Khasare Equation of State for Molecular Cluster Study of Some Organic Liquids

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ABSTRACT

Comparative study of second generation and third generation Khasare’s EOS are carried out at critical temperature. Third generation of EOS is used to study the correlation of structural properties and thermodynamic behavior in terms of liquid clusters. Computations are based on $\zeta$, a new parameter introduced to obtain the unique solution. All computations are carried at from 283.15 K to 343.15 K. The value of $\zeta$ is attributed to cluster forming/breaking. Present calculation is based upon the sample thermodynamic data such as ultrasonic wave, density, volume expansion coefficient and ratio of specific heat (1.3).

Key Words: Equation of State, LJ Potential, Computer Algebra, Molecular Clusters.

PACS: 51.30.+i Thermodynamic properties, equations of state
PACS: 36.40.Ei Phase transitions in clusters
PACS: 05.70.Ce thermodynamics

INTRODUCTION

Study of liquids finds immense importance in the physical and chemical sciences. Large experimental data is published over the years. Also many eminent workers established different significant theories for understanding the behavior of pure liquids, solutions, and liquid mixtures. Structurally related organic liquids and their mixtures find enormous attention in recent years as they have vast applicability in chemical industries. Scaled Particle Theory (SPT) serves as a starting point to develop further insight in the subject. Earlier reasonable theoretical approach for extended scaled particle theory is developed (first generation EOS) in earlier several papers [1-11]. The Equation of State [EOS] [12-18] is developed based upon this idea. Many workers have tested its utility for real liquids in their studies. Using the perception of hard sphere with perturbation view Khasare-Deshpande obtained following second generation EOS [19]

$$
z := \frac{-\frac{3}{2} \eta^2 - \frac{5}{4} \eta - 1}{\left(\frac{3}{4} \eta - 1\right)^2} + \frac{3432 \eta}{35 \zeta^2 \left(\frac{3}{4} \eta - 1\right)}
$$

[1]
This was used to carry out the study of nano-cavity [20-22].

The above expression was modified further by putting the constraint of lattice concept by aptly introducing the parameter \( \lambda \) which is defined as

\[
\lambda = (1 + \frac{f \eta}{\eta}) \quad \text{with} \quad m = \frac{3}{4}; \quad f_{fc} = 0.337817454; \quad f_{bcc} = 0.437135330; \quad \text{[2]}
\]

With this adaptation, third generation equation becomes as [23-24]

\[
z := \frac{(8 \lambda^2 m + (-8 m - 9) \lambda + 2 m + 6) \eta^2 + (4 \lambda^2 m + (-2 - 4 m) \lambda + m) \eta - \lambda}{((1 - 2 \lambda)^2 m \eta - \lambda) (\eta - 1)^2} - \frac{1056 ((1 - 2 \lambda)^2 m - 4 \lambda) \eta}{35 \tau^2 ((1 - 2 \lambda)^2 m \eta - \lambda)} \quad \text{[3]}
\]

This paper mainly delineates study of the pure organic liquids listed below with molecular weights shown in brackets.

1) 1-4 Dioxane (88) 2) Methyl alcohol (32) 3) Benzene (78) 4) Tetrahydrofuran (72) 5) Carbon-tetrachloride (154) 6) Cyclohexanol (100) 7) Methyl-cyclohexane (98) 8) Cyclohexane (84) 9) Tetrahydro pyrrrole (71).

Here computational technique is being developed to obtain some results by considering aggregation of molecular clustering in the liquid state. The properties of hard sphere and concept of revised scaled particle theory is employed to work out thermodynamic parameters. The paper presents mathematical computations in detail.

Two parameters, namely radius and binding energy of molecule are necessary for real fluids. Authors used equation of state for a strong repulsive potential together with a weak attractive potential. Authors used equation of state for a strong repulsive potential together with a weak attractive potential. Dimensional less variable packing fraction (\( \eta \)) and temperature (\( \tau = \frac{k_B T}{\epsilon} \)) are required for calculating ultrasonic wave velocity, density, and volume expansion coefficient.

Hence we have following set of equations containing thermodynamic reduced variable [\( \eta, \tau \)].

\[
\frac{\beta P}{\varphi P} = Z(\eta, \beta \epsilon) = \xi(\eta, \tau) \quad \text{[4]}
\]

\[
\frac{M u^2}{\varphi R T} = -\frac{\partial (Z \eta)}{\partial \eta} = \psi(\eta, \tau) \quad \text{[5]}
\]

\[
\frac{M u^2 dT}{\varphi R T} = -\frac{\partial (Z T)}{\partial T} = \alpha(\eta, \tau) \quad \text{[6]}
\]

To obtain the unique mathematical solution of above set of equations new variable \( \xi \) is brought in to picture. Clustering of molecules is taken into account to associate model parameters in terms of \( \xi \) for real fluids. These model parameters have link with properties of liquids such as ultrasonic velocity, bulk density and volume expansion coefficient.

**Mathematical model for Fluid**

A compressibility factor \( Z \) for Lennard-Jones fluids is

\[
Z(\eta, \tau) = \frac{\beta P}{\varphi P}, \quad \beta = \frac{1}{k_B T}, \quad \beta \epsilon = \frac{1}{\tau}, \quad \eta = \frac{\nu}{V} = \frac{\pi \rho d^3}{6}, \quad 0 < \xi < 1 \quad \text{[7]}
\]
Where $v$ is volume of cavity containing few chemical units, $V$ is volume, $P$ is a pressure, $\rho = N/V$ is the density, $T$ is temperature, $\varepsilon$ is binding energy of cluster containing chemical units, $\zeta$ parameter used to obtain the solution and $k_B$ is Boltzmann constant.

Final expression for equation of state for a fluid is expressed as

$$\frac{\beta P}{\zeta \rho} = \frac{Z(\eta, \tau)}{\eta} = z$$

[8]

Where, $z$ is given by eq. [3]

Now $m_\parallel$ and $\lambda$ (eq. [2]) for face centre lattice are given by following equation

So that eq. (8) become

$$z := (-2 (1 + f \eta) \eta - 9 (1 + f \eta) \eta^2 + 8 \eta^2 (1 + f \eta)^2 m - 4 \eta (1 + f \eta) m$$

$$+ 4 \eta (1 + f \eta)^2 m - 8 \eta^2 (1 + f \eta) m + 6 \eta^2 + 2 m \eta^2 + m \eta - 1 - f \eta) / ((\eta - 1)^2$$

$$- \frac{1056 (4 (1 + f \eta)^2 m + m - 4 - 4 f \eta - 4 (1 + f \eta) m) \eta}{35 \tau^2 (4 \eta (1 + f \eta)^2 m + m \eta - 4 \eta (1 + f \eta) m - 1 - f \eta)}$$

From above, we get eq. [9] and eq. [10]

$$\frac{\mu^2}{\zeta RT} = \frac{\partial (Z \eta)}{\partial \eta} = y$$

[9]

Where

$$y := \left(\begin{array}{c}
-4 f \eta - 2 - 9 f \eta^2 - 18 (1 + f \eta) \eta + 16 \eta (1 + f \eta)^2 m + 16 \eta^2 (1 + f \eta) m f \\
-4 (1 + f \eta) m - 4 f \eta m + 4 (1 + f \eta)^2 m + 8 \eta (1 + f \eta) m f - 16 \eta (1 + f \eta) m \\
-8 \eta^2 (f m + 12 \eta + 4 m \eta + m - f) / ((\eta - 1)^2$$

$$- (4 \eta (1 + f \eta)^2 m + m \eta - 4 \eta (1 + f \eta) m - 1 - f \eta)) - 2 (-2 (1 + f \eta) \eta$$

$$- 9 (1 + f \eta) \eta^2 + 8 \eta^2 (1 + f \eta)^2 m - 4 \eta (1 + f \eta) m + 4 \eta (1 + f \eta)^2 m$$

$$- 8 \eta^2 (1 + f \eta) m + 6 \eta^2 + 2 m \eta^2 + m \eta - 1 - f \eta) / ((\eta - 1)^3$$

$$- (4 \eta (1 + f \eta)^2 m + m \eta - 4 \eta (1 + f \eta) m - 1 - f \eta)) - (-2 (1 + f \eta) \eta$$

$$- 9 (1 + f \eta) \eta^2 + 8 \eta^2 (1 + f \eta)^2 m - 4 \eta (1 + f \eta) m + 4 \eta (1 + f \eta)^2 m$$

$$- 8 \eta^2 (1 + f \eta) m + 6 \eta^2 + 2 m \eta^2 + m \eta - 1 - f \eta)$$

$$+ 1056 (4 (1 + f \eta)^2 m + m - 4 - 4 f \eta - 4 (1 + f \eta) m) \eta$$

$$- \frac{1056 (4 (1 + f \eta)^2 m + m - 4 - 4 f \eta - 4 (1 + f \eta) m) \eta}{35 \tau^2 (4 \eta (1 + f \eta)^2 m + m \eta - 4 \eta (1 + f \eta) m - 1 - f \eta)} + 1056$$
\[
(4 (1 + f\eta)^2 m + m - 4 - 4 f\eta - 4 (1 + f\eta) m)\eta \\
\frac{(4 (1 + f\eta)^2 m + 8 \eta (1 + f\eta) m + m - 4 (1 + f\eta) m - 4 f\eta m - f)}{(35 \tau^2)} \\
(4 \eta (1 + f\eta)^2 m + m - 4 \eta (1 + f\eta) m - 1 - f\eta) \eta + (-2 (1 + f\eta) \eta \\
- 9 (1 + f\eta) \eta^2 + 8 \eta^2 (1 + f\eta)^2 m - 4 \eta (1 + f\eta) m + 4 \eta (1 + f\eta)^2 m \\
- 8 \eta^2 (1 + f\eta) m + 6 \eta^2 + 2 m \eta^2 + m \eta - 1 - f\eta) / ((\eta - 1)^2) \\
(4 \eta (1 + f\eta)^2 m + m - 4 \eta (1 + f\eta) m - 1 - f\eta)) \\
\frac{1056 (4 (1 + f\eta)^2 m + m - 4 - 4 f\eta - 4 (1 + f\eta) m)\eta}{35 \tau^2 (4 \eta (1 + f\eta)^2 m + m - 4 \eta (1 + f\eta) m - 1 - f\eta)}
\]

And

\[
\frac{\mu c\alpha T}{\zeta \beta T} = \frac{\partial (ZT)}{\partial T} = x \quad [10]
\]

Where

\[
x := \frac{1056 (4 (1 + f\eta)^2 m + m - 4 - 4 f\eta - 4 (1 + f\eta) m)\eta}{35 \tau^2 (4 \eta (1 + f\eta)^2 m + m - 4 \eta (1 + f\eta) m - 1 - f\eta)} + (-2 (1 + f\eta) \eta \\
- 9 (1 + f\eta) \eta^2 + 8 \eta^2 (1 + f\eta)^2 m - 4 \eta (1 + f\eta) m + 4 \eta (1 + f\eta)^2 m \\
- 8 \eta^2 (1 + f\eta) m + 6 \eta^2 + 2 m \eta^2 + m \eta - 1 - f\eta) / ((\eta - 1)^2) \\
(4 \eta (1 + f\eta)^2 m + m - 4 \eta (1 + f\eta) m - 1 - f\eta))
\]

It is important to note that in above set of equations \(Z(\eta, \xi, \tau, \psi)\) nearest pole for fcc \(\eta_{\text{max}} = 0.7404804897\) and for bcc \(\eta_{\text{max}} = 0.6801747616\), \(R = (8.314)10^7\) J/mole K; \(N_A = (6.02215)10^{23}\) mol⁻¹; pressure = (101.2928) kPa.

For fluid, present equation of state is tested by considering \(\eta = v/V\), and \(\tau > 0\). The term \(v/V\) is taken as the probability for creating a cavity in fluid, assuming presence of group of molecules in cavity.

Boundary condition for gas phase can be put as

\[
\text{if} \quad \frac{\beta p}{\gamma} = Z(\eta, \beta e) = \zeta(\eta, \tau) = 1, \text{then} \zeta = 1
\]

For deviation of \(\zeta\) from 1 can be attributed to liquid phase hence we define Ordering= \([1-\zeta]\).

**RESULTS**

The EOS, data, results and molecular cluster are presented in the tabular form.

<table>
<thead>
<tr>
<th>S. No.</th>
<th>(\eta)</th>
<th>(Z(\text{MD}))</th>
<th>(Z(\text{BH2}))</th>
<th>(Z_\alpha(\tau))</th>
<th>(Z_\beta(\tau))</th>
<th>(Z_{\Omega(\tau)})</th>
<th>(Z_{\Omega(\text{cl})})</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.052</td>
<td>0.72</td>
<td>0.74</td>
<td>0.7542</td>
<td>0.75</td>
<td>0.7135</td>
<td>0.7436</td>
</tr>
<tr>
<td>2</td>
<td>0.105</td>
<td>0.52</td>
<td>0.52</td>
<td>0.5368</td>
<td>0.54</td>
<td>0.4601</td>
<td>0.5231</td>
</tr>
<tr>
<td>3</td>
<td>0.157</td>
<td>0.35</td>
<td>0.36</td>
<td>0.3765</td>
<td>0.38</td>
<td>0.2667</td>
<td>0.3650</td>
</tr>
<tr>
<td>4</td>
<td>0.209</td>
<td>0.27</td>
<td>0.26</td>
<td>0.2996</td>
<td>0.30</td>
<td>0.1561</td>
<td>0.2938</td>
</tr>
<tr>
<td>5</td>
<td>0.262</td>
<td>0.30</td>
<td>0.27</td>
<td>0.3546</td>
<td>0.35</td>
<td>0.1776</td>
<td>0.3614</td>
</tr>
<tr>
<td>6</td>
<td>0.288</td>
<td>0.41</td>
<td>0.35</td>
<td>0.4519</td>
<td>0.45</td>
<td>0.2615</td>
<td>0.4708</td>
</tr>
<tr>
<td>7</td>
<td>0.340</td>
<td>0.80</td>
<td>0.74</td>
<td>0.8467</td>
<td>0.87</td>
<td>0.6521</td>
<td>0.9199</td>
</tr>
<tr>
<td>8</td>
<td>0.393</td>
<td>1.73</td>
<td>1.64</td>
<td>1.6502</td>
<td>1.73</td>
<td>1.5393</td>
<td>1.8814</td>
</tr>
<tr>
<td>9</td>
<td>0.445</td>
<td>3.37</td>
<td>3.36</td>
<td>3.0614</td>
<td>3.35</td>
<td>3.2829</td>
<td>3.7202</td>
</tr>
<tr>
<td>10</td>
<td>0.497</td>
<td>6.32</td>
<td>6.32</td>
<td>5.4691</td>
<td>6.33</td>
<td>6.7099</td>
<td>7.2791</td>
</tr>
</tbody>
</table>

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Here we used $\lambda = \lambda_{\text{fcc}}$ or $\lambda = \lambda_{\text{bcc}}$ so that $\eta = 0.74$ or $\eta = 0.68$ for solid-state as a boundary condition can be imposed which similar to $\eta = 0$, for $Z = 1.0$ for gas-state, where following is the suitable empirical function.

$$
\lambda_{\text{fcc}} = (1+0.337817454 \eta); \lambda_{\text{bcc}} = (1+0.437135330 \eta);
$$

[11]

$Z_0(\tau_c)$ [SBK-MSD], $\tau$ (critical) = 3.312373150; $\eta$(critical) = 0.1572541882; rms-deviation$_1 = 0.2890522064$.
$Z_1(\tau_c)$ [SBK], $\tau$ (critical) = 3.258762327; $\eta$(critical) = 0.1579722415; rms-deviation$_1 = 0.0036835$, $Z_i(\tau_c)$ [BH2], rms-deviation$_1 = 0.041593$;
$Z_2(\tau_c)$ [SBK], $\tau$ (critical) = 3.164; $\eta = 0.1546269541;$ rms-deviation$_2 = 0.3299431994$
$Z_3(\tau_c)$ [SBK], $\tau$ (bcc) = 3.242842579; $\eta = 0.1538974793; $ rms-deviation$_3 = 0.5974345121$.
Table 2: Thermodynamic data such as Velocity, density and volume expansion coefficient (alpha) data in terms of temperature (\( t = \) degree centigrade), ratio of specific heat=1.3:

<table>
<thead>
<tr>
<th>Liquid(1):=1-4 Dioxane;</th>
<th>temp:=(273.16+te) m/mol=88; gamma=1.3; dens:=(1039.9751-0.9151<em>te)/100; alpha:=(diff(ln(dens),te)); te:=10; den:=dens; vel:=(1450.9465-4.2447</em>te)<em>100; alpha1:=alpha; alphat:=temp</em>alpha1;</th>
</tr>
</thead>
<tbody>
<tr>
<td>Liquid(2):=Methyl alcohol;</td>
<td>temp:=(273.16+te) m/mol=32; gamma=1.3; dens:=(800.9381-0.8353<em>te)/100; alpha:=(diff(ln(dens),te)); te:=10; den:=dens; vel:=(1183.6869-3.2527</em>te)<em>100; alpha1:=alpha; alphat:=temp</em>alpha1;</td>
</tr>
<tr>
<td>Liquid(3):=Benzene;</td>
<td>temp:=(273.16+te) m/mol=78.00; gamma=1.3; dens:=(891.9408-0.8938<em>te)/100; alpha:=(diff(ln(dens),te)); te:=10; den:=dens; vel:=(1095.3231-4.2713</em>te)<em>100; alpha1:=alpha; alphat:=temp</em>alpha1;</td>
</tr>
<tr>
<td>Liquid(4):=Tetrahydrofuran;</td>
<td>temp:=(273.16+te) m/mol=72.00; gamma=1.3; dens:=(906.8611-1.0315<em>te)/100; alpha:=(diff(ln(dens),te)); te:=10; den:=dens; vel:=(1389.7431-4.4833</em>te)<em>100; alpha1:=alpha; alphat:=temp</em>alpha1;</td>
</tr>
<tr>
<td>Liquid(5):=Carbon tetrachloride;</td>
<td>temp:=(273.16+te) m/mol=154; gamma=1.3; dens:=(1626.3210-1.7205<em>te)/100; alpha:=(diff(ln(dens),te)); te:=10; den:=dens; vel:=(1391.9295-4.1947</em>te)<em>100; alpha1:=alpha; alphat:=temp</em>alpha1;</td>
</tr>
<tr>
<td>Liquid(6):=Cyclohexanol;</td>
<td>temp:=(273.16+te) m/mol=110; gamma=1.3; dens:=(953.6185-0.6605<em>te)/100; alpha:=(diff(ln(dens),te)); te:=10; den:=dens; vel:=(1645.2765-6.4587</em>te)<em>100; alpha1:=alpha; alphat:=temp</em>alpha1;</td>
</tr>
<tr>
<td>Liquid(7):=Methylcyclohexane;</td>
<td>temp:=(273.16+te) m/mol=98; gamma=1.3; dens:=(780.3847-0.8120<em>te)/100; alpha:=(diff(ln(dens),te)); te:=10; den:=dens; vel:=(1314.8365-4.1947</em>te)<em>100; alpha1:=alpha; alphat:=temp</em>alpha1;</td>
</tr>
<tr>
<td>Liquid(8):=Cyclohexane;</td>
<td>temp:=(273.16+te) m/mol=84; gamma=1.3; dens:=(786.6264-0.8367<em>te)/100; alpha:=(diff(ln(dens),te)); te:=10; den:=dens; vel:=(1364.5498-4.6480</em>te)<em>100; alpha1:=alpha; alphat:=temp</em>alpha1;</td>
</tr>
<tr>
<td>Liquid(9):=Tetrahydropyrole;</td>
<td>temp:=(273.16+te) m/mol=71; gamma=1.3; dens:=(813.0460-0.8273<em>te)/100; alpha:=(diff(ln(dens),te)); te:=10; den:=dens; vel:=(1474.1564-4.2247</em>te)<em>100; alpha1:=alpha; alphat:=temp</em>alpha1;</td>
</tr>
</tbody>
</table>

Graph-2: Molecular Cluster (\( \zeta^4 \)) at various temperatures
Table 3: Molecular Cluster ($\zeta$) at various temperatures

<table>
<thead>
<tr>
<th>S. No.</th>
<th>Temp</th>
<th>$\zeta^{-1}$ (1)</th>
<th>$\zeta^{-1}$ (2)</th>
<th>$\zeta^{-1}$ (3)</th>
<th>$\zeta^{-1}$ (4)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>10</td>
<td>14994.92125</td>
<td>14991.40215</td>
<td>8511.093768</td>
<td>3778.478406</td>
</tr>
<tr>
<td>2</td>
<td>20</td>
<td>13179.85076</td>
<td>11361.03671</td>
<td>6814.077945</td>
<td>2073.623731</td>
</tr>
<tr>
<td>3</td>
<td>30</td>
<td>11397.18539</td>
<td>7884.969336</td>
<td>5162.862540</td>
<td>767.2047032</td>
</tr>
<tr>
<td>4</td>
<td>40</td>
<td>9648.222005</td>
<td>4697.233040</td>
<td>3572.815969</td>
<td>287.4672091</td>
</tr>
<tr>
<td>5</td>
<td>50</td>
<td>7935.442610</td>
<td>2241.990557</td>
<td>2095.451566</td>
<td>160.5869371</td>
</tr>
<tr>
<td>6</td>
<td>60</td>
<td>6263.171842</td>
<td>1050.958923</td>
<td>934.4160265</td>
<td>110.4755936</td>
</tr>
<tr>
<td>7</td>
<td>70</td>
<td>4641.868253</td>
<td>616.0957465</td>
<td>400.8569412</td>
<td>84.58877970</td>
</tr>
</tbody>
</table>

Table 4: Molecular Cluster ($\zeta$) at various temperatures

<table>
<thead>
<tr>
<th>S. No.</th>
<th>Temp</th>
<th>$\zeta^{-1}$ (5)</th>
<th>$\zeta^{-1}$ (6)</th>
<th>$\zeta^{-1}$ (7)</th>
<th>$\zeta^{-1}$ (8)</th>
<th>$\zeta^{-1}$ (9)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>10</td>
<td>5769.107053</td>
<td>23249.39901</td>
<td>4827.727689</td>
<td>4940.599525</td>
<td>11817.82899</td>
</tr>
<tr>
<td>2</td>
<td>20</td>
<td>4237.428281</td>
<td>21720.58188</td>
<td>3667.696146</td>
<td>3590.014627</td>
<td>9962.382333</td>
</tr>
<tr>
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<td>30</td>
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<td>20211.22899</td>
<td>2553.230564</td>
<td>2306.973957</td>
<td>8146.456918</td>
</tr>
<tr>
<td>4</td>
<td>40</td>
<td>1453.468783</td>
<td>18721.72838</td>
<td>1522.041792</td>
<td>1180.463736</td>
<td>6374.650827</td>
</tr>
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<td>17251.88243</td>
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<td>4657.671575</td>
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<tr>
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<td>15802.51821</td>
<td>319.1034686</td>
<td>241.0072790</td>
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<tr>
<td>7</td>
<td>70</td>
<td>162.7288078</td>
<td>14373.69369</td>
<td>184.1863833</td>
<td>155.1250789</td>
<td>1591.371641</td>
</tr>
</tbody>
</table>

DISCUSSION

Calculations show that Cyclohexanol [23249, 14374, 61.8%, 1-4 Dioxane [14995, 4642, 30.9%], methyalcohol [14991, 616, 4.1%] and Tetra hydro pyrrol [11818, 1591, 13.5%] are highly associative while Benzene [8511, 401, 4.7%] shows moderate clustering. Carbon tetrachloride [5769, 163, 2.8%], Cyclohexane [4941, 155, 3.1%], Methylcyclohexane [4828, 184, 3.8%], Tetra hydro furan [3778, 84, 2.2%] seems to remain less associative.

In the given set of liquids, Cyclohexanol [61.8%, 1-4 Dioxane [30.9%], Tetra hydro pyrrol [13.5%], Benzene [4.7%], methyalcohol [4.1%], Methylcyclohexane [3.8%], Cyclohexane [3.1%], Carbon tetrachloride [2.8%], Tetra hydro furan [2.2%] forms groups based on definition of cluster decay rate as $[\zeta^{-1}(\text{minimum}) \times 100 / \zeta^{-1}(\text{maximum})]$ descending order over temperature range 283.15 K to 343.15 K.
We have limited to qualitative results hence there is a scope for comparison with experiments and other models in the literature.

CONCLUSION

Each calculation shows unique solution of $\eta$ and $\tau$ due to occurrence of parameter $\zeta$. Here $\zeta^{-1}$ is associated to cluster size, so that built up picture seems to be virtually reliable.

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REFERENCES