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Measurement of Thermal Conductivity of 1-Butyl-3-Methylimidazolium

L-tryptophan + Water + Ethanol Mixtures at T = (283.15 to 333.15) K

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Thermal conductivities of 1-butyl-3-methylimidazolium L-tryptophan Abstract:

([BMIM][L-trp]), water, ethanol, [BMIM][L-trp] + water, [BMIM][L-trp] + ethanol, water +

ethanol and [BMIM][L-trp] + water + ethanol were investigated from 283.15 K to 333.15 K

covering the whole scale of concentrations at atmospheric pressure with transient hot wire

method. The thermal conductivities of pure [BMIM][L-trp] decease linearly from 0.180 to

0.177 W·m<sup>-1</sup>·K<sup>-1</sup> with increasing temperature. The uncertainty of the measurement was

less than 2% at 0.95 confident level. The experimental data of binary and ternary mixtures

were correlated by second-order Scheffé polynomial as a function of composition and

temperature. The average relative deviation of the calculated values with experiment data

was 0.58%.

1. Introduction

Ionic liquids (ILs) have attracted widespread attention in recent years as environmental

friendly solvents and were utilized in extraction, gas absorption, chemical catalysis and

other fields, because of their negligible vapor pressure, higher thermal stability, good solubility and adjustable structure.<sup>1-3</sup> Thermal conductivity is the measurement of the heat transfer ability of the materials and the study of thermal conductivities is significant for scale-up and industrialization of the chemical engineering process, so as for the application of ILs.<sup>4-7</sup> Hot wire method is an important technique of thermal conductivity measurement, which was considered as the most stable and accurate method for fluid measurement.<sup>8-10</sup> For example, Tomida et al.<sup>11</sup> studied the thermal conductivities of several kinds of imidazolium-based ionic liquids with different alkyl chain lengths by hot wire method and the pressure dependences of the thermal conductivity of ILs. Castro et al.<sup>12</sup> measured the thermal conductivities of several kinds of alkyl-methylimidazolium ionic liquids and corresponding IoNanofluids which is composed by ionic liquids with a few multiwall carbon nanotubes (MWCNTs) dispersed. The thermal conductivity enhancement by the addition of MWCNTs and the temperature dependence of the IoNanofluids system were also investigated.

lonic liquids, especially chiral ionic liquids, are mainly combined with other solvents when applied in chemical process to reduce the viscosity. In consideration of the surroundings in the industrial scale process, Ge et al.<sup>13</sup> investigated the thermal conductivities of [BMIM][OTf] + water, [EMIM][EtSO<sub>4</sub>] + water binary mixtures and correlated the data by the Jamieson correlation equation. Chen et al.<sup>14</sup> studied the thermal conductivities of [MMIM][DMP] + water and [MMIM][DMP] + methanol binary mixtures and fitted the data with higher accuracy. Besides that, several other ionic liquid binary mixture systems were measured mainly by hot wire method recent years.<sup>15-19</sup>

Amino acid ionic liquid is an important kind of ionic liquids. As chiral molecular, it has the general characteristics of chiral molecules and well chiral selectivity. Recently, amino acid ionic liquids have been widely applied in extraction separation and asymmetric synthesis process, with scale-up potential.<sup>20-24</sup> There are some published works about the density and viscosity measurement of amino acid ionic liquids, 25-28 but the thermal conductivities measurements of those have been rarely reported. Only Gardas et al.29 studied the thermal conductivities of several kinds of ammonium- and phosphonium- based amino acid ionic liquids and correlated the experiment data by group contribution method. In extraction process, in addition to binary mixtures system, sometimes the separation process is carried out through ternary mixtures system by the addition of co-solvent like alcohols or weak acids, to improve the solubility of the extracted substances. 30, 31 In this work, the thermal conductivities of [BMIM][L-trp], water, ethanol, their binary mixtures and ternary mixtures from 283.15 K to 333.15 K within the whole scale of concentrations have been determined at room pressure and the experimental data were correlated by second-order Scheffé polynomial. 32-34

### 2. Experimental section

### 2.1 Materials

The supplier and purity grades (expressed as mass fraction) of chemical reagents used in this work are shown in Table 1.

Ultrapure water purchased from Wahaha Group Co., Ltd. was further purified by lab ultrapure water purification system (resistivity > 18.2  $M\Omega$ ·cm at room temperature).

1-Butyl-3-methylimidazolium L-tryptophan, as shown in Figure 1, was purchased from

Shanghai Chengjie Chemical Co., Ltd. Mass content of water for the sample analyzed by Karl Fisher titration (Metrohm 870 KF Titrino Plus) was lower than 500 ppm. The bromine contents were below the detection limit (< 200 ppm) determined by titration with AgNO<sub>3</sub>. The structure of the ionic liquid was confirmed by <sup>1</sup>HNMR (AVANCE III 500 MHz Digital NMR Spectrometer). The weights of material were recorded by an analytical balance (Mettler Toledo XS205 Dual Range) to a precision of ± 0.1 mg.

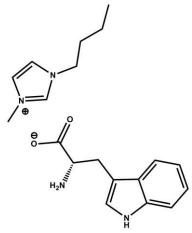


Figure 1. The structure of 1-butyl-3-methylimidazolium L-tryptophan

### 2.2 Methods

The thermal conductivity measuring instrument (Xi'an Xiatech Electronic Technology Co., Ltd., TC 3000L) was used to collect the thermal data of pure components and mixtures by transient hot wire method. Detailed descriptions of the apparatus and measuring theory can be found in previous references including our works. The length of tantalum wires were 29 mm and 58 mm, respectively. An automatic Wheatstone-type electronic bridge was used to measure the time evolution of temperature of the wires during the application of a constant heat flux to the transient hot wire instrument. The isothermal environment for the thermal cell was provided by a

thermostatic bath (Hui Chuang, YHX 2014, uncertainty of ± 0.1°C) and the temperature of the sample was measured by the platinum resistance thermometer of the apparatus automatically. The total uncertainty of the temperature for thermal conductivity measurement is less than ± 20 mK. The injection volume of sample of each different components mixture is 40 cm<sup>3</sup> approximately. The data acquisition time is 1 second. The heating voltage is adjusted for each sample within the range from 1.2 V (for pure ethanol) to 2.2 V (for pure water), to keep the transient temperature rise at approximately 3 K. All measurements were repeated at least five times for each data point. The thermal conductivity of deionized water, pure ethanol and pure toluene were chosen to check the accuracy and stability of the instrument at the selected temperature range. The detected results had good reproducibility within ± 0.73% and were in well agreement with the reference standard data,38 from which the maximum deviation and average relative deviation were 1.02% and 0.62% for water, 1.95% and 1.42% for ethanol, 2.24% and 1.60% for toluene, respectively. Accounting for all the random errors of measurement, the overall uncertainty of the present thermal conductivity data was estimated to be less than 2.0% with a coverage factor of k = 2, at a 0.95 confidence interval.

### 3. Results and Discussion

# 3.1 Pure components

The experimental and reference thermal conductivities of pure components including [BMIM][L-trp], water and ethanol are listed in Table 2 for comparison and correlation. The reproducibility of pure components is smaller than 0.5% and the uncertainty is less than 2% and ± 0.0015 W·m<sup>-1</sup>·K<sup>-1</sup>. The thermal conductivities of [BMIM][L-trp] are between 0.180

and 0.177 W·m<sup>-1</sup>·K<sup>-1</sup> from 283.15 K to 343.15 K, similar with those of ammonium- and phosphonium- based amino acid ionic liquids reported by Gardas et al.<sup>26</sup> The thermal conductivities decrease linearly with the increase of temperature, which is in agreement with the tendency of most ionic liquids from published references. <sup>39, 40</sup> So we correlate the thermal conductivity of [BMIM][L-trp] as a linear function of temperature here.

$$\lambda_i = a_0 + a_i T \tag{1}$$

The thermal conductivities of water and ethanol at different temperature have been studied by many researchers and can be correlated as a function of temperature using a second-order polynomial.<sup>34,41</sup>

$$\lambda_i = a_0 + a_1 T + a_2 T^2 \tag{2}$$

Where  $\lambda_i$  (W·m<sup>-1</sup>·K<sup>-1</sup>) is the thermal conductivity of pure component i, T (K) is the temperature, subscript i represents each pure component as 1 for [BMIM][L-trp], 2 for water and 3 for ethanol.  $a_0$ ,  $a_1$  and  $a_2$  are the correlation coefficients. As for ionic liquid system, equation 2 is also suitable when  $a_2$  = 0. The parameters  $a_0$ ,  $a_1$ ,  $a_2$  for equation 2, the values of average absolute relative deviation (AARD) and standard deviation (SD) are listed in Table 3.

# 3.2 Binary systems

The thermal conductivities data of binary mixtures [BMIM][L-trp] + water, [BMIM][L-trp] + ethanol, water + ethanol measured from 283.15 K to 333.15 K at approximately 10 K interval are listed in Table 4, Table 5 and Table 6 respectively. The thermal conductivities of [BMIM][L-trp] + water increase with the increase of the temperature in the tested concentration range, and those increase with the increase of water content. Similarly with

the [BMIM][L-trp] + water mixture system, the thermal conductivities of water + ethanol mixture increase with the increase of the mass fraction of water and temperature when the mass fraction of water is more than 0.3 and those decrease with the temperature increasing while the mass fraction of water is less than 0.3, which is consistent with the published works. The thermal conductivities of [BMIM][L-trp] + ethanol are less than 0.2 W·m-1·K-1 in the whole concentration range and decrease with the increase of temperature and the mass fraction of [BMIM][L-trp].

The empirical correlation equation second-order Scheffé polynomial, which can well correlate most binary mixtures from pure component and directly calculate the values for ternary data with parameters correlated from binary mixtures with simple forms, was applied in this work.

The equation of second-order Scheffé polynomial for binary mixture is

$$\lambda_{ij} = \lambda_i \mathbf{w}_i^2 + \lambda_j \mathbf{w}_i^2 + 2\beta_{ij} \lambda_i \lambda_j \tag{3}$$

where subscripts i and j represent two different components as 1 for [BMIM][L-trp], 2 for water, 3 for ethanol, respectively. The  $\lambda_{ij}$  (W·m<sup>-1</sup>·K<sup>-1</sup>) is the thermal conductivity of binary mixture of component i and j.  $\lambda_i$  (W·m<sup>-1</sup>·K<sup>-1</sup>) is the thermal conductivity of pure component i, and  $w_i$  is the mass fraction of component i in the mixture.  $\beta_{ij}$  is the nonlinear mixing effect between component i and j. The parameter  $\beta_{ij}$  is expected to be a function of temperature and can be assumed as a linear dependence on temperature,<sup>44</sup>

$$\beta_{ii} = A_{ii} + B_{ii}T \tag{4}$$

where  $A_{ij}$  and  $B_{ij}$  is correlation coefficients.

The thermal conductivities of binary mixtures [BMIM][L-trp] + water, [BMIM][L-trp] +

ethanol, water + ethanol were correlated by equations 3 and 4. The coefficients  $A_{ij}$ ,  $B_{ij}$  for three binary mixtures systems together with fitting AARD and SD are listed in Table 7.

# 3.3 Ternary systems

For ternary mixtures of [BMIM][L-trp] + water + ethanol, the thermal conductivities data of 36 different compositions measured from 283.15 K to 333.15 K at approximately 10 K interval at atmosphere were list in Table 8. Overall, because the thermal conductivities of water are much higher than that of organic compounds in the experiment temperature range, the thermal conductivities of the ternary mixtures were mainly decided by the mass fraction of water content, and increase with the increase of the mass fraction of water. When the mass fraction of water is constant, the thermal conductivities of mixtures slightly decreased with the increase of mass fraction of ethanol. Besides, the thermal conductivities of ternary mixtures increase with the increase of temperature when the mass fraction of water is higher than 0.2 and decrease with the increase of temperature when the mass fraction of water is lower than 0.2.

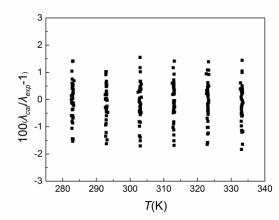
The previously mentioned second-order Scheffé polynomial was used to calculate the ternary mixture data and can be expanded as

$$\lambda_{\text{ternary}} = \lambda_1 W_1^2 + \lambda_2 W_2^2 + \lambda_3 W_3^2 + 2\lambda_1 \lambda_2 \beta_{12} + 2\lambda_1 \lambda_3 \beta_{13} + 2\lambda_2 \lambda_3 \beta_{23}$$
 (5)

where  $\lambda_{ternary}$  (W·m<sup>-1</sup>·K<sup>-1</sup>) is the thermal conductivity of the ternary mixtures,  $\lambda$  (W·m<sup>-1</sup>·K<sup>-1</sup>) and w is the thermal conductivity and mass fraction of pure component. Subscript 1, 2, 3 represent [BMIM][L-trp], water, and ethanol, respectively.  $\beta$  is the nonlinear mixing effect between two components that calculated from their binary mixtures.

The thermal conductivities of [BMIM][L-trp] + water + ethanol ternary mixtures can be

calculated by equations 4 and 5 with the parameters listed in Table 7. Figure 2 shows the relative deviations between experimental data and calculated values with the change of temperature. The AARD and SD are 0.58% and 0.0018 W·m<sup>-1</sup>·K<sup>-1</sup>, respectively. The result indicates that the second-order Scheffé polynomial can be used to estimate the thermal conductivity of [BMIM][L-trp] + water + ethanol ternary mixtures with high accuracy from experimental data of their binary mixtures.



**Figure 2.** Relative deviations  $100(\lambda_{cal}/\lambda_{exp}-1)$  between experimental data  $\lambda_{exp}$  and the values  $\lambda_{cal}$  calculated by equations 4 and 5 for [BMIM][L-trp] + water + ethanol from 283.15 K to 333.15 K at pressure p = 0.1 MPa. The average absolute relative deviation (AARD) is 0.58% and maximum absolute deviation is 1.83%.  $\blacksquare$ , this work.

# Conclusion

The thermal conductivities of [BMIM][L-trp], water, ethanol, their binary mixtures and ternary mixtures were measured by the instrument with transient hot wire method over the whole concentration range from 283.15 K to 333.15 K. The pure component data were correlated by empirical equation as a function of temperature and the binary mixtures data were correlated as the function of temperature and compositions by second-order Scheffé polynomial. The thermal conductivities data of ternary mixtures were directly calculated by the coefficient correlated from data of their binary mixtures through second-order Scheffé polynomial, and were in good agreement with the experiment results.

## Acknowledgement

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# **List of Tables**

**Table 1. Chemical Sample Description** 

chemical names	CAS	mass mass		purification	purity analysis		
chemical names	CAS	supplier	fraction	method	method		
1-butyl-3-methylimidazolium		Chengjie Chemical	0.99	none	LIDI Ca		
L-tryptophan		Co., Ltd.,China	0.99	none	HPLC		
ethanol	64-17-5	Aladdin Chemical	0.998	none	GCÞ		
ешапо	04-17-5	Co., Ltd.	0.996	none	HPLC <sup>a</sup> GC <sup>b</sup> GC <sup>b</sup>		
m othydb on zon o	108-88-3	Sinopharm Chemical	0.995	none	GC <sup>b</sup>		
methylbenzene	100-00-3	Reagent Co., Ltd.	0.995	none			
silver nitrate	7761-88-8	Sinopharm Chemical	0.998	nono	CCb		
	1101-00-0	Reagent Co., Ltd.	0.990	none	GC <sup>3</sup>		

<sup>&</sup>lt;sup>a</sup>High performance liquid chromatography. <sup>b</sup>Gas chromatography

Table 2. Experimental and Reference Thermal Conductivities Data of Pure Components from 283.15 K to 343.15 K at Pressure  $p = 0.1 \text{ MPa}^a$ 

[E	BMIM][L-trp]		water		ethanol		
T(K)	λ(W·m <sup>-1</sup> ·K <sup>-1</sup> )	T(K)	$T(K)$ $\lambda(W \cdot m^{-1} \cdot K^{-1})$		T(K)	λ(W·m <sup>-1</sup> ·K <sup>-1</sup> )	
_	exp.		exp.	ref. <sup>b</sup>	•	ехр.	ref. <sup>b</sup>
283.92	0.180	283.10	0.585	0.5800	283.54	0.168	0.1687
293.50	0.180	293.05	0.602	0.5983	293.31	0.166	0.1663
303.46	0.179	303.17	0.618	0.6155	303.28	0.163	0.1640
313.48	0.179	313.34	0.633	0.6309	313.25	0.160	0.1617
323.45	0.178	323.19	0.646	0.6436	323.07	0.158	0.1595
333.58	0.178	332.85	0.656	0.6541	332.97	0.154	0.1573
343.39	0.177	343.02	0.664	0.6630	342.82	0.152	0.1551

<sup>&</sup>lt;sup>a</sup>The expanded uncertainties U (0.95 level of confidence, k = 2) are  $U(\lambda) = 0.02\lambda$ , U(T) = 20 mK and U(p) = 0.002 MPa.

Table 3. Correlation coefficient  $a_0$ ,  $a_1$ ,  $a_2$ , Average Absolute Relative Deviation (AARD) and Standard Deviation (SD) of Pure Components

	<b>a</b> <sub>0</sub>	a <sub>1</sub>	<b>a</b> <sub>2</sub>	AARD(%)	SD(W·m <sup>-1</sup> ·K <sup>-1</sup> )
[BMIM][L-trp]	1.938×10 <sup>-1</sup>	-4.889×10 <sup>5</sup>		0.052	0.0001
water	-6.634×10 <sup>-1</sup>	6.942×10 <sup>-3</sup>	-8.951×10 <sup>6</sup>	0.035	0.0002
ethanol	2.091×10 <sup>-1</sup>	-2.404×10 <sup>5</sup>	-4.228×10 <sup>7</sup>	0.116	0.0002

<sup>&</sup>lt;sup>b</sup>Reference 38.

Table 4. Experimental Thermal Conductivities Data of [BMIM][L-trp] (1) + Water (2) from 283.15 K to 333.15 K at Pressure  $p = 0.1 \text{ MPa}^a$ 

W <sub>1</sub>	T(K)	λ(W·m <sup>-1</sup> ·K <sup>-1</sup> )	<b>W</b> <sub>1</sub>	T(K)	λ(W·m <sup>-1</sup> ·K <sup>-1</sup> )	<b>W</b> <sub>1</sub>	T(K)	λ(W·m <sup>-1</sup> ·K <sup>-1</sup> )
0.1000	282.90	0.528	0.2000	283.16	0.476	0.3000	283.00	0.427
	293.16	0.543		292.90	0.488		293.22	0.437
	303.09	0.556		303.35	0.501		302.99	0.447
	312.97	0.568		312.97	0.510		313.37	0.456
	322.88	0.578		322.95	0.520		323.07	0.463
	333.27	0.587		333.10	0.528		333.09	0.469
0.3999	282.92	0.379	0.4999	283.29	0.335	0.5998	283.11	0.295
	293.22	0.388		293.22	0.342		293.08	0.299
	303.20	0.396		303.08	0.347		303.08	0.303
	313.33	0.403		313.34	0.353		313.15	0.307
	323.33	0.409		322.94	0.357		323.07	0.311
	333.20	0.414		332.98	0.361		333.18	0.314
0.6998	283.35	0.259	0.7997	283.41	0.228	0.8998	283.00	0.200
	293.17	0.262		293.29	0.229		293.09	0.201
	303.22	0.265		303.33	0.230		303.13	0.201
	312.97	0.266		312.96	0.231		313.28	0.202
	323.09	0.269		323.05	0.232		323.08	0.202
	333.08	0.271		333.10	0.234		333.11	0.202

<sup>&</sup>lt;sup>a</sup>The expanded uncertainties U (0.95 level of confidence, k = 2) are  $U(\lambda) = 0.02\lambda$ , U(T) = 20 mK, U(p) = 0.002 MPa and U(w) = 0.0001.

Table 5. Experimental Thermal Conductivities Data of [BMIM][L-trp] (1) + Ethanol (3) from 283.15 K to 333.15 K at Pressure  $p = 0.1 \text{ MPa}^a$ 

W <sub>1</sub>	T(K)	λ(W·m <sup>-1</sup> ·K <sup>-1</sup> )	<b>W</b> <sub>1</sub>	T(K)	λ(W·m <sup>-1</sup> ·K <sup>-1</sup> )	<b>W</b> <sub>1</sub>	T(K)	λ(W·m <sup>-1</sup> ·K <sup>-1</sup> )
0.0999	283.04	0.171	0.2000	283.13	0.172	0.3000	283.18	0.173
	292.94	0.169		293.27	0.170		293.01	0.171
	303.07	0.166		303.21	0.168		302.82	0.170
	313.10	0.163		313.26	0.166		312.97	0.167
	323.23	0.161		323.22	0.163		322.98	0.164
	333.16	0.158		333.26	0.160		333.35	0.163
0.3995	282.86	0.175	0.5000	282.99	0.175	0.5997	283.39	0.176
	293.32	0.173		293.22	0.174		293.36	0.175
	303.14	0.171		302.88	0.172		303.45	0.174
	313.27	0.169		313.11	0.170		312.99	0.172
	323.07	0.168		323.14	0.169		323.04	0.171
	333.27	0.165		333.31	0.167		332.89	0.170
0.6998	283.23	0.177	0.7996	282.95	0.177	0.8998	283.06	0.177
	293.03	0.176		293.34	0.177		292.84	0.177
	303.08	0.175		303.15	0.176		302.99	0.178
	313.34	0.174		312.91	0.175		312.92	0.176
	323.05	0.171		323.12	0.174		323.09	0.175
	333.09	0.171		332.87	0.172		332.94	0.174

<sup>&</sup>lt;sup>a</sup>The expanded uncertainties U (0.95 level of confidence, k = 2) are  $U(\lambda) = 0.02\lambda$ , U(T) = 20 mK, U(p) = 0.002 MPa and U(w) = 0.0001.

Table 6. Experimental Thermal Conductivities Data of Water (2) + Ethanol (3) from 283.15 K to 333.15 K at Pressure  $p = 0.1 \text{ MPa}^a$ 

$W_2$	T(K)	$\lambda(W \cdot m^{-1} \cdot K^{-1})$	$W_2$	T(K)	$\lambda(W \cdot m^{-1} \cdot K^{-1})$	<i>W</i> <sub>2</sub>	T(K)	λ(W·m <sup>-1</sup> ·K <sup>-1</sup> )
0.8999	282.71	0.516	0.8000	282.89	0.455	0.7001	282.92	0.403
	292.96	0.530		292.86	0.467		292.60	0.412
	302.89	0.546		303.04	0.480		303.05	0.420
	312.70	0.559		312.98	0.491		313.03	0.427
	322.88	0.568		323.02	0.499		323.12	0.434
	333.00	0.577		333.09	0.505		333.14	0.438
0.5999	283.04	0.356	0.4993	283.23	0.311	0.4000	283.02	0.273
	293.26	0.362		293.19	0.314		293.03	0.274
	303.05	0.367		303.43	0.318		303.15	0.275
	313.15	0.371		313.23	0.319		313.00	0.276
	322.94	0.375		323.01	0.321		323.33	0.277
	333.13	0.379		333.26	0.323		333.32	0.277
0.3000	283.10	0.240	0.1996	283.07	0.212	0.1000	282.85	0.189
	293.16	0.240		293.13	0.211		293.16	0.186
	303.19	0.240		303.12	0.210		303.11	0.184
	313.02	0.240		313.19	0.208		313.18	0.182
	323.05	0.239		323.19	0.207		323.15	0.180
	333.14	0.238		333.26	0.206		333.15	0.178

<sup>&</sup>lt;sup>a</sup>The expanded uncertainties U (0.95 level of confidence, k = 2) are  $U(\lambda) = 0.02\lambda$ , U(T) = 20 mK, U(p) = 0.002 MPa and U(w) = 0.0001.

Table 7. Correlation Parameters, Average Absolute Relative Deviation (AARD) and Standard Deviation (SD) of Binary Mixtures for equations 3 and 4

		$A_{ij}$	$B_{ij}$	AARD(%)	SD( W·m <sup>-1</sup> ·K <sup>-1</sup> )
[BMIM][L-trp] + water	i = 1, j = 2	1.914×10 <sup>-1</sup>	3.407×10 <sup>-4</sup>	0.778	0.0027
[BMIM][L-trp] + ethanol	i = 1, j = 3	2.233×10 <sup>-1</sup>	-1.647×10 <sup>-4</sup>	0.421	0.0009
water + ethanol	i = 2, j = 3	2.429×10 <sup>-1</sup>	8.334×10 <sup>-6</sup>	0.459	0.0016

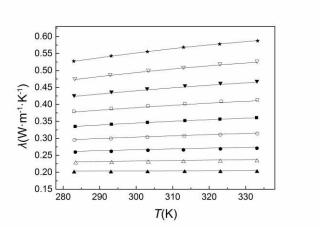
Table 8. Experimental Thermal Conductivities Data of [BMIM][L-trp] (1) + Water (2) + Ethanol (3) from 283.15 K to 333.15 K at Pressure p = 0.1 MPa<sup>a</sup>

$W_1, W_2$	T(K)	$\lambda(W \cdot m^{-1} \cdot K^{-1})$	$W_1, W_2$	T(K)	$\lambda(W \cdot m^{-1} \cdot K^{-1})$	$W_1,W_2$	T(K)	λ(W·m <sup>-1</sup> ·K <sup>-1</sup> )
0.7998	282.99	0.201	0.6992	282.88	0.225	0.6999	283.12	0.197
0.1002	292.91	0.201	0.2005	293.16	0.226	0.0999	292.77	0.198
	303.02	0.202		303.03	0.227		303.02	0.197
	313.24	0.202		313.03	0.228		312.98	0.197
	323.10	0.202		323.03	0.229		323.04	0.197
	333.09	0.202		333.37	0.230		333.46	0.197
0.5997	282.97	0.255	0.5994	283.13	0.226	0.5999	282.77	0.197
0.3002	292.98	0.257	0.2004	293.20	0.227	0.0999	292.90	0.197
	303.02	0.259		302.93	0.228		303.03	0.196
	313.05	0.261		313.10	0.228		312.91	0.196
	322.88	0.263		323.32	0.229		323.18	0.194
_	333.06	0.264		333.24	0.229		333.00	0.195
0.4993	282.78	0.291	0.4991	282.96	0.254	0.5000	282.99	0.222
0.4009	292.76	0.294	0.3004	292.97	0.256	0.2000	292.89	0.221
	302.81	0.298		303.03	0.258		302.80	0.222
	312.75	0.301		313.08	0.260		312.96	0.223
	322.93	0.304		322.87	0.261		323.15	0.223
_	333.15	0.306		333.13	0.261		333.20	0.223
0.4997	282.60	0.196	0.4001	282.86	0.329	0.3998	283.12	0.287
0.1002	292.95	0.195	0.4999	293.39	0.335	0.4004	292.89	0.290
	302.76	0.195		303.26	0.340		302.74	0.293
	312.96	0.194		313.18	0.344		312.97	0.296
	323.17	0.193		323.04	0.349		323.10	0.299
	333.31	0.192		333.03	0.352		333.04	0.301
0.3999	282.82	0.253	0.4000	283.02	0.220	0.3999	282.97	0.195
0.2999	293.06	0.255	0.2003	292.97	0.220	0.1002	292.69	0.194
	303.03	0.256		302.82	0.221		302.86	0.193

	312.67	0.257		312.81	0.220		313.10	0.192
	322.68	0.259		323.15	0.220		323.03	0.191
	333.39	0.260		333.16	0.220		333.34	0.190
0.3000	282.58	0.372	0.2997	282.99	0.325	0.2985	282.95	0.284
0.6001	292.91	0.381	0.5004	292.67	0.330	0.3985	292.82	0.287
	302.36	0.387		303.09	0.335		303.36	0.290
	312.53	0.395		312.98	0.339		313.18	0.292
	322.62	0.402		323.12	0.343		323.28	0.294
	332.71	0.405		333.04	0.346		333.04	0.296
0.2984	283.26	0.250	0.3000	282.88	0.219	0.3000	282.79	0.194
0.3035	293.15	0.251	0.2000	293.06	0.219	0.1000	292.96	0.193
	302.96	0.252		302.77	0.218		303.02	0.192
	312.90	0.253		312.91	0.218		312.89	0.190
	323.17	0.254		323.25	0.217		323.05	0.189
	333.14	0.254		333.51	0.217		333.23	0.187
0.1992	282.94	0.418	0.1998	283.07	0.369	0.1999	282.90	0.321
0.6986	292.93	0.427	0.6006	293.00	0.376	0.5004	293.06	0.325
	303.31	0.437		302.98	0.382		302.93	0.329
	313.08	0.444		312.97	0.389		312.97	0.333
	323.35	0.454		323.08	0.393		323.04	0.336
	333.26	0.458		332.81	0.398		333.07	0.338
0.1995	283.06	0.283	0.1999	283.13	0.246	0.1998	282.86	0.217
0.4011	293.09	0.285	0.3000	293.00	0.247	0.2006	292.92	0.217
	303.11	0.287		302.97	0.248		302.99	0.216
	313.03	0.289		312.99	0.249		312.84	0.216
	323.03	0.291		323.13	0.249		323.34	0.215
	333.14	0.292		333.08	0.249		333.33	0.214
0.2000	282.73	0.193	0.1000	282.69	0.465	0.1000	282.61	0.411
0.0998	292.82	0.191	0.8000	292.98	0.480	0.6999	293.07	0.420

	303.02	0.190		302.88	0.491		302.71	0.428
	313.04	0.188		313.03	0.502		312.97	0.435
	323.33	0.187		323.14	0.508		323.07	0.443
	333.24	0.185		333.08	0.516		332.95	0.448
0.1000	283.03	0.362	0.0999	283.15	0.317	0.0999	283.35	0.278
0.5999	292.63	0.368	0.5001	292.98	0.320	0.4002	292.88	0.280
	302.79	0.374		303.16	0.324		303.23	0.282
	312.96	0.380		313.11	0.327		313.14	0.283
	322.75	0.384		323.04	0.330		323.01	0.285
	333.01	0.388		333.15	0.332		333.13	0.286
0.1000	282.86	0.244	0.0998	282.96	0.216	0.0999	283.07	0.192
0.3000	293.01	0.244	0.2003	292.81	0.214	0.1007	292.93	0.189
	303.11	0.245		302.96	0.214		302.97	0.188
	313.01	0.245		312.79	0.213		313.12	0.186
	323.13	0.245		322.98	0.212		323.26	0.184
	333.30	0.244		333.22	0.210		333.25	0.182

<sup>&</sup>lt;sup>a</sup>The expanded uncertainties U (0.95 level of confidence, k = 2) are  $U(\lambda) = 0.02\lambda$ , U(T) = 20 mK, U(p) = 0.002 MPa and U(w) = 0.0001.



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