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Temperature Dependence of Viscosities of Heptamethylene Dibromide Solutions in Ethanol at 288-323 K

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The densities and viscosities of heptamethylene dibromide in ethanol had been determined from (288.15 to 323.15) K. The relative viscosities were correlated using the Surtherland-Wassiljewa equation. The results showed that the model agreed well with the experimental data.

Keywords: Heptamethylene dibromide, Densities, Viscosities, Correlation, Surtherland-Wassiljewa equation.

INTRODUCTION

Heptamethylene dibromide is an important pharmaceutical intermediate, commonly used in drugs, chiral macrocyclic ligands, long-chain fatty alcohol and the synthesis of cationic surfactant and is widely used in the fields of pharmacy, bionic chemical, petroleum, food and cosmetics. In the synthesis and purification process of heptamethylene dibromide, it is useful to know the basic data of densities and viscosities of heptamethylene dibromide and its solution. The densities and viscosities are very important data in chemical engineering design, process optimization and molecular thermodynamic study of solution. In this study, based on the densities and viscosities of heptamethylene dibromide[1] and its solution from (288.15 to 323.15) K, the relative viscosities of heptamethylene dibromide in ethanol are calculated and correlated using the Surtherland-Wassiljewa equation. Results are fit to obtain the adjustable parameters and standard deviations between the measured and fitted values. These parameters had certain practical value for the design and synthesis of heptamethylene dibromide.

EXPERIMENTAL

Heptamethylene dibromide and ethanol were of AR grade and obtained from Shanghai Chemical Reagent Co. All the liquids were stored in dark bottles over 0.4 nm molecular sieves to reduce the water content and were degassed before use. The estimated purities as per gas chromatographic analysis were better than 99.5 mol % for all liquid samples. Further, the purities of liquids were checked by comparing the measured densities and viscosities with those reported in the literature[2,3]. The double-distilled and degassed water used in the experiments was deionized and its conductivity was less than 5 μS m^{-1}.

Measurements of densities: The density of the mixtures and the corresponding pure substances were measured with an Anton Paar Model DMA 5000 digital vibrating U-tube densimeter, with automatic viscosity correction[1] and a stated accuracy of ± 5 × 10^{-6} g cm^{-3}. The temperature in the cell was regulated to ± 0.001 K with a built-in solid-state thermostat. It was measured by means of two integrated Pt 100 platinum thermometers and its stability was better than ± 0.002 K. The reliability of the apparatus was verified daily with dry air and distilled freshly degassed water. To minimize the errors in composition, all mixtures were prepared by mass using the cell and the procedure described by Roberto *et al.*[4] and a Mettler AG 204 balance with a precision of 1 × 10^{-4} g. The uncertainty of the mole fraction calculation was less than ± 1 × 10^{-4}. All molar quantities were based on the IUPAC relative atomic mass table. The experimental uncertainty in density was about ± 1 × 10^{-4} g cm^{-3}.

Measurements of viscosities: Viscosity was measured using an Ubbelohde-type glass capillary viscometer of 0.6 mm diameter (type 1836-A, Shanghai Glass Instruments Factory, China), calibrated with double-distilled water at (288.15 and 323.15) K[1]. A thoroughly cleaned and perfectly dried viscometer, filled with experimental solution, was placed exactly vertical in an insulated jacket, wherein constant temperature (± 0.02 K) was maintained by circulating water from a thermoelectric controller (type 501, Shanghai Laboratory Instrument Works Co., Ltd.) at the required temperature. After thermal stability was attained, the flow times of the solutions were recorded with an electronic digital stopwatch correct to ± 0.01

s. At least five repetitions of each datum point obtained were reproducible to ± 0.06 s and the results were averaged. Because all flow times were greater than 150 s and the capillary diameter (0.6 mm) was far less than its length (120 mm), the kinetic energy and end corrections, respectively, were found to be negligible. The viscosity was then calculated from the fundamental relationship[5].

The values of viscosity and density of pure water obtained from the literature[2]. The uncertainty in the viscosity measurement is estimated to be ± 0.006 mPa s.

Experiment reliability proof: The densities and viscosities, water and ethanol or pure heptamethylene dibromide were measured and compared with literature values[2,3]. The results were listed in Table-1. It could be seen that the present experimental values of densities and viscosities were in good agreement with those reported in the literature[2,3].

RESULTS AND DISCUSSION

The measured densities and viscosities of heptamethylene dibromide in ethanol at various temperatures and mole fraction x of heptamethylene dibromide were listed in Table-2. It can

TABLE-1
COMPARISON OF EXPERIMENTAL DATA AND LITERATURE DATA FOR DENSITIES AND VISCOSITIES OF ETHANOL OR WATER OR HEPTAMETHYLENE DIBROMIDE

Substance	ρ (g cm^{-3})	ρ(lit) (g cm^{-3})	100 RD	η (mPa s)	η (lit) (mPa s)	100 RD
Water	0.9982	0.99820 (293.15 K) [Ref. 2]	0.00	0.8000	0.7977 (303.15 K) [Ref. 2]	0.28
Ethanol	0.7893	0.78940 (293.15 K) [Ref. 2]	-0.01	1.0760	1.0740 (298.15 K) [Ref. 2]	0.19
Heptamethylene dibromide	1.5124	1.51300 (293.15 K) [Ref. 3]	0.04	-	-	-

TABLE-2
DENSITIES AND VISCOSITIES FOR HEPTAMETHYLENE DIBROMIDE IN ETHANOL AT VARIOUS TEMPERATURES AND MOLE FRACTION x

x	ρ (g cm^{-3})	η (mPa s)	100 RD	ρ (g cm^{-3})	η (mPa s)	100 RD
	T = 288.15 K			T = 293.15 K		
0.0992	0.9787	1.672	0.60	0.9744	1.503	0.56
0.1985	1.1087	2.071	-1.69	1.1045	1.856	-0.74
0.2970	1.2062	2.554	0.63	1.2014	2.242	0.15
0.3949	1.2778	2.952	-0.22	1.2745	2.601	-0.05
0.4945	1.3392	3.449	2.06	1.3335	2.991	0.75
0.5919	1.3892	3.734	-1.23	1.3824	3.268	-1.71
0.6870	1.4275	4.158	-0.17	1.4228	3.706	1.04
0.7857	1.4616	4.523	-0.76	1.4561	4.035	0.34
0.8829	1.4907	4.967	0.62	1.4858	4.351	-0.36
	T = 298.15 K			T = 303.15 K		
0.0992	0.9700	1.356	0.14	0.9650	1.237	0.63
0.1985	1.0987	1.655	-1.07	1.0944	1.48771	-1.88
0.2970	1.1961	2.009	1.09	1.1905	1.80074	0.17
0.3949	1.2694	2.301	0.14	1.2640	2.059	-0.83
0.4945	1.3266	2.606	-0.22	1.3219	2.3569	0.00
0.5919	1.3758	2.908	-0.32	1.3706	2.659	1.10
0.6870	1.4170	3.233	0.59	1.4108	2.864	-1.05
0.7857	1.4503	3.493	-0.77	1.4440	3.153	-0.42
0.8829	1.4795	3.833	0.35	1.4732	3.434	0.05
	T = 308.15 K			T = 313.15 K		
0.0992	0.9598	1.120	0.90	0.9556	1.027	-0.84
0.1985	1.0890	1.347	-1.22	1.0858	1.227	-0.88
0.2970	1.1853	1.618	0.25	1.1820	1.457	0.96
0.3949	1.2581	1.857	-0.27	1.2542	1.671	1.16
0.4945	1.3157	2.119	0.29	1.3112	1.876	0.40
0.5919	1.3642	2.354	-0.15	1.3601	2.111	1.19
0.6870	1.4043	2.614	0.72	1.3989	2.230	-3.26
0.7857	1.4381	2.822	-0.67	1.4345	2.538	0.19
0.8829	1.4674	3.086	0.14	1.4637	2.787	0.77
	T = 318.15 K			T = 323.15 K		
0.0992	0.9512	0.938	0.09	0.9466	0.861	0.41
0.1985	1.0795	1.120	-0.89	1.0752	1.015	-0.88
0.2970	1.1757	1.332	0.65	1.1702	1.198	0.51
0.3949	1.2480	1.522	0.28	1.2433	1.365	0.23
0.4945	1.3068	1.719	0.10	1.3005	1.522	-1.02
0.5919	1.3535	1.920	0.28	1.3463	1.735	1.29
0.6870	1.3934	2.093	-0.77	1.3883	1.877	-0.49
0.7857	1.4284	2.312	-0.06	1.4216	2.065	-0.23
0.8829	1.4575	2.523	0.26	1.4529	2.257	0.15

TABLE-3
REGRESSION COEFFICIENTS AND STANDARD DEVIATION OF HEPTAMETHYLENE DIBROMIDE IN ETHANOL

Temperature (K)	A_{11}	A_{12}	A_{22}	100 RMSD	100 RAD
288.15	1.0408	0.9411	0.8887	4.03	0.89
293.15	1.1863	1.1338	0.9624	3.12	0.63
298.15	1.3817	1.3415	1.0391	0.21	0.52
303.15	1.5463	1.4883	1.1418	2.03	0.68
308.15	1.7274	1.6898	1.2557	1.22	0.51
313.15	1.9616	2.2051	1.2817	3.02	1.10
318.15	2.1533	2.2713	1.4390	0.82	0.38
323.15	2.4330	2.6577	1.5478	1.13	0.58

be seen that the densities and viscosities of heptamethylene dibromide in ethanol decrease with the increase of temperature. The relation of the densities and temperature have good linear relationship. The viscosities for heptamethylene dibromide in ethanol at various temperatures and mole fraction x of heptamethylene dibromide also have good linear relationship, it could be found that the viscosities increased with increasing mole fraction of heptamethylene dibromide at constant temperature and decreased with increasing temperature at a fixed mole fraction of heptamethylene dibromide for heptamethylene dibromide in ethanol. The viscosities for heptamethylene dibromide in ethanol were calculated from the Surtherland-Wassiljewa equation of the binary non-electrolyte mixture[6].

$$\eta_m = \sum_i \frac{x_i \eta_i}{\sum_i A_{ij} x_j} \quad (1)$$

where x_i is mole fraction of component i and A_{ij} is the Wassiljewa coefficient interpreted as the ratio of the efficiencies with which molecules 'j' and 'i' impede the transport of momentum by molecules 'i'.

The Wassiljewa coefficient A_{ij} is independent of composition and the temperature dependence of A_{ij} is smaller than the experimental error.

Wassiljewa coefficients obtained by a computerized least squares procedure from the experimental data were listed in Table-3 along with the RMSD and RAD.

The root-mean-square deviation (RMSD) was defined by Li *et al.*[7].

$$RMSD = \left[\frac{1}{N-1} \sum_{i=1}^{N} (\eta_{ci} - \eta_i)^2 \right]^{1/2} \quad (2)$$

where N is the number of experimental points, η_{ci} represents the viscosities calculated from equations and η_i represents the experimental viscosity values.

The relative average deviations (RAD) was defined by Li *et al.*[7].

$$RAD = \frac{1}{N} \sum_{i=1}^{N} \left| \frac{\eta_i - \eta_{ci}}{\eta_i} \right| \quad (3)$$

The relative deviations between the experimental value and calculated value were listed in Table-2. Relative deviations (RD) were calculated according to:

$$RD = \frac{\eta - \eta_c}{\eta} \quad (4)$$

where η_c represents the viscosities calculated from equations and η represents the experimental viscosity values.

The Wassiljewa coefficient values obtained at various temperatures were listed in Table-3.

From Table-2, it can be found that the calculated viscosities showed good agreement with the experimental data, the absolute value of relative deviations by eqn. 1 among all of these value did not exceed 3.26 %. Table-3 showed that the relative average deviations was less than 1.10 %. The RMSD was less than 4.03 %, which indicated that the Surtherland-Wassiljewa equation was suited to correlate the viscosity data of heptamethylene dibromide in ethanol.

Conclusion

The densities and viscosities of heptamethylene dibromide in ethanol had been determined from (288.15 to 323.15) K. The viscosities were correlated using the Surtherland-Wassiljewa equation, it appeared the absolute value of relative deviation among all these values did not exceed 3.26 % and the average relative deviation was 0.66 %, the viscosities calculated by the model showed good agreement with the experimental data.

REFERENCES

1. H. Li, H.K. Wang and X.S. Chen, *Exp. Therm. Fluid Sci.*, **35**, 1480 (2011).
2. J.A. Dean, Lange's Handbook of Chemistry, McGraw-Hill: New York, edn 15 (1999).
3. Handbook of Fine Chemicals, Sigma-Aldrich Group: USA (2008).
4. F.P. Roberto, A.H. Harvey and D.A. Palmer, Aqueous Systems at Elevated Temperatures and Pressures, Academic Press (2004).
5. J.Y. Wang, F.A. Wang, P. Zhang, C. Li and B. Ren, *J. Chem. Eng. Data*, **53**, 648 (2008).
6. R. Dey, A.K. Singh and J.D. Pandey, *J. Mol. Liq.*, **137**, 88 (2008).
7. H. Li, F. Guo, G.Q. Hu, L. Zhao and Y. Zhang, *J. Chem. Eng. Data*, **54**, 2100 (2009).