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Excess molar volume along with viscosity, refractive index and relative permittivity for binary mixtures of *exo*-tetrahydrodicyclopentadiene with four octane isomers

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ABSTRACT

The fundamental physical properties including density, viscosity, refractive index and relative permittivity, have been measured for binary mixtures of *exo*-tetrahydrodicyclopentadiene (JP-10) with four octane isomers (*n*-octane, 3-methylheptane, 2,4-dimethylhexane and 2,2,4-trimethylpentane) over the whole composition range at temperatures $T = (293.15 \text{ to } 313.15)$ K and pressure $p = 0.1$ MPa. The values of excess molar volume $\left(V_m^E\right)$, viscosity deviation $(\Delta\eta)$, refractive index deviation (Δn_D) and relative permittivity deviation $(\Delta\varepsilon_r)$ are then calculated. All of the values of V_m^E and $\Delta\eta$ are observed to be negative, while those of Δn_D and $\Delta\varepsilon_r$ are close to zero. The effects of temperature and composition on the variation of V_m^E values are discussed. The negative values of V_m^E and $\Delta\eta$ are conductive to high-density and low-resistance of fuels, which is favorable for the design and preparation of advanced hydrocarbon fuels.

1. Introduction

An appropriate liquid endothermic hydrocarbon fuel is designed to be used as both propellant and coolant for advanced hypersonic aircrafts [1–3]. *exo*-tetrahydrodicyclopentadiene (JP-10, $C_{10}H_{16}$) is the candidate of such a functional fuel, and it has been widely studied recently because of its high density, suitable flash point, low freezing point, high thermal stability and high heat sink capacity [4,5]. However, the relatively high viscosity and large C/H ratio of JP-10 lead to its unsatisfactory properties of fluidity, ignition and combustion [6,7]. In order to improve the performance of JP-10, the addition of hydrocarbon components with relatively high volatility and low viscosity [8], such as normal alkane, isoalkane and cycloalkane, is an effectively practical method. Hence, the measurements on the physical properties of the mixtures of JP-10 with alkane components are a fundamental work to be beneficial to the composition optimization.

Isoalkanes are important components of the military fuels, such as JP-7, RP-1 and Jet-A [9,10]. Especially, isoalkanes make up the largest fraction of alkane components in Jet-A. In comparison with normal alkanes, the existence of tertiary carbons (from branching) in isoalkanes is able to enhance the cracking reactivity of hydrocarbon fuels [11], and isoalkanes generally own the properties of higher volatility and lower viscosity. The addition of an isoalkane to JP-10 with an appropriate fraction can improve the performance of JP-10 in fluidity, ignition and combustion. The isomers of octane can be found in gasoline, diesel, and jet fuels [12–14]. In this work, densities, viscosities, refractive indices and relative permittivities have been measured for binary mixtures of JP-10 with four octane isomers (*n*-octane, 3-methylheptane, 2,4-dimethylhexane and 2,2,4-trimethylpentane) over the whole composition range at temperature $T = (293.15 \text{ to } 313.15)$ K and pressure $p = 0.1$ MPa. The excess molar volume $\left(V_m^E\right)$ of these four binary mixtures are then calculated and discussed on the basis of the steric configurations and intermolecule forces. The results are expected to provide some important information for optimum design of advanced hydrocarbon fuels.

2. Experimental

2.1. Materials

JP-10 (CAS Registry No. 2825-82-3, mass fraction purity (wt%) > 0.98) is supplied by Liming Research Institute of Chemical Industry (LRICI). *n*-Octane (CAS Registry No. 111-65-9, wt% > 0.99) and 2,2,4-trimethylpentane (CAS Registry No. 540-84-1, wt% > 0.995) are supplied by Aladdin Chemical Reagent Company. 3-Methylheptane (CAS Registry No. 589-81-1, wt% > 0.99) and

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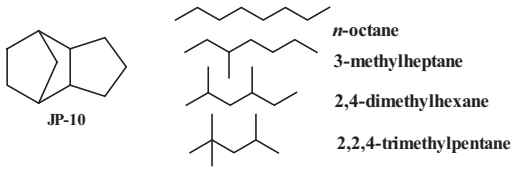

FIGURE 1. Chemical structures of JP-10 and four octane isomers.

2,4-dimethylhexane (CAS Registry No. 589-43-5, wt% > 0.99) are supplied by Sinopharm Chemical Reagent Company. The chemical structures of the compounds are shown in figure 1. The reagents are checked by GC–MS (7890A/5975C, Agilent) and used without further purification. The specifications of these chemicals are listed in table 1. The binary mixtures are prepared with the weighing method. The precision of Mettler balance used is 0.0001 g. The uncertainty of the mole fraction is estimated to be within ±0.0001.

2.2. Methods

The densities of pure compounds and binary mixtures were measured by using an Anton Paar DMA 5000 M densimeter at five temperatures in the range T = (293.15 to 313.15) K and pressure p = 0.1 MPa. The automatic control system of the apparatus kept the temperature balance with a precision of 0.01 K. The atmospheric pressure was recorded from a Fortin barometer with an uncertainty of 2.0 kPa. The uncertainty of the density measurements is ±0.00005 g · cm^{-3}.

The viscosities were measured by using an Anton Paar AMVn viscometer at five temperatures in the range T = (293.15 to 313.15) K and pressure p = 0.1 MPa. The precision of the efflux time was ±0.001 s, and the apparatus could keep the temperature varying within ±0.01 K. The calculation procedure is shown in the Supporting Information. The uncertainty of the viscosity measurement is within 0.5%.

The refractive indices were measured by using a WAY-2S refractometer at five temperatures in the range T = (293.15 to 313.15) K. A HAAKE circulator with circulating water was used to maintain the temperatures with a precision of ±0.01 K. The uncertainty of the refractive index is ±0.0005.

The relative permittivity was measured using a direct capacitance method with a concentric cylinder capacitor. The cell capacitance in air (C_0) and the capacitance of the pure liquid (C) were measured by a PCM-1A precision LCR meter (Nanda Wanhe Technology Corporation) at 50 kHz. Then the relative permittivity, ε_r was given by

$$\varepsilon_r = C/C_0. \quad (1)$$

The working temperatures were (293.15, 303.15 and 313.15) K, which were controlled by a HAAKE circulator with a precision of ±0.01 K. The uncertainty of the relative permittivity is ±0.01.

3. Results and discussion

The experimental values of density, viscosity, refractive index and relative permittivity of pure compounds measured in this work at T = 293.15 K and p = 0.1 MPa are compared with the literature

TABLE 1
Specification of chemicals in this work.

Chemical name	Source	Provided mass fraction purity	Purification method	Measured mass fraction purity	Analysis method
JP-10	LRICI	>0.98	None	0.990	GC–MS
n-octane	Aladdin	>0.99	None	0.995	GC–MS
3-methylheptane	Sinopharm	>0.99	None	0.992	GC–MS
2,4-dimethylhexane	Sinopharm	>0.99	None	0.993	GC–MS
2,2,4-trimethylpentane	Aladdin	>0.995	None	0.998	GC–MS

TABLE 2
Densities (ρ), viscosities (η), refractive indices (n_D) and relative permittivities (ε_r) of pure compounds at T = 293.15 K and p = 0.1 MPa.[a]

Compound	ρ/g · cm^{-3}		η/mPa · s		n_D		ε_r	
	Exptl	Lit	Exptl	Lit	Exptl	Lit	Exptl	Lit
JP-10	0.93566	0.9357[b] 0.93572[c]	2.974	3.0752[b] 2.992[c]	1.4871	1.4874[c] 1.4878[d]	2.19	–
n-octane	0.70282	0.7027[e] 0.70277[i]	0.547	0.541[f] 0.538[g]	1.3969	1.39742[h] 1.3978[i]	1.96	1.968[i]
3-methylheptane	0.70637	0.7058[e]	0.512	0.492[j]	1.3957_t	1.3960_t[k]	1.95	–
2,4-dimethylhexane	0.70057	0.7004[e]	0.476	0.461[j]	1.3947	1.39534[l]	1.96	–
2,2,4-trimethylpentane	0.69189	0.6919[e]	0.518	0.5125[m]	1.3906	1.3912[n]	1.94	1.94[o]

t Values are given at temperature T = 298.15 K.
[a] Standard uncertainties u are $u(T)$ = 0.01 K, $u(p)$ = 2.0 kPa, $u(\rho)$ = 0.00005 g · cm^{-3}, $u(\eta)$ = 0.005 mPa · s, $u(n_D)$ = 0.0005 and $u(\varepsilon_r)$ = 0.01.
[b] Reference [15].
[c] Reference [16].
[d] Reference [17].
[e] Reference [18].
[f] Reference [19].
[g] Reference [20].
[h] Reference [21].
[i] Reference [22].
[j] Reference [23].
[k] Reference [24].
[l] Reference [25].
[m] Reference [26].
[n] Reference [27].
[o] Reference [28].