On the Prediction of Critical Temperatures of Ionic Liquids: Model Development and Evaluation

Mehdi Sattari,^{*,a} Arash Kamari,^a Amir H. Mohammadi,^{*,a,b} Deresh Ramjugernath,^{*,a}

^aThermodynamics Research Unit, School of Engineering, University of KwaZulu-Natal, Howard College Campus, King George V Avenue, Durban 4041, South Africa

^bInstitut de Recherche en Génie Chimique et Pétrolier (IRGCP), Paris Cedex, France

Abstract – In this study, the Guggenheim equation was used to estimate the critical temperature (T_c) of 106 ionic liquids using experimental surface tension data as inputs. A group contribution (GC) and a Quantitative Structure–Property Relationship (QSPR) model were also developed to correlate/predict the T_c of ionic liquids. It was shown that a lack of sufficiently large database for T_c lead to the development of models with low prediction capability. The model's output as well as the T_c values estimated from the surface tension data were compared with the critical temperatures calculated by the Valderrama *et al.* method. The results showed that the Valderrama *et al.* method produces different data values compared with the values calculated by the Guggenheim equation. Neither the GC, QSPR, nor Valderrama's method is capable of reliable prediction of the T_c of ionic liquids. Consequently, the calculated T_c values are not reliable enough to be used in the development of corresponding state models for prediction of other thermophysical properties of ionic liquids. Any usage of critical properties of ionic liquids should be done with a serious caution.

Keywords: Critical Temperature, T_c , Ionic Liquid, Group Contribution, GC, QSPR, Model.

*Corresponding authors: Email: sattarim@ukzn.ac.za, a.h.m@irgcp.fr, and ramjuger@ukzn.ac.za

1. Introduction

Over the last few decades, researchers from around the world have undertaken numerous studies on ionic liquids (ILs) and demonstrated their potential use in various industrial applications. Ionic liquids are defined as molten salts which are generally liquid at or near room temperature (typically below 100 °C) due to the poor coordination of ions [1]. In general, they show unusual, but interesting properties such as extremely low saturation vapor pressure and negligible volatility, wide liquidus range, nonflammability, high thermal conductivity, and high physical and chemical stability [2]. These unique properties make them potential replacement solvents for conventional volatile and commonly toxic and flammable organic solvents in numerous industrial applications such as extraction and separation processes [3-5], battery industry [6, 7], solar panels [8, 9], waste recycling [10, 11], lubricants [12-15], fuel cells [16, 17], polymer and biopolymer processing [18-20], electroplating [21, 22], gas separation and CO₂ capturing [23-30], catalysis [31-33], and other processes [34-37].

In order to understand the behaviour of ILs in such applications, thermodynamic models and property estimation methods are required. The critical properties, especially the critical temperature (T_c), are used commonly in the development of the corresponding state models. The critical temperature of a substance is the temperature at and above which vapor of the substance cannot be liquefied, no matter how much pressure is applied. The behavior of a fluid near its critical point is a specific property necessary to develop the thermodynamic models for fluids [38]. Due to presence of high electrostatic interactions and Coulombic forces, as well as short-range van der Waals interactions in ionic liquids, the critical properties of ionic liquids, cannot be measured as they are decomposed before their normal boiling temperature (T_b) are reached [39, 40]. As a result, experimental data of critical properties of ILs as well as their T_b are not available in the literature and they can only be estimated in theory.

Despite this limitation for the ionic liquids, some researchers have tried to use the available correlations and estimation methods of common organic compounds to estimate the critical properties of ILs. The most accepted approach is to use the relationship between critical temperature, density, and surface tension and thereafter, estimate the T_c of ionic liquids. According to the fact that the surface tension becomes zero at the critical temperature, two correlations were presented by Eötvös [41] and Guggenheim [42] which are shown in equation (1) and equation (2), respectively.

$$\gamma \left(\frac{M}{\rho} \right)^{2/3} = k(T_c - T) \quad (1)$$

$$\gamma = K(T_c - T)^{11/9} \quad (2)$$

where γ is surface tension, ρ is density, M is molar mass, k and K are two different constants. These equations usually can estimate the T_c of organic compounds pretty well; so it is assumed that they are applicable for ionic liquids too. This approach has been followed by the majority of researchers [38, 40, 43-47] to calculate and report the critical temperature of ionic liquids.

Another approach was followed by Valderrama *et al.* [39] where they used the Lydersen group contribution method to estimate the critical pressure and critical volume, and the Joback and Reid group contribution method to calculate the normal boiling temperature and the critical temperature of ionic liquids. They combined the best results of Lydersen's method with the best results of the Joback-Reid method to propose a "modified Lydersen-Joback-Reid" method and stated that this modified method had good results for molecules of high molecular weight. Thereafter, Valderrama *at al.* performed a consistency test and used a correlation for density to validate the estimated critical properties of ionic liquids. This correlation was developed earlier by Valderrama and Abu-Sharkh [48] to relate the critical

properties of saturated liquids and petroleum fractions to their density. Consequently, they published the results of their calculations for 1130 ionic liquids [49].

Despite their interesting approach, there is unsatisfactory agreement between the values of T_c estimated by their method and the approach using Guggenheim equations for most of the ionic liquids. Nonetheless, these calculated critical properties were used by several researchers to develop corresponding state models for prediction of thermophysical properties of ionic liquids [50-57].

In this study, the available experimental data of surface tension of ionic liquids were used to estimate the critical temperature. Thereafter, a group contribution (GC) and a Quantitative Structure–Property Relationship (QSPR) models were developed to correlate/predict the T_c of ionic liquids. The results were compared with the values calculated by Valderrama *et al.*

2. Model Development Methodology

2.1 Data preparation

The NIST Standard Reference Database #103b [58] and some newly published papers [59-63] were used to extract experimental data for surface tension of ionic liquids. In the next step, the data gathered were analyzed and screened to remove duplicates and outliers. As the surface tension is temperature dependent, data analysis was undertaken as follows:

- 1) Where there were several reported values of the desired property for a single temperature, the values were plotted against temperature to find and remove the sources that their results had no agreement with others.

- 2) If there were only two sources, the values with the lowest uncertainty were incorporated into dataset utilized.
- 3) If the reported values had equal uncertainties, the latest published values were utilized.
- 4) To verify the potential outliers in the final dataset, the target values were plotted against temperature and a (non-)linear curve fitting algorithm was applied to fit the data. The data points which were “far” from the curve fitted were considered as outliers and omitted from the dataset.

The result of the screening process was 1513 data points for 139 ionic liquids constituted from 63 types of cations and 40 types of anions. Figure 1 shows the number of ionic liquids in each family. In addition, the names and structures of cations and anions are available in Table S1 and Table S2 in the supplementary materials.

Figure 1

2.2 T_c Calculation

As mentioned before, the most realistic value of critical temperature should be calculated from the Eötvös and/or Guggenheim equations. Previous studies [38, 40] showed that the T_c calculated by these equations are in fair agreement with each other (less than 100 °C in most cases); however the Eötvös equation is more prone to deviations due to use of two sources of experimental data as inputs (surface tension and density). In addition, it is difficult to find experimental data for surface tension and density measured by the same laboratories at the same conditions. As a result, the Guggenheim equation was chosen for the estimation of critical temperature of ionic liquids. Unfortunately, for 33 ILs there was only one data point available and thus the T_c could not be calculated for them. Consequently, the critical temperature was calculated for 106 ionic liquids.

2.3 Model Development

The GC and QSPR approaches were followed in the development of the models. The common approach in GC modeling is to use the linear summation of functional groups to develop a model. This approach is beneficial because of its simplicity, but its disadvantage is the weakness in the prediction of properties for compounds which exhibit complex behavior, have isomers, etc. [64-70]. The Quantitative Structure-Property Relationship is a well-established and highly respected technique to correlate diverse simple and complex physicochemical properties of a component by its molecular structure and interactions among different molecular groups based on their connectivities [71-73]. In this approach, it is assumed that the molecular features which are called “molecular descriptors” affect directly the properties of compounds. As a result, there are some descriptors which can deal with isomers and proximity effects (inter/intra-molecular interactions). This feature is the most important advantage of the QSPR method over the GC method. In addition, QSPR models usually have less parameters than GC models for a similar accuracy, which indicates that the descriptors can correlate the target property better than simple functional groups [68-70, 72, 74].

To calculate the functional groups as well as the descriptors, the SMILES formula of cations and anions were used separately and the functional groups and 2D descriptors were calculated using Dragon software [75]. After calculating the structure-based variables for the cations and anions, they were collected into one dataset; two prefixes were added to the name of GCs/descriptors to make the cations and anions variables distinguishable. For the QSPR model development, pair correlation was undertaken for all descriptors. Accordingly, pairs of descriptors with a correlation coefficient greater than 0.9 were removed and the remainders used in the model development [73].

As the final step of model development, the experimental data was divided in two subsets. One was used to develop and train the model which is named the training set, the other for determining the prediction capability of the model for new compounds which were not used in model development (training set). For

this purpose, K-means clustering is used to select the training and test sets. K-means clustering is a method of cluster analysis which aims to partition n observations into k clusters in which each observation belongs to the cluster with the nearest mean. As a result, 20% of the ILs were kept for the test set and remainder used as the training set to develop the model.

3. Results and discussion

To assess the possibility of developing a predictive model for estimating the T_c of ionic liquids, a 30-parameter GC and a 25-parameter QSPR models were developed. The GC model has an Average Absolute Relative Deviation (AARD) of 5.17% for the 106 data points, and the QSPR model has an AARD% of 4.69% (Table 1). As a result, the models can calculate the training set and predict the test set fairly well. The models parameters as well as their outputs are available in the supplementary materials.

To compare the model output for other ionic liquids, the T_c for 33 additional ionic liquids were calculated. As mentioned before, these ionic liquids had only one experimental surface tension data point; so it was not possible to fit the Guggenheim equation and find these critical temperature. Table 2 shows the outputs of the GC and QSPR models for these ionic liquids. Unfortunately, Valderrama *et al.* did not report the coefficients for the functional groups in their published paper [49] and it was therefore not possible to calculate the T_c for these ionic liquids. The T_c of only some of them were reported by Valderrama *et al.*

As seen in Table 2, for some of the ionic liquids there is an agreement between the GC, QSPR, and Valderrama *et al.* methods, e.g. 1-hexyl-3-methylimidazolium nitrate. On the other hand, the T_c of some ionic liquids calculated by the GC and QSPR models are similar, but different from that obtained by Valderrama's method, e.g. 1-ethyl-3-methylimidazolium acetate; and some are altogether different for all methods, e.g. 1-ethyl-3-methylimidazolium bis[(pentafluoroethyl)sulfonyl]amide. The worst agreement amongst methods are for ionic liquids with bis[1-methylimidazolium] cations. The outputs of the GC and

QSPR models are different values and the trends are also not similar. In addition, the GC model produces negative values of T_c which are obviously meaningless and erroneous. In these cases, the QSPR model has better output compared with the GC model, but the trends are still not acceptable.

For ionic liquids with 3,3'-(1,10-decanediyl)bis[1-methylimidazolium] as the cation and bis(trifluoromethylsulfonyl)imide (AKA 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide) and tetrafluoroborate, and as the anion, the values of T_c are 915.6 K, 964.9 K respectively; but for the 1,1,2,2,2-pentafluoro-N-[(1,1,2,2,2-pentafluoroethyl)sulfonyl] ethanesulfonamide (AKA bis(pentafluoroethylsulfonyl)imide) anion, the T_c is calculated as 1961.2 K by the QSPR model. According to Table S2 in supplementary materials, the later has four additional fluorine atom compared with bis(trifluoromethylsulfonyl)imide anion; but the molecular structures are similar. In addition, the surface tension of these two ionic liquids does not have a noticeable different at the same temperature (less than 8%); so this small difference in their surface tension cannot lead to 1000 K jump in the critical temperature estimation. For this ionic liquid, the GC model produces a negative value (-825.86 K), as mentioned before. As a result, it is concluded that both model fails to estimate the T_c of this ionic liquid due to lack of experimental surface tension data and consequently, its absence in training set. Similar effect is observed for other ionic liquids with abovementioned anion as there is not any surface tension data for them; however the temperature jump is less than 500 K.

As the number of data points used in the model development procedure is not large enough, it is not possible to develop a model with a wide range of applicability and high prediction ability. Large deviations are expected and inevitable and currently it is not possible to develop a quality model with the available experimental datasets for surface tension.

To check the validity of the Valderrama's method, the values of T_c calculated by the Guggenheim equation and the outputs of the GC model as well as QSPR were compared with the Valderrama *et al.*

values in the supplementary materials. According to the data provided, the comparison can be done for only 51 ionic liquids because the coefficients for functional groups are not available for Valderrama's model [49]. Regarding to Figure 2, it is clear that most of the T_c values calculated by Valderrama's method do not agree with the values calculated using the surface tension data.

Figure 2

The results provided in the supplementary materials can be visualized for specific cations and different anions. For example, Figure 3 shows the critical temperatures calculated by the Guggenheim equation, GC, QSPR, and Valderrama's methods for 1-ethyl-3-methylimidazolium ionic liquids. Accordingly, Valderrama's T_c values do not have agreement with other models. In addition to the deviations in the values of T_c , the model also fails to estimate the T_c in a reasonable trend according to the output of Guggenheim equation.

In another comparison, the T_c values of 1-butyl-3-methylimidazolium ionic liquids are compared and the results are shown in Figure 4. Accordingly, similar fluctuations are observed in Valderrama's model which indicates the disagreement with the Guggenheim model.

Figure 3

Figure 4

As discussed earlier, the QSPR model developed is more reliable than the GC model as the later calculates negative T_c values for some ionic liquids. Thus, the QSPR model is chosen to calculate the T_c for 1130 ionic liquids which were used by Valderrama *et al.* [49]. According to the data provided in the supplementary materials, there are some ionic liquids for which the QSPR model produces negative or very high values of T_c . As discussed before, it is not possible to develop a comprehensive model using

such a small number of data points. In this study, the QSPR model has been developed using 41 cations and 34 anions, while Valderrama's database consists of 484 cations and 113 anions. It is thus expected that the QSPR model developed would not be reliable for calculation of values for some ionic liquids as their cation and/or anion have not been used in the "training" subset.

To have a better comparison, the calculated T_c of 1-ethyl-3-methylimidazolium ionic liquids with 45 different anions is shown in Figure 5. According to Figure 3, the average critical temperature of 1-ethyl-3-methylimidazolium ionic liquids is approximately 1200 K, which is shown by a red tie line in Figure 5. Accordingly, the QSPR model provides similar results and only four deviations are observed; two for around 700 K and two for over 1800 K. Valderrama's model has more fluctuations between 600 K and 1000 K. Despite the better results for the QSPR model proposed, both models seem to be not reliable enough for use in developing accurate corresponding state models; however the QSPR model seems to have better predictions for the ionic liquids for which their cation and anion exist in the "training" set.

Figure 5

For further comparison, the effect of side-chain length on the T_c value is investigated for a certain anion and cation core. Rebelo *et al.* [40] used both Guggenheim and Eötvös equations and calculated the critical temperatures for 15 1-alkyl-3-methylimidazolium ionic liquids with different anions. They observed that the longer side-chain imidazolium ionic liquids had lower critical temperature. They interpreted that longer side-chains in the 1-alkyl-3-methylimidazolium cation decreased the relative importance of the Coulomb forces which led to the smaller values of T_c . In another study, Zaitsau *et al.* [76] measured the vapor pressure of four 1-alkyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide ionic liquids and used the Antoine equation to extrapolate the vapor pressure data to atmospheric pressure and estimated the T_b of ionic liquids studied. They also observed the same decrease in T_b while the length of side-chain

was increased. As the T_b of majority of chemical compounds lie around 0.6 of T_c , it can be concluded that their work confirmed the Zaitsau *et al.* interpretation.

In this regard, the effect of aliphatic side-chain length for 1-alkyl-3-methylimidazolium ionic liquids with bis[(trifluoromethyl)sulfonyl]amide and chloride anions are shown in Figure 6 and Figure 7, respectively. Regarding to these figures, the Guggenheim equation and QSPR model show a decrease in T_c while the length of side-chain increases. On the contrary, Valderrama's model shows an increase in T_c proportional to the length of side-chain, which opposes the abovementioned findings. This incompatible behavior is due to the nature of compounds used by Valderrama *et al.* to develop their models. As mentioned before, they have used high molecular weight (non-ionic) compounds to develop the models in which the T_b and consequently, T_c increases proportionally to the side-chain length and molecular weight of compounds. As a result, Valderrama's model produces inaccurate T_c values which should be considered if one wants to use this model to estimate the critical temperature of ionic liquids.

Figure 6

Figure 7

According to the papers published by Valderrama *et al.* [39, 49, 77], a density correlation was used to validate the calculated critical properties and normal boiling points of ionic liquids which had been developed for saturated liquids and petroleum fractions [48].

$$\rho = \left(\frac{A}{B}\right) + \left(\frac{2}{7}\right) \{(A \ln B)/B\} \frac{T-T_b}{T_c-T_b} \quad (3)$$

$$A = a + bM/V_c$$

$$B = \left(\frac{c}{V_c} + \frac{d}{M}\right)V_c^\delta$$

$$a = 0.3411, \quad b = 2.0443, \quad c = 0.5386$$

$$d = 0.0393, \quad \delta = 1.0476$$

It was reported that the density calculated using the above-mentioned correlation had an average deviation of less than 19%. As a result, Valderrama *et al.* concluded that the estimated critical properties as well as the normal boiling point were valid and reliable. In this study, it was shown that the critical temperatures calculated by Valderrama's model were mostly doubtful compared with the T_c calculated using the experimental surface tension of ionic liquids. Thus, the estimated T_b , V_c , other critical properties, and the validation technique could be questionable and these data should be used with great care.

In recent years, some corresponding state models [50-57] have been developed by several researchers to model other thermophysical properties of ionic liquids using the critical properties estimated by Valderrama *et al.* models. According to the results of this study, these models are also questionable and should be used with great care. The development of models for critical properties of ionic liquids and use of them for subsequent development of corresponding state models therefore needs more research and consideration. Moreover, the estimation of the critical temperature of ionic liquids using surface tension data is highly dependent on the quality of measurements and uncertainty of surface tension data. In addition, further model development requires larger datasets of experimental data for surface tension. At this time, large reliable datasets for surface tension are lacking, which limits the development of models in term of prediction reliability.

4- Conclusions

The theoretical critical temperature of ionic liquids was calculated using experimental data for surface tension of ionic liquids by means of the Guggenheim equation. Thereafter, two different GC and QSPR models were developed to assess the prediction ability of the models and compare the results with the

pioneering work of Valderrama *et al.* [39, 49, 77]. This study showed that the QSPR model provided better results compared with the GC model in terms of prediction and meaningful results. In addition, it was shown that the critical temperatures calculated by Valderrama's model had relatively large deviations compared with values estimated from surface tension data. Furthermore, Valderrama's model failed to represent the effect of side-chain length on critical temperature of ionic liquids. Consequently, one can question the validation method used by Valderrama *et al.* and thus one can conclude that the reported critical properties are probably not of suitable reliability to be used for developing corresponding state models for different thermophysical properties of ionic liquids.

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Figure 1: The number of ionic liquids in different families used for modeling the critical temperature.

Figure 2: A comparison between the T_c estimated by Guggenheim equation and other methods.

Figure 3: Estimated T_c of 1-ethyl-3-methylimidazolium ILs by different models.

Figure 4: Estimated T_c of 1-butyl-3-methylimidazolium ILs by different models.

Figure 5: T_c of 1-ethyl-3-methylimidazolium ionic liquids with 45 different anions calculated by the QSPR and Valderrama *et al.* models.

Table 1: Statistical parameters of GC and QSPR models

Table 2: Comparison of estimated T_c of ionic liquids by different methods.

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Figure 6: Estimated T_c of 1-alkyl-3-methylimidazolium bis[(trifluoromethyl)sulfonyl]imide ILs by different models.

Figure 7: Estimated T_c of 1-alkyl-3-methylimidazolium Chloride ILs by different models.

Table 1: Statistical parameters of GC and QSPR models

<i>Statistical Parameter</i>	GC Model	QSPR Model
<i>training set</i>		
R ² ^a	0.925	0.934
Average absolute relative deviation ^b	5.19	4.95
Standard deviation error ^c	69.57	65.32
Root mean square error ^d	69.60	65.34
N	82	82
<i>test set</i>		
R ²	0.911	0.941
Average absolute relative deviation	5.12	3.84
Standard deviation error	77.46	64.58
Root mean square error	77.72	64.65
N	24	24
<i>total</i>		
R ²	0.921	0.935
Average absolute relative deviation	5.17	4.70
Standard deviation error	71.52	65.18
Root mean square error	71.52	65.18
N	106	106

$$^a R^2 = 1 - \frac{\sum_{i=1}^N [y(i)_{calc} - y(i)_{exp}]^2}{\sum_{i=1}^N [y(i)_{calc} - \bar{y}_{exp}]^2}$$

$$^b AARD\% = \frac{100}{N} \sum_{i=1}^N \left| \frac{y(i)_{calc} - y(i)_{exp}}{y(i)_{exp}} \right|$$

$$^c SDEC = \sqrt{\frac{1}{N} \sum_{i=1}^N [e(i) - \bar{e}]^2}, (e = y_{calc} - y_{exp})$$

$$^d RMSE = \sqrt{\frac{1}{N} \sum_{i=1}^N [y(i)_{calc} - y(i)_{exp}]^2}$$

Table 2: Comparison of estimated T_c of ionic liquids by different methods.

No.	Name	T_c			
		Guggenheim Equation	GC Model	QSPR Model	Valderrama <i>et al.</i> [49]
1	1-(2-aminoethyl)-3-methylimidazolium tetrafluoroborate	1086.1	1119.0	1093.0	n.a.
2	1-(2-hydroxyethyl)-3-methylimidazolium tetrafluoroborate	1506.2	1506.2	1506.2	691.9
3	1-(3-aminopropyl)-3-methylimidazolium tetrafluoroborate	1115.7	1023.1	1134.2	n.a.
4	1,2-dimethyl-3-propylimidazolium bis[(trifluoromethyl)sulfonyl]amide	n.a.	536.5	543.8	1269.7
5	1,3-diethylimidazolium bis[(trifluoromethyl)sulfonyl]amide	1354.6	1372.0	1363.1	1259.3
6	1,3-dimethylimidazolium dimethylphosphate	636.5	635.8	646.2	n.a.
7	1,3-dimethylimidazolium methyl sulfate	1220.3	1230.1	1215.2	1040
8	1-butyl-1-methylpyrrolidinium bis[(trifluoromethyl)sulfonyl]amide	1014.3	1110.9	1103.6	1093.1
9	1-butyl-1-methylpyrrolidinium dicyanamide	1015.2	1094.2	1100.2	n.a.
10	1-butyl-1-methylpyrrolidinium thiocyanate	736.0	574.4	579.5	n.a.
11	1-butyl-1-methylpyrrolidinium trifluoroacetate	1431.0	1401.0	1479.0	n.a.
12	1-butyl-1-methylpyrrolidinium tris(pentafluoroethyl)trifluorophosphate	n.a.	1058.0	1037.2	n.a.
13	1-butyl-2,3-dimethylimidazolium bis(trifluoromethylsulfonyl)imide	553.1	553.1	553.1	1281.1
14	1-butyl-3-(6-hydroxyhexyl)-imidazolium chloride	456.4	434.2	475.2	n.a.
15	1-butyl-3-methylimidazolium acetate	1381.8	1391.0	1335.1	847.3
16	1-butyl-3-methylimidazolium Aspartate	677.1	675.5	718.3	n.a.
17	1-butyl-3-methylimidazolium bis[(trifluoromethyl)sulfonyl]amide	1187.6	1173.7	1186.1	1269.9
18	1-butyl-3-methylimidazolium chloride	1171.8	1177.0	1171.0	789
19	1-butyl-3-methylimidazolium dicyanamide	1322.5	1157.0	1182.7	1035.8
20	1-butyl-3-methylimidazolium glutamine	471.3	462.1	466.8	n.a.
21	1-butyl-3-methylimidazolium glycine	683.1	700.5	626.0	n.a.
22	1-butyl-3-methylimidazolium glycolate	1053.6	1105.7	1019.8	n.a.
23	1-butyl-3-methylimidazolium hexafluorophosphate	1183.9	1177.0	1217.4	719.4
24	1-butyl-3-methylimidazolium iodide	1082.9	1177.0	1137.4	871.2
25	1-butyl-3-methylimidazolium lactate	1176.5	1105.7	1136.0	n.a.
26	1-butyl-3-methyl-imidazolium L-lactate	1276.3	1105.7	1136.0	n.a.
27	1-butyl-3-methylimidazolium methylsulfate	1242.9	1266.2	1252.0	1081.6
28	1-butyl-3-methylimidazolium nitrate	n.a.	1102.1	1174.2	954.8
29	1-butyl-3-methylimidazolium octylsulfate	849.3	861.2	868.8	1189.8
30	1-butyl-3-methylimidazolium tetrafluoroborate	1141.1	1177.0	1210.8	643.2
31	1-butyl-3-methylimidazolium tetrakisothiocyanatocobaltate(II)	1247.2	1270.8	1247.6	n.a.
32	1-butyl-3-methylimidazolium thiocyanate	594.0	637.3	662.0	1047.4
33	1-butyl-3-methylimidazolium trifluoromethanesulfonate	1447.5	1520.5	1508.1	1023.5
34	1-butyl-3-methylpyridinium bis[(trifluoromethyl)sulfonyl]amide	800.1	892.3	805.5	1240.5
35	1-butyl-4-methylpyridinium thiocyanate	513.8	607.9	602.0	n.a.
36	1-butylpyridinium bis[(trifluoromethyl)sulfonyl]amide	1151.8	1148.9	1127.2	1229.1
37	1-butylpyridinium heptachlorodialuminate	1089.1	1089.1	1085.9	n.a.
38	1-butylpyridinium nitrate	1089.9	1077.2	1115.3	n.a.
39	1-decyl-3-methylimidazolium bis(trifluoromethylsulfonyl)amide	875.8	923.3	802.9	n.a.

40	1-dodecyl-3-methylimidazolium hexafluorophosphate	n.a.	901.2	829.1	857.6
41	1-dodecyl-3-methylimidazolium tetrafluoroborate	n.a.	901.2	822.5	784.6
42	1-ethyl-3-(6-hydroxyhexyl)-imidazolium chloride	505.0	527.2	460.9	n.a.
43	1-ethyl-3-methylimidazolium methylsulfate	1313.5	1275.9	1275.6	1053.6
44	1-ethyl-3-methylimidazolium 1,1,2,2-tetrafluoroethanesulfonate	1180.0	1184.6	1186.3	n.a.
45	1-ethyl-3-methylimidazolium acetate	n.a.	1400.7	1358.7	807.1
46	1-ethyl-3-methylimidazolium bis[(pentafluoroethyl)sulfonyl]amide	n.a.	492.3	1732.5	1231.4
47	1-ethyl-3-methylimidazolium bis[(trifluoromethyl)sulfonyl]amide	1177.5	1183.4	1209.7	1249.3
48	1-ethyl-3-methylimidazolium dicyanamide	1262.5	1166.7	1206.3	999
49	1-ethyl-3-methylimidazolium diethylphosphate	1115.7	1116.4	1106.0	877.2
50	1-ethyl-3-methylimidazolium ethyl sulfate	1227.6	1275.9	1244.7	1067.5
51	1-ethyl-3-methylimidazolium hexylsulfate	n.a.	870.9	1025.5	n.a.
52	1-ethyl-3-methylimidazolium L-lactate	926.0	1115.4	1159.6	n.a.
53	1-ethyl-3-methylimidazolium octyl sulfate	n.a.	870.9	892.4	n.a.
54	1-ethyl-3-methylimidazolium tetrachloroindate	1244.7	1314.1	1304.0	n.a.
55	1-ethyl-3-methylimidazolium tetracyanoborate	620.4	646.9	620.4	n.a.
56	1-ethyl-3-methylimidazolium tetrafluoroborate	1322.2	1186.7	1234.4	596.2
57	1-ethyl-3-methylimidazolium trifluoromethanesulfonate	1716.8	1530.2	1531.7	992.3
58	1-ethyl-3-methylimidazolium tris(pentafluoroethyl)trifluorophosphate	1057.3	1130.5	1143.3	n.a.
59	1-ethylpyridinium bis[(trifluoromethyl)sulfonyl]amide	1391.1	1312.8	1390.7	1207.9
60	1-heptyl-3-methylimidazolium bis(trifluoromethylsulfonyl)amide	925.4	961.2	1006.4	1305
61	1-hexyl-3-methylimidazolium bis[(trifluoromethyl)sulfonyl]amide	1056.7	1063.5	1056.0	1292.8
62	1-hexyl-3-methylimidazolium chloride	1163.2	1066.8	1040.8	829.2
63	1-hexyl-3-methylimidazolium hexafluorophosphate	1030.4	1066.8	1087.3	764.9
64	1-hexyl-3-methylimidazolium iodide	1012.4	1066.8	1007.3	n.a.
65	1-hexyl-3-methylimidazolium nitrate	n.a.	991.9	1044.1	991.8
66	1-hexyl-3-methylimidazolium tetrafluoroborate	1155.8	1066.8	1080.6	690
67	1-hexyl-3-methylimidazolium trifluoromethanesulfonate	1301.1	1410.2	1378.0	1055.6
68	1-hexyl-3-methylimidazolium tris(pentafluoroethyl)trifluorophosphate	950.0	1010.6	989.6	n.a.
69	1-hexylpyridinium bis(trifluoromethylsulfonyl)imide	1224.9	1108.2	1140.9	1252.3
70	1-isobutenyl-3-methylimidazolium tetrafluoroborate	n.a.	561.5	1133.3	n.a.
71	1-methyl-1-propylpyrrolidinium bis[(trifluoromethyl)sulfonyl]amide	1069.2	1107.1	1016.7	n.a.
72	1-methyl-3-hexylimidazolium chloroindium	1172.9	1194.1	1148.3	n.a.
73	1-octyl-3-methylimidazolium chloride	1000.8	980.9	992.1	869.4
74	1-methyl-3-pentylimidazolium 1,1,2,2,2-pentafluoro-N-[(1,1,2,2,2-pentafluoroethyl)sulfonyl]ethanesulfonamide	n.a.	371.4	1616.6	n.a.
75	1-methyl-3-pentylimidazolium aluminum tetrachloride	1213.8	1193.1	1184.2	n.a.
76	1-methyl-3-pentylimidazolium gallium tetrachloride	1247.8	1193.1	1190.8	n.a.
77	1-methyl-3-pentylimidazolium nitrate	n.a.	990.8	1082.0	n.a.
78	1-methyl-3-pentylimidazolium tetrachloroindate	1208.3	1193.1	1188.2	n.a.
79	1-methyl-3-pentylimidazolium tetrafluoroborate	993.1	1065.7	1118.5	666.6
80	1-methyl-3-propylimidazolium bis(pentafluoroethylsulfonyl)imide	n.a.	466.0	1642.8	n.a.
81	1-methyl-3-propylimidazolium bis[(trifluoromethyl)sulfonyl]amide	1107.6	1157.1	1120.0	1259.3

82	1-methyl-3-propylimidazolium hexafluorophosphate	1175.0	1160.4	1151.3	696.7
83	1-methyl-3-propylimidazolium nitrate	n.a.	1085.5	1108.1	n.a.
84	1-octyl-3-methylimidazolium bis[(trifluoromethyl)sulfonyl]amide	918.0	977.6	1008.7	1317.8
85	1-octyl-3-methylimidazolium bromide	n.a.	980.9	981.3	912.3
86	1-octyl-3-methylimidazolium hexafluorophosphate	1053.3	980.9	1040.0	810.8
87	1-octyl-3-methylimidazolium tetrafluoroborate	1044.6	980.9	1033.4	737
88	1-pentyl-3-methylimidazolium bis(trifluoromethylsulfonyl)amide	1051.2	1062.5	1095.8	1281.1
89	1-pentylpyridinium bis(trifluoromethylsulfonyl)imide	1152.8	1107.2	1128.0	n.a.
90	1-pentylpyridinium tetraoxorhenate	989.0	960.6	999.2	n.a.
91	1-propyl-3-methylimidazolium glutamate	538.9	529.9	539.5	n.a.
92	1-propyl-3-methylimidazolium tetrafluoroborate	1089.5	1160.4	1147.1	619.7
93	1-propylpyridinium tetrafluoroborate	1102.3	1289.8	1093.9	n.a.
94	2-hydroxy ethylammonium formate	1480.1	1494.6	1480.2	571.3
95	3-(6-hydroxyhexyl)-1-methylimidazolium chloride	554.3	540.7	553.9	n.a.
96	3-(6-hydroxyhexyl)-imidazolium chloride	547.3	560.8	573.0	n.a.
97	3,3'-(1,10-decanediyl)bis[1-methylimidazolium] 1,1,2,2,2-pentafluoro-N-[(1,1,2,2,2-pentafluoroethyl)sulfonyl]ethanesulfonamide	n.a.	-825.9	1961.2	n.a.
98	3,3'-(1,10-decanediyl)bis[1-methylimidazolium] bis(trifluoromethylsulfonyl)imide	n.a.	556.3	915.6	n.a.
99	3,3'-(1,10-decanediyl)bis[1-methylimidazolium] tetrafluoroborate	n.a.	562.9	964.9	n.a.
100	3,3'-(1,12-dodecanediyl)bis[1-methylimidazolium] 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	n.a.	531.0	908.5	n.a.
101	3,3'-(1,12-dodecanediyl)bis[1-methylimidazolium] 1,1,2,2,2-pentafluoro-N-[(1,1,2,2,2-pentafluoroethyl)sulfonyl]ethanesulfonamide	n.a.	-851.2	1955.6	n.a.
102	3,3'-(1,12-dodecanediyl)bis[1-methylimidazolium] tetrafluoroborate	n.a.	537.6	957.8	n.a.
103	3,3'-(1,5-pentanediy)bis[1-methylimidazolium] 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	n.a.	755.0	896.9	n.a.
104	3,3'-(1,5-pentanediy)bis[1-methylimidazolium] 1,1,2,2,2-pentafluoro-N-[(1,1,2,2,2-pentafluoroethyl)sulfonyl]ethanesulfonamide	n.a.	-627.2	1942.5	n.a.
105	3,3'-(1,6-hexanediy)bis[1-methylimidazolium] 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	n.a.	636.0	1133.0	n.a.
106	3,3'-(1,6-hexanediy)bis[1-methylimidazolium] 1,1,2,2,2-pentafluoro-N-[(1,1,2,2,2-pentafluoroethyl)sulfonyl]ethanesulfonamide	n.a.	-746.2	2181.1	n.a.
107	3,3'-(1,8-octanediy)bis[1-methylimidazolium] 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	n.a.	610.7	892.5	n.a.
108	3,3'-(1,9-nonanediy)bis[1-methylimidazolium] 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	n.a.	569.0	907.6	n.a.
109	3,3'-(1,9-nonanediy)bis[1-methylimidazolium] 1,1,2,2,2-pentafluoro-N-[(1,1,2,2,2-pentafluoroethyl)sulfonyl]ethanesulfonamide	n.a.	-813.2	1955.2	n.a.
110	3,3'-(1,9-nonanediy)bis[1-methylimidazolium] tetrafluoroborate	n.a.	575.5	956.9	n.a.
111	3-butyl-1-methylimidazolium benzoate	1287.4	1262.0	1265.6	n.a.
112	3-ethyl-1-methylimidazolium butyl sulfate	n.a.	1068.9	1486.6	n.a.
113	3-hexyl-1-methylimidazolium 1,1,2,2,2-pentafluoro-N-[(1,1,2,2,2-pentafluoroethyl)sulfonyl]ethanesulfonamide	n.a.	372.4	1576.8	n.a.
114	3-methyl-1-propylpyridinium bis(trifluoromethylsulfonyl)imide	1180.4	1030.0	1123.5	1228.9

115	butylammonium formate	n.a.	1441.2	1093.4	546.7
116	butyltrimethylammonium bis(trifluoromethylsulfonyl)imide	1007.7	1052.9	1013.6	1038.7
117	decyl(trimethyl)ammonium bis(trifluoromethylsulfonyl)imide	935.1	914.8	815.9	1136.3
118	hexyltrimethylammonium bis[(trifluoromethyl)sulfonyl]amide	982.4	1043.2	1102.4	1173.9
119	methyltrioctylammonium bis(trifluoromethylsulfonyl)imide	753.7	746.7	696.0	n.a.
120	N,N-dimethyl-N-propyl-1-butanaminium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1111.9	947.7	991.5	n.a.
121	N,N-dimethyl-N-propyldecanaminium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	818.9	726.3	888.0	n.a.
122	N,N-dimethyl-N-propylhexanaminium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	879.6	907.1	918.3	n.a.
123	N-butyl-3-methylpyridinium dicyanamide	721.1	875.6	802.1	n.a.
124	N-butyl-4-methylpyridinium tetrafluoroborate	1300.4	1147.6	1150.8	625.8
125	N-octyl-3-methylpyridinium tetrafluoroborate	698.1	757.6	753.4	n.a.
126	tetradecyltriethylphosphonium bromide	846.9	895.9	843.3	n.a.
127	triethyl-1-decanaminium bis(trifluoromethylsulfonyl)imide	751.9	765.3	756.0	n.a.
128	triethyl-1-dodecanammonium bis(trifluoromethylsulfonyl)imide	727.2	740.0	732.4	n.a.
129	triethyl-1-pentylammonium bis(trifluoromethylsulfonyl)imide	902.7	916.0	894.0	1102.5
130	triethylhexylammonium bis(trifluoromethylsulfonyl)imide	813.2	806.7	847.5	1119.2
131	triethyloctylammonium bis(trifluoromethylsulfonyl)imide	775.8	819.7	775.9	1153.7
132	triethyl(tetradecyl)phosphonium bis[(trifluoromethyl)sulfonyl]imide	869.5	892.7	870.7	n.a.
133	triethyl(tetradecyl)phosphonium chloride	819.7	895.9	855.6	n.a.
134	triethyl(tetradecyl)phosphonium dicyanamide	916.4	875.9	867.3	n.a.
135	triethyl(tetradecyl)phosphonium tris(pentafluoroethyl)trifluorophosphate	945.9	839.7	804.3	n.a.
136	triethyltetradecylphosphonium bis(2,4,4-trimethylpentyl)phosphinate	784.1	783.7	805.9	n.a.
137	triethyltetradecylphosphonium decanoate	864.4	842.9	842.3	n.a.
138	triethyltetradecylphosphonium dicyanamide	831.2	875.9	867.3	n.a.
139	triethyltetradecylphosphonium methanesulfonate	842.3	821.0	943.5	n.a.