*J. Chem. Eng. Data* **2006,** *51,* 671−675

# Densities, Viscosities, and Ultrasonic Velocity Studies of Binary Mixtures of Chloroform with Pentan-1-ol, Hexan-1-ol, and Heptan-1-ol at (303.15 and 313.15) K

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Densities, viscosities, and ultrasonic velocities of binary mixtures of chloroform with pentan-1-ol, hexan-1-ol, and heptan-1-ol have been measured over the entire range of composition at (303.15 and 313.15) K and at atmospheric pressure. From the experimental values of density, viscosity, and ultrasonic velocity, the excess molar volumes ($V^E$), deviations in viscosity ($\Delta\eta$), and excess isentropic compressibility ($\kappa_s^E$) have been calculated. The excess molar volumes ($V^E$) are positive for all the three binaries studied over the whole composition, the excess isentropic compressibilities ($\kappa_s^E$) are also positive except for low mole fractions of chloroform, while deviations in viscosities ($\Delta\eta$) are negative for all the three binary mixtures. The excess molar volumes, deviations in viscosity, and excess isentropic compressibility have been fitted to the Redlich−Kister polynomial equation. McAllister's three-body interaction model has been used to correlate the kinematic viscosities of binary liquid mixtures with mole fraction. The very recently proposed Jouyban−Acree model is used to correlate the experimental values of density, viscosity, and ultrasonic velocity at different temperatures.

## Introduction

Studies on thermodynamic and transport properties of binary liquid mixtures provide information on the nature of interactions in the constituent binaries. Literature provides extensive data on the density and viscosity of liquid mixtures, but a combined study of density, viscosity, and ultrasonic velocity is quite scarce. The effect of molecular size, shape, chain length, and degree of molecular association of normal alkanols and branched alkanols on the volumetric, viscometric, and acoustic properties of binary mixtures containing acetonitrile, dimethyl sulfoxide, ethyl acetate, and benzonitrile have been reported earlier.[1−5] Alkanols and chloroform are widely used industrial chemicals and solvents. Alkanols are self-associated, and there is a decrease in the self-association when they are mixed with chloroform as a result of hydrogen-bonded interaction between hydroxyl oxygen of alkanols and chloroform and due to the presence of specific interaction between hydroxyl oxygen of alkanols with the chlorine of chloroform. In the present paper, we report density, viscosity, and ultrasonic velocity data for the binary mixtures of chloroform with pentan-1-ol, hexan-1-ol, and heptan-1-ol at 303.15 K and 313.15 K.

## Experimental Section

Pentan-1-ol (E. Merck, purity 99.5 %), hexan-1-ol (s.d. fine chem., purity 99 %), and heptan-1-ol (s.d. fine chem., purity 99 %) were used after a single distillation. Chloroform (s.d. fine chem., purity 99 %) was shaken several times with distilled water to remove ethanol, dried over anhydrous calcium chloride, and then fractionally distilled. The purity of the solvents, after purification, was ascertained by comparing their densities, viscosities, and ultrasonic velocities with the corresponding literature values at 303.15 K (Table 1). Binary mixtures were prepared by mass in airtight stoppered glass bottles. The masses were recorded on an Adairdutt balance to an accuracy of ± 1 × $10^{-4}$ g. Care was taken to avoid evaporation and contamination during mixing. The estimated uncertainty in mole fraction was <1 × $10^{-4}$.

**Table 1. Comparison of Experimental Density, Viscosity, and Ultrasonic Velocity of Pure Liquids with Literature Values at 303.15 K**

| | $\rho \times 10^{-3}$/(kg·m$^{-3}$) | | $\eta$/(mPa·s) | | $u$/(m·s$^{-1}$) | |
|---|---|---|---|---|---|---|
| pure liquid | exptl | lit | exptl | lit | exptl | lit |
| chloroform | 1.46921 | 1.47060[a]<br>1.4692[b] | 0.534 | 0.514[a]<br>0.534[b] | 969 | 968[c] |
| pentan-1-ol | 0.80860 | 0.80720[a]<br>0.8079[d] | 3.017 | 2.933[e] | 1264 | 1263[f] |
| hexan-1-ol | 0.81165 | 0.81184[a]<br>0.8116[g] | 3.801 | 3.765[a]<br>3.792[h] | 1289 | 1289[g] |
| heptan-1-ol | 0.81494 | 0.8148[d] | 5.043 | 5.03[i] | 1313 | 1313[j] |

[a] Ref 11. [b] Ref 20. [c] Ref 21. [d] Ref 22. [e] Ref 23. [f] Ref 24. [g] Ref 25. [h] Ref 26. [i] Ref 27. [j] Ref 28.

Densities were determined by using 15 cm$^3$ bicapillary pycnometer with capillary bore with an internal diameter of 2 mm and a length of 15 cm$^3$ as described earlier.[6,7] The pycnometer was calibrated using conductivity water with 0.99705 g·cm$^{-3}$ as its density[8] at 298.15 K. The pycnometer filled with air bubble free experimental liquids was kept in a transparent walled water bath (maintained constant to ± 0.01 K) for (10 to 15) min to attain thermal equilibrium. The positions of the liquid levels in the two arms were recorded with the help of travelling microscope, which could read to 0.01 mm. The estimated uncertainty of density measurements of solvent and binary mixtures was 0.00005 g·cm$^{-3}$. At least three to four measurements were made, which had an average deviation of ± 0.00005 g·cm$^{-3}$.

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10.1021/je0504459 CCC: $33.50

**Table 2. Density ($\rho$), Viscosity ($\nu$), Ultrasonic Velocity ($u$), and Isentropic Compressibility ($\kappa_s$) for Chloroform (1) + Alkanols (2) at (303.15 and 313.15) K**

| | $T$ = 303.15 K | | | | $T$ = 313.15 K | | | | | $T$ = 303.15 K | | | | $T$ = 313.15 K | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $x_1$ | $\rho \times 10^{-3}$ / kg·m$^{-3}$ | $\nu$ / mm$^2$·s$^{-1}$ | $u$ / m·s$^{-1}$ | $\kappa_s$ / TPa$^{-1}$ | $\rho \times 10^{-3}$ / kg·m$^{-3}$ | $\nu$ / mm$^2$·s$^{-1}$ | $u$ / m·s$^{-1}$ | $\kappa_s$ / TPa$^{-1}$ | $x_1$ | $\rho \times 10^{-3}$ / kg·m$^{-3}$ | $\nu$ / mm$^2$·s$^{-1}$ | $u$ / m·s$^{-1}$ | $\kappa_s$ / TPa$^{-1}$ | $\rho \times 10^{-3}$ / kg·m$^{-3}$ | $\nu$ / mm$^2$·s$^{-1}$ | $u$ / m·s$^{-1}$ | $\kappa_s$ / TPa$^{-1}$ |
| Chloroform (1) + Pentan-1-ol (2) | | | | | | | | | | | | | | | | | |
| 0.0000 | 0.80860 | 3.731 | 1264 | 774 | 0.80099 | 2.890 | 1228 | 828 | 0.5498 | 1.12144 | 0.931 | 1068 | 782 | 1.10855 | 0.802 | 1032 | 847 |
| 0.0603 | 0.83865 | 3.293 | 1241 | 774 | 0.83058 | 2.560 | 1206 | 828 | 0.6001 | 1.15525 | 0.827 | 1053 | 781 | 1.14178 | 0.722 | 1017 | 847 |
| 0.1009 | 0.85939 | 3.022 | 1226 | 774 | 0.85098 | 2.355 | 1191 | 828 | 0.6513 | 1.19080 | 0.724 | 1038 | 779 | 1.17665 | 0.643 | 1002 | 846 |
| 0.1484 | 0.88422 | 2.697 | 1209 | 774 | 0.87542 | 2.116 | 1173 | 830 | 0.7003 | 1.22593 | 0.657 | 1025 | 776 | 1.21112 | 0.585 | 989 | 844 |
| 0.1999 | 0.91183 | 2.371 | 1190 | 774 | 0.90258 | 1.878 | 1154 | 832 | 0.7510 | 1.26353 | 0.585 | 1012 | 773 | 1.24797 | 0.530 | 977 | 839 |
| 0.2517 | 0.94034 | 2.084 | 1171 | 776 | 0.93067 | 1.661 | 1135 | 834 | 0.8000 | 1.30108 | 0.530 | 1001 | 767 | 1.28481 | 0.483 | 966 | 834 |
| 0.2999 | 0.96760 | 1.827 | 1153 | 777 | 0.95742 | 1.475 | 1117 | 837 | 0.8503 | 1.34102 | 0.487 | 991 | 759 | 1.32397 | 0.448 | 956 | 826 |
| 0.3492 | 0.99623 | 1.607 | 1135 | 779 | 0.98558 | 1.308 | 1099 | 840 | 0.9004 | 1.38224 | 0.442 | 982 | 750 | 1.36437 | 0.411 | 947 | 817 |
| 0.3998 | 1.02646 | 1.392 | 1118 | 779 | 1.01529 | 1.150 | 1082 | 841 | 0.9520 | 1.42640 | 0.405 | 974 | 739 | 1.40756 | 0.375 | 938 | 807 |
| 0.4500 | 1.05732 | 1.218 | 1101 | 780 | 1.04559 | 1.018 | 1065 | 843 | 1.0000 | 1.46921 | 0.363 | 969 | 725 | 1.44974 | 0.339 | 934 | 791 |
| 0.5004 | 1.08921 | 1.067 | 1084 | 781 | 1.07695 | 0.903 | 1048 | 845 | | | | | | | | | |
| Chloroform (1) + Hexan-1-ol (2) | | | | | | | | | | | | | | | | | |
| 0.0000 | 0.81165 | 4.683 | 1289 | 742 | 0.80424 | 3.631 | 1256 | 788 | 0.5520 | 1.10094 | 1.144 | 1087 | 769 | 1.08853 | 0.950 | 1051 | 832 |
| 0.0497 | 0.83307 | 4.356 | 1271 | 743 | 0.82531 | 3.213 | 1238 | 791 | 0.6000 | 1.13301 | 0.987 | 1070 | 771 | 1.12000 | 0.833 | 1034 | 835 |
| 0.1004 | 0.85562 | 3.881 | 1253 | 744 | 0.84751 | 2.892 | 1220 | 793 | 0.6540 | 1.17075 | 0.852 | 1052 | 772 | 1.15700 | 0.735 | 1016 | 837 |
| 0.1500 | 0.87854 | 3.445 | 1236 | 745 | 0.87006 | 2.594 | 1201 | 797 | 0.7001 | 1.20457 | 0.746 | 1038 | 771 | 1.19018 | 0.649 | 1002 | 837 |
| 0.2006 | 0.90279 | 3.044 | 1217 | 748 | 0.89394 | 2.311 | 1182 | 801 | 0.7530 | 1.24539 | 0.650 | 1023 | 767 | 1.23025 | 0.582 | 986 | 836 |
| 0.2506 | 0.92771 | 2.671 | 1198 | 751 | 0.91840 | 2.051 | 1163 | 805 | 0.7992 | 1.28269 | 0.582 | 1010 | 764 | 1.26683 | 0.522 | 974 | 832 |
| 0.3005 | 0.95348 | 2.336 | 1180 | 753 | 0.94371 | 1.825 | 1143 | 811 | 0.8511 | 1.32707 | 0.508 | 997 | 758 | 1.31035 | 0.470 | 961 | 826 |
| 0.3497 | 0.98004 | 2.044 | 1161 | 757 | 0.96985 | 1.604 | 1125 | 815 | 0.8996 | 1.37059 | 0.450 | 987 | 749 | 1.35295 | 0.426 | 950 | 819 |
| 0.4004 | 1.00841 | 1.774 | 1142 | 760 | 0.99766 | 1.409 | 1105 | 821 | 0.9502 | 1.41868 | 0.406 | 977 | 738 | 1.40010 | 0.381 | 941 | 807 |
| 0.4516 | 1.03838 | 1.531 | 1123 | 764 | 1.02709 | 1.233 | 1086 | 826 | 1.0000 | 1.46921 | 0.363 | 969 | 725 | 1.44974 | 0.339 | 934 | 791 |
| 0.4996 | 1.06763 | 1.338 | 1106 | 766 | 1.05584 | 1.089 | 1069 | 829 | | | | | | | | | |
| Chloroform (1) + Heptan-1-ol (2) | | | | | | | | | | | | | | | | | |
| 0.0000 | 0.81494 | 6.188 | 1312 | 713 | 0.80777 | 4.588 | 1278 | 758 | 0.5517 | 1.08209 | 1.352 | 1107 | 754 | 1.06943 | 1.133 | 1072 | 814 |
| 0.0487 | 0.83337 | 5.582 | 1296 | 714 | 0.82581 | 4.167 | 1262 | 760 | 0.6002 | 1.11383 | 1.174 | 1089 | 757 | 1.10051 | 1.001 | 1054 | 818 |
| 0.1002 | 0.85369 | 4.978 | 1277 | 718 | 0.84575 | 3.743 | 1244 | 764 | 0.6539 | 1.15117 | 0.976 | 1070 | 759 | 1.13719 | 0.845 | 1035 | 821 |
| 0.1498 | 0.87420 | 4.410 | 1260 | 721 | 0.86580 | 3.344 | 1226 | 768 | 0.6994 | 1.18484 | 0.851 | 1054 | 760 | 1.17019 | 0.741 | 1019 | 823 |
| 0.2006 | 0.89615 | 3.862 | 1241 | 725 | 0.88732 | 2.954 | 1207 | 774 | 0.7449 | 1.22055 | 0.740 | 1039 | 759 | 1.20518 | 0.659 | 1004 | 823 |
| 0.2516 | 0.91927 | 3.381 | 1222 | 728 | 0.90996 | 2.612 | 1187 | 780 | 0.8000 | 1.26683 | 0.633 | 1022 | 756 | 1.25050 | 0.569 | 987 | 821 |
| 0.3003 | 0.94239 | 2.930 | 1204 | 732 | 0.93257 | 2.293 | 1168 | 786 | 0.8465 | 1.30867 | 0.558 | 1008 | 752 | 1.29164 | 0.509 | 972 | 819 |
| 0.3538 | 0.96909 | 2.521 | 1183 | 737 | 0.95873 | 1.993 | 1147 | 793 | 0.9003 | 1.36081 | 0.481 | 993 | 745 | 1.34282 | 0.445 | 957 | 813 |
| 0.4003 | 0.99352 | 2.179 | 1165 | 742 | 0.98267 | 1.750 | 1129 | 798 | 0.9521 | 1.41486 | 0.420 | 979 | 737 | 1.39616 | 0.388 | 943 | 805 |
| 0.4466 | 1.01910 | 1.894 | 1147 | 746 | 1.00769 | 1.536 | 1111 | 804 | 1.0000 | 1.46921 | 0.363 | 969 | 725 | 1.44974 | 0.339 | 934 | 791 |
| 0.5001 | 1.05023 | 1.605 | 1126 | 751 | 1.03822 | 1.321 | 1091 | 809 | | | | | | | | | |

The kinematic viscosities were measured using an Ubbelohde suspended level viscometer,[7] calibrated with conductivity water. An electronic digital stop watch with readability of ± 0.01 s was used for the flow time measurements. At least three repetitions of each data reproducible to ± 0.05 s were obtained, and the results were averaged. Since all flow times were greater than 200 s and capillary radius (0.5 mm) was far less than its length (50 to 60) mm, the kinetic energy and end corrections, respectively, were found to be negligible. The uncertainties in kinematic viscosities are of the order of ± 0.003 mm$^2$·s$^{-1}$.

The ultrasonic velocities ($u$) were measured at a frequency of 2 MHz in these solutions using an interferometric method, Mittal's F-81 model (with a precision of ± 0.8 m·s$^{-1}$), at (303.15 and 313.15) K (± 0.05 K). The uncertainty in velocity measurements is ± 0.1 %.The other experimental details are the same as reported earlier.[2−4]

## Results and Discussion

Experimental values of densities ($\rho$), viscosities ($\eta$), and ultrasonic velocities ($u$) of mixtures at (303.15 and 313.15) K are listed as a function of mole fraction in Table 2. The density values have been used to calculate excess molar volumes ($V^E$) using the following equation:

$$V^E = (x_1M_1 + x_2M_2)/\rho_{12} - (x_1M_1/\rho_1) - (x_2M_2/\rho_2) \qquad (1)$$

where $\rho_{12}$ is the density of the mixture and $x_1$, $M_1$, $\rho_1$, and $x_2$, $M_2$, $\rho_2$ are the mole fraction, the molecular weight, and the density of pure components 1 and 2, respectively.

The viscosity deviations $\Delta\eta$ were calculated using

$$\Delta\eta = \eta_{12} - x_1\eta_1 - x_2\eta_2 \qquad (2)$$

where $\eta_{12}$ is the viscosity of the mixture and $x_1$, $x_2$ and $\eta_1$, $\eta_2$ are the mole fraction and the viscosity of pure components 1 and 2, respectively. The excess isentropic compressibility ($\kappa_s^E$) was obtained using the relation

$$\kappa_s^E = \kappa_s - \kappa_s^{id} \qquad (3)$$

where $\kappa_s$ is the isentropic compressibility and was calculated using the Laplace relation, that is $\kappa_s = (1/u^2\rho)$ and $\kappa_s^{id}$ was calculated from the relation:[9,10]

$$\kappa_s^{id} = \sum\phi_i[\kappa_{s,i} + TV^\circ_i(\alpha^{\circ 2}_i)/C_{p,i}] - [T(\sum x_iV^\circ_i)(\sum\phi_i\alpha^\circ_i)^2/\sum x_iC_{p,i}] \qquad (4)$$

where $\phi_i$ is the volume fraction of the component $i$ in the mixture stated, $T$ is the temperature, and $\kappa_{s,i}$, $V^\circ_i$, $\alpha^\circ_i$, and $C_{p,i}$ are the isentropic compressibility, molar volume, coefficient of thermal expansion, and molar heat capacity, respectively, for pure component $i$. The values required were taken from literature.[11,12]

The excess molar volumes and excess isentropic compressibility and deviations in viscosity were fitted to a Redlich−

**Table 3. Parameters and Standard Deviations ($\sigma$) of Equations 5 and 6 for Chloroform + Pentan-1-ol, Chloroform + Hexan-1-ol, and Chloroform + Heptan-1-ol**

| | $T$/K | $a_0$ | $a_1$ | $a_2$ | $a_3$ | $a_4$ | $\sigma$ |
|---|---|---|---|---|---|---|---|
| | | | Chloroform + Pentan-1-ol | | | | |
| $V^E/(\mathrm{cm^3 \cdot mol^{-1}})$ | 303.15 | 0.6162 | 0.44 | −0.0237 | 0.1140 | 0.1765 | 0.001 |
| | 313.15 | 0.716 | 0.4196 | −0.1465 | 0.3035 | 0.5155 | 0.004 |
| $\Delta\eta/(\mathrm{mPa \cdot s})$ | 303.15 | −2.4633 | 0.1267 | 0.7690 | −0.1152 | 0.1722 | 0.005 |
| | 313.15 | −1.72730 | 0.1234 | 0.5993 | | | 0.003 |
| $\kappa_s^E/(\mathrm{TPa^{-1}})$ | 303.15 | 40.682 | 77.534 | 12.253 | | | 0.74 |
| | 313.15 | 58.681 | 97.474 | 8.048 | | | 0.89 |
| | | | Chloroform + Hexan-1-ol | | | | |
| $V^E/(\mathrm{cm^3 \cdot mol^{-1}})$ | 303.15 | 0.6615 | 0.4607 | 0.0703 | 0.1684 | | 0.003 |
| | 313.15 | 0.8130 | 0.5010 | −0.1483 | 0.2311 | 0.3732 | 0.004 |
| $\Delta\eta/(\mathrm{mPa \cdot s})$ | 303.15 | −2.941 | 0.3304 | −0.1865 | −1.7920 | 2.4707 | 0.019 |
| | 313.15 | −2.2591 | −0.0377 | 0.8425 | 0.9304 | −1.1704 | 0.009 |
| $\kappa_s^E/(\mathrm{TPa^{-1}})$ | 303.15 | 53.877 | 102.779 | −3.524 | −29.594 | | 0.63 |
| | 313.15 | 87.270 | 106.732 | −25.515 | 36.634 | 70.135 | 0.68 |
| | | | Chloroform + Heptan-1-ol | | | | |
| $V^E/(\mathrm{cm^3 \cdot mol^{-1}})$ | 303.15 | 0.9579 | 0.6297 | 0.0435 | | | 0.004 |
| | 313.15 | 1.4535 | 0.7301 | −0.0889 | 0.0676 | 0.2863 | 0.002 |
| $\Delta\eta/(\mathrm{mPa \cdot s})$ | 303.15 | −4.4316 | 0.238 | 0.9355 | −0.1590 | 0.1911 | 0.007 |
| | 313.15 | −2.9144 | 0.0905 | 0.6213 | −0.0812 | 0.1953 | 0.006 |
| $\kappa_s^E/(\mathrm{TPa^{-1}})$ | 303.15 | 42.113 | 63.468 | −21.756 | | | 0.34 |
| | 313.15 | 108.818 | 91.703 | −45.353 | 59.927 | 85.518 | 0.80 |

Kister[13] equation of the type

$$Y = x_1 x_2 \sum_{i}^{n} a_i (x_1 - x_2)^i \tag{5}$$

where $Y$ is either $V^E$, $\Delta\eta$, or $\kappa_s^E$ and $n$ is the degree of polynomial. Coefficients $a_i$ were obtained by fitting eq 5 to experimental results using a least-squares regression method. In each case, the optimum number of coefficients is ascertained from an examination of the variation in standard deviation ($\sigma$).

$\sigma$ was calculated using the relation

$$\sigma(Y) = \left[\frac{\sum (Y_{\mathrm{expt}} - Y_{\mathrm{calc}})^2}{N - n}\right]^{1/2} \tag{6}$$

where $N$ is the number of data points and $n$ is the number of coefficients. The calculated values of the coefficients ($a_i$) along with the standard deviations ($\sigma$) are given in Table 3.

The variation of $V^E$ with the mole fraction $x_1$ of chloroform for pentan-1-ol, hexan-1-ol, and heptan-1-ol at 303.15 K is represented in Figure 1. The observed positive excess molar volumes in the present investigation may be discussed in terms of several effects.[14] These may be divided into three types; chemical, physical, and structural. Changes in the associative equilibria of alkan-1-ol molecules may lead to contributions of all the three types. The disruption of alkanol aggregates through the breaking of hydrogen bonds makes $V^E$ positive since aggregates have smaller volumes than the sum of their components. As the chain length in alkanols increases, the proton-donating ability and the strength and extent of H-bonds decrease. Thus, the mixtures of chloroform with alkanols show the trend heptan-1-ol > hexan-1-ol > pentan-1ol.

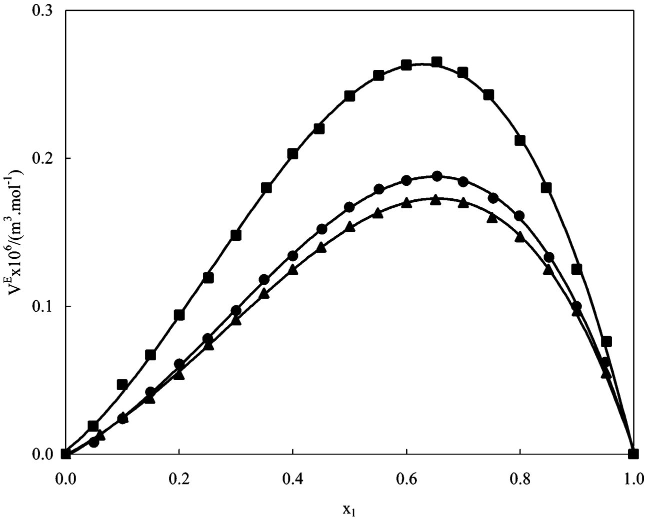

**Figure 1.** Excess molar volumes ($V^E$) at 303.15 K for $x_1$ chloroform + (1 − $x_1$) alkanols: ▲, pentan-1-ol; ●, hexan-1-ol; ■, heptan-1-ol.

Figure 2 depicts the variation of $\Delta\eta$ with the mole fraction $x_1$ of chloroform. $\Delta\eta$ values are negative in all systems and become more negative with an increase in chain length of alkanols, suggesting a decrease in heteroassociation of molecules with an increase in molar mass of alkanols.

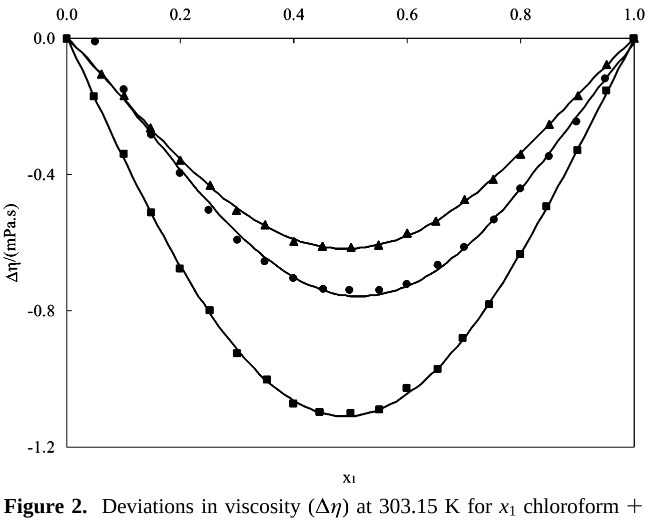

**Figure 2.** Deviations in viscosity ($\Delta\eta$) at 303.15 K for $x_1$ chloroform + (1 − $x_1$) alkanols: ▲, pentan-1-ol; ●, hexan-1-ol; ■, heptan-1-ol.

Kinematic viscosities ($\nu$) of the binary liquid mixtures were obtained from their dynamic viscosities and densities. McAllister's three-body interaction model[15] has been used to correlate the kinematic viscosities of binary liquid mixtures:

$$\ln \nu = x_1^3 \ln \nu_1 + x_2^3 \ln \nu_2 + 3x_1^2 x_2 \ln \nu_{12} + 3x_1 x_2^2 \ln \nu_{21} - \ln[x_1 + (x_2 M_2/M_1)] + 3x_1^2 x_2 \ln[(2/3) + (M_2/3M_1)] + 3x_1 x_2^2 \ln[(1/3) + (2M_2/3M_1)] + x_2^3 \ln(M_2/M_1) \tag{7}$$

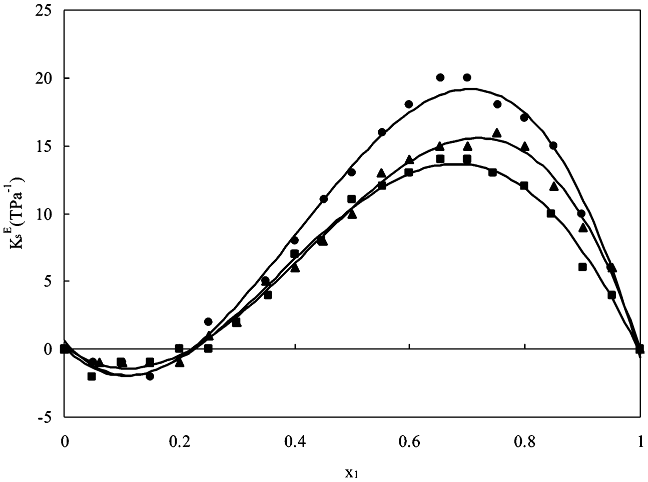

**Figure 3.** Excess isentropic compressibility ($\kappa_s^E$) at 303.15 K for $x_1$ chloroform + (1 − $x_1$) alkanols: ▲, pentan-1-ol; ●, hexan-1-ol; ■, heptan-1-ol.

**Table 4. Parameters of McAllister's Model and Standard Percentage Deviation for Kinematic Viscosities at (303.15 and 313.15) K**

| system | $T$/K | $\nu_{12}$ | $\nu_{21}$ | $\sigma$ % |
|---|---|---|---|---|
| chloroform + pentan-1-ol | 303.15 | 0.6419 | 1.838 | 2.43 |
| | 313.15 | 0.5942 | 1.4315 | 2.41 |
| chloroform + hexan-1-ol | 303.15 | 0.6929 | 2.6757 | 1.17 |
| | 313.15 | 0.6872 | 1.7232 | 1.58 |
| chloroform +heptan-1-ol | 303.15 | 0.8777 | 3.1193 | 1.28 |
| | 313.15 | 0.7882 | 2.3793 | 1.46 |

where $\nu_{12}$ and $\nu_{21}$ are model parameters. The percentage standard deviation was calculated by using the following equation:

$$\sigma\,\% = \sum[(100(\nu_{\mathrm{exptl}} - \nu_{\mathrm{calcd}})/\nu_{\mathrm{exptl}})^2/(n - m)]^{1/2} \qquad (8)$$

where $n$ represents the number of experimental points and $m$ represents the number of coefficients. Table 4 includes the different parameters and percentage standard deviations. From Table 4, it is clear that McAllister's three-body interaction model is suitable for correlating the kinematic viscosities of the binary mixtures studied.

The variation of $\kappa_s^E$ with composition of mixture ($x_1$ of chloroform) is represented in Figure 3. Kiyohara and Benson[16] have suggested that $\kappa_s^E$ is the result of several opposing effects. A strong molecular interaction through charge transfer, dipole−induced dipole and dipole−dipole[17] interactions, interstitial accommodation, and orientational ordering lead to a more compact structure making $\kappa_s^E$ negative, and a break-up of the alkanol structures tends to make $\kappa_s^E$ positive. The magnitudes of the various contributions depend mainly on the relative molecular size of the components. The positive values of $\kappa_s^E$ for mixtures of chloroform with pentan-1-ol, hexan-1-ol, and heptan-1-ol signify decreasing dipole−dipole interactions due to less decreasing proton-donating abilities with increasing chain length of alkan-1-ols. Declustering of alkan-1-ols in the presence of chloroform may also lead to positive $\kappa_s^E$ values.

Recently Jouyban and Acree and co-workers[18,19] proposed a model for correlating the density and viscosity of liquid mixtures at various temperatures. The proposed equation is

$$\ln y_{m,T} = f_1 \ln y_{1,T} + f_2 \ln y_{2,T} + f_1 f_2 \sum[A_j (f_1 - f_2)^j / T] \qquad (9)$$

**Table 5. Parameters of Jouyban−Acree Model and Average Percentage Deviation for Densities, Viscosities, and Ultrasonic Velocities**

| system | $A_0$ | $A_1$ | $A_2$ | APD |
|---|---|---|---|---|
| | Density | | | |
| chloroform + pentan-1-ol | 51.448 | −12.226 | 2.327 | 0.02 |
| chloroform + hexan-1-ol | 50.565 | −11.779 | 2.665 | 0.01 |
| chloroform + heptan-1-ol | 48.486 | −11.262 | 2.999 | 0.02 |
| | Viscosity | | | |
| chloroform + pentan-1-ol | −119.068 | −106.471 | 162.075 | 0.91 |
| chloroform + hexan-1-ol | −35.269 | −150.167 | 56.033 | 1.70 |
| chloroform + heptan-1-ol | 14.902 | −140.685 | 74.045 | 0.88 |
| | Ultrasonic Velocity | | | |
| chloroform + pentan-1-ol | −25.184 | −22.169 | −6.363 | 0.05 |
| chloroform + hexan-1-ol | −14.807 | −25.395 | −6.829 | 0.09 |
| chloroform + heptan-1-ol | −0.844 | −23.273 | −6.364 | 0.05 |

where $y_{m,T}$, $y_{1,T}$, and $y_{2,T}$ are density, or viscosity of the mixture and solvents 1 and 2 at temperature $T$, respectively; $f_1$and $f_2$ are the volume fractions of solvents in case of density and mole fraction in case of viscosity; and $A_j$ is the model constants.

The correlating ability of the Jouyban−Acree model was tested by calculating the average percentage deviation (APD) between the experimental and calculated density and viscosity as

$$\mathrm{APD} = (100/N)\sum[(|y_{\mathrm{exptl}} - y_{\mathrm{calcd}}|)/\,y_{\mathrm{exptl}})] \qquad (10)$$

where $N$ is the number of data points in each set. The optimum numbers of constants $A_j$, in each case, were determined from the examination of the average percentage deviation value.

The Jouyban−Acree model was not previously applied to ultrasonic velocity measurements. We extend the Jouyban−Acree model (eq 9) to ultrasonic velocity of the liquid mixtures with $f$ as the mole fraction and again apply eq 10 for the correlating ability of the model.

The constants $A_j$ calculated from the least-squares analysis are presented in Table 5 along with the average percentage deviation (APD). The proposed model provides reasonably accurate calculations for the density, viscosity, and ultrasonic velocity of binary liquid mixtures at various temperatures, and the model could be used in data modeling.

### Acknowledgment

The authors thank the Principal of M. S. G. College for the facilities provided.

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Received for review October 21, 2005. Accepted January 23, 2006. U.B.K. thanks University Grants Commission for the award of a teacher fellowship.

JE0504459