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Densities and Viscosities of [Bmim][PF_6] and Binary Systems [Bmim][PF_6] + Ethanol, [Bmim][PF_6] + Benzene at Several Temperatures and Pressures: Determined by the Falling-Ball Method

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ABSTRACT: A falling-body viscometer was designed and manufactured to determine the densities and viscosities of liquids at high temperatures and pressures. The densities and viscosities for pure [bmim][PF_6], [bmim][PF_6] + ethanol, and [bmim][PF_6] + benzene binary systems were determined in the temperature range of (313.2 to 413.2) K and in the pressure range of (0.1 to 25.0) MPa. The viscosities of [bmim][PF_6] + ethanol, and [bmim][PF_6] + benzene binary systems were correlated with temperature, pressure, and composition by correlation equations. The correlation coefficients (R) are 0.999 and 0.999 for [bmim][PF_6] + ethanol and [bmim][PF_6] + benzene systems, respectively.

INTRODUCTION

Ionic liquids (ILs) are a novel class of room temperature molten salts with melting points near ambient temperature. They are composed entirely of anions and cations. Because of the beneficial properties such as negligible vapor pressure, high heat capacity, high thermal conductivity, and a wide temperature range for liquids, ILs have a diversity of applications: thermal storage media,[1] heat transfer fluids,[2] electrolytic media,[3] and extraction processes.[4,5]

The transport properties such as the viscosity and density of fluids are important for engineering and equipment design. The viscosities of ILs are usually very high, which leads to many difficulties in processes of pumping, mixing, and stirring and makes a decrease of mass transfer and heat transfer.[6] Temperature and pressure are two factors influencing the viscosity. The viscosity of ILs will also change obviously when they are mixed with other compounds. To take full advantage of ILs, the influence of temperature, pressure, and other compounds on the viscosity of ILs should be studied carefully. Some research has been done for the viscosity of pure ILs and their binary systems with organic compounds,[7−11] but little work has been done on the research of IL + organic compound binary systems in both large temperature and pressure ranges.

As one of the most important traditional ILs, [bmim][PF_6] has been widely used in the fields of separation, catalysis, and synthesis.[12−16] The structure of [bmim][PF_6] is shown in Figure 1. Therefore, it is necessary to determine the viscosities of the mixtures containing [bmim][PF_6]. Geng et al.[17] measured densities and viscosities of [bmim][PF_6] + *N*,*N*-dimethylformamide binary mixtures at (293.15 to 318.15) K. Fan et al.[18] measured densities and viscosities for the [bmim][PF_6] + methyl methacrylate binary system, over the whole concentration range in the temperature range from (283.15 to 353.15) K. Zhu et al.[19] measured viscosities of [bmim][PF_6] + butanone and [bmim][PF_6] + acetone binary systems over the whole concentration range at 298.15 K. However, there is no literature reported on the viscosities of [bmim][PF_6] + ethanol and [bmim][PF_6] + benzene binary systems which are also important for the application of [bmim][PF_6].

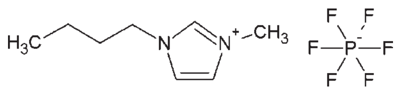

Figure 1. Structure of [bmim][PF_6].

In this work an apparatus set was designed and manufactured for measuring the viscosities and densities of ILs at high temperatures and pressures. The density and viscosity data of pure [bmim][PF_6], [bmim][PF_6] + ethanol, and [bmim][PF_6] + benzene binary systems were measured using the apparatus. Then, the viscosity data were fitted with temperature, pressure, and the mole fraction of organic compounds by equations.

EXPERIMENTAL SECTION

Materials. Ethanol and benzene were both purchased from Tianjin Guangfu Technology Development Co. Ltd., China with quoted purities of > 99.7 % and > 99.5 %. [bmim][PF_6] with a purity higher than 99 % and water mass fraction of less than 0.01 was supplied by Henan Lihua Pharmaceutical Co. Ltd., China. Viscosity calibration fluid was purchased from Brookfield, USA.

Apparatus and Procedure. A schematic diagram of the falling-body viscometer is shown in Figure 2. The viscometer contains four parts: viscometer body, temperature control system, high pressure part, and timer system. The viscometer body

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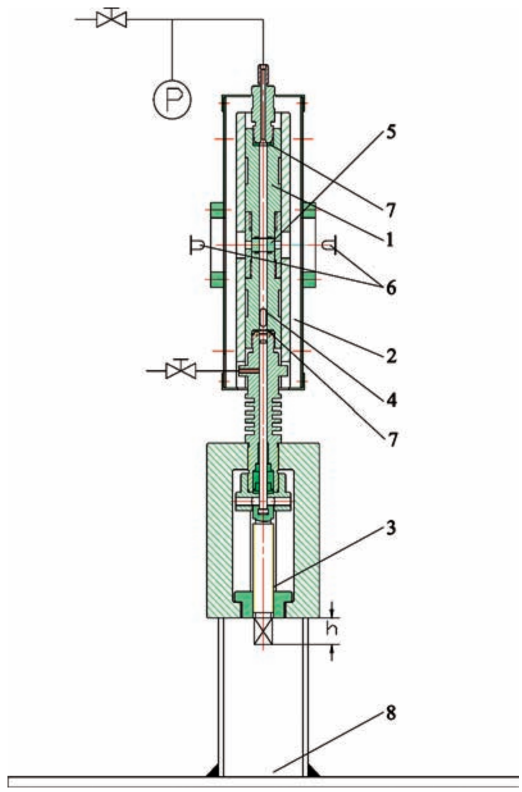

Figure 2. Falling-body viscometer: 1, viscometer body; 2, heater; 3, piston shaft; 4, falling body; 5, sapphire window; 6, laser transmitter and receiver; 7, copper piece; 8, bracket of the viscometer.

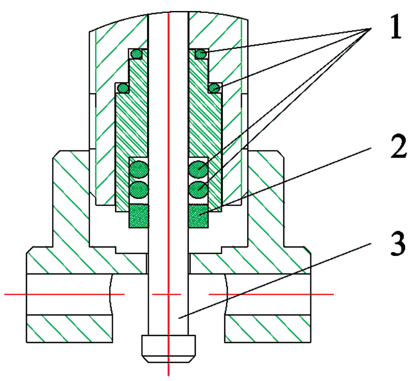

Figure 3. Pressurized structure of the piston shaft: 1, fluorine rubber ring; 2, polyimide ring; 3, piston shaft.

is a stainless steel tube which is 13 cm long with an inner diameter of 0.588 cm. The falling-body which is 0.728 cm long with a diameter of 0.550 cm is made of the same material as viscometer body tube. A sapphire window is 1 cm long with an inner diameter of 0.588 cm and is installed in the main tube to measure the falling time of the falling body. The main tube is wrapped by an aluminum block equipped with a heater. The heater is controlled by an XMTA-808 temperature controller (Yuyao Changjiang Merer Co. Ltd., China) with the precision of ± 0.10 K. The timer system contains a ST-1670 laser emitter, a ST-JS01A laser acceptor, and a MUJ-6B computer time counter (Qingfeng Instrument Plant, Beijing, China) with the accuracy of

Table 1. Viscosity of Standard Liquid Measured by the Rheometer

	η/(mPa·s)		
T/K	9.50	97.00	990.0
298.15	9.50	97.00	989.8
303.15	8.71	88.66	899.8
313.15	7.39	73.78	755.8
323.15	6.30	61.91	629.9
333.15	5.45	52.55	536.9
343.15	4.73	44.63	455.9
353.15	4.15	38.51	395.9
363.15	3.66	33.59	344.9

0.0001 s. The laser transmitter and receiver are fixed on both sides of the sapphire window. The pressures of liquid are controlled by the piston shaft at the bottom of the device, and it is measured with YB-150A precision pressure gauge (Tianlin Pressure Gauge Plant, Shanghai, China) with an accuracy of 0.1 MPa. The pressurized structure of the piston shaft is shown in Figure 3.

The samples were first prepared and fed into the viscometer. Then the temperature was adjusted, and the piston pressure gauge was turned on to change the system pressure. When the temperature and pressure were stable, the laser emitter, the photoelectric conversion circuit, and the computer timer were turned on. Then the main tube was whirled 180 degrees and fixed with a pin. The timer recorded the time of the falling body passing through the sapphire window, and the temperature and pressure were written down at the same time. The falling procedure was repeated six times at each temperature and pressure, and the average data were considered as the experimental result. In Figure 2 h was measured three times, and the average data were recorded as the result.

There are three steps to gain the viscosity of a sample:

1 To measure the body-falling time in the viscosity calibration fluids as described above and calculate the apparatus parameters;
2 To measure the body-falling time in the samples as described above;
3 To calculate the viscosity of the samples according to the body-falling time and the apparatus parameters.

There are many equations that can be used for the falling-body viscometer. Formula 1[20] is a relatively simple equation, but it cannot reflect the impact of temperature and pressure.

$$\eta = [k/V(t)](\rho_s - \rho_f) \tag{1}$$

In this work the viscosity was correlated with temperature and pressure by a more complex eq 2.[21]

$$\eta = \frac{t(1 - \rho_l/\rho_s)}{A[1 + 2\alpha(T - T_r)][1 - 2\beta(p - p_r)]} \tag{2}$$

where t is the body-falling time; α and β are the linear expansion coefficient and compressibility, respectively, and are 0.0000168 K^{-1} and 0.000002 Pa^{-1}, respectively, for the 304 stainless steel material used in this device; T_r and p_r are the reference temperature and pressure; T and p are the experimental temperature and pressure; ρ_s and ρ_l are densities of the falling body

Table 2. Comparison of Measured Densities and Viscosities of [bmim][PF_6] with Literature Values at Atmospheric Pressure

	ρ/(g·cm^{-3})		η/(mPa·s)	
T/K	expt	lit.	expt	lit.
313.2	1.358	1.3543,[25] 1.35717,[26] 1.35335,[27] 1.35453,[28] 1.354195,[29] 1.35495,[24] 1.3528,[30] 1.3533,[31] 1.355087[8]	109.2	109,[23] 120,[24] 110.79,[32] 123.4[8]
333.2	1.340	1.34502,[27] 1.33783,[28] 1.33858,[24] 1.3369,[30] 1.3352,[29] 1.338696[8]	45.2	59,[23] 49,[24] 50.38[8]
353.2	1.325	1.32238,[24] 1.3211,[30] 1.322473[8]	24.0	25.5,[24] 25.77[8]

Table 3. Densities of Pure IL [bmim][PF_6]

	ρ/(g·cm^{-3})					
p/MPa	T = 313.2 K	T = 333.2 K	T = 353.2 K	T = 373.2 K	T = 393.2 K	T = 413.2 K
25.0	1.372	1.356	1.340	1.322	1.307	1.291
20.0	1.371	1.354	1.337	1.320	1.304	1.289
15.0	1.368	1.351	1.335	1.318	1.302	1.287
10.0	1.366	1.349	1.332	1.315	1.299	1.284
5.0	1.363	1.346	1.329	1.312	1.295	1.282
0.1	1.358	1.340	1.325	1.309	1.291	1.276

Table 4. Viscosities of Pure IL [bmim][PF_6]

	η/(mPa·s)					
p/MPa	T = 313.2 K	T = 333.2 K	T = 353.2 K	T = 373.2 K	T = 393.2 K	T = 413.2 K
25.0	132.3	58.2	30.8	18.3	12.5	9.2
20.0	127.3	56.4	29.6	17.8	11.9	8.5
15.0	124.3	54.5	29.0	16.6	11.5	7.9
10.0	118.0	49.6	27.9	15.9	10.9	7.4
5.0	113.0	47.0	26.2	15.3	10.7	7.2
0.1	109.2	45.2	24.0	14.8	10.3	7.1

and the sample liquid, respectively. ρ_s which changes with temperature and pressure can be expressed as follows:

$$\rho_s = \frac{\rho_{sr}}{[1 + 3\alpha(T - T_r)][1 - 3\beta(p - p_r)]} \quad (3)$$

where ρ_{sr} is the density of falling body at T_r and p_r.

A is the apparatus constant, and it is correlated to $t(1 - \rho_l/\rho_s)$.[22] In this paper A is expressed as follows:

$$A = A_0 + B_0[t(1 - \rho_l/\rho_s)]^N \quad (4)$$

A_0, B_0, and N are instrumental constants determined by calibration with liquids of known viscosity. In this paper A_0, B_0, and N are −0.00607, 0.0685, and 0.11895, respectively. They were determined by three viscosity calibration fluids. Their viscosities at 25 °C are 9.50 mPa·s, 97.00 mPa·s, and 990.0 mPa·s, respectively. The viscosities of the three viscosity calibration fluids were determined at different temperatures and atmospheric pressure by DV-III ULTRA rheometry (Brookfield, USA). The results are shown in Table 1.

The density of the sample is necessary in the falling-body method. The density is calculated by the mass and volume of the sample at different temperatures and pressures. The volume of the sample is expressed as eq 5:

$$V/\text{mL} = A(T/\text{K} - 303.15) + Bp/\text{MPa} + Ch/\text{cm} + D \quad (5)$$

D is the minimum volume that the piston shaft could be compressed; A, B, and C are volume parameters; h is shown in Figure 2. A, B, C, and D are 0.0032217, 0.0065488, 0.27889, and 8.729, respectively, which were derived by calibrating with deionized water.

In the experimental, the uncertainties of h, T, and p are 0.002 cm, 0.1 K, and 0.1 MPa, respectively. Therefore, the volume accuracy of the sample is 0.0015 mL. The experimental uncertainty for mass was 10^{-4} g. The uncertainty of density is about 0.0015 g·cm^{-3}. The experimental accuracy for body falling time is less than 1 %, which leads to about 1 % uncertainty for viscosity. The sample concentration uncertainty is ± 0.0001.

Table 5. Densities of [bmim][PF_6] (1) + Ethanol (2) System

	ρ/(g·cm^{-3})					
T/K	p = 25.0 MPa	p = 20.0 MPa	p = 15.0 MPa	p = 10.0 MPa	p = 5.0 MPa	p = 0.1 MPa
			x_2 = 0.1000			
313.2	1.353	1.352	1.349	1.346	1.343	1.340
333.2	1.335	1.333	1.330	1.328	1.325	1.320
353.2	1.318	1.316	1.314	1.311	1.308	
373.2	1.302	1.300	1.297	1.295	1.292	
393.2	1.286	1.284	1.281	1.278	1.275	
			x_2 = 0.2000			
313.2	1.329	1.327	1.325	1.322	1.320	1.315
333.2	1.312	1.310	1.307	1.305	1.302	1.298
353.2	1.295	1.293	1.291	1.288	1.285	
373.2	1.279	1.277	1.275	1.272	1.269	
			x_2 = 0.2892			
313.2	1.314	1.312	1.310	1.308	1.305	1.300
333.2	1.299	1.296	1.294	1.291	1.288	1.284
353.2	1.283	1.280	1.278	1.275	1.272	
			x_2 = 0.4035			
313.2	1.276	1.274	1.272	1.269	1.267	1.262
333.2	1.260	1.257	1.255	1.253	1.250	1.246
			x_2 = 0.4959			
313.2	1.249	1.247	1.245	1.242	1.240	1.235
333.2	1.233	1.231	1.228	1.226	1.223	1.219

RESULTS AND DISCUSSION

To illustrate the reliability of the viscosimeter, densities and viscosities of pure IL [bmim][PF_6] at atmospheric pressure were measured and compared with literature values. The results were presented in Table 2. The viscosity at 313.2 K agrees well with

Table 6. Viscosities of [bmim][PF_6] (1) + Ethanol (2) System

	η/(mPa·s)					
T/K	p = 25.0 MPa	p = 20.0 MPa	p = 15.0 MPa	p = 10.0 MPa	p = 5.0 MPa	p = 0.1 MPa
			x_2 = 0.1000			
313.2	77.4	75.6	74.6	73.0	70.6	68.5
333.2	40.0	38.0	36.9	34.9	33.4	31.1
353.2	21.6	19.8	18.9	18.3	17.4	
373.2	12.4	11.8	11.5	11.0	10.5	
393.2	7.9	7.6	7.0	6.8	6.7	
			x_2 = 0.2000			
313.2	57.1	54.0	52.4	49.1	47.9	46.6
333.2	28.1	26.8	26.0	24.9	24.2	23.1
353.2	15.4	14.8	14.2	13.8	13.3	
373.2	8.0	7.7	7.5	6.8	6.5	
			x_2 = 0.2892			
313.2	29.8	28.8	27.4	26.2	25.8	25.3
333.2	17.3	16.4	15.3	14.6	14.2	12.6
353.2	9.3	8.8	8.2	7.6	7.3	
			x_2 = 0.4035			
313.2	20.7	19.1	18.9	17.7	17.1	15.6
333.2	10.8	10.2	9.5	9.1	8.7	8.2
			x_2 = 0.4959			
313.2	17.4	16.3	15.6	14.5	13.9	13.2
333.2	9.1	8.9	8.1	7.9	7.7	7.3

Table 7. Densities of [bmim][PF_6] (1) + Benzene (2) System

	ρ/(g·cm^{-3})					
T/K	p = 25.0 MPa	p = 20.0 MPa	p = 15.0 MPa	p = 10.0 MPa	p = 5.0 MPa	p = 0.1 MPa
			x_2 = 0.0999			
313.2	1.347	1.346	1.344	1.342	1.339	1.335
333.2	1.330	1.328	1.326	1.324	1.321	1.317
353.2	1.312	1.310	1.308	1.306	1.304	
373.2	1.296	1.294	1.292	1.290	1.287	
393.2	1.281	1.278	1.277	1.274	1.271	
413.2	1.266	1.263	1.261	1.259	1.256	
			x_2 = 0.2002			
313.2	1.325	1.324	1.322	1.320	1.318	1.314
333.2	1.309	1.307	1.305	1.303	1.300	1.296
353.2	1.292	1.290	1.288	1.286	1.284	
			x_2 = 0.3003			
313.2	1.302	1.300	1.298	1.296	1.293	1.289
333.2	1.285	1.283	1.281	1.279	1.276	1.272
353.2	1.268	1.267	1.265	1.262	1.260	
			x_2 = 0.3953			
313.2	1.274	1.272	1.270	1.268	1.265	1.260
333.2	1.256	1.254	1.253	1.250	1.247	1.242
353.2	1.240	1.238	1.236	1.233	1.231	
			x_2 = 0.5001			
313.2	1.239	1.237	1.236	1.233	1.231	1.226
333.2	1.223	1.221	1.219	1.216	1.213	1.210
			x_2 = 0.6008			
313.2	1.200	1.198	1.196	1.193	1.190	1.186
333.2	1.184	1.182	1.179	1.177	1.174	
			x_2 = 0.6779			
313.2	1.162	1.160	1.158	1.156	1.153	1.149

Table 8. Viscosities of [bmim][PF_6] (1) + Benzene (2) System

	η/(mPa·s)					
T/K	p = 25.0 MPa	p = 20.0 MPa	p = 15.0 MPa	p = 10.0 MPa	p = 5.0 MPa	p = 0.1 MPa
			x_2 = 0.0999			
313.2	74.6	69.0	64.4	60.7	58.0	54.8
333.2	35.6	33.5	31.1	29.1	27.7	26.9
353.2	18.9	18.0	17.2	16.7	16.4	
373.2	12.2	11.8	11.5	11.3	11.0	
393.2	8.6	8.4	8.1	7.8	7.5	
413.2	6.9	6.7	6.5	6.3	6.1	
			x_2 = 0.2002			
313.2	50.7	48.3	46.2	43.7	42.2	40.7
333.2	27.2	26.0	25.2	24.3	23.0	22.0
353.2	16.6	16.1	15.3	14.8	14.4	
			x_2 = 0.3003			
313.2	35.0	33.5	32.2	30.9	29.8	29.0
333.2	20.9	19.4	18.1	17.0	16.0	15.1
353.2	11.3	10.5	10.0	9.6	9.0	
			x_2 = 0.3953			
313.2	23.2	22.1	21.2	20.4	19.1	18.5
333.2	13.1	12.4	11.7	11.0	10.4	9.6
353.2	8.1	7.8	7.3	6.8	6.5	
			x_2 = 0.5001			
313.2	15.3	14.2	12.9	12.3	11.6	11.2
333.2	9.1	8.7	8.4	8.1	8.0	7.6
			x_2 = 0.6008			
313.2	11.8	10.8	10.0	9.2	8.6	7.7
333.2	7.2	6.8	6.5	6.1		
			x_2 = 0.6779			
313.2	10.3	9.8	9.0	8.4	7.8	7.2

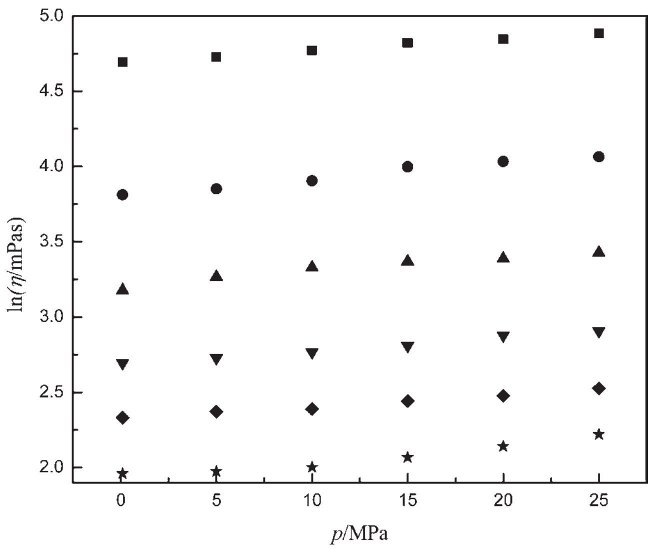

Figure 4. Logarithm values of viscosities vs pressure of pure IL [bmim][PF_6] at different temperatures: ■, 313.2 K; ●, 333.2 K;▲, 353.2 K; ▼, 373.2 K; ◆, 393.2 K; ★, 413.2 K.

ref 23. The viscosity data of [bmim][PF_6] are about 10 % lower than the value of refs 8 and 24, which may be due to the different water content in the ILs. A small change in water content will lead to great change in viscosity. [bmim][PF_6] used in this paper was

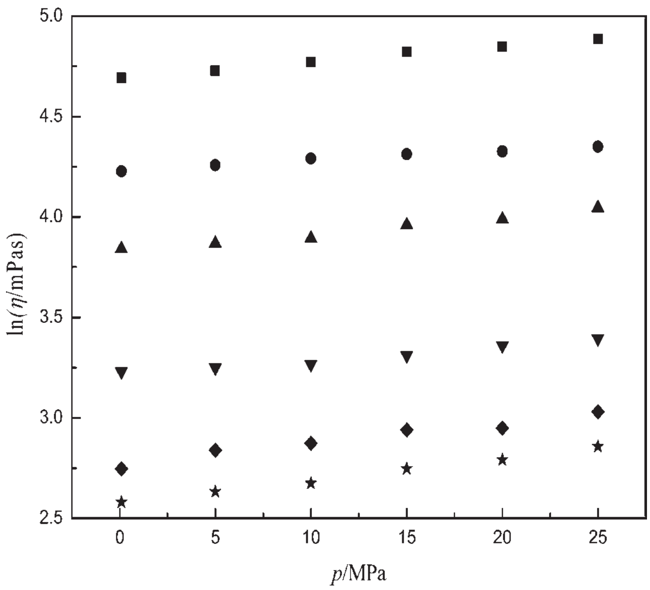

Figure 5. Logarithm values of viscosities vs pressure of different [bmim][PF$_6$] (1) + alcohol (2) mixtures at 313.2 K: ■, x_2 = 0.0000; ●, x_2 = 0.1000; ▲, x_2 = 0.2000; ▼, x_2 = 0.2892; ◆, x_2 = 0.4035; ★, x_2 = 0.4959.

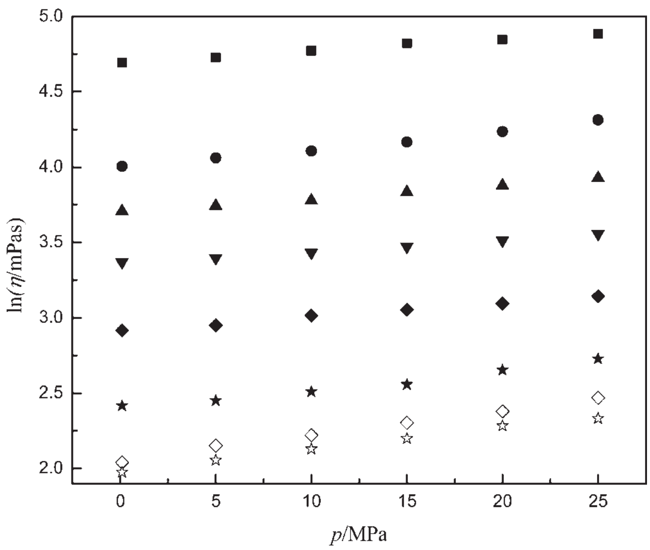

Figure 6. Logarithm values of viscosities vs pressure of different [bmim][PF$_6$] (1) + benzene (2) mixtures at 313.2 K: ■, x_2 = 0.0000; ●, x_2 = 0.0999; ▲, x_2 = 0.2002; ▼, x_2 = 0.3003; ◆, x_2 = 0.3953; ★, x_2 = 0.5001; ◇, x_2 = 0.6008; ☆, x_2 = 0.6779.

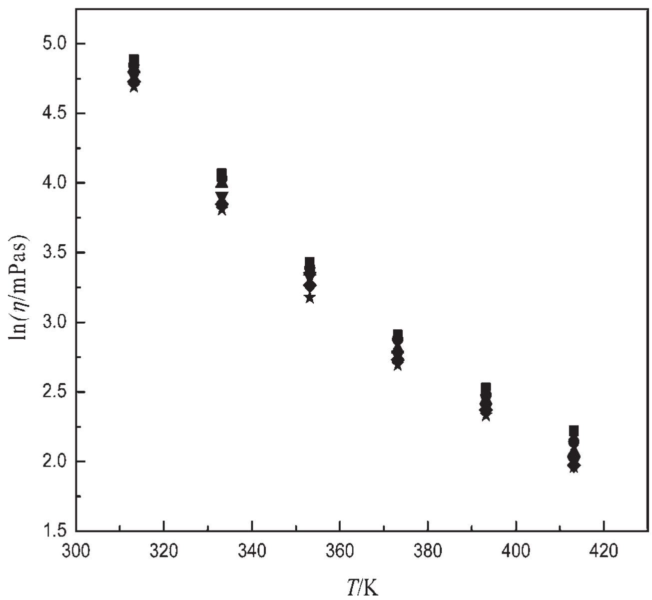

Figure 7. Logarithm values of viscosities vs temperature of pure IL [bmim][PF$_6$] at different pressures: ■, 25 MPa; ●, 20 MPa; ▲, 15 MPa; ▼, 10 MPa; ◆, 5 MPa; ★, 0.1 MPa.

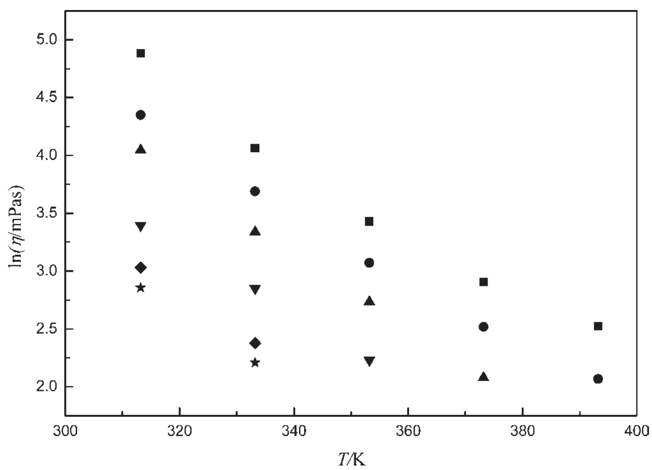

Figure 8. Logarithm values of viscosities vs temperature of different [bmim][PF$_6$] (1) + alcohol (2) mixtures at 25 MPa: ■, x_2 = 0.0000; ●, x_2 = 0.1000; ▲, x_2 = 0.2000; ▼, x_2 = 0.2892; ◆, x_2 = 0.4035; ★, x_2 = 0.4959.

not dried before use, while [bmim][PF$_6$] used in refs 8 and 24 was dried under vacuum. The water content in ref 8 is below 0.01 % which is lower than 1 % in our work. The experimental density and viscosity data of [bmim][PF$_6$] were shown in Tables 3 and 4, respectively. The density and viscosity data of [bmim][PF$_6$] + ethanol binary system were shown in Tables 5 and 6, respectively. The density and viscosity data of [bmim][PF$_6$] + benzene binary system were listed in Tables 7 and 8, respectively.

Effect of Pressure on Viscosity. The curves of logarithm values of viscosities to pressure for [bmim][PF$_6$], [bmim][PF$_6$] + ethanol, and [bmim][PF$_6$] + benzene are presented in Figures 4, 5, and 6, respectively. The figures show that the viscosities increase while pressures increase at a constant pressure and the logarithm values of viscosities are linear functions of pressure.

Effect of Temperature on Viscosity. The curves of logarithm values of viscosities to temperature of [bmim][PF$_6$], [bmim]-[PF$_6$] + ethanol, and [bmim][PF$_6$] + benzene are shown in Figures 7, 8, and 9, respectively. The figures show that the viscosities decrease while temperatures increase at a constant temperature and the logarithm values of viscosities are parabolic functions of temperature.

The viscosity data are functions of both temperature and pressure for the experimental systems. They can be regressed by

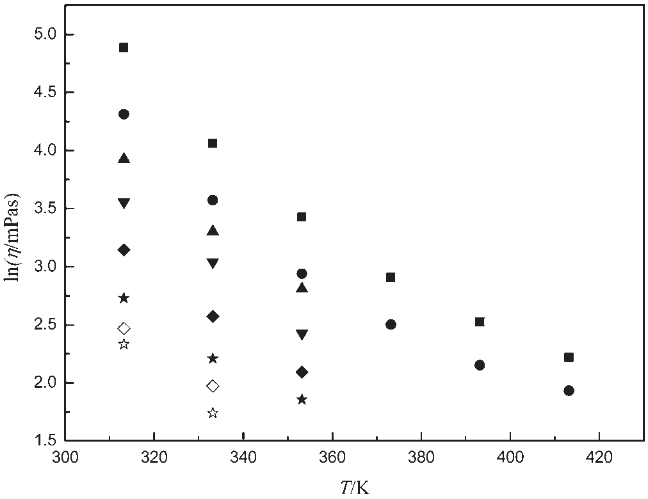

Figure 9. Logarithm values of viscosities vs temperature of different [bmim][PF_6] (1) + benzene (2) mixtures at 25 MPa: ■, x_2 = 0.0000; ●, x_2 = 0.0999; ▲, x_2 = 0.2002; ▼, x_2 = 0.3003; ◆, x_2 = 0.3953; ★, x_2 = 0.5001; ◇, x_2 = 0.6008; ☆, x_2 = 0.6779.

Table 9. Parameters of Correlation

system	*a*	*b*	*c*	*d*
[bmim][PF_6] + ethanol	50.744963	−286.255471	485.044093	381.562517
[bmim][PF_6] + benzene	28.431726	40.087317	−202.3226	13.435419
system	*e*	*f*	*g*	*h*
[bmim][PF_6] + ethanol	−283.367407	−0.257946	1.886176	−4.015434
[bmim][PF_6] + benzene	0.096877	−0.116316	−0.263373	1.152587
system	*i*	*j*	*k*	*D*
[bmim][PF_6] + ethanol	0.000337	−0.00284	0.006113	0.009215
[bmim][PF_6] + benzene	0.000123	0.000439	−0.001766	0.010330

the following equation:

$$\ln(\eta/\text{mPa}\cdot\text{s}) = A + B(T/\text{K}) + C(T/\text{K})^2 + D(p/\text{MPa}) \quad (6)$$

$$A = a + bx + cx^2 + dx^3 + ex^4 \quad (7)$$

$$B = f + gx + hx^2 \quad (8)$$

$$C = i + jx + kx^2 \quad (9)$$

where T is the absolute temperature; p is pressure; x is the mole fraction of organic compounds.

The average absolute deviation (AAD) for the correlation was defined as:

$$\text{AAD} = \left(\sum_i \frac{|\eta_{\exp,i} - \eta_{\text{reg},i}|}{\eta_{\exp,i}} \cdot 100\ \%\right)/N \quad (10)$$

where $\eta_{\exp,i}$ and $\eta_{\text{reg},i}$ are the experimental data and regression data, respectively. N is the number of data points .

The parameters for eq 6 are shown in Table 9. For the [bmim][PF_6] + ethanol system, R and AAD are 0.999 and 2.04 %, respectively. For the [bmim][PF_6] + benzene system, R and AAD are 0.999 and 2.86 %, respectively.

CONCLUSION

In this work, a falling-body viscometer was built. The viscometer can be used to measure density and viscosity at high temperatures and pressures. The viscosities and densities of [bmim][PF_6], [bmim][PF_6] + ethanol, and [bmim][PF_6] + benzene binary systems were measured and correlated at different temperatures and pressures. The results show that the logarithm values of viscosities of pure [bmim][PF_6] and its binaries decrease linearly with pressure while they are approximately parabola functions of temperature. The viscosities of [bmim] [PF_6] + ethanol and [bmim] [PF_6] + benzene binary systems could be well fitted with temperatures, pressures, and the mole fraction of organic compounds. The average correlation coefficient for the two systems is 0.999.

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