.** The corresponding evaluated **'η'** values for the present mixtures at temperature 300K under study are given in **table 3**.Some related thermodynamic parameters for pure constituents are presented in **table-4.**

**Table 1:** Molecular assignment for different shapes

| Shape | Size | R | S | $V_H$ |
|---|---|---|---|---|
| Sphere | Radius=r | r | $4\pi r^2$ | $(4/3)\pi r^3$ |
| Cube | Side=r | (3/4)r | $6r^2$ | $r^3$ |
| Tetrahedron | Side=r | $3r(\arctan\sqrt{2})/2\pi$ | $\sqrt{3}r^2$ | $(\sqrt{2})r^3/12$ |
| Discs: Radius=r and Depth=l | | | | |
| Disc 1 | l=2r | $(\pi+2)r/4$ | $6\pi r^2$ | $2\pi r^3$ |
| Disc2 | l= (3/2)r | $(\pi+1.5)r/4$ | $5\pi r^2$ | $(3/2)r^3$ |
| Disc3 | l=r | $(\pi+1)r/4$ | $4\pi r^2$ | $\pi r^3$ |
| Disc4 | l= (1/2)r | $(\pi+0.50)r/4$ | $3\pi r^2$ | $(1/2)\pi r^3$ |
| Disc5 | l= (1/4)r | $(\pi+0.25)r/4$ | $(5/2)\pi r^2$ | $(1/4)\pi r^3$ |
| Disc6 | l= (1/10)r | $(\pi+0.10)r/4$ | $(11/5)\pi r^2$ | $(1/10)\pi r^3$ |

**Table 2:** Shape parameters

| Shape | $X=RS/V_H$ | $Y=R\,V_H^{-1/3}$ | $Z=SR^{-2}$ |
|---|---|---|---|
| Sphere | 3.0000 | 0.6204 | 12.5664 |
| Cube | 4.5000 | 0.7500 | 10.6666 |
| Tetrahedron | 6.7035 | 0.9303 | 8.3247 |
| Disc 1 | 3.8562 | 0.6966 | 11.4084 |
| Disc2 | 3.8680 | 0.6921 | 11.6656 |
| Disc3 | 4.1416 | 0.7070 | 11.7218 |
| Disc4 | 5.4624 | 0.7832 | 11.3712 |
| Disc5 | 8.4790 | 0.9190 | 10.9244 |
| Disc6 | 17.8274 | 1.1920 | 10.5253 |

**Table 3:** Microscopic dimensions of pure liquid molecule at 300K

| Liquid | Shape | $R*10^{-10}$ (m) | $S*10^{-19}$ ($m^2$) | $V_H*10^{-29}$ ($m^3$) | η |
|---|---|---|---|---|---|
| DMAc | Sphere | 2.6492 | 8.8192 | 7.7860 | 0.4904 |
| | Cube | 3.0600 | 9.9881 | 6.7920 | 0.4278 |
| | Tetrahedron | 3.5987 | 10.7810 | 5.7885 | 0.3645 |
| | Disc 1 | 2.8947 | 9.5594 | 7.1756 | 0.4519 |
| | Disc2 | 2.8750 | 9.6423 | 7.1681 | 0.4514 |
| | Disc3 | 2.9136 | 9.9507 | 6.9989 | 0.4408 |
| | Disc4 | 3.1172 | 11.0496 | 6.3051 | 0.3970 |
| | Disc5 | 3.4301 | 12.8532 | 5.1996 | 0.3275 |
| | Disc6 | 3.8837 | 15.8756 | 3.4587 | 0.2178 |
| | | | | | |
| CF | Sphere | 2.4655 | 7.6388 | 6.2763 | 0.4514 |
| | Cube | 2.8361 | 8.5795 | 5.4072 | 0.3888 |
| | Tetrahedron | 3.3200 | 9.1759 | 4.5452 | 0.3269 |
| | Disc 1 | 2.6873 | 8.2384 | 5.7409 | 0.4130 |
| | Disc2 | 2.6689 | 8.3093 | 5.7343 | 0.4124 |
| | Disc3 | 2.7028 | 8.5627 | 5.5868 | 0.4018 |
| | Disc4 | 2.8828 | 9.4500 | 4.9868 | 0.3586 |
| | Disc5 | 3.1553 | 10.8765 | 4.0475 | 0.2911 |
| | Disc6 | 3.5388 | 13.1807 | 2.6165 | 0.1882 |

**Table 4:** Some related parameters for pure components

| Liquid | $\rho_N*10^{27}$ ($m^{-3}$) | ϒ | L |
|---|---|---|---|
| DMAc | 6.2979 | 1.2316 | 0.1311 |
| CF | 7.1919 | 1.1105 | 0.1582 |

The theoretical speeds based on SPT are computed for the DMAc + CF binary mixture by considering different shapes, viz., sphere, cube, tetrahedron, disc 1, disc 2, disc 3 disc 4, disc 5and disc 6 for both the participating components. At each temperature, for DMAc + CF binary mixture 9 × 9 combinations of the different shapes are possible. Of these 81 combinations the best-fit combination of shapes of the participating component molecules is arrived at, using Chi-square test ($\chi^2$ ). At 300 K, the theoretical ultrasonic speeds calculated using SPT for the combinations spherical + disc 5 (SP-D5), is found to have lowest $\chi^2$ value. Therefore in **table 5**, the theoretical and experimental ultrasonic speeds for all possible shape combinations with spherical shape for DMAc and other possible shapes (viz., sphere, cube, tetrahedron, disc 1, disc 2, disc 3, disc 4, disc 5 and disc 6) for CF are presented.

**Table 5**

| $X_2$ | $\varphi_2$ | $U_{(Exp)}$ | $U_{(SP-SP)}$ | $U_{(SP-CU)}$ | $U_{(SP-TH)}$ |
|---|---|---|---|---|---|
| 0.1 | 0.0887 | 1378.2 | 1386.3144 | 1358.8031 | 1387.5261 |
| 0.2 | 0.1796 | 1320 | 1340.5872 | 1339.5750 | 1342.3804 |
| 0.3 | 0.2729 | 1272.4 | 1294.9225 | 1293.4600 | 1296.8147 |
| 0.4 | 0.3686 | 1228.6 | 1249.1739 | 1247.3513 | 1250.8232 |
| 0.5 | 0.4669 | 1159.7 | 1203.1950 | 1201.1407 | 1204.3922 |
| 0.6 | 0.5678 | 1107.5 | 1156.8310 | 1154.7093 | 1157.4906 |
| 0.7 | 0.6714 | 1073.4 | 1109.9061 | 1107.9140 | 1110.0553 |
| 0.8 | 0.7779 | 1035.4 | 1062.2034 | 1060.5660 | 1061.9709 |
| 0.9 | 0.8874 | 998.7 | 1013.4315 | 1012.3966 | 1013.0339 |
| $\chi^2$ | | | 6.8614 | 6.4052 | 7.1857 |

**Table 5:** Continued…

| $U_{(SP-D1)}$ | $U_{(SP-D2)}$ | $U_{(SP-D3)}$ | $U_{(SP-D4)}$ | $U_{(SP-D5)}$ | $U_{(SP-D6)}$ |
|---|---|---|---|---|---|
| 1385.8382 | 1385.7641 | 1385.6651 | 1385.2571 | 1385.5833 | 1387.0276 |
| 1339.6781 | 1339.5429 | 1339.3583 | 1338.8384 | 1339.0334 | 1341.2990 |
| 1293.6479 | 1293.4647 | 1293.2140 | 1292.4538 | 1292.5633 | 1295.1685 |
| 1247.6245 | 1247.4067 | 1247.1153 | 1246.1614 | 1246.1288 | 1248.7159 |
| 1201.4845 | 1201.2458 | 1200.9444 | 1199.8659 | 1199.6775 | 1201.9969 |
| 1155.0949 | 1154.8487 | 1154.5733 | 1153.4595 | 1153.1388 | 1155.0329 |
| 1108.2994 | 1108.0593 | 1107.8498 | 1106.8076 | 1106.4099 | 1107.7982 |
| 1060.8980 | 1060.6773 | 1060.5772 | 1059.7271 | 1059.3337 | 1060.1989 |
| 1012.6124 | 1012.4241 | 1012.1377 | 1011.9514 | 1011.6632 | 1012.0383 |
| $\chi^2$ 6.2874 | 6.2037 | 6.1129 | 5.7758 | 5.7011 | 6.3872 |

At 300 K, the theoretical ultrasonic speeds calculated using SPT for the combinations cubical+ disc 6 (CU-D6), is found to have lowest $\chi^2$ value. Therefore in **table 6**, the theoretical and experimental ultrasonic speeds for all possible shape combinations with cubical shape for DMAc and other possible shapes (viz., sphere, cube, tetrahedron, disc 1, disc 2, disc 3, disc 4, disc 5 and disc 6) for CF are presented.

**Table 6**

| $U_{(Exp)}$ | $U_{(CU-SP)}$ | $U_{(CU-CU)}$ | $U_{(CU-TH)}$ | $U_{(CU-D1)}$ | $U_{(CU-D2)}$ |
|---|---|---|---|---|---|
| 1378.2 | 1387.0697 | 1385.5232 | 1385.5241 | 1386.0018 | 1386.0008 |
| 1320 | 1342.2945 | 1339.4137 | 1339.3180 | 1340.3039 | 1340.2990 |
| 1272.4 | 1297.5618 | 1293.5038 | 1293.2508 | 1294.7241 | 1294.7123 |
| 1228.6 | 1252.3685 | 1247.6383 | 1247.2039 | 1249.0924 | 1249.0706 |
| 1159.7 | 1206.8086 | 1201.6611 | 1201.0577 | 1203.2374 | 1203.2027 |
| 1107.5 | 1160.5653 | 1155.4067 | 1154.6818 | 1156.9787 | 1156.9281 |
| 1073.4 | 1113.3993 | 1108.9873 | 1107.9221 | 1110.1141 | 1110.0446 |
| 1035.4 | 1065.0312 | 1061.2723 | 1060.5795 | 1062.4001 | 1062.3087 |
| 998.7 | 1015.1114 | 1012.8555 | 1012.3755 | 1013.5199 | 1013.4039 |
| $\chi^2$ | 8.1580 | 6.3770 | 6.1413 | 6.8810 | 6.8606 |


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**Table 6:** Continued..

| U (CU-D3) | U (CU-D4) | U (CU-D5) | U (CU-D6) |
|---|---|---|---|
| 1385.8291 | 1385.1002 | 1384.4883 | 1384.6866 |
| 1339.9821 | 1338.6237 | 1337.4604 | 1337.6721 |
| 1294.2832 | 1292.4184 | 1290.7963 | 1290.9000 |
| 1248.5688 | 1246.3448 | 1244.3865 | 1244.3188 |
| 1202.6746 | 1200.2622 | 1198.1184 | 1197.8669 |
| 1156.4268 | 1154.0198 | 1151.8664 | 1151.4632 |
| 1109.6297 | 1107.4431 | 1105.4779 | 1104.9928 |
| 1062.0459 | 1060.3136 | 1058.7516 | 1058.2850 |
| 1013.3635 | 1012.3340 | 1011.4025 | 1011.0780 |
| $\chi^2$ 6.6986 | 5.9177 | 5.2651 | 5.1718 |

At 300 K, the theoretical ultrasonic speeds calculated using SPT for the combinations tetrahedral + disc 6 (TH-D6), is found to have lowest $\chi^2$ value. Therefore in **table 7**, the theoretical and experimental ultrasonic speeds for all possible shape combinations with tetrahedral shape for DMAc and other possible shapes (viz., sphere, cube, tetrahedron, disc 1, disc 2, disc 3, disc 4, disc 5 and disc 6) for CF are presented.

**Table 7**

| U (Exp) | U (TH-SP) | U (TH-CU) | U (TH-TH) | U (TH-D1) | U (TH-D2) |
|---|---|---|---|---|---|
| 1378.2 | 1389.1568 | 1386.6909 | 1384.9402 | 1387.5776 | 1387.6733 |
| 1320 | 1346.4262 | 1341.7748 | 1338.5256 | 1343.4370 | 1343.6135 |
| 1272.4 | 1303.3564 | 1296.8714 | 1292.4210 | 1299.1735 | 1299.4133 |
| 1228.6 | 1259.6509 | 1251.7691 | 1246.4635 | 1254.5466 | 1254.8297 |
| 1159.7 | 1131.3503 | 1206.2513 | 1200.4888 | 1209.3067 | 1209.6093 |
| 1107.5 | 1169.0326 | 1160.0875 | 1154.3219 | 1163.1862 | 1163.4803 |
| 1073.4 | 1121.3794 | 1113.0222 | 1107.7649 | 1115.8877 | 1116.1400 |
| 1035.4 | 1071.5759 | 1064.7560 | 1060.5760 | 1067.0655 | 1067.2364 |
| 998.7 | 1019.0704 | 1014.9147 | 1012.4366 | 1016.2960 | 1016.3381 |
| $\chi^2$ | 9.7362 | 7.9552 | 5.9905 | 9.1235 | 9.2347 |

**Table 7:** Continued…..

| U (TH-D3) | U (TH-D4) | U (TH-D5) | U (TH-D6) |
|---|---|---|---|
| 1387.4819 | 1386.4424 | 1385.2964 | 1384.6582 |
| 1343.2533 | 1341.2934 | 1339.1320 | 1337.8507 |
| 1298.9146 | 1296.1868 | 1293.1829 | 1291.3137 |
| 1254.2312 | 1250.9263 | 1247.2976 | 1244.9535 |
| 1208.9601 | 1205.3110 | 1201.3227 | 1198.6721 |
| 1162.8405 | 1159.1277 | 1155.0942 | 1152.3568 |
| 1115.5819 | 1112.1378 | 1108.4242 | 1105.8668 |
| 1066.8455 | 1064.0589 | 1061.0810 | 1059.0117 |
| 1016.2139 | 1014.5324 | 1012.7549 | 1011.5157 |
| $\chi^2$ 8.9941 | 7.6158 | 6.2504 | 5.4153 |

At 300 K, the theoretical ultrasonic speeds calculated using SPT for the combinations disc 1 + disc 5 (D1-D5), is found to have lowest $\chi^2$ value. Therefore in **table 8**, the theoretical and experimental ultrasonic speeds for all possible shape combinations with disc 1 shape for DMAc and other possible shapes (viz., sphere, cube, tetrahedron, disc 1, disc 2, disc 3, disc 4, disc 5 and disc 6) for CF are presented.

**Table 8**

| U (Exp) | U (D1-SP) | U (D1-CU) | U (D1-TH) | U (D1-D1) | U (D1-D2) |
|---|---|---|---|---|---|
| 1378.2 | 1386.6142 | 1385.4433 | 1386.0862 | 1385.7598 | 1385.7302 |
| 1320 | 1341.3815 | 1339.1918 | 1340.1997 | 1339.7889 | 1339.7319 |
| 1272.4 | 1296.1570 | 1293.1398 | 1294.2874 | 1293.9682 | 1293.8866 |
| 1228.6 | 1250.7616 | 1247.1488 | 1248.2621 | 1248.1459 | 1248.0429 |
| 1159.7 | 1205.0152 | 1201.0794 | 1202.0345 | 1202.1695 | 1202.0485 |
| 1107.5 | 1158.7284 | 1154.7824 | 1155.5036 | 1155.8774 | 1155.7424 |
| 1073.4 | 1111.6912 | 1108.0857 | 1108.5432 | 1109.0860 | 1108.9413 |
| 1035.4 | 1063.6536 | 1060.7740 | 1060.9806 | 1061.5698 | 1061.4203 |
| 998.7 | 1014.2948 | 1012.5542 | 1012.5622 | 1013.0281 | 1012.8788 |
| $\chi^2$ | 7.4981 | 6.1652 | 6.4350 | 6.5202 | 6.4723 |

**Table 8:** Continued….

| U (D1-D3) | U (D1-D4) | U (D1-D5) | U (D1-D6) |
|---|---|---|---|
| 1385.5819 | 1385.0167 | 1384.6801 | 1385.3140 |
| 1339.4585 | 1338.3975 | 1337.7183 | 1338.6620 |
| 1293.5175 | 1292.0526 | 1291.0601 | 1292.0730 |
| 1247.6134 | 1245.8586 | 1244.6145 | 1245.5310 |
| 1201.6001 | 1199.6906 | 1198.2864 | 1199.0069 |
| 1155.3222 | 1153.4124 | 1151.9659 | 1152.4484 |
| 1108.6018 | 1106.8637 | 1105.5147 | 1105.7658 |
| 1061.2183 | 1059.8382 | 1058.7442 | 1058.8108 |
| 1012.8747 | 1012.0493 | 1011.3799 | 1011.3407 |
| $\chi^2$ 6.3413 | 5.7363 | 5.3063 | 5.4910 |

At 300 K, the theoretical ultrasonic speeds calculated using SPT for the combinations disc 2 + disc 5 (D2-D5), is found to have lowest $\chi^2$ value. Therefore in **table 9**, the theoretical and experimental ultrasonic speeds for all possible shape combinations with disc 2 shape for DMAc and other possible shapes (viz., sphere, cube, tetrahedron, disc 1, disc 2, disc 3, disc 4, disc 5 and disc 6) for CF are presented.

**Table 9**

| U (Exp) | U (D2-SP) | U (D2-CU) | U (D2-TH) | U (D2-D1) | U (D2-D2) |
|---|---|---|---|---|---|
| 1378.2 | 1386.3989 | 1385.2989 | 1386.0933 | 1385.5830 | 1385.5417 |
| 1320 | 1341.1764 | 1339.1137 | 1340.3810 | 1339.6535 | 1339.5756 |
| 1272.4 | 1295.9656 | 1293.1165 | 1294.5916 | 1293.8702 | 1293.7607 |
| 1228.6 | 1250.5874 | 1247.1682 | 1248.6407 | 1248.0805 | 1247.9451 |
| 1159.7 | 1204.8616 | 1201.1289 | 1202.4423 | 1202.1315 | 1201.9764 |
| 1107.5 | 1158.5990 | 1154.8490 | 1155.8988 | 1155.8609 | 1155.6928 |
| 1073.4 | 1111.5893 | 1108.1562 | 1108.8876 | 1109.0847 | 1108.9108 |
| 1035.4 | 1063.5827 | 1060.8346 | 1061.2395 | 1061.5767 | 1061.4046 |
| 998.7 | 1014.2578 | 1012.5913 | 1012.7047 | 1013.0355 | 1012.8735 |
| $\chi^2$ | 7.4418 | 6.1782 | 6.5612 | 6.5056 | 6.4467 |

**Table 9:** Continued……

| U (D2-D3) | U (D2-D4) | U (D2-D5) | U (D2-D6) |
|---|---|---|---|
| 1385.3885 | 1384.8309 | 1384.5065 | 1385.1502 |
| 1339.2933 | 1338.2456 | 1337.5867 | 1338.5456 |
| 1293.3797 | 1291.9318 | 1290.9645 | 1291.9944 |
| 1247.5018 | 1245.7660 | 1244.5489 | 1245.4818 |
| 1201.5133 | 1199.6229 | 1198.2450 | 1198.9796 |
| 1155.2582 | 1153.3662 | 1151.9430 | 1152.4364 |
| 1108.5583 | 1106.8352 | 1105.5049 | 1105.7634 |
| 1061.1926 | 1059.8234 | 1058.7424 | 1058.8132 |
| 1012.8636 | 1012.0439 | 1011.3813 | 1011.3436 |
| $\chi^2$ 6.3113 | 5.7137 | 5.2918 | 5.4798 |

At 300 K, the theoretical ultrasonic speeds calculated using SPT for the combinations disc 3 + disc 5 (D3-D5), is found to have lowest $\chi^2$ value. Therefore in **table 10**, the theoretical and experimental ultrasonic speeds for all possible shape combinations with disc 3 shape for DMAc and other possible shapes (viz., sphere, cube, tetrahedron, disc 1, disc 2, disc 3, disc 4, disc 5 and disc 6) for CF are presented.


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**Table 10**

| $U_{(Exp)}$ | $U_{(D3-SP)}$ | $U_{(D3-CU)}$ | $U_{(D3-TH)}$ | $U_{(D3-D1)}$ | $U_{(D3-D2)}$ |
|---|---|---|---|---|---|
| 1378.2 | 1386.9124 | 1385.7440 | 1386.4734 | 1386.0545 | 1386.0087 |
| 1320 | 1341.7976 | 1339.6087 | 1340.7695 | 1340.1962 | 1340.1100 |
| 1272.4 | 1296.6762 | 1293.6542 | 1294.9999 | 1294.4719 | 1294.3512 |
| 1228.6 | 1251.3599 | 1247.7335 | 1249.0689 | 1248.7210 | 1248.5723 |
| 1159.7 | 1205.6587 | 1201.6990 | 1202.8792 | 1202.7825 | 1202.6129 |
| 1107.5 | 1159.3732 | 1155.3935 | 1156.3231 | 1156.4857 | 1156.3030 |
| 1073.4 | 1112.2824 | 1108.6370 | 1109.2688 | 1109.6385 | 1109.4512 |
| 1035.4 | 1064.1260 | 1061.2073 | 1061.5396 | 1062.0070 | 1061.8243 |
| 998.7 | 1014.5729 | 1012.8052 | 1012.8792 | 1013.2830 | 1013.1148 |
| $\chi^2$ | 7.7331 | 6.3678 | 6.7144 | 6.7274 | 6.6627 |

**Table 10:** Continued……

| $U_{(D3-D3)}$ | $U_{(D3-D4)}$ | $U_{(D3-D5)}$ | $U_{(D3-D6)}$ |
|---|---|---|---|
| 1385.8370 | 1385.2143 | 1384.7805 | 1385.2397 |
| 1339.7938 | 1338.6286 | 1337.7785 | 1338.4278 |
| 1293.9242 | 1292.3193 | 1291.1044 | 1291.7507 |
| 1248.0747 | 1246.1557 | 1244.6588 | 1245.1772 |
| 1202.0910 | 1200.0054 | 1198.3388 | 1198.6648 |
| 1155.8099 | 1153.7258 | 1152.0276 | 1152.1493 |
| 1109.0455 | 1107.1499 | 1105.5806 | 1105.5307 |
| 1061.5701 | 1060.0660 | 1058.8040 | 1058.6516 |
| 1013.0803 | 1012.1828 | 1011.4189 | 1011.2620 |
| $\chi^2$ 6.5055 | 5.8373 | 5.3265 | 5.3975 |

At 300 K, the theoretical ultrasonic speeds calculated using SPT for the combinations disc 4 + disc 6 (D4-D6), is found to have lowest $\chi^2$ value. Therefore in **table 11**, the theoretical and experimental ultrasonic speeds for all possible shape combinations with disc 4 shape for DMAc and other possible shapes (viz., sphere, cube, tetrahedron, disc 1, disc 2, disc 3, disc 4, disc 5 and disc 6) for CF are presented.

**Table 11**

| $U_{(Exp)}$ | $U_{(D4-SP)}$ | $U_{(D4-CU)}$ | $U_{(D4-TH)}$ | $U_{(D4-D1)}$ | $U_{(D4-D2)}$ |
|---|---|---|---|---|---|
| 1378.2 | 1387.6300 | 1386.0755 | 1386.2504 | 1386.5462 | 1386.5087 |
| 1320 | 1343.2760 | 1340.3681 | 1340.5820 | 1341.2482 | 1341.1764 |
| 1272.4 | 1298.8142 | 1294.8005 | 1294.9514 | 1296.0139 | 1295.9115 |
| 1228.6 | 1254.0153 | 1249.1942 | 1249.2154 | 1250.6489 | 1250.5203 |
| 1159.7 | 1208.6439 | 1203.3689 | 1203.2300 | 1204.9563 | 1204.8066 |
| 1107.5 | 1162.4507 | 1157.1344 | 1156.8420 | 1158.7283 | 1158.5635 |
| 1073.4 | 1115.1620 | 1110.2775 | 1109.8757 | 1111.7345 | 1111.5617 |
| 1035.4 | 1066.4623 | 1062.5432 | 1062.1131 | 1063.7033 | 1063.5306 |
| 998.7 | 1015.9658 | 1013.6028 | 1013.2610 | 1014.2909 | 1014.1276 |
| $\chi^2$ | 8.8614 | 6.9324 | 6.8549 | 7.4850 | 7.4232 |

**Table 11:** Continued….

| $U_{(D4-D3)}$ | $U_{(D4-D4)}$ | $U_{(D4-D5)}$ | $U_{(D4-D6)}$ |
|---|---|---|---|
| 1386.2813 | 1385.4111 | 1384.5597 | 1384.3275 |
| 1340.7563 | 1339.1376 | 1337.5465 | 1337.0221 |
| 1295.3407 | 1293.1203 | 1290.9319 | 1290.1051 |
| 1249.8487 | 1247.2003 | 1244.5875 | 1243.4933 |
| 1204.0927 | 1201.2171 | 1198.3822 | 1197.0966 |
| 1157.8745 | 1155.0007 | 1152.1732 | 1150.8084 |
| 1110.9738 | 1108.3579 | 1105.7923 | 1104.4910 |
| 1063.1288 | 1061.0526 | 1059.0247 | 1057.9542 |
| 1014.0049 | 1012.7722 | 1011.5737 | 1010.9192 |
| $\chi^2$ 7.1892 | 6.2272 | 5.3512 | 4.9669 |

At 300 K, the theoretical ultrasonic speeds calculated using SPT for the combinations disc 5 + disc 6 (D5-D6), is found to have lowest $\chi^2$ value. Therefore in **table 12**, the theoretical and experimental ultrasonic speeds for all possible shape combinations with disc 5 shape for DMAc and other possible shapes (viz., sphere, cube, tetrahedron, disc 1, disc 2, disc 3, disc 4, disc 5 and disc 6) for CF are presented.

**Table-12**

| $U_{(Exp)}$ | $U_{(D5-SP)}$ | $U_{(D5-CU)}$ | $U_{(D5-TH)}$ | $U_{(D5-D1)}$ | $U_{(D5-D2)}$ |
|---|---|---|---|---|---|
| 1378.2 | 1389.1242 | 1387.099 | 1386.5812 | 1387.7666 | 1387.7388 |
| 1320 | 1346.2489 | 1342.4309 | 1341.4174 | 1343.6836 | 1343.6293 |
| 1272.4 | 1303.0804 | 1297.7610 | 1296.3041 | 1299.4981 | 1299.4186 |
| 1228.6 | 1259.3140 | 1252.8560 | 1251.0397 | 1254.9538 | 1254.8512 |
| 1159.7 | 1214.6254 | 1207.4749 | 1205.4179 | 1209.7837 | 1209.6608 |
| 1107.5 | 1168.6611 | 1161.3607 | 1159.2194 | 1163.7019 | 1163.5621 |
| 1073.4 | 1121.0274 | 1114.2285 | 1112.1998 | 1116.3917 | 1116.2399 |
| 1035.4 | 1071.2743 | 1065.7483 | 1064.0701 | 1067.4892 | 1067.3315 |
| 998.7 | 1018.8713 | 1015.5149 | 1014.4660 | 1016.5550 | 1016.3993 |
| $\chi^2$ | 11.37787 | 8.5449 | 7.6484 | 9.3234 | 9.2643 |

**Table 12:** Continued…

| $U_{(D5-D3)}$ | $U_{(D5-D4)}$ | $U_{(D5-D5)}$ | $U_{(D5-D6)}$ |
|---|---|---|---|
| 1387.4424 | 1386.2664 | 1384.8928 | 1383.7848 |
| 1343.0754 | 1340.8746 | 1338.3228 | 1336.2587 |
| 1298.6555 | 1295.6144 | 1292.1169 | 1289.2867 |
| 1253.9382 | 1250.2789 | 1246.1083 | 1242.7391 |
| 1208.6700 | 1204.6568 | 1200.1280 | 1196.4829 |
| 1162.5800 | 1158.5244 | 1153.9964 | 1150.3722 |
| 1115.3690 | 1111.6333 | 1107.5099 | 1104.2339 |
| 1066.6921 | 1063.6922 | 1060.4211 | 1057.8464 |
| 1016.1297 | 1014.3354 | 1012.4049 | 1010.9044 |
| $\chi^2$ 8.8906 | 7.3973 | 5.8918 | 4.8156 |

At 300 K, the theoretical ultrasonic speeds calculated using SPT for the combinations disc 6 + disc 6 (D6-D6), is found to have lowest $\chi^2$ value. Therefore in **table 13**, the theoretical and experimental ultrasonic speeds for all possible shape combinations with disc 6 shape for DMAc and other possible shapes (viz., sphere, cube, tetrahedron, disc 1, disc 2, disc 3, disc 4, disc 5 and disc 6) for CF are presented.

**Table 13**

| $U_{(Exp)}$ | $U_{(D6-SP)}$ | $U_{(D6-CU)}$ | $U_{(D6-TH)}$ | $U_{(D6-D1)}$ | $U_{(D6-D2)}$ |
|---|---|---|---|---|---|
| 1378.2 | 1391.8937 | 1389.4074 | 1388.1888 | 1390.2690 | 1390.2470 |
| 1320 | 1351.6969 | 1346.9276 | 1344.6084 | 1348.5721 | 1348.52799 |
| 1272.4 | 1310.9460 | 1304.1730 | 1300.9110 | 1306.4954 | 1306.42934 |
| 1228.6 | 1269.2021 | 1260.8036 | 1256.8055 | 1263.6654 | 1263.5780 |
| 1159.7 | 1225.9663 | 1216.4492 | 1211.9797 | 1219.6694 | 1219.5618 |
| 1107.5 | 1180.6615 | 1170.6972 | 1166.0903 | 1174.0422 | 1173.9163 |
| 1073.4 | 1132.6104 | 1123.0785 | 1118.7480 | 1126.2498 | 1126.1087 |
| 1035.4 | 1081.0099 | 1073.0473 | 1069.4967 | 1075.6683 | 1075.5171 |
| 998.7 | 1024.9050 | 1019.9526 | 1017.7806 | 1021.5578 | 1021.4044 |
| $\chi^2$ | 17.1154 | 12.2455 | 10.2620 | 13.7919 | 13.7266 |

**Table 13:** Continued…..

| $U_{(D6-D3)}$ | $U_{(D6-D4)}$ | $U_{(D6-D5)}$ | $U_{(D6-D6)}$ |
|---|---|---|---|
| 1389.8754 | 1388.3775 | 1386.4427 | 1384.3674 |
| 1347.8199 | 1344.9702 | 1341.3280 | 1337.4724 |
| 1305.4320 | 1301.4213 | 1296.3535 | 1291.0651 |
| 1262.3541 | 1257.4293 | 1251.2826 | 1244.9676 |
| 1218.1940 | 1212.6718 | 1205.8704 | 1198.9992 |
| 1172.5124 | 1166.7959 | 1159.8547 | 1152.9675 |
| 1124.8075 | 1119.4052 | 1112.9437 | 1106.6553 |
| 1074.4959 | 1070.0414 | 1064.7980 | 1059.7999 |
| 1020.8856 | 1018.1567 | 1014.9996 | 1012.0601 |
| $\chi^2$ 13.0783 | 10.5576 | 7.8513 | 5.5593 |


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## 4. Conclusion

The experimental values of ultrasonic speed, for the binary mixtures of N, N dimethylacetamide (DMAc) with chloroform (CF) at 300 K and at atmospheric pressure over the entire composition range of DMAc have been used to study the intermolecular interactions in the mixture. Theoretical ultrasonic speeds for the present binary mixtures are estimated using SPT and compared with experimental speeds. Close analysis of various combinational configurations with the help of $\chi^2$ fit values, reveals that disc 5+disc-6 combination gives appropriate shape of constituent liquid molecules out of all possible configurations. The shapes of the participating molecules are analyzed using SPT at temperature 300K in the present binary system, and it was found that due to the presence of varying intermolecular interactions in the liquid mixtures the shapes of the constituent molecules change at any given temperature under study.

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