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Excess molar volume along with refractive index for binary systems of dimethoxymethylphenylsilane with dimethyldimethoxysilane, dimethyldiethoxysilane, methylvinyl-diethoxysilane and ethenyltrimethoxysilane

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ABSTRACT

The density and refractive index were determined for four binary mixtures of dimethoxymethylphenylsilane with dimethyldimethoxysilane, dimethyldiethoxysilane, methylvinyl-diethoxysilane and ethenyltrimethoxysilane at different temperatures $T = (298.15, 303.15, 308.15, 313.15 \text{ and } 318.15) \text{ K}$ and atmospheric pressure using a DMA4500/RXA170 combined system. The corresponding derived properties were computed from the experimental data. The results were fitted by means of the Redlich–Kister equation and used to estimate the binary interaction parameters and standard deviations. The factors that affect these excess quantities have been discussed.

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1. Introduction

One general class of monomers and oligomers with a large variety of organic functionalization, called alkoxy-silanes, were identified early by researchers as excellent coupling agents, a material which assists in adhesive bonding between dissimilar surfaces, allowing for better bulk and interface properties [1]. In continuation of our study on mixing and excess properties of binary mixtures contain alkoxy-silanes [2], the density and refractive index were determined for four binary mixtures of dimethoxymethylphenylsilane with dimethyldimethoxysilane, dimethyldiethoxysilane, methylvinyl-diethoxysilane and ethenyl-trimethoxysilane at different temperatures $T = (298.15, 303.15, 308.15, 313.15 \text{ and } 318.15) \text{ K}$ and atmospheric pressure. In addition, the isobaric coefficient of thermal expansion (α), excess molar volume (V_m^E), the deviations in refraction indices (Δn_D), molar refractions (R_m) and the deviations in molar refraction (ΔR_m) for these binary systems were calculated and correlated using these data.

2. Experimental

2.1. Chemicals

Dimethoxymethylphenylsilane, dimethyldimethoxysilane, dimethyldiethoxysilane and methylvinyl-diethoxysilane were obtained from the Shandong Wanda Chemical Company Ltd. Ethenyltrimethoxysilane was provided by Nanjing Xiangqian Chemical Company Ltd. To eliminate the influence of small insoluble particles on densities and refractive index, all chemicals used were dried using $4 \times 10^{-8} \text{ cm}$ (4 \AA) molecular sieves and filtered through a $0.45 \mu\text{m}$ filter paper. Their mass fraction purities (Table 1) were determined by a gas chromatograph equipped with a HP-5 column and a flame ionization detector (FID). All chemicals were degassed using an ultrasonic bath prior to use. The densities and refractive indices were obtained for all solvents at the temperatures, $T = (293.15 \text{ or } 298.15) \text{ K}$, and compared with those reported in the literatures (Table 2) [3–6]. The binary solutions were prepared in airtight-stoppered glass bottles to prevent evaporation. The mass of each sample was determined using an analytical balance (Sartorius, model BS 224 S, $\pm 0.1 \text{ mg}$). Both of the uncertainties in the determination of the molar fraction basis and the volume fraction basis were ~ 0.0001 .

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Table 1
Sample description.

Chemical name	CAS registry number	Source	Mass fraction purity	Analysis method
Dimethoxymethylphenylsilane	3027-21-2	Shandong Wanda Chemical	0.999	GC ^a
Dimethyldimethoxysilane	1112-39-6	Shandong Wanda Chemical	0.999	GC ^a
Dimethyldiethoxysilane	78-62-6	Shandong Wanda Chemical	0.999	GC ^a
Methylvinyl-diethoxysilane	5507-44-8	Shandong Wanda Chemical	0.999	GC ^a
Ethyltrimethoxysilane	2768-02-7	Nanjing Xiangqian Chemical	0.999	GC ^a

^a Gas–liquid chromatography.**Table 2**
Experimental densities (ρ) and refractive index (n_D) of the pure liquid components and their literature values at $p = (103 \pm 2)$ kPa.

Chemical name	T/K	$\rho/\text{g}\cdot\text{cm}^{-3}$		n_D	
		exp	lit	exp	lit
Dimethyldimethoxysilane	298.15	0.8579	0.861 [3]	1.36816	1.3699 [3]
Dimethyldiethoxysilane	293.15	0.84011	0.8401 [4]	1.38452	1.3814 [4]
Methylvinyl-diethoxysilane	293.15	0.86221	0.8620 [5]	1.40033	1.4001 [5]
Ethyltrimethoxysilane	298.15	0.96569	0.9669 [6]	1.39022	1.3910 [6]

Standard uncertainties are $u(T) = 0.03$ K, $u(x) = 0.0001$, $u(\rho) \approx 0.2 \text{ kg}\cdot\text{m}^{-3}$ and $u(n_D) \approx 0.002$.

2.2. Density and refractive index measurements

The density and refractive index of the pure components and their mixtures at different temperatures were automatically analysed at atmospheric pressure, (103 ± 2) kPa (Weather bureau of Hangzhou) using a DMA4500/RXA170 combined system (Anton Paar) with a density uncertainty of $u(\rho) \approx 0.2 \text{ kg}\cdot\text{m}^{-3}$ and a refractive index uncertainty of $u(n_D) \approx 0.002$. The combined system was calibrated periodically using ultra-pure water and dry air [1]. Two integrated Pt 100 platinum thermometers ($u(T) = 0.03$ K) together with Peltier elements provided precise temperature control. The estimated uncertainty of V_m^E was $\pm 0.005 \text{ cm}^3\cdot\text{mol}^{-1}$. The uncertainty in the calculation of the deviations in refraction indices (Δn_D), the molar refraction (R_m) and the deviation in molar refraction (ΔR_m) were estimated to be ± 0.0003 , $\pm 0.004 \text{ cm}^3\cdot\text{mol}^{-1}$ and $\pm 0.005 \text{ cm}^3\cdot\text{mol}^{-1}$ respectively.

3. Results and discussion

3.1. Thermodynamic properties

3.1.1. Excess molar volume

The density of the pure components and their binary mixtures were used to determine the excess molar volumes (V_m^E) presented in Table 3 using Eq. (1).

$$V_m^E = (x_1 M_1 + x_2 M_2) / \rho - x_1 M_1 / \rho_1 - x_2 M_2 / \rho_2 \quad (1)$$

where x_i , ρ_i and M_i represent the mole fraction, the density and the molecular weight of the pure components respectively. ρ represents the density of the mixture.

The composition dependence of V_m^E can be represented by the Redlich–Kister equation [7]:

$$V_m^E = x_1 x_2 \sum_{i=0}^n A_i (x_1 - x_2)^i \quad (2)$$

where x_1 is the mole fraction of dimethoxymethylphenylsilane, A_i the adjustable parameters and $n + 1$ the number of the fitted parameters.

The Redlich–Kister equation was fitted using the least square fit method and the results are listed in Table 4. Eq. (3) was used to calculate the standard deviation $\sigma(Y)$:

$$\sigma(Y) = \left[\sum_{i=1}^n (Y_{\text{exp}} - Y_{\text{cal}})^2 / (n - m) \right]^{1/2} \quad (3)$$

where n is the total number of experimental points for each data set and m the number of coefficients in Eq. (2). The standard deviations of V_m^E for all the binary mixtures are shown in Table 4.

The excess molar volumes (V_m^E) of the four binary systems at 298.15 K are shown as an example in Fig. 1. It can be seen that all of the excess molar volumes for the four systems are negative. The values of V_m^E decrease in the following order: ethyltrimethoxysilane > methylvinyl-diethoxysilane > dimethyldimethoxysilane > dimethyldiethoxysilane. All the maximum absolute values of V_m^E of these four binary systems at a given temperature are at mole fraction x_1 from 0.4 to 0.6 of dimethoxymethylphenylsilane. The trend of V_m^E as a function of the composition of the binary system {dimethoxymethylphenylsilane(1) + dimethyldimethoxysilane(2)} at (298.15, 303.15, 308.15, 313.15 and 318.15) K are shown in Fig. 2 to illustrate the effect of temperature on V_m^E . With the increase of temperature, the values of V_m^E change in decreasing trends.

The excess molar volume of the binary mixtures studied is a result of the chemical, physical and structural characteristics of the liquids used [8]. Considering there are no chemical interaction forces in organic silicon compounds, the excess molar volume is the result of the balance between the physical intermolecular forces (mainly the dispersion force) and the structural effect [9]. A negative value indicates a net packing effect resulting from structural effects arising from interstitial accommodation [10]. The structural contributions are mostly negative and are due to interstitial accommodation and geometrical fitting of one component into another due to the differences in the molar volume and free volume between components.

3.1.2. Partial excess volume at infinite dilution

To investigate the contraction and expansion behaviour of a binary mixture due to the interactions between the solute and solvent, the values of the partial excess volume at infinite dilution ($\bar{V}_i^{E,\infty}$) can be calculated using the adjustable parameters of the Redlich–Kister equation when $x_1 \rightarrow 0$ and $x_2 \rightarrow 1$. Under such circumstances, the partial excess volumes were obtained using Redlich–Kister Eqs. (4) and (5).

$$\bar{V}_1^{E,\infty} = A_0 - A_1 + A_2 - A_3 + A_4 \quad (4)$$

$$\bar{V}_2^{E,\infty} = A_0 + A_1 + A_2 + A_3 + A_4 \quad (5)$$

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