Thermochimica Acta 511 (2010) 119–123

Contents lists available at ScienceDirect

Thermochimica Acta

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

Thermodynamic properties of 1-butyl-3-methylimidazolium trifluoromethanesulfonate ionic liquid in the condensed state

Yauheni U. Paulechka*, Sviataslau V. Kohut, Andrey V. Blokhin, Gennady J. Kabo

Chemistry Faculty, Belarusian State University, Leningradskaya 14, 220030 Minsk, Belarus

ARTICLE INFO

Article history:
Received 16 April 2010
Accepted 4 August 2010
Available online 12 August 2010

Keywords:
Ionic liquids
Thermodynamic properties
1-Butyl-3-methylimidazolium trifluoromethanesulfonate
Solid–liquid phase change entropy
Correlation equations

ABSTRACT

Heat capacity for 1-butyl-3-methylimidazolium trifluoromethanesulfonate [C$_4$mim]OTf in the temperature range of (5–370) K has been measured in an adiabatic calorimeter. The temperature $T_{\text{fus}} = (290.98 \pm 0.01)$ K and the enthalpy of fusion $\Delta_{\text{fus}}H^{\circ}_{\text{m}} = (19.43 \pm 0.02)$ kJ mol^{-1} were determined. A solid-phase transition was observed near $T = 120$ K. Thermodynamic functions for the compound in the condensed state were calculated. Trends in the solid–liquid phase change entropies, $\sum\Delta_{\text{tr}}S_{\text{m}}$, for 1-alkyl-3-methylimidazolium salts [C$_n$mim]An were analyzed. The increment to $\sum\Delta_{\text{tr}}S$ was shown to increase with n. It was found that $\sum\Delta_{\text{tr}}S_{\text{m}} = 66.4 \pm 1.3$ J K^{-1} mol^{-1} for all the studied [C$_4$mim]An ionic liquids except [C$_4$mim]NTf$_2$. This difference can be partly explained by formation of two distinguishable conformers of the NTf$_2$ anion in the liquid state.

1. Introduction

The interest to room-temperature ionic liquids (ILs) remains stable, and the number of papers on this subject published annually has been increasing. During the last years, various applications have been proposed for these compounds [1,2]. The parameters of fusion of ILs are among the properties determining their applicability. While general trends in the temperatures of fusion of ILs are known (for example, Chapter 3.1 of [1]), no effective method for quantitative prediction of the temperatures of fusion has been proposed. The enthalpies of fusion of the most studied 1-butyl-3-methylimidazolium ILs, [C$_4$mim]An, are normally within (18–24) kJ mol^{-1} [3–10]. However, no procedure for estimation of the enthalpies or entropies of fusion has been developed even for this group of ILs. The additive predictive procedure has been demonstrated to work better for a sum of entropies of solid-phase transitions and fusion (solid–liquid phase change entropy), $\sum\Delta_{\text{tr}}S_{\text{m}}$, than for the entropy of fusion of a given compound [11]. So, it seems reasonable to analyze solid–liquid phase change entropies for the studied ILs.

This work continues a cycle of papers from our laboratory on investigation of 1-butyl-3-methylimidazolium ILs by adiabatic calorimetry [3–10]. Here we report thermodynamic properties for 1-butyl-3-methylimidazolium trifluoromethanesulfonate, [C$_4$mim]OTf, based on the measurements by adiabatic calorimetry in the temperature range of (5–370) K. Trends in the solid–liquid phase change entropy for 1-alkyl-3-methylimidazolium salts were analyzed and two correlation equations for estimation of this quantity were proposed.

2. Experimental

A commercial sample of [C$_4$mim]OTf (Solvent Innovation, stated purity >0.99) was purified by exposition to a vacuum of 1 mPa for 33 h at T rising from (292 to 373) K. This period was long enough to get mass of the sample constant within the weighing uncertainty of $\pm 5 \times 10^{-5}$ g. The mole fraction purity of [C$_4$mim]OTf was determined by the fractional-melting technique in an adiabatic calorimeter to be 0.996.

Heat capacities of [C$_4$mim]OTf in a range of temperatures of (5–370) K and enthalpy of fusion were measured in a Termis TAU-10 adiabatic calorimeter. The calorimeter and the procedure of measurements were described in [12]. The maximum error in heat-capacity measurements with this calorimeter did not exceed $\pm 4 \times 10^{-3} C_p$ in the main temperature range of (20–370) K, $\pm 1 \times 10^{-2} C_p$ in the range of (10–20) K, and $\pm 2 \times 10^{-2} C_p$ at $T < 10$ K. The [C$_4$mim]OTf mass corrected for buoyancy was 0.9922 g.

3. Results

The experimental heat capacities for [C$_4$mim]OTf in the condensed state in a range of temperatures of (5–370) K are presented

---

* Corresponding author. Tel.: +375 17 2095197; fax: +375 17 2003916.
E-mail address: paulechka@bsu.by (Y.U. Paulechka).

0040-6031/$ – see front matter © 2010 Elsevier B.V. All rights reserved.
doi:10.1016/j.tca.2010.08.002

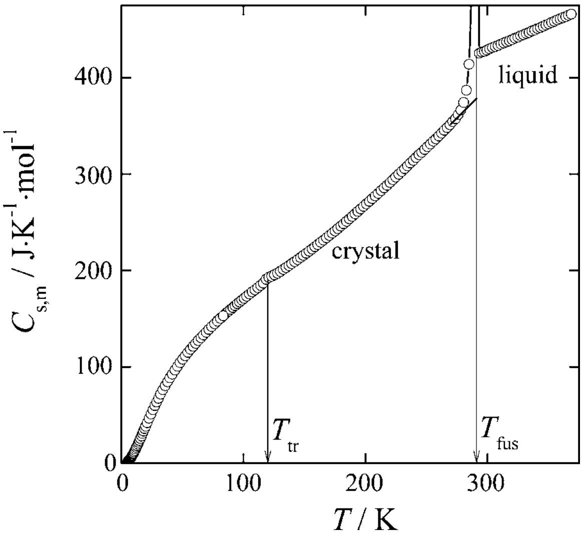

Fig. 1. Experimental heat capacities of [C_4mim]OTf between (5 and 370) K.

in Fig. 1 and Table S.1. We have reported the liquid-phase heat capacity for this compound [3]. In the subsequent calculations both the data from this work and [3] were used.

The heat capacity of liquid [C_4mim]OTf was studied by differential scanning calorimetry in [13–17]. The heat capacities from [14] differ from those reported in this work by $<8 \times 10^{-3} C_p$. The deviation of the results [17] does not exceed $0.03C_p$. The deviation of the values from Refs. [15,16] is $\leq 0.043C_p$. The results [13] have the largest deviation of up to $0.10C_p$.

Table 1
Determination of the molar enthalpy of fusion for [C_4mim]OTf.

Series no.	T_i (K)	T_f (K)	Q (J mol^{-1})	$\Delta_{fus}H_m^\circ$ (J mol^{-1})
1	268.65	293.45	28,613	19,429[a]
2	269.62	292.60	27,894	19,412[a]
3	269.38	294.41	28,774	19,438
4	269.28	293.27	28,334	19,447
Average				19,432± 15

[a] From the fractional-melting experiments.

The triple-point temperature T_{fus} = (290.98 ± 0.01) K was determined from the fractional-melting experiments (Fig. 2 and Table S.2) with the use of van't Hoff equation

$$T = T_{fus} - \frac{RT_{fus}^2(1-x)}{\Delta_{fus}H_m^\circ}\frac{1}{f}, \qquad (1)$$

where T_{fus} is a triple-point temperature; f is an equilibrium fraction of a melt at temperature T; $\Delta_{fus}H_m^\circ$ is the standard molar enthalpy of fusion for a pure compound; x is a mole fraction of the main component in a sample. The enthalpy of fusion for [C_4mim]OTf $\Delta_{fus}H_m^\circ = (19.43 \pm 0.02)$ kJ mol^{-1} was determined (Table 1) using the equation

$$\Delta_{fus}H_m^\circ = Q - \int_{T_i}^{T_{fus}} C_{p,m}(\text{crystal})\,dT - \int_{T_{fus}}^{T_f} C_{p,m}(\text{liquid})\,dT, \qquad (2)$$

where Q is the energy required to heat 1 mol of substance from T_i to T_f. Initial T_i and final T_f temperatures lay outside the melting range. Heat capacities of the crystal and the liquid were described by the following equations obtained from the experimental heat capacities in the temperature ranges of (220–269) K and (292–367) K, respectively:

$$C_{p,m}(\text{crystal})(\text{J K}^{-1}\,\text{mol}^{-1}) = 63.55 + 0.8806T(\text{K}) + 6.936 \times 10^{-4}T(\text{K})^2 \qquad (3)$$

$$C_{p,m}(\text{liquid})(\text{J K}^{-1}\,\text{mol}^{-1}) = 295.6 + 0.3643T(\text{K}) + 2.636 \times 10^{-4}T(\text{K})^2 \qquad (4)$$

The heat-capacity anomaly was observed in the temperature range of (114–130) K (Fig. 3). This anomaly was reproducible in series 1 and 3. The heat-capacity peak was very smooth due to a large intramolecular vibrational contribution $C_{vib,m}$. To make the peak strongly pronounced the vibrational contribution was substracted from the experimental heat capacities (Fig. 4). The obtained residual values were designated $C_{res,m}$. Frequencies of normal vibrations for the ions were calculated for their most stable conformers (Fig. 5) at the B3LYP/6-31+G(2df,p) theory level using Firefly software [18] and are reported in Supplementary Material. The frequencies were scaled with the frequency-dependent factors

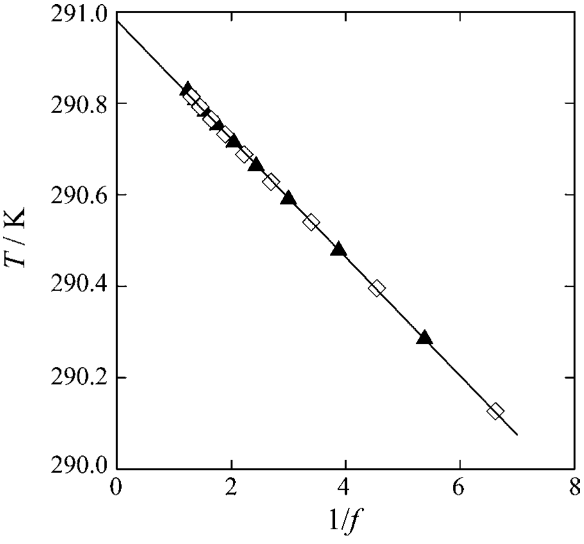

Fig. 2. Results of the fractional-melting experiments for [C_4mim]OTf: ▲, series 1; □, series 2.

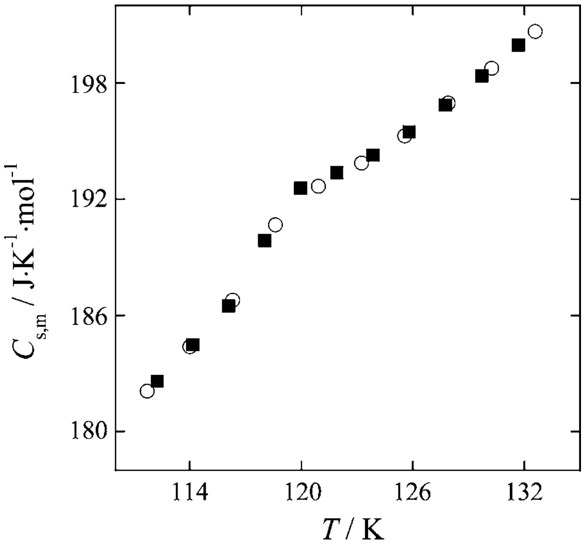

Fig. 3. Heat capacity of crystalline [C_4mim]OTf] in the solid-phase transition region: ○, series 1; ■, series 3.

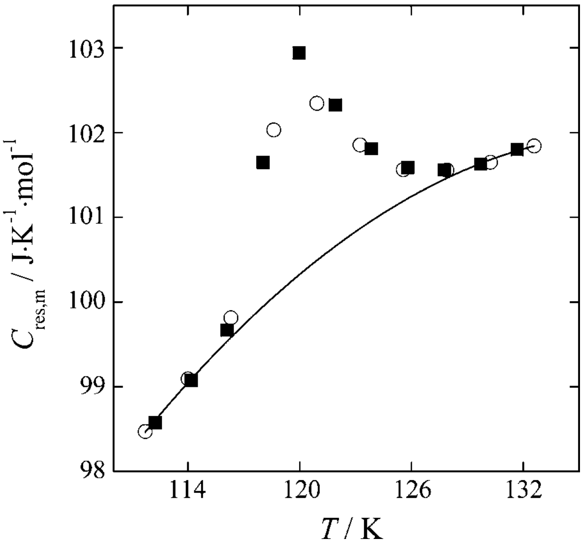

Fig. 4. Residual heat capacity of [C$_4$mim]OTf in the temperature range of (111–133) K: ○, series 1; ■, series 3; a solid line is a baseline for the solid-phase transition.

obtained in [19] for the [C$_4$mim]$^+$ and NTf_{2-} ions. The temperature $T_{\mathrm{tr}} = (120 \pm 1)$ K corresponding to a maximum in the $C_{\mathrm{res,m}}(T)$ curve was assumed to be the temperature of the phase transition. The enthalpy and the entropy of the phase transition $\Delta_{\mathrm{tr}}H_{\mathrm{m}} = 13 \pm 1\,\mathrm{J\,mol^{-1}}$, $\Delta_{\mathrm{tr}}S_{\mathrm{m}} = 0.11 \pm 0.01\,\mathrm{J\,K^{-1}\,mol^{-1}}$ were estimated by numerical integration of excess $C_{\mathrm{s,m}}$ and $C_{\mathrm{s,m}}/T$ in the temperature range of (114–130) K (Fig. 4).

For calculation of entropy and enthalpy for the phases the experimental heat capacities are to be extrapolated below $T = 5$ K. The extrapolation was performed with the use of the empirical equation:

$$C_{\mathrm{s,m}} \approx C_{\mathrm{v,m}} = D_3(\theta_{\mathrm{D}}) + 3E(\theta_{\mathrm{E}}), \qquad (5)$$

where D is a Debye heat-capacity function for three degrees of freedom, E is an Einstein heat-capacity function for one degree of freedom, θ_{D} and θ_{E} are corresponding characteristic temperatures. The parameters were obtained by the least-squares fitting of the experimental $C_{\mathrm{s,m}}$ values in the temperature range of (5.20–9.66) K: $\theta_{\mathrm{D}} = 54.7$ K and $\theta_{\mathrm{E}} = 59.2$ K. The deviation of the experimental values from those obtained from Eq. (5) was $<0.01C_p$ and did not exceed the experimental uncertainty in this interval. The smoothed values of the heat capacity and the derived thermodynamic functions are presented in Table 2. The standard thermodynamic functions of liquid [C$_4$mim]OTf at $T = 298.15$ K are equal to:

$$C^{\circ}_{p,\mathrm{m}} = (427.7 \pm 1.7)\,\mathrm{J\,K^{-1}\,mol^{-1}},$$

$$S^{\circ}_{\mathrm{m}} = (523.9 \pm 2.3)\,\mathrm{J\,K^{-1}\,mol^{-1}},$$

$$\Delta_0^T H^{\circ}_{\mathrm{m}}/T = (279.0 \pm 1.2)\,\mathrm{J\,K^{-1}\,mol^{-1}},$$

$$\Phi^{\circ}_{\mathrm{m}} = (244.9 \pm 2.6)\,\mathrm{J\,K^{-1}\,mol^{-1}}$$

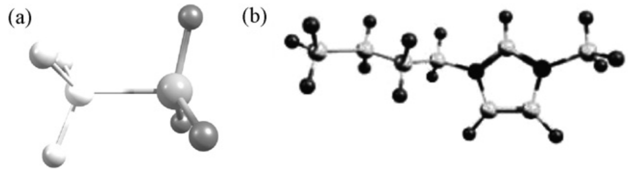

Fig. 5. Most stable conformers of the (a) OTf$^-$ and (b) [C$_4$mim]$^+$ ions.

Table 2
Molar thermodynamic functions of [C$_4$mim]OTf in the condensed state.

T (K)	$C^{\circ}_{p,\mathrm{m}}$ (J K^{-1} mol^{-1})	$\Delta_0^T H^{\circ}_{\mathrm{m}}/T$ (J K^{-1} mol^{-1})	S°_{m} (J K^{-1} mol^{-1})	$\Phi^{\circ}_{\mathrm{m}}$ [a] (J K^{-1}mol^{-1})
Crystal				
0	0	0	0	0
5	1.486	0.3706	0.4944	0.1239
10	10.20	2.798	3.77	0.9728
15	23.78	7.456	10.39	2.930
20	38.56	13.39	19.26	5.868
25	52.98	19.88	29.42	9.546
30	66.38	26.53	40.29	13.76
35	78.37	33.10	51.44	18.34
40	88.95	39.43	62.61	23.18
45	98.67	45.48	73.65	28.17
50	107.5	51.25	84.51	33.27
55	115.5	56.73	95.14	38.41
60	123.0	61.94	105.5	43.57
65	130.0	66.91	115.6	48.73
70	136.6	71.65	125.5	53.86
80	148.9	80.55	144.6	64.02
90	160.0	88.77	162.8	73.99
100	170.5	96.42	180.2	83.74
110	180.5	103.6	196.9	93.27
120	192.4	110.5	213.0	102.6
130	198.6	117.0	228.7	111.7
140	206.9	123.1	243.7	120.6
150	216.1	129.0	258.3	129.3
160	225.6	134.7	272.5	137.8
170	235.5	140.4	286.5	146.1
180	245.9	145.9	300.3	154.3
190	256.7	151.5	313.8	162.3
200	267.8	157.0	327.3	170.3
210	279.3	162.6	340.6	178.1
220	290.9	168.1	353.9	185.7
230	302.8	173.7	367.1	193.3
240	314.9	179.4	380.2	200.9
250	327.1	185.0	393.3	208.3
260	339.4	190.7	406.4	215.7
270	(351.9)[b]	196.5	419.4	223.0
280	(364.5)[b]	202.2	432.5	230.2
290	(377.3)[b]	208.1	445.5	237.4
290.98	(378.5)[b]	208.6	446.8	238.1
Liquid				
290.98	423.9	275.4	513.6	238.1
298.15	427.7	279.0	523.9	244.9
300	428.6	280.0	526.6	246.6
310	433.9	284.8	540.7	255.9
320	439.2	289.6	554.6	265.0
330	444.6	294.2	568.2	274.0
340	450.0	298.7	581.5	282.8
350	455.4	303.1	594.7	291.6
360	460.9	307.4	607.6	300.2
370	(466.4)[b]	311.6	620.3	308.6

[a] $\Phi^{\circ}_{\mathrm{m}} = -(G^{\circ}_{\mathrm{m}}(T) - H^{\circ}_{\mathrm{m}}(0))/T = (\Delta_0^T S^{\circ}_{\mathrm{m}} - \Delta_0^T H^{\circ}_{\mathrm{m}})/T$.
[b] Extrapolated values.

4. Discussion

The heat-capacity data from liquid helium temperatures and the parameters of solid-phase transitions and fusion determined by adiabatic calorimetry are available for 1-alkyl-3-methylimidazolium ILs presented in Table 3. The entropies of fusion, $\Delta_{\mathrm{fus}}S_{\mathrm{m}}$, of [C$_n$mim]Br increase with the increase in a number of atoms in the alkyl chain. The different increments when going from [C$_2$mim]Br to [C$_3$mim]Br and from [C$_3$mim]Br to [C$_4$mim]Br may be attributed to the odd–even effect. At the same time, the entropies of fusion of [C$_n$mim]NTf$_2$ change irregularly and it seems impossible to find out the correlation between $\Delta_{\mathrm{fus}}S_{\mathrm{m}}$ and the number of carbon atoms in the alkyl chain. No correlation with the anion properties was also found.

The solid–liquid phase change entropy, $\sum\Delta_{\mathrm{tr}}S_{\mathrm{m}}$, for ILs (Table 3 and Fig. 6) increase with the increase of the alkyl

Table 3
Parameters of phase transitions for 1-alkyl-3-methylimidazolium compounds.

Substance	Crystal phase	T_{fus} (K)	$\Delta_{fus}S_m$ (J K^{-1} mol^{-1})	$\sum\Delta_{tr}S_m$ (J K^{-1} mol^{-1})	Reference
[C_2mim]Br	cr	349.81	52.6 ± 0.3	52.9 ± 0.4	[4]
[C_3mim]Br	crII	309.58	62.7 ± 0.3	62.7 ± 0.3	[3]
[C_4mim]Br	cr	351.35	65.1 ± 0.1	65.1 ± 0.1	[4]
[C_4mim]CF_3COO	cr	296.42	66.6 ± 0.3	66.6 ± 0.3	[5]
[C_4mim]$N(CN)_2$	cr	270.83	65.7 ± 0.4	65.7 ± 0.4	[3]
[C_4mim]NO_3	cr	309.16	58.2 ± 0.3	67.4 ± 0.3	[6]
[C_4mim]OTf	cr	290.98	66.8 ± 0.1	66.9 ± 0.1	This work
[C_4mim]PF_6	crI	283.51	69.1 ± 0.1	69.1 ± 0.1	[7]
[C_4mim]Tos[a]	crI	343.9	62.7 ± 0.2	64.0 ± 0.2	[8]
[C_2mim]NTf_2	crIV	256.91	84.7 ± 0.5	84.7 ± 0.5	[9]
	crIII	263.0	85.7 ± 0.8	85.7 ± 0.8	
	crI	271.44	80.6 ± 0.1	80.6 ± 0.1	
	crI	271.4	78.5	78.5	[20]
[C_4mim]NTf_2	cr	270.22	88.0 ± 0.1	90.5 ± 0.2[b]	[10]
	cr	270.4	88.0	90.5	[21]
[C_6mim]NTf_2	crI	272.03	103.3 ± 0.3	103.3 ± 0.3	[12]
	crI	272.1	104.1	104.1	[22]
[C_8mim]NTf_2	crIII	251.42		113.3 ± 0.5	[9]
	crII	255.9		124.1 ± 0.4	
	crI	263.96	95.4 ± 0.5	115.2 ± 0.8	
[C_{18}mim]NTf_2	cr	327.1	222	241	[20]

[a] 1-Butyl-3-methylimidazolium tosylate.
[b] Taking into account $S_0 = 2.5$ J K^{-1} mol^{-1}.

chain length. The butyl moieties in a half of cations in the crystalline [C_4mim]NTf_2 are disordered: 70% of them are in the g′t conformation and 30% are in the gt conformation [23]. So, the crystalline [C_4mim]NTf_2 has a residual entropy of $S_{0,m} = -0.5R(0.3\ln 0.3 + 0.7\ln 0.7) = 2.5$ J K^{-1} mol^{-1}. Since $\sum\Delta_{tr}S_m$ characterize a total entropy change when going from ordered crystal to liquid, $S_{0,m}$ was added to $\sum\Delta_{tr}S_m$ for this compound.

The $\sum\Delta_{tr}S_m$ values for [$C_n$mim]NTf_2 is a non-linear function of n. The observed dependence was fitted by the quadratic function

$$\sum\Delta_{tr}S_m/\mathrm{J\,K^{-1}\,mol^{-1}} = 83.8 + 0.4897n^2 \qquad (6)$$

The increment per CH_2 group calculated as $d(\sum\Delta_{tr}S_m)/dn = 0.979n$ J K^{-1} mol^{-1} becomes comparable with that of n-alkanes (11 J K^{-1} mol^{-1} as determined from the recommended data [24]) only at $n > 10$ and it is much lower for short-chained ILs.

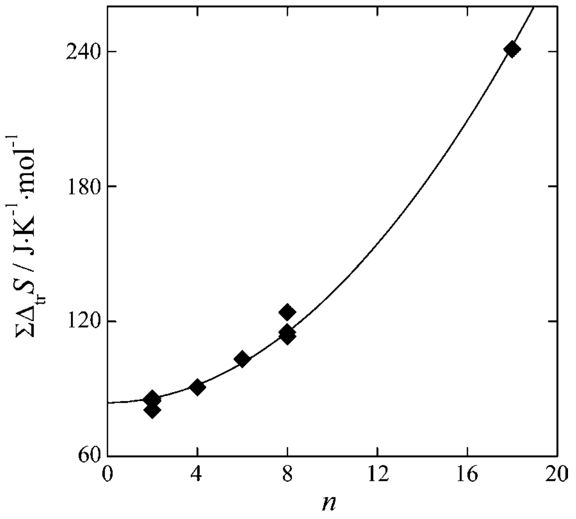

Fig. 6. $\sum\Delta_{tr}S_m$ values for [$C_n$mim]NTf_2, a line is a function described by Eq. (6).

The values of $\sum\Delta_{tr}S_m$ for all 1-butyl-3-methylimidazolium ILs except [C_4mim]NTf_2 are very close, and the average value is

$$\sum\Delta_{tr}S_m = 66.4 \pm 1.3\,\mathrm{J\,K^{-1}\,mol^{-1}} \qquad (7)$$

The maximum deviation from this value of 2.7 J K^{-1} mol^{-1} is observed for [C_4mim]PF_6. Eqs. (6) and (7) can be jointly used for estimation of $\sum\Delta_{tr}S_m$, which is equal to $\Delta_{fus}S_m$ for many compounds, for 1-alkyl-3-methylimidazolium ILs with the anions presented in Table 3 except NTf_{2-}.

Unlike all the anions mentioned in Table 3, the NTf_{2-} anion forms distinguishable conformers, cis and trans (Fig. 7). This might be a possible cause of such a large difference in $\sum\Delta_{tr}S_m$ between [$C_n$mim]NTf_2 and the other considered ILs. Only cis conformer was observed in the crystal of [C_4mim]NTf_2 [23]. Above T_{fus}, the equilibrium mixture of trans- and cis-conformers is formed, and each conformer is a mixture of equal amounts of chiral counterparts. The mole fractions of the conformers, $x_{cis} = 0.33$ and $x_{trans} = 0.67$, were calculated assuming that the equilibrium mixture of the conformers is formed at $T_{fus} = 270.22$ K. The value of ΔH(trans–cis) = 4.0 kJ mol^{-1} obtained by averaging of the experimental values [25,26] was accepted in the calculations ΔS^0_m(trans–cis) = 9 J K^{-1} mol^{-1} was found from the entropy values of the conformers in the ideal-gas state [19]. The corresponding entropy of mixing is

$$\Delta_{mix}S = -R\left(0.33\ \ln\left(\frac{0.33}{2}\right) + 0.67\ \ln\left(\frac{0.67}{2}\right)\right)$$
$$= 11.0\,\mathrm{J\,K^{-1}\,mol^{-1}} \qquad (8)$$

Since the molar entropies of the conformers are not equal, an additional contribution of $0.33 \times 9 + 0.67 \times 0 - 9 = -6$ J K^{-1} mol^{-1}

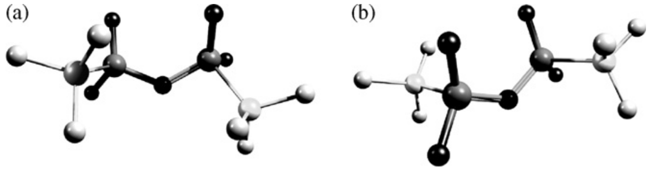

Fig. 7. Conformers of the NTf_2 anion: (a) cis and (b) trans.

appears. Therefore, the resulting entropy change due to formation of distinguishable conformers is $5\,\mathrm{J\,K^{-1}\,mol^{-1}}$. It means that the conformational contribution is not the only contribution explaining the high $\sum\Delta_{\mathrm{tr}}S_{\mathrm{m}}$ value for [C_4mim]NTf_2.

5. Conclusion

In this work heat capacities in the temperature range of (5–370) K and parameters of a solid-phase transition and fusion were determined for the 1-butyl-3-methylimidazolium trifluoromethanesulfonate. Its thermodynamic properties in the crystal and liquid states were calculated from those data. The trends in the solid–liquid phase change entropy for 1-alkyl-3-methylimidazolium salts [$C_n$mim]An were analyzed. Two correlations for estimation of this quantity were proposed.

Appendix A. Supplementary data

Supplementary data associated with this article can be found, in the online version, at doi:10.1016/j.tca.2010.08.002.

References

[1] P. Wasserscheid, T. Welton (Eds.), Ionic Liquids in Synthesis, second ed., Wiley-VCH, Weinheim, Germany, 2008.
[2] N.V. Plechkova, K.R. Seddon, Chem. Soc. Rev. 37 (2008) 123–150.
[3] Y.U. Paulechka, A.G. Kabo, A.V. Blokhin, G.J. Kabo, M.P. Shevelyova, J. Chem. Eng. Data 55 (2010) 2719–2724.
[4] Y.U. Paulechka, G.J. Kabo, A.V. Blokhin, A.S. Shaplov, E.I. Lozinskaya, Y.S. Vygodskii, J. Chem. Thermodyn. 39 (2006) 158–166.
[5] A.A. Strechan, Y.U. Paulechka, A.V. Blokhin, G.J. Kabo, J. Chem. Thermodyn. 34 (2008) 632–639.
[6] A.A. Strechan, A.G. Kabo, Y.U. Paulechka, A.V. Blokhin, G.J. Kabo, A.S. Shaplov, E.I. Lozinskaya, Thermochim. Acta 474 (2008) 25–31.
[7] G.J. Kabo, A.V. Blokhin, Y.U. Paulechka, A.G. Kabo, M.P. Shymanovich, J.W. Magee, J. Chem. Eng. Data 49 (2004) 453–461.
[8] A.A. Strechan, Y.U. Paulechka, A.G. Kabo, A.V. Blokhin, G.J. Kabo, J. Chem. Eng. Data 52 (2007) 1791–1799.
[9] Y.U. Paulechka, A.V. Blokhin, G.J. Kabo, A.A. Strechan, J. Chem. Thermodyn. 39 (2007) 866–877.
[10] A.V. Blokhin, Y.U. Paulechka, A.A. Strechan, G.J. Kabo, J. Phys. Chem. B 112 (2008) 4357–4364.
[11] J.S. Chickos, W.E. Acree Jr., J.F. Liebman, J. Phys. Chem. Ref. Data 28 (1999) 1535–1673.
[12] A.V. Blokhin, G.J. Kabo, Y.U. Paulechka, J. Chem. Eng. Data 51 (2006) 1377–1388.
[13] R. Ge, C. Hardacre, J. Jacquemin, P. Nancarrow, D.W. Rooney, J. Chem. Eng. Data 53 (2008) 2148–2153.
[14] G. García-Miaja, J. Troncoso, L. Romaní, J. Chem. Thermodyn. 41 (2009) 161–166.
[15] Y.-H. Yu, A.N. Soriano, M.-H. Li, Thermochim. Acta 482 (2009) 42–48.
[16] C.P. Fredlake, J.M. Crosthwaite, D.G. Hert, S.N.V.K. Aki, J.F. Brennecke, J. Chem. Eng. Data 49 (2004) 954–964.
[17] A. Diedrichs, J. Gmehling, Fluid Phase Equilib. 244 (2006) 68–77.
[18] A.A. Granovsky, Firefly version 7.1.G, http://classic.chem.msu.su/gran/firefly/index.html.
[19] Y.U. Paulechka, G.J. Kabo, V.N. Emel'yanenko, J. Phys. Chem. B 112 (2008) 15708–15717.
[20] Y. Shimizu, Y. Ohte, Y. Yamamura, K. Saito, Chem. Phys. Lett. 470 (2009) 295–299.
[21] Y. Shimizu, Y. Ohte, Y. Yamamura, K. Saito, Chem. Lett. 36 (2007) 1484–1485.
[22] Y. Shimizu, Y. Ohte, Y. Yamamura, K. Saito, T. Atake, J. Phys. Chem. B 110 (2006) 13970–13975.
[23] Y.U. Paulechka, G.J. Kabo, A.V. Blokhin, A.S. Shaplov, E.I. Lozinskaya, D.G. Golovanov, K.A. Lyssenko, A.A. Korlyukov, Ya.S. Vygodskii, J. Phys. Chem. B 113 (2009) 9538–9546.
[24] M. Frenkel, R.D. Chirico, V. Diky, C.D. Muzny, E.W. Lemmon, A. Kazakov, NIST ThermoData Engine, NIST Standard Reference Database 103b – Pure compounds, Version 4.0, NIST, Boulder, CO, 2009, http://www.nist.gov/srd/nist103b.htm.
[25] J.C. Lassegues, J. Grondin, R. Holomb, P. Johansson, J. Raman Spectrosc. 38 (2007) 551–558.
[26] K. Fujii, T. Fujimori, T. Takamuku, R. Kanzaki, Y. Umebayashi, S. Ishiguro, J. Phys. Chem. B 110 (2006) 8179–8183.