Journal of Molecular Liquids 196 (2014) 192–197

Contents lists available at ScienceDirect

Journal of Molecular Liquids

journal homepage: www.elsevier.com/locate/molliq

Volumetric, viscosimetric and spectroscopic studies for aqueous solution of ethylene glycol monoethyl ether

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ARTICLE INFO

Article history:
Received 8 December 2013
Received in revised form 17 February 2014
Accepted 26 March 2014
Available online 8 April 2014

Keywords:
Ethylene glycol monoethyl ether
Density
Viscosity
Spectroscopic study

ABSTRACT

As a continuation of the systematic study on thermodynamic properties for the aqueous solution of alkoxyethanols, this paper reports new measurements of densities and viscosities for the aqueous solution of ethylene glycol monoethyl ether ($CH_3CH_2OCH_2CH_2OH$) covering the whole composition range at $T = (293.15, 303.15, 313.15, 323.15, 333.15)$ K under atmospheric pressure. The thermal expansion coefficient and Grunberg–Nissan interaction parameter were calculated. Excess properties including excess molar volumes, viscosity deviations, and excess energies of activation for viscous flow were calculated according to the experimental results. These data have been correlated by the Redlich–Kister type equations to obtain their coefficients and standard deviations. UV–vis spectra and fluorescence emission of probe pyrene were recorded to reflect molecular interactions and the polarity change of micro environment in an aqueous solution with varied concentration of ethylene glycol monoethyl ether. The results indicate that molecular interaction between ethylene glycol monoethyl ether and water is weaker than that between diethylene glycol monoethyl ether and triethylene glycol monoethyl ether with water.

1. Introduction

Alkoxyethanols are a very interesting class of solvents due to the presence of the ether, alcohol and hydrocarbon chain in the same molecule [1]. This unique characteristic leads to self-association behavior of alkoxyethanols in water via the formation of intra- and intermolecular hydrogen bonds. Thus, they are used in various biotechnical and biomedical applications, constituting a simple model of biological systems [2]. They can also be used as valid model for the research of the hydration of polyether (PEO) which is important in many industrial, environmental, and biological applications. Most of the interesting physical properties of PEO solution to a large extent depend on the polymer's interaction with water [3]. PEO is used as side chain of synthetic polymers in biotechnology applications owing to its properties of uncharged, nontoxic, nonimmunogenic, and FDA-approved. In addition, PEO can also be used in the construction of functional polymers, hydrogels, microgels, polymer brushes, nanohybrid materials, and bioactive surfaces based on its excellent thermoresponsive and biocompatible properties [4]. On the other hand, alkoxyethanols find wide use as important industrial solvents such as scrubbing liquids in the cleaning of exhaust air and gas streams from industrial production plants. Therefore the study of alkoxyethanols in pure as well as in aqueous mixtures is significant from both the theoretical and industrial points of view [5].

Various physicochemical and spectroscopic techniques had been used to investigate the interesting properties of the alkoxyethanol aqueous solution, including Raman, FT-IR, NMR spectroscopies as well as MD simulations. 1H NMR spectra of the aqueous solutions of some n-alkoxyethanols (C_1Em, $m = 1, 2, 3$) over the whole composition rang at 298.15 K had been used to study the behavior of binary liquid mixtures. Spectroscopic results confirm the strong interactions between components involving hydrogen bonds [6]. Katsumoto et al. [7] had investigated the molecular interaction occurring in the mixed system of 2-butoxyethanol with water by infrared (IR) spectroscopy combined with quantum chemical calculations. They found that the blue shift of the ν_{CH} bands due to the butoxy group of C_4E_1 originates mainly from the formation of H-bonds between the ether oxygen atom and water molecules.

In recent years, we have measured densities and viscosities for the aqueous solutions of several alkoxyethanols at different temperatures with the purpose of obtaining accurate thermophysical property data for industrial process design requirement. These macroscopic properties combined with spectroscopic techniques supply useful information to understand the intermolecular interaction and molecular aggregation that exist in the aqueous solution of alkoxyethanols and their sensitivities to composition, temperature, and the molecular structure of the pure components [8]. As a continuation, this paper focuses on thermodynamic and spectroscopic studies for the aqueous solution of ethylene glycol monoethyl ether (EGMEE). EGMEE, also called 2-ethoxyethanol, is widely used as a solvent for nitrocellulose, dyes, inks, resins, lacquers, paints, and varnishes. It can also be used as

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http://dx.doi.org/10.1016/j.molliq.2014.03.042
0167-7322/

Table 1
Comparison of measured densities (ρ) and viscosities (η) of EGMEE with literature values at $T = (293.15, 298.15, 303.15, 313.15, 323.15)$ K.

T/K	ρ/g cm^{-3}		η/mPa s	
	This work	Lit	This work	Lit
293.15	0.9296	0.929545[a]	2.054	2.077[d]
		0.9297[d]		2.142[i]
		0.92908[g]		
298.15	0.9251	0.925027[a]	1.814	1.848[i]
		0.92515[e]		2.054[j]
		0.92502[f]		1.784[k]
		0.92515[g]		1.850[l]
303.15	0.9205	0.920457[a]	1.612	1.6541[b]
		0.92119[b]		1.6543[c]
		0.92118[c]		1.612[d]
		0.92050[g]		1.646[i,j]
		0.9205[h]		
313.15	0.9119	0.91158[b]	1.306	1.3055[b]
		0.91229[c]		1.293[c]
		0.91138[g]		1.240[d]
		0.9122[h]		
323.15	0.9036	0.90345[b]	1.065	1.1156[b]
		0.9038[h]		1.026 [d]

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a component of many cleaning agents, anti-icing fuel additive in aviation. In addition, EGMEE is a chemical intermediate in the production of ethylene glycol monoethyl ether acetate. To the best of our knowledge, there has been no literature report on a systematic investigation for the thermodynamic and spectroscopic properties for the aqueous solution of EGMEE. This paper aims to measure the density, viscosity, as well as spectroscopic properties of the system.

2. Experimental

2.1. Materials

Ethylene glycol monoethyl ether (EGMEE, CAS 110-80-5) was purchased from Acros, and its mass fraction purity was >99%. Prior to measurements, it was dried over 0.4 nm molecular sieves and partially degassed under vacuum. Pyrene (CAS 129-00-0) was purchased from Acros with mass fraction purity 98%. Pyrene was recrystallized from ethanol before use. Doubly distilled water with its conductivity lower than $10^{-7}\ \Omega^{-1}\ cm^{-1}$ was used.

2.2. Apparatus and procedure

The methods for measuring density and viscosity have been escribed elsewhere [9]. The binary mixtures were prepared by mass, using an electronic analytical balance (HANGPING FA2104, Shanghai, China) with a precision of ±0.0001 g. The uncertainty of the mole fraction was estimated to be ±0.0001. All samples were carefully stored to protect from atmospheric moisture and CO_2 as far as possible. The densities were measured with a 10 cm^3 capillary pycnometer. The viscosities were determined with a capillary viscometer of Ubbelohde type. The flow-time measurements were determined using an accurate stopwatch with a precision of ±0.01 s. Degassed doubly distilled water was used as calibrating substances. The experimental temperature was controlled to ±0.01 K by using a water bath. The uncertainties of the density were estimated to be ±0.0001 g cm^{-3} while the uncertainties of the viscosity measurements were estimated to be better than ±0.2%.

In order to investigate the effect of composition on the molecular interaction, UV–vis spectra for the aqueous solution of EGMEE with varied concentration were recorded at room temperature on a TU-1901 UV–vis spectrophotometer by using 1 cm quartz cuvette covering the wave length region of 190–350 nm. A baseline correction was made for the spectra recorded in distilled water.

The polarity of the solution was investigated by using the pyrene I_1/I_3 ratio method [10,11]. The procedure has been described previously [12]. A predetermined amount of pyrene acetone solution with its concentration 0.05 mol cm^{-3} was input into sample bottles, and then acetone was evaporated completely, followed by the addition of the EGMEE aqueous solution with different composition. The final concentration of pyrene in each sample solution was maintained to be around 0.001 mol cm^{-3}. Each sample was stirred at least 24 h for equilibration prior to measurements. Fluorescence emission was recorded in a Hitachi F-4500 spectrofluorometer at room temperature. The excitation wavelength of 335 nm was adopted while the slit width was kept at 2.5 nm during the measurements.

3. Results and discussion

The molecular structure of EGMEE is relatively simple which has only one oxyethylene unit. There are some literature reports on density and viscosity for pure EGMEE at different temperature. A comparison of the experimental values of density and viscosity with the data found in

Table 2
Densities ρ and viscosities η for the mixture of EGMEE (1) + water (2) at $T = (293.15, 303.15, 313.15, 323.15, 333.15)$ K.

	ρ/g cm^{-3}					η/mPa s				
x_1	T/K = 293.15	303.15	313.15	323.15	333.15	293.15	303.15	313.15	323.15	333.15
0.0000	0.9982	0.9957	0.9922	0.9881	0.9832	1.005	0.8007	0.656	0.5494	0.4688
0.02202	0.9987	0.9954	0.9912	0.9865	0.9811	1.422	1.097	0.8665	0.6974	0.5649
0.04761	1.0010	0.9963	0.9908	0.9855	0.9794	2.020	1.485	1.140	0.8748	0.6870
0.07883	1.0015	0.9952	0.9891	0.9827	0.9755	2.731	1.928	1.456	1.105	0.8344
0.1177	0.9998	0.9929	0.9854	0.9779	0.9699	3.402	2.355	1.727	1.320	0.9896
0.1666	0.9939	0.9865	0.9786	0.9706	0.9623	3.943	2.703	1.967	1.479	1.100
0.2304	0.9858	0.9779	0.9699	0.9621	0.9538	4.205	2.920	2.124	1.613	1.202
0.3180	0.9751	0.9667	0.9585	0.9504	0.9420	4.219	2.951	2.140	1.656	1.235
0.4441	0.9628	0.9539	0.9455	0.9371	0.9285	3.838	2.746	2.011	1.591	1.203
0.5303	0.9559	0.9469	0.9384	0.9301	0.9215	3.471	2.547	1.900	1.514	1.150
0.6418	0.9481	0.9391	0.9304	0.9219	0.9134	3.081	2.280	1.731	1.398	1.075
0.7202	0.9431	0.9340	0.9253	0.9169	0.9085	2.836	2.126	1.614	1.324	1.028
0.8271	0.9369	0.9279	0.9192	0.9109	0.9025	2.502	1.912	1.491	1.212	0.9614
0.9078	0.9331	0.9240	0.9154	0.9071	0.8988	2.270	1.764	1.399	1.133	0.9164
1.0000	0.9296	0.9205	0.9119	0.9036	0.8953	2.054	1.612	1.306	1.065	0.8673