咪唑基离子液体的物理化学性质估算及预测

刘青山¹ 杨 淼¹ 谭志诚^{1,2,*} WELZ-BIERMANN Urs^{1,*}⁽¹⁾ 中国科学院大连化学物理研究所, 中国离子液体实验室, 辽宁 大连 116023;⁽²⁾ 中国科学院大连化学物理研究所, 热化学实验室, 辽宁 大连 116023)

摘要: 根据经验和半经验方程及空隙模型理论, 可以估算及预测离子液体在 298.15 K 的物理化学性质. 本文讨论了离子液体的分子体积, 密度, 标准熵, 晶格能, 表面张力, 等张比容, 摩尔蒸发焓, 空隙体积, 空隙率和热膨胀系数. 通过实验测得的三种离子液体 1-乙基-3-甲基咪唑硫酸乙酯([C₂mim][EtSO₄]), 1-丁基-3-甲基咪唑硫酸辛酯([C₄mim][OcSO₄])和 1-乙基-3-甲基咪唑双三氟甲磺酰亚胺盐([C₂mim][NTf₂])的密度和表面张力估算了它们的其它物理化学性质. 由这三种离子液体的分子体积及等张比容预测了同系列中其它离子液体[C_nmim][EtSO₄], [C_nmim][OcSO₄]和[C_nmim][NTf₂](*n*=1–6)的分子体积及等张比容, 由此计算出它们的密度及表面张力. 进而预测了它们的物理化学性质. 将预测的离子液体[C_nmim][NTf₂]和[C₂mim][OcSO₄]的密度值与文献报导的实验值进行比较, 其偏差在实验误差范围内. 最后, 将由 Kabo 经验方程计算的七个离子液体[C₂mim][EtSO₄], [C₄mim][OcSO₄], [C₂mim][NTf₂], [C₄mim][NTf₂], 丁基三甲基铵双三氟甲磺酰亚胺盐([N₄₁₁][NTf₂]), 甲基三辛基铵双三氟甲磺酰亚胺盐([N₈₈₁][NTf₂])和 1-辛基-3-甲基吡啶四氟硼酸盐([m₃opy][BF₄])的摩尔蒸发焓与由 Verevkin 简单规则预测的摩尔蒸发焓进行比较, 发现两者符合很好. 因此, 在缺乏密度和表面张力实验数据的情况下, 可以用 Verevkin 简单规则来预测离子液体的摩尔蒸发焓.

关键词: 离子液体; 密度; 表面张力; 等张比容; 蒸发焓; 分子体积

中图分类号: O642

Estimation and Prediction of the Physicochemical Properties of Imidazolium-Based Ionic Liquids

LIU Qing-Shan¹ YANG Miao¹ TAN Zhi-Cheng^{1,2,*} WELZ-BIERMANN Urs^{1,*}

⁽¹⁾China Ionic Liquid Laboratory, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian 116023, Liaoning Province, P. R. China; ⁽²⁾Thermochemistry Laboratory, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian 116023, Liaoning Province, P. R. China)

Abstract: The physicochemical properties of ionic liquids (ILs) at 298.15 K could be estimated and predicted in terms of empirical and semi-empirical equations as well as by interstice model theory. In this paper, the molecular volume, density, standard molar entropy, lattice energy, surface tension, parachor, molar enthalpy of vaporization, interstice volume, interstice fraction, and thermal expansion coefficient are discussed. These properties were first estimated by experimentally determining the density and surface tension for 1-ethyl-3-methylimidazolium ethylsulfate ([C₂mim][EtSO₄]), 1-butyl-3-methylimidazolium octylsulfate ([C₄mim][OcSO₄]), and 1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide ([C₂mim][NTf₂]). The molecular volume and parachor of the three homologues of the imidazolium-based ILs [C_nmim][EtSO₄], [C_nmim][OcSO₄], and [C_nmim][NTf₂] (*n*=1–6) were predicted and their densities and surface tensions were obtained. Other properties were also calculated using the obtained density and surface tension values. The predicted density was compared to the experimental values for [C₄mim][NTf₂] and [C₂mim][OcSO₄], which shows that the deviation between experimental and predicted data are within experimental error. Finally, we compared the values for the molar enthalpy of vaporization estimated by Kabo's empirical equation with those predicted by Verevkin's simple rule for [C₂mim][EtSO₄], [C₄mim][OcSO₄], [C₂mim][NTf₂], [C₄mim][NTf₂], *N*-butyltrimethyla-

Received: November 9, 2009; Revised: February 2, 2010; Published on Web: April 9, 2010.

*Corresponding authors. Email: tzc@dicp.ac.cn, uw@dicp.ac.cn

© Editorial office of Acta Physico-Chimica Sinica

ammonium bis(trifluoromethylsulfonyl)imide [N_{4111}][NTf₂], *N*-methyltriocetyl ammonium bis(trifluoromethylsulfonyl)imide ([N_{8881}][NTf₂]), and *N*-octyl-3-methylpyridinium tetrafluoroborate ([m_3opy][BF₄]) and found that the values obtained by these two equations were in good agreement with each other. Therefore, we suggest that the molar enthalpy of vaporization of ILs can be predicted by Verevkin's simple rule when experimental data for density and surface tension are not available.

Key Words: Ionic liquids; Density; Surface tension; Parachor; Enthalpy of vaporization; Molecular volume

ILs as organic salts, often exhibit interesting properties, such as low melting points, good solvation properties, and non-volatility, which are required both by industrial and scientific communities for their broad application range as electrolytes in batteries and supercapacitors^[1-2], reaction media in nanoscience^[3], physical chemistry^[4-5] and many other areas. Therefore, the data of physicochemical properties of ILs are fundamental for their future application and valuable for an insight into the origins of their unique behavior. Recently, more and more publications reported the experimental physicochemical properties of various ILs^[6-15]. Although there is a significant amount of data related to imidazolium-based ILs, properties of homologue of [C_n mim][EtSO₄], [C_n mim][OcSO₄], and [C_n mim][NTf₂] ($n=1-6$) covered in this publication are still limited^[16-17]. In this regard, we estimated various physicochemical properties of [C_2 mim][EtSO₄], [C_4 mim][OcSO₄], and [C_2 mim][NTf₂] by using their experimental density and surface tension data. In the next step, the physicochemical properties of their homologues [C_n mim][EtSO₄], [C_n mim][OcSO₄], and [C_n mim][NTf₂] ($n=1-6$) were predicted from the estimated values of their molecular volumes and parachors. In the present paper, the ionic liquid cations are 1-alkyl-3-methylimidazolium ([C_n mim]⁺), tetra-alkyl ammonium ([TAA]⁺), *N*-octyl-3-methylpyridinium ([m_3opy]⁺); the anions of the ILs are ethylsulfate ([EtSO₄]⁻), octylsulfate ([OcSO₄]⁻), bis(trifluoromethylsulfonyl)imide ([NTf₂]⁻), and tetrafluoroborate ([BF₄]⁻).

1 Volumetric, entropy and lattice energy

The molecular volume, V_m , can be calculated from experimental density using the following equation:

$$V_m = M / (N \cdot \rho) \quad (1)$$

where M is molar mass, ρ is density, and N is Avogadro's constant.

According to Glasser's theory^[18], the standard molar entropy, $S^\ominus$, could be estimated from the following equation:

$$S^\ominus(298.15\text{ K}) = 1246.5V_m + 29.5 \quad (2)$$

The lattice energy, U_{pot} , was estimated according to the following equation^[18]:

$$U_{\text{pot}}(298.15\text{ K}) = 1981.2(\rho/M)^{1/3} + 103.8 \quad (3)$$

The contribution methylene ($-\text{CH}_2-$) group to the molecular volume is 0.0272 nm³ for [C_n mim][BF₄]^[18], 0.0282 nm³ for [C_n mim][NTf₂]^[18], 0.0270 nm³ for [C_n mim][AlCl₄]^[15], and 0.0278 nm³ for [C_n mim][Ala]^[14]. Due to the similar values of the contribution of per $-\text{CH}_2-$ to the molecular volume, the group of methylene in the alkyl chains of the imidazolium-based ILs could be considered to have the similar chemical environment. Hence,

the mean value of the contribution can be calculated to be 0.0275 nm³, the physicochemical properties (density, standard entropy, lattice energy) of the homologues of [C_n mim][EtSO₄] and [C_n mim][OcSO₄] ($n=1-6$) could be predicted. Using the value 0.0282 nm³ for the contribution of per $-\text{CH}_2-$ to the molecular volume for the homologues of [C_n mim][NTf₂] ($n=1-6$)^[18], the physicochemical properties of all IL homologues can be predicted. The calculated density value (1.4381 g·cm⁻³) for [C_3 mim][NTf₂] is in good agreement with the experimental values (1.4366 g·cm⁻³^[6], 1.43410 and 1.43573 g·cm⁻³^[19]). The predicted density value (1.0881 g·cm⁻³) for [C_2 mim][OcSO₄] is also in good agreement with the experimental value of 1.0942 g·cm⁻³^[20].

All of these estimated and predicted physicochemical property data are listed in Tables 1–3.

Based on the plots of $S^\ominus$ against the number of the carbons, n , in the alkyl chain of the ILs (see Fig.1), the contribution of per methylene group to $S^\ominus$ was calculated to be 35.1 J·K⁻¹·mol⁻¹ for [C_n mim][NTf₂], 34.3 J·K⁻¹·mol⁻¹ for [C_n mim][EtSO₄], and 34.3 J·K⁻¹·mol⁻¹ for [C_n mim][OcSO₄]. The above calculated values are in good agreement with the literature values of 35.1 J·K⁻¹·mol⁻¹ for [C_n mim][NTf₂]^[18], 33.9 J·K⁻¹·mol⁻¹ for [C_n mim][BF₄]^[18], 33.7 J·K⁻¹·mol⁻¹ for [C_n mim][AlCl₄]^[15], and 34.6 J·K⁻¹·mol⁻¹ for [C_n mim][Ala]^[14]. According to these various values for the contribution of per methylene group to the standard molar entropy in the homologue series with different anions, it could be concluded that these contributions are relatively similar for all imidazolium-based ILs.

2 Parachors and molar enthalpy of vaporization

The parachor, P , was estimated from the following equation^[21]:

$$P = M\gamma^{1/4}/\rho \quad (4)$$

where γ is the surface tension.

According to literature^[15], the contribution of per methylene ($-\text{CH}_2-$) group to parachor is 31.1. The values of parachors for the homologue series of the imidazolium-based ILs [C_n mim][EtSO₄], [C_n mim][OcSO₄], and [C_n mim][NTf₂] ($n=1-6$) were predicted.

The values of molar enthalpies of vaporization were estimated in terms of Kabo's empirical equation^[22]:

$$\Delta_f H_m^\ominus(298.15\text{ K}) = 0.01121(\gamma V^{2/3} N^{1/3}) + 2.4 \quad (5)$$

where V is molar volume.

According to Eq.(4), the surface tension can be calculated from predicted density and parachor data. The calculated value (31.71 mJ·m⁻²) for the surface tension of [C_4 mim][NTf₂] is in good agreement with the experimental value (31.71 mJ·m⁻²)^[23].

Table 1 Estimated and predicted values of physicochemical properties of $[C_n\text{mim}][\text{EtSO}_4]$ ($n=1-6$) at 298.15 K

	V_m nm ³	ρ (g·cm ⁻³)	$S^\ominus$ (J·K ⁻¹ ·mol ⁻¹)	U_{ps} (kJ·mol ⁻¹)	V (cm ³ ·mol ⁻¹)	P	$\Delta_f^\ominus H_m^\ominus$ (kJ·mol ⁻¹)	$10^{23}v$ cm ³	$\sum v$ cm ³	$10^2 \sum v/V$	$10^4 \alpha$ K ⁻¹	γ (mJ·m ⁻²)
$[C_1\text{mim}][\text{EtSO}_4]^b$	0.2880	1.2784	389.5	459	173.9	463.2	151.0	15.86	19.10	10.98	5.53	50.38
$[C_2\text{mim}][\text{EtSO}_4]^a$	0.3163	1.2411 ^[6]	423.7	448	190.4	494.3	144.7	18.52	22.30	11.71	5.89, 5.58 ^[6]	45.44 ^[6]
$[C_3\text{mim}][\text{EtSO}_4]^b$	0.3438	1.2094	458.0	439	207.0	525.4	139.9	21.19	25.52	12.33	6.20	41.53
$[C_4\text{mim}][\text{EtSO}_4]^b$	0.3713	1.1826	492.3	430	223.5	556.5	136.3	23.82	28.68	12.83	6.45	38.42
$[C_5\text{mim}][\text{EtSO}_4]^b$	0.3988	1.1593	526.6	423	240.1	587.6	133.6	26.38	31.76	13.23	6.66	35.89
$[C_6\text{mim}][\text{EtSO}_4]^b$	0.4263	1.1393	560.9	416	256.6	618.7	131.5	28.89	34.78	13.55	6.82	33.78

^a Property data for this IL were estimated values; ^b property data for this IL were predicted values.**Table 2** Estimated and predicted values of physicochemical properties of $[C_n\text{mim}][\text{NTf}_2]$ ($n=1-6$) at 298.15 K

	V_m nm ³	ρ (g·cm ⁻³)	$S^\ominus$ (J·K ⁻¹ ·mol ⁻¹)	U_{ps} (kJ·mol ⁻¹)	V (cm ³ ·mol ⁻¹)	P	$\Delta_f^\ominus H_m^\ominus$ (kJ·mol ⁻¹)	$10^{23}v$ cm ³	$\sum v$ cm ³	$10^2 \sum v/V$	$10^4 \alpha$ K ⁻¹	γ (mJ·m ⁻²)
$[C_1\text{mim}][\text{NTf}_2]^b$	0.3998	1.5676	527.9	422	240.7	598.7	142.6	23.94	28.82	11.98	6.02	38.29
$[C_2\text{mim}][\text{NTf}_2]^a$	0.4280	1.5187 ^[6]	563.0	415	257.7	629.8	139.2	26.59	32.01	12.43	6.25, 6.66 ^[6]	35.70 ^[6]
$[C_3\text{mim}][\text{NTf}_2]^b$	0.4562	1.4759	598.2	409	274.6	660.9	136.5	29.20	35.16	12.80	6.44	33.54
$[C_4\text{mim}][\text{NTf}_2]^b$	0.4844	1.4381	633.3	403	291.6	692.0	134.4	31.76	38.24	13.11	6.60	31.71
$[C_5\text{mim}][\text{NTf}_2]^a$	0.4849	1.4366 ^[6]	633.9	402	291.9	698.6	139.0	30.19	36.35	12.45	6.27, 6.73 ^[6]	32.80 ^[6]
$[C_6\text{mim}][\text{NTf}_2]^a$	0.4857	1.43410 ^[9]	635.0	402	292.4							
$[C_6\text{mim}][\text{NTf}_2]^a$	0.4852	1.43573 ^[9]	634.3	402	292.1							
$[C_3\text{mim}][\text{NTf}_2]^b$	0.5126	1.4044	668.5	397	308.6	723.1	132.7	34.26	41.25	14.13	6.72	30.15
$[C_6\text{mim}][\text{NTf}_2]^b$	0.5408	1.3743	703.6	392	325.6	754.2	131.4	36.70	44.18	14.32	6.83	28.80

^a Property data for this IL were estimated values; ^b property data for this IL were predicted values.**Table 3** Estimated and predicted values of the physicochemical properties of $[C_n\text{mim}][\text{OCSO}_4]$ ($n=1-6$) at 298.15 K

	V_m nm ³	ρ (g·cm ⁻³)	$S^\ominus$ (J·K ⁻¹ ·mol ⁻¹)	U_{ps} (kJ·mol ⁻¹)	V (cm ³ ·mol ⁻¹)	P	$\Delta_f^\ominus H_m^\ominus$ (kJ·mol ⁻¹)	$10^{23}v$ cm ³	$\sum v$ cm ³	$10^2 \sum v/V$	$10^4 \alpha$ K ⁻¹	γ (mJ·m ⁻²)
$[C_1\text{mim}][\text{OCSO}_4]^b$	0.4617	1.1025	605.0	407	277.9	651.5	124.1	34.19	41.17	14.81	7.45	30.19
$[C_2\text{mim}][\text{OCSO}_4]^b$	0.4892	1.0881	639.3	402	294.5	682.6	123.3	36.58	44.05	14.96	7.52	28.86
$[C_3\text{mim}][\text{OCSO}_4]^a$	0.4866	1.0942 ^[20]	636.0	402	293.0							
$[C_3\text{mim}][\text{OCSO}_4]^b$	0.5167	1.0753	673.6	396	311.1	713.7	122.8	38.86	46.79	15.04	7.57	27.72
$[C_4\text{mim}][\text{OCSO}_4]^a$	0.5442	1.0638 ^[6]	707.8	391	327.6	744.8	122.6	41.09	49.47	15.10	7.59, 6.21 ^[6]	26.71 ^[6]
$[C_5\text{mim}][\text{OCSO}_4]^b$	0.5717	1.0534	742.1	387	344.2	775.9	122.5	43.20	52.02	15.11	7.60	25.83
$[C_6\text{mim}][\text{OCSO}_4]^b$	0.5992	1.0439	776.4	382	360.7	807.0	122.6	45.24	54.47	15.10	7.60	25.05

^a Property data for this IL were estimated values; ^b property data for this IL were predicted values.

reement with the experimental value (32.80 mJ·m⁻²)^[6]. The molar enthalpy of vaporization, $\Delta_f^\ominus H_m^\ominus$, then can be obtained based on the predicted density and surface tension data.

All of these data are listed in Tables 1–4.

Fig.1 Plots of $S^\ominus$ against the number of the carbon (n) in the alkyl chain of the ILs at 298.15 K

- (a) $S^\ominus=570.7+34.27n$, $R=0.9999$ for $[C_n\text{mim}][\text{OCSO}_4]$;
 (b) $S^\ominus=492.7+35.14n$, $R=0.9999$ for $[C_n\text{mim}][\text{NTf}_2]$;
 (c) $S^\ominus=355.2+34.29n$, $R=0.9999$ for $[C_n\text{mim}][\text{EtSO}_4]$

The plots of density, ρ , and surface tension, γ , against the number of carbon, n , in alkyl chain of ILs at 298.15 K are shown in Figs.2 and 3.

From the Figs.2 and 3, it can be seen that as for density: $[C_n\text{mim}][\text{NTf}_2] > [C_n\text{mim}][\text{EtSO}_4] > [C_n\text{mim}][\text{OCSO}_4]$ and as for surface tension: $[C_n\text{mim}][\text{EtSO}_4] > [C_n\text{mim}][\text{NTf}_2] > [C_n\text{mim}][\text{OCSO}_4]$.

3 Interstice model theory

According to the interstice model^[23-24], the interstice volume, v , could be estimated by classical statistical mechanics:

$$v=0.6791(k_B T/\gamma)^{3/2} \quad (6)$$

where k_B is the Boltzmann constant, T is the thermodynamic temperature.

The molar volume of ionic liquids, V , consists of the inherent volume, V_p , and the volume of the interstice; whereas the molar volume of the interstice is $\sum v=2Nv$:

$$V=V_p+2Nv \quad (7)$$

If the expansion volume of IL only results from the expansion of the interstice when the temperature increases, then, the thermal expansion coefficient, α , can be predicted from the interstice model:

Table 4 Values of the molar enthalpies of vaporization of ILs at 298.15 K

	ρ (g·cm ⁻³)	γ (mJ·m ⁻²)	$\Delta_f^\circ H_m^\ominus$ (kJ·mol ⁻¹)	$\Delta_f^\circ H_m^\ominus$ (kJ·mol ⁻¹)
[C ₂ mim][EtSO ₄]	1.2411 ^[6]	45.44 ^[6]	158.8	144.7
[C ₂ mim][NTf ₂]	1.5187 ^[6]	35.70 ^[6]	132.9	139.3
[C ₄ mim][NTf ₂]	1.4366 ^[6]	32.80 ^[6]	137.9	139.0
[C ₄ mim][OcSO ₄]	1.0638 ^[6]	26.71 ^[6]	178.8	122.5
[N ₄₁₁₁][NTf ₂]	1.3940 ^[6]	32.46 ^[6]	136.2	135.3
[N ₈₈₈₁][NTf ₂]	1.1046 ^[6]	27.93 ^[6]	181.2	187.8
[m ₃ opy][BF ₄]	1.0945 ^[8]	36.51 ^[8]	166.2 ^a	167.4 ^b

^a data predicted from Eq.(9); ^b data estimated from Eq.(5) **Fig.2** Plots of density (ρ) against n ($n=1-6$) at 298.15 K

$$\alpha=(1/V)(\partial V/\partial T)_p=3Nv/VT \quad (8)$$

All data obtained by this estimation and prediction are listed in Tables 1–3.

The prediction and estimation values of the thermal expansion coefficients in Tables 1–3 are in good agreement with experimental values. It also can be noticed that the values of interstice fractions, $\sum v/V$, differentiate only about 10%–15% for all ILs studied in the present article and these values are in good agreement with the values of volume expansion in the process from solid to liquid state for the majority of materials. Therefore the interstice model is applicable and the interstice model theory can be used to calculate the thermal expansion coefficient of imidazolium-based ILs.

4 Prediction of enthalpy of vaporization

Recently, Verevkin^[25] has published an article titled “Predicting enthalpy of vaporization of ionic liquids: a simple rule for a complex property”, in which he predicted molar enthalpy of vaporization of ILs by a simple rule in case of lack of experimental data. He proposed the following simple rule:

$$\Delta_f^\circ H_m^\ominus(\text{IL})=\sum n_i\Delta H_i+\sum n_j\Delta H_j \quad (9)$$

where ΔH_i is the contribution of the i th element, n_i is the number of the element of the i th type in ILs, ΔH_j is the contribution of the j th structural correction and n_j is the number of the element of the j th structural correction in ILs. The parameters^[25] for predicting the molar enthalpy of vaporization of ILs are listed in Table 5.

Verevkin pointed out that “a special structural correction could

Table 5 Parameters for predicting the enthalpy of vaporization of ILs at 298.15 K^[25]

Parameter	Value	Parameter	Value
$\Delta H_c/(\text{kJ}\cdot\text{mol}^{-1})$	2.5	$\Delta H_p/(\text{kJ}\cdot\text{mol}^{-1})$	4.1
$\Delta H_N/(\text{kJ}\cdot\text{mol}^{-1})$	26.3	$\Delta H_S/(\text{kJ}\cdot\text{mol}^{-1})$	−8.2
$\Delta H_O/(\text{kJ}\cdot\text{mol}^{-1})$	23.6	$\Delta H_{\text{CS}}/(\text{kJ}\cdot\text{mol}^{-1})$	−63.1
$\Delta H_B/(\text{kJ}\cdot\text{mol}^{-1})$	23.0	$\Delta H_{\text{mg}}/(\text{kJ}\cdot\text{mol}^{-1})$	27.1
$\Delta H_r/(\text{kJ}\cdot\text{mol}^{-1})$	13.7

Fig.3 Plots of surface tension (γ) against n ($n=1-6$) at 298.15 K

be also necessary for quaternary ammonium based ILs”^[25]. Herein, the structure of the quaternary ammonium cation is regarded to be the ring of imidazolium cation, therefore, its structural correction parameter is $\Delta H=27.1$ kJ·mol⁻¹. The predicted data are listed in Table 4. From this table, the values of the molar enthalpies of vaporization, $\Delta_f^\circ H_m^\ominus$, predicted by Eq.(9) are in good agreement with the values estimated by Eq.(5) except for [C₄mim][OcSO₄]. This is because that the Eq.(5) is valid mainly for ILs [C_{*n*}mim][NTf₂]. Indeed, the assumption to consider the quaternary ammonium cation as a ring system needs confirmation.

5 Conclusions

The physicochemical properties (molecular volume, molar volume, parachor, interstice volume, interstice fraction, thermal expansion coefficient, standard entropy, lattice energy, and molar enthalpy of vaporization) of [C₂mim][EtSO₄], [C₄mim][OcSO₄], and [C₂mim][NTf₂] were estimated by using their experimental data of density and surface tension. Based on the estimated data of the molecular volume and parachor, the physicochemical properties (density, surface tension and all of the properties mentioned above) for their homologue series [C_{*n*}mim][EtSO₄], [C_{*n*}mim][OcSO₄], and [C_{*n*}mim][NTf₂] ($n=1-6$) were predicted.

We compared the values of molar enthalpies of vaporization for [C₂mim][EtSO₄], [C₄mim][OcSO₄], [C₂mim][NTf₂], [C₄mim][NTf₂], [N₄₁₁₁][NTf₂], [N₈₈₈₁][NTf₂], and [m₃opy][BF₄], estimated by Kabo’s empirical equation with those predicted by Verevkin’s simple rule, and found that the values calculated in terms of the two approaches are in good agreement with each other. Hence, it is suggested that the molar enthalpy of vaporization of ILs could be estimated in terms of Verevkin’s simple rule when the experimental data are not available.

References

- 1 Tsunashima, K.; Sugiya, M. *Electrochem. Commun.*, **2007**, **9**: 2353
- 2 Seki, S.; Kobayashi, Y.; Miyashiro, H.; Ohno, Y.; Usami, A.; Mita, Y.; Watanabe, M.; Terada, N. *Chem. Commun.*, **2006**: 544
- 3 Itoh, H.; Naka, K.; Chujo, Y. *J. Am. Chem. Soc.*, **2004**, **126**: 3026
- 4 Du, Z.; Yu, Y. L.; Wang, J. H. *Chem. Eur. J.*, **2007**, **13**: 2130
- 5 Endres, F.; Abedin, S. Z. E. *Phys. Chem. Chem. Phys.*, **2006**, **8**: 2101
- 6 Wandschneider, A.; Lehmann, J. K.; Heintz, A. *J. Chem. Eng. Data*, **2008**, **53**: 596
- 7 Bandres, I.; Giner, B.; Artigas, H.; Lafuente, C.; Royo, F. M. *J. Chem. Eng. Data*, **2009**, **54**: 236
- 8 Sun, J.; Forsyth, M.; MacFarlane, D. R. *J. Phys. Chem. B*, **1998**, **102**: 8858
- 9 Tokuda, H.; Hayamizu, K.; Ishii, K.; Susan, M. A. B. H.; Watanabe, M. *J. Phys. Chem. B*, **2004**, **108**: 16593
- 10 Tokuda, H.; Ishii, K.; Susan, M. A. B. H.; Tsuzuki, S.; Hayamizu, K.; Watanabe, M. *J. Phys. Chem. B*, **2006**, **110**: 2833
- 11 Bandrés, I.; Giner, B.; Artigas, H.; Royo, F. M.; Lafuente, C. *J. Phys. Chem. B*, **2008**, **112**: 3077
- 12 Tong, J.; Liu, Q. S.; Guan, W.; Yang, J. Z. *J. Phys. Chem. B*, **2007**, **111**: 3197
- 13 Tong, J.; Liu, Q. S.; Zhang, P.; Yang, J. Z. *J. Chem. Eng. Data*, **2007**, **52**: 1497
- 14 Fang, D. W.; Guan, W.; Tong, J.; Wang, Z. W.; Yang, J. Z. *J. Phys. Chem. B*, **2008**, **112**: 7499
- 15 Tong, J.; Liu, Q. S.; Xu, W. G.; Fang, D. W.; Yang, J. Z. *J. Phys. Chem. B*, **2008**, **112**: 4381
- 16 Fernández, A.; Torrecilla, J. S.; García, J.; Rodríguez, F. *J. Chem. Eng. Data*, **2007**, **52**: 1979
- 17 Fernández, A.; García, J.; Torrecilla, J. S.; Oliet, M.; Rodríguez, F. *J. Chem. Eng. Data*, **2008**, **53**: 1518
- 18 Glasser, L. *Thermochim. Acta*, **2004**, **421**: 87
- 19 Troncoso, J.; Cerdeirina, C. A.; Sanmamed, Y. A.; Romani, L.; Rebelo, L. P. N. *J. Chem. Eng. Data*, **2006**, **51**: 1856
- 20 Hasse, B.; Lehmann, J.; Assenbaum, D.; Wasserscheid, P.; Leipertz, A.; Froba, A. P. *J. Chem. Eng. Data*, **2009**, **54**: 2576
- 21 Deetlefs, M.; Seddon, K. R.; Shara, M. *Phys. Chem. Chem. Phys.*, **2006**, **8**: 642
- 22 Zaitsau, D. H.; Kabo, G. J.; Strechan, A. A.; Paulechka, Y. U.; Tschersich, A.; Verevkin, S. P.; Heintz, A. *J. Phys. Chem. A*, **2006**, **110**: 7303
- 23 Yang, J. Z.; Lu, X. M.; Gui, J. S.; Xu, W. G. *Green Chem.*, **2004**, **6**: 541
- 24 Zhang, Q. G.; Yang, J. Z.; Lu, X. M.; Gui, J. S.; Huang, M. *Fluid Phase Equilib.*, **2004**, **226**: 207
- 25 Verevkin, S. P. *Angew. Chem. Int. Edit.*, **2008**, **47**: 5071