

# Physical Properties of Ionic Liquids: Database and Evaluation

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A comprehensive database on physical properties of ionic liquids (ILs), which was collected from 109 kinds of literature sources in the period from 1984 through 2004, has been presented. There are 1680 pieces of data on the physical properties for 588 available ILs, from which 276 kinds of cations and 55 kinds of anions were extracted. In terms of the collected database, the structure-property relationship was evaluated. The correlation of melting points of two most common systems, disubstituted imidazolium tetrafluoroborate and disubstituted imidazolium hexafluorophosphate, was carried out using a quantitative structure-property relationship method. © 2006 American Institute of Physics. [DOI: 10.1063/1.2204959]

Key words: ionic liquid; database; properties; melting point; QSPR.

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## 1. Introduction

Although the first room temperature ionic liquids (ILs) were first observed in the middle of the 19th Century,<sup>2</sup> only since the 1980s have room temperature ILs attracted a significant and growing interest. Now, ILs, as green solvents, have been studied extensively<sup>56,82,42,126</sup> thanks to their tempting properties such as negligible vapor pressure, large liquidus range, high thermal stability, high ionic conductivity, large electrochemical window, and ability to solvate compounds of widely varying polarity.<sup>111,37,29,32</sup> Utilizing ILs is one of the goals of green chemistry because they create a cleaner and more sustainable chemistry and are receiving increasing interest as environmental friendly solvents for many synthetic and catalytic processes.<sup>36,43,56,53</sup> An intriguing characteristic is to fine tune the physical-chemical prop-

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erties by suitable choice of cations and anions. Therefore, ILs have been recognized as “designer-solvents.”<sup>29</sup>

To optimize the use of ILs and design the desirable ILs, knowledge of the physical and chemical properties of ILs is essentially important. From the industrial viewpoint, a fundamental understanding of the chemical and physical properties of ILs should be known before its industrial application. Physical properties such as melting point, density, and viscosity, are related to the mechanical and engineering components associated with a process.<sup>63</sup> For academic research, physical and chemical properties are also indispensable to validate the theoretical models or select proper ILs. For example, densities, viscosities, and surface tensions determine important parameters including rates of liquid-liquid phase separation, mass transfer, power requirements of mixing, and pumping. Other physical properties, such as refractive index, are related to certain chemical properties despite providing a bulk property description.<sup>7</sup>

Most of the recent work with ILs has focused on the characterization and application of certain kinds of ILs, and provided a large amount of useful data as well as regulations. However, there is not a comprehensive database publicly available for researchers to consult. Although we can find some data of ILs from some databases (e.g., Beilstein<sup>127</sup>), the data are limited and most of them are bromides with high melting points (over 100 °C). There are also ionic liquid databases developed by companies such as Merck,<sup>128</sup> but these are not complete and most of them are products of company.

In this work, we establish a database of physical properties of ILs from the open literature from 1980 through 2004. Based on the database, the structure-property relationships of ILs and the variations of properties with the change of cations and anions are studied. Models with good correlation of melting points for two kinds of ILs are developed by using the quantitative structure-property relationship (QSPR) method.

## 2. The Classification of ILs

There are comparatively abundant data available for imidazolium salts from monosubstituted to pentasubstituted compounds. The data on ammonium, pyridinium, isoquinolinium, sulfonium, phosphonium, pyrrolidinium, and other complex compounds are also available. In Table 1, the cations and anions extracted from the reported ILs are tabulated by a code. In property tables the cations and anions are represented by codes and abbreviations which are consistent with the classification presented in Table 1.

The cations and anions are coded according to their types. For cations, when the code contains no more than three digits the first number is its type number. For example, “201” means the cation is disubstituted imidazolium and the number “01” reflects the least molecular weight in this type. Since some ILs are retrieved later (after a series of codes was established), their codes do not exactly reflect their molecular weight. The type number is listed from 1 to 19. Thus,

when the code of a cation comes to four digits the first two digits describes its type. For example, for the cation coded “1109” the type number is “11” which means pyridinium. There are also four-digit identification numbers when the type number is “2” because of the variety of this type. Therefore, the code beginning with “2” means the cation is disubstituted imidazolium. For the anions, the code is similar except that we added “0” before each identification number of anions to differentiate them from cations.

## 3. Phase Transition Temperature: Melting Point ( $T_m$ ), Glass Transition Point ( $T_g$ ), Decomposition Point ( $T_d$ ), Freezing Point ( $T_f$ ), and Clearing Point ( $T_c$ )

Data on melting point ( $T_m$ ) and glass transition point ( $T_g$ ) are tabulated in Table 2, whereas the decomposition point ( $T_d$ ), the freezing point ( $T_f$ ), and the clearing point ( $T_c$ ) are tabulated in Tables 3–5, respectively. Melting happens when the molecules or ions fall out of their crystal structures, and become disordered liquid. The glass transition is a transition which happens from solid state to amorphous solid; but even crystalline solids may have some amorphous portion. This is why the same sample of ILs may have both a glass transition temperature and a melting temperature. Freezing point has the same meaning as melting point but an opposite process. Some salts with long chains are low melting solids which display enantiotropic mesomorphism with extensive thermotropic mesophase range<sup>37</sup> with the lower limit, melting point and upper limit, clearing point.

The phase transition temperature of ILs is governed by van der Waals forces and electrostatic interaction force,<sup>10,15,26</sup> and the impact of the two forces play different roles for different kinds of ILs. It has been pointed out that the  $T_m$  of quaternary ammonium type ionic liquid is governed by the van der Waals force rather than the electrostatic interaction force,<sup>18</sup> i.e., for such kind of cations, the change of phase transition temperature with the anions is not as great as cations. The ionic liquids of imidazolium containing symmetric cations such as 1,3-dimethylimidazolium (c201), 1,3-diethylimidazolium (c207), 1,2,3-trimethylimidazolium (c32), and 1,2-dimethyl-3-ethylimidazolium (c33), show higher melting points than those containing asymmetric cations.<sup>97</sup> The phenomena can be observed in Fig. 1. ILs with symmetric cation (c201) exhibit the highest melting points; the melting points appear to fall steadily with increasing alkyl chain length; when the carbon number ( $n$ ) in the branch of  $[C_n\text{MIM}]X^-$  (1-alkyl-3-methylimidazolium,  $X^- = \text{BF}_4^-, \text{PF}_6^-, \text{Cl}^-$ ) comes to 4–9 there is a platform, then the melting points increase with the carbon number. The variation of melting points with anions was shown in Fig. 2. The radii of the anions were calculated at B3LYP/6-31G level. The results are as follows:  $a_0(\text{Cl}) = 2.70 \text{ \AA}$ ;  $a_0(\text{Br}) = 3.12 \text{ \AA}$ ;  $a_0(\text{PF}_6) = 3.60 \text{ \AA}$ ;  $a_0(\text{BF}_4) = 3.44 \text{ \AA}$ ;  $a_0(\text{TfO}, [\text{CF}_3\text{SO}_3]) = 3.79 \text{ \AA}$ ; and  $a_0(\text{TFSI}, [(\text{CF}_3\text{SO}_2)_2\text{N}]) = 4.39 \text{ \AA}$ . The melting temperatures are generally decreased with increasing anion radius except for  $\text{PF}_6$ . It is because the larger anion radius

TABLE 1. Cations and Anions

ID	Abbreviation	Name	Formula	M/g mol <sup>-1</sup>
<b>Cations</b>				
297	NPEMI	3-[2-(4-nitro-phenyl)-2-oxoethyl]-1-methylimidazolium	C <sub>12</sub> H <sub>14</sub> N <sub>3</sub> O <sub>2</sub>	232.26
264	CPOEMI	3-[2-(3-chlorophenyl)-2-oxoethyl]-1-methylimidazolium	C <sub>12</sub> H <sub>12</sub> ClN <sub>2</sub> O	235.69
265	C'POEMI	3-[2-(4-chlorophenyl)-2-oxoethyl]-1-methylimidazolium	C <sub>12</sub> H <sub>12</sub> ClN <sub>2</sub> O	235.69
293	EONiBeI	1-ethyloxy-3-[4-nitrobenzyl]imidazolium	C <sub>12</sub> H <sub>14</sub> N <sub>3</sub> O <sub>3</sub>	248.26
290	MOPOEI	1-methyloxy-3-[2-(4-chlorophenyl)-2-oxoethyl]imidazolium	C <sub>12</sub> H <sub>12</sub> ClN <sub>2</sub> O <sub>2</sub>	251.69
267	NPOEMI	3-[2-(4-nitro-phenyl)-2-oxoethyl]-1-methylimidazolium	C <sub>12</sub> H <sub>12</sub> N <sub>3</sub> O <sub>3</sub>	246.25
295	EtODBeI	1-etheneoxy-3-[2,4-dichlorobenzyl]imidazolium	C <sub>12</sub> H <sub>11</sub> Cl <sub>2</sub> N <sub>2</sub> O	270.14
294	EODBeI	1-ethyloxy-3-[2,4-dichlorobenzyl]imidazolium	C <sub>12</sub> H <sub>13</sub> Cl <sub>2</sub> N <sub>2</sub> O	272.15
266	PECl <sub>2</sub> MI	3-[2-(3,4-dichlorophenyl)-2-oxoethyl]-1-methylimidazolium	C <sub>12</sub> H <sub>11</sub> Cl <sub>2</sub> N <sub>2</sub> O	270.14
236	C <sub>9</sub> MI	1-hydrocinnamyl-3-methylimidazolium	C <sub>13</sub> H <sub>17</sub> N <sub>2</sub>	201.29
234	C <sub>9</sub> MI	1-nonyl-3-methylimidazolium	C <sub>13</sub> H <sub>25</sub> N <sub>2</sub>	209.35
235	C <sub>2</sub> C <sub>8</sub> I	1-octyl-3-ethylimidazolium	C <sub>13</sub> H <sub>25</sub> N <sub>2</sub>	209.35
237	DBOMI	1,3-di-(1-butoxymethyl)imidazolium	C <sub>13</sub> H <sub>25</sub> N <sub>2</sub> O <sub>2</sub>	241.35
268	MOTEI	1-Methyl-3-(2-oxo-2-o-tolyl-ethyl)-imidazolium	C <sub>13</sub> H <sub>15</sub> N <sub>2</sub> O	215.27
219	MOBMI	1-(4-methoxybutyl)-3-methylimidazolium	C <sub>9</sub> H <sub>17</sub> N <sub>2</sub> O	169.25
220	C5O2MI	1-[2-(2-methoxyethoxy)ethyl]-3-methylimidazolium	C <sub>9</sub> H <sub>17</sub> N <sub>2</sub> O <sub>2</sub>	185.25
275	DBI	1,3-dibenzylimidazolium	C <sub>10</sub> H <sub>10</sub> N <sub>2</sub>	158.20
221	C6MI	1-hexyl-3-methylimidazolium	C <sub>10</sub> H <sub>19</sub> N <sub>2</sub>	167.27
222	PEMI	1-[2-phenyl-2-oxethyl]-3-methylimidazolium	C <sub>10</sub> H <sub>11</sub> N <sub>2</sub> O	175.21
276	CPCEI	1-(3-cyano-propyl)-3-(2-cyano-ethyl)imidazolium	C <sub>10</sub> H <sub>13</sub> N <sub>4</sub>	189.24
292	FOEMI	1-(2-Furan-2-yl-2-oxo-ethyl)-3-methylimidazolium	C <sub>10</sub> H <sub>11</sub> N <sub>2</sub> O <sub>2</sub>	191.21
299	HyDBeI	1-hydroxy-3-[2,4-dichlorobenzyl]imidazolium	C <sub>10</sub> H <sub>9</sub> Cl <sub>2</sub> N <sub>2</sub> O	244.10
2100	BenMI	1-benzyl-3-methylimidazolium	C <sub>11</sub> H <sub>13</sub> N <sub>2</sub>	173.24
282	BenHMI	1-benzyl-3-methylimidazolium	C <sub>11</sub> H <sub>13</sub> N <sub>2</sub>	173.24
224	C7MI	1-heptyl-3-methylimidazolium	C <sub>11</sub> H <sub>21</sub> N <sub>2</sub>	181.30
225	C2C6I	1-hexyl-3-ethylimidazolium	C <sub>11</sub> H <sub>21</sub> N <sub>2</sub>	181.30
226	C4C4I	1,3-dibutylimidazolium	C <sub>11</sub> H <sub>21</sub> N <sub>2</sub>	181.30
228	MPMI	1-(4-methoxyphenyl)-3-methylimidazolium	C <sub>11</sub> H <sub>13</sub> ON <sub>2</sub>	189.24
230	C8pMI	phenemyl-3-methylimidazolium	C <sub>12</sub> H <sub>15</sub> N <sub>2</sub>	187.26
286	M3BzMI	1-methyl-3-(3-methyl-benzyl)-imidazolium	C <sub>12</sub> H <sub>15</sub> N <sub>2</sub>	187.26
287	M2BzMI	1-methyl-3-(2-methyl-benzyl)-imidazolium	C <sub>12</sub> H <sub>15</sub> N <sub>2</sub>	187.26
291	PEBrMI	3-[2-(4-bromo-phenyl)-2-oxoethyl]-1-methylimidazolium	C <sub>12</sub> H <sub>12</sub> BrN <sub>2</sub> O	280.14
229	C8MI	1-octyl-3-methylimidazolium	C <sub>12</sub> H <sub>23</sub> N <sub>2</sub>	195.33
232	C8OPI	phenylethanoyl-3-propylimidazolium	C <sub>12</sub> H <sub>15</sub> N <sub>2</sub> O	203.26
231	C8OMI	heptoxymethyl-3-methylimidazolium	C <sub>12</sub> H <sub>23</sub> N <sub>2</sub> O	211.33
263	PE(o-F)MI	3-[2-(2-florophenyl)-2-oxoethyl]-1-methylimidazolium	C <sub>12</sub> H <sub>12</sub> FN <sub>2</sub> O	219.24
233	PBOMI	1-(1-propoxymethyl)-3-(1-butoxymethyl)imidazolium	C <sub>12</sub> H <sub>23</sub> N <sub>2</sub> O <sub>2</sub>	227.33
297	NPEMI	3-[2-(4-nitro-phenyl)-2-oxoethyl]-1-methylimidazolium	C <sub>12</sub> H <sub>14</sub> N <sub>3</sub> O <sub>2</sub>	232.26
264	CPOEMI	3-[2-(3-chlorophenyl)-2-oxoethyl]-1-methylimidazolium	C <sub>12</sub> H <sub>12</sub> ClN <sub>2</sub> O	235.69
265	C'POEMI	3-[2-(4-chlorophenyl)-2-oxoethyl]-1-methylimidazolium	C <sub>12</sub> H <sub>12</sub> ClN <sub>2</sub> O	235.69
293	EONiBeI	1-ethyloxy-3-[4-nitrobenzyl]imidazolium	C <sub>12</sub> H <sub>14</sub> N <sub>3</sub> O <sub>3</sub>	248.26
290	MOPOEI	1-methyloxy-3-[2-(4-chlorophenyl)-2-oxoethyl]imidazolium	C <sub>12</sub> H <sub>12</sub> ClN <sub>2</sub> O <sub>2</sub>	251.69
267	NPOEMI	3-[2-(4-nitro-phenyl)-2-oxoethyl]-1-methylimidazolium	C <sub>12</sub> H <sub>12</sub> N <sub>3</sub> O <sub>3</sub>	246.25
295	EtODBeI	1-etheneoxy-3-[2,4-dichlorobenzyl]imidazolium	C <sub>12</sub> H <sub>11</sub> Cl <sub>2</sub> N <sub>2</sub> O	270.14
294	EODBeI	1-ethyloxy-3-[2,4-dichlorobenzyl]imidazolium	C <sub>12</sub> H <sub>13</sub> Cl <sub>2</sub> N <sub>2</sub> O	272.15
266	PECl <sub>2</sub> MI	3-[2-(3,4-dichlorophenyl)-2-oxoethyl]-1-methylimidazolium	C <sub>12</sub> H <sub>11</sub> Cl <sub>2</sub> N <sub>2</sub> O	270.14
236	C <sub>9</sub> MI	1-hydrocinnamyl-3-methylimidazolium	C <sub>13</sub> H <sub>17</sub> N <sub>2</sub>	201.29
234	C <sub>9</sub> MI	1-nonyl-3-methylimidazolium	C <sub>13</sub> H <sub>25</sub> N <sub>2</sub>	209.35
235	C <sub>2</sub> C <sub>8</sub> I	1-octyl-3-ethylimidazolium	C <sub>13</sub> H <sub>25</sub> N <sub>2</sub>	209.35
237	DBOMI	1,3-di-(1-butoxymethyl)imidazolium	C <sub>13</sub> H <sub>25</sub> N <sub>2</sub> O <sub>2</sub>	241.35
268	MOTEI	1-Methyl-3-(2-oxo-2-o-tolyl-ethyl)-imidazolium	C <sub>13</sub> H <sub>15</sub> N <sub>2</sub> O	215.27
290	CBMI	3-(4-Cyano-benzoyl)-1-methylimidazolium	C <sub>13</sub> H <sub>12</sub> N <sub>3</sub> O	226.26
269	MOPOMI	3-[2-(4-Methyloxyphenyl)-2-oxoethyl]-1-methylimidazolium	C <sub>13</sub> H <sub>15</sub> N <sub>2</sub> O <sub>2</sub>	231.27
270	M'OPOMI	3-[2-(2-Methyloxyphenyl)-2-oxoethyl]-1-methylimidazolium	C <sub>13</sub> H <sub>15</sub> N <sub>2</sub> O <sub>2</sub>	231.27
298	EOPOEI	1-ethyloxy-3-[2-(4-chlorophenyl)-2-oxoethyl]imidazolium	C <sub>13</sub> H <sub>14</sub> ClN <sub>2</sub> O <sub>2</sub>	265.72
2102	HyTMOBI	1-hydroxy-3-(3,4,5-trimethyloxybenzyl)imidazolium	C <sub>13</sub> H <sub>17</sub> N <sub>2</sub> O <sub>4</sub>	265.29
2103	EBPOEI	1-ethyl-3-[2-(4-bromo-phenyl)-2-oxoethyl]imidazolium	C <sub>13</sub> H <sub>14</sub> BrN <sub>2</sub> O	294.17
240	MDI	1-methyl-3-[2,6-(S)-dimethylocten-2-yl]imidazolium	C <sub>14</sub> H <sub>25</sub> N <sub>2</sub>	221.37
238	C <sub>3</sub> C <sub>8</sub> I	1-octyl-3-propylimidazolium	C <sub>14</sub> H <sub>27</sub> N <sub>2</sub>	223.38

TABLE I. Cations and Anions—Continued

ID	Abbreviation	Name	Formula	M/g mol <sup>-1</sup>
239	C <sub>10</sub> MI	1-decyl-3-methylimidazolium	C <sub>14</sub> H <sub>27</sub> N <sub>2</sub>	223.38
271	PEMe <sub>2</sub> MI	3-[2-(1,2-dimethoxyphenyl)-2-oxoethyl]-1-methylimidazolium	C <sub>14</sub> H <sub>17</sub> N <sub>2</sub> O	229.30
296	DMPEMI	3-(1,1-dimethyl-2-phenyl-2-oxoethyl)-1-methylimidazolium	C <sub>14</sub> H <sub>17</sub> N <sub>2</sub> O	229.30
278	MOPOEMI	3-[2-(3,5-dimethoxyphenyl)-2-oxoethyl]-1-methylimidazolium	C <sub>14</sub> H <sub>17</sub> N <sub>2</sub> O <sub>3</sub>	261.30
272	PEMe <sub>2</sub> MI	3-[2-(3,4-Dimethoxyphenyl)-2-oxoethyl]-1-methylimidazolium	C <sub>14</sub> H <sub>17</sub> N <sub>2</sub> O	229.30
241	NOMMI	1-(1-nonoxymethyl)-3-methylimidazolium	C <sub>14</sub> H <sub>27</sub> N <sub>2</sub> O	239.38
273	PE(OEt)MI	3-[2-(3-ethoxyphenyl)-2-oxoethyl]-1-methylimidazolium	C <sub>14</sub> H <sub>17</sub> N <sub>2</sub> O <sub>2</sub>	245.30
274	POEMI	3-[2-(4-ethoxyphenyl)-2-oxoethyl]-1-methylimidazolium	C <sub>14</sub> H <sub>17</sub> N <sub>2</sub> O <sub>2</sub>	245.30
242	ABOMI	1-(1-amyloxymethyl)-3-butoxymethyl imidazolium	C <sub>14</sub> H <sub>27</sub> N <sub>2</sub> O <sub>2</sub>	255.38
288	ABMI	1-amy-3-benzylimidazolium	C <sub>15</sub> H <sub>21</sub> N <sub>2</sub>	229.35
245	HxBOMI	1-(1-hexyloxymethyl)-3-(1-butoxymethyl) imidazolium	C <sub>15</sub> H <sub>29</sub> N <sub>2</sub> O <sub>2</sub>	269.41
243	C11MI	1-undecyl-3-methylimidazolium	C <sub>15</sub> H <sub>29</sub> N <sub>2</sub>	237.41
244	DOMMI	1-(1-decyloxymethyl)-3-methylimidazolium	C <sub>15</sub> H <sub>29</sub> N <sub>2</sub> O	253.41
279	PPOMI	3-[2-(3-propyloxyphenyl)-2-oxoethyl]-1-methyl imidazolium	C <sub>15</sub> H <sub>19</sub> N <sub>2</sub> O <sub>2</sub>	259.33
280	MOOIPi	3-[2-(3-methoxyloxyphenyl)-2-oxoethyl]-1-isopropylimidazolium	C <sub>15</sub> H <sub>19</sub> N <sub>2</sub> O <sub>2</sub>	259.33
281	PE(Me)3MI	3-[2-(2,4,6-trimethoxyphenyl)-2-oxoethyl]-1-methylimidazolium	C <sub>15</sub> H <sub>19</sub> N <sub>2</sub> O <sub>2</sub>	259.33
2107	α-NOEMI	3-[2-α-naphthyl-2-oxoethyl]-1-methylimidazolium	C <sub>16</sub> H <sub>15</sub> N <sub>2</sub> O	251.31
248	HpBOMI	1-(1-heptyloxymethyl)-3-(1-butoxymethyl) imidazolium	C <sub>16</sub> H <sub>31</sub> N <sub>2</sub> O <sub>2</sub>	283.43
246	C12MI	1-dodecyl-3-methylimidazolium	C <sub>16</sub> H <sub>31</sub> N <sub>2</sub>	251.44
247	UOMMI	1-(1-undecyloxymethyl)-3-methylimidazolium	C <sub>16</sub> H <sub>31</sub> N <sub>2</sub> O	267.43
277	POCPOEI	1-(2,2-dimethylpropionyloxy)-3-[2-(4-chlorophenyl)-2-oxoethyl]imidazolium	C <sub>16</sub> H <sub>18</sub> ClN <sub>2</sub> O <sub>3</sub>	321.78
250	DOMMI	1-(1-dodecyloxymethyl)-3-methylimidazolium	C <sub>17</sub> H <sub>33</sub> N <sub>2</sub> O	281.46
249	C13MI	1-tridecyl-3-methylimidazolium	C <sub>17</sub> H <sub>33</sub> N <sub>2</sub>	265.46
2104	BODCBI	1-benzoyloxy-3-(2,4-dichlorobenzyl)imidazolium	C <sub>17</sub> H <sub>15</sub> Cl <sub>2</sub> N <sub>2</sub> O	334.22
284	BoBzYMI	1-(4-Benzoyl-benzyl)-3-methyl-imidazolium	C <sub>18</sub> H <sub>17</sub> N <sub>2</sub> O	277.35
251	C14MI	1-tetradecyl-3-methylimidazolium	C <sub>18</sub> H <sub>35</sub> N <sub>2</sub>	279.49
2101	MOPOPI	3-[2-(3-methoxyloxyphenyl)-2-oxoethyl]-1-phenylimidazolium	C <sub>18</sub> H <sub>17</sub> N <sub>2</sub> O <sub>2</sub>	293.35
252	NBOMI	1-(1-nonyloxymethyl)-3-(1-butoxymethyl)imidazolium	C <sub>18</sub> H <sub>33</sub> N <sub>2</sub> O <sub>2</sub>	311.49
2105	PEODCBI	1-(2-phenylethoxy)-3-(2,5-dichlorobenzyl)imidazolium	C <sub>18</sub> H <sub>17</sub> Cl <sub>2</sub> N <sub>2</sub> O	348.25
298	POPOEI	1-[2,4-dichlorophenylmethoxy]-3-[2-(4-chlorophenyl)-2-oxoethyl]imidazolium	C <sub>18</sub> H <sub>14</sub> Cl <sub>3</sub> N <sub>2</sub> O	396.68
253	C15MI	1-pentadecyl-3-methylimidazolium	C <sub>19</sub> H <sub>37</sub> N <sub>2</sub>	293.52
2106	PDAOI	1-phenyloxy-3-[2-(4-Dimethylamino-phenyl)-2-oxoethyl]imidazolium	C <sub>19</sub> H <sub>20</sub> N <sub>3</sub> O <sub>2</sub>	322.39
256	DBOMI	1-(1-decyloxymethyl)-3-(1-butoxy methyl)imidazolium	C <sub>19</sub> H <sub>37</sub> N <sub>2</sub> O <sub>2</sub>	325.51
255	C16MI	1-hexadecyl-3-methylimidazolium	C <sub>20</sub> H <sub>39</sub> N <sub>2</sub>	307.54
254	DOMHI	1-(1-decyloxymethyl)-3-hexyl imidazolium	C <sub>20</sub> H <sub>39</sub> N <sub>2</sub> O	323.54
257	UBOMI	1-(1-undecyloxymethyl)-3-(1-butoxy methyl)imidazolium	C <sub>20</sub> H <sub>39</sub> N <sub>2</sub> O <sub>2</sub>	339.54
258	UOMHI	1-(1-undecyloxymethyl)-3-hexyl imidazolium	C <sub>21</sub> H <sub>41</sub> N <sub>2</sub> O	337.57
259	C18MI	1-octadecyl-3-methylimidazolium	C <sub>22</sub> H <sub>43</sub> N <sub>2</sub>	335.60
260	C20MI	1-cosyl-3-methylimidazolium	C <sub>24</sub> H <sub>47</sub> N <sub>2</sub>	363.65
261	PEOI-I	1-(2-(2-(2-(2-(2-(2-(methacryloyloxy)ethoxy)ethoxy)ethoxy)ethoxy)ethoxy)ethoxy)-3-ethylimidazolium	C <sub>25</sub> H <sub>45</sub> O <sub>9</sub> N <sub>2</sub>	517.64
262	PEOII-I	polymer of PEOimidazolium		
337	DHBrI	1,3-dihydroxy-2-bromoimidazolium	C <sub>3</sub> H <sub>4</sub> BrN <sub>2</sub> O <sub>2</sub>	179.98
327	DMCII	1,3-dimethyl-5-chlorideimidazolium	C <sub>5</sub> H <sub>8</sub> ClN <sub>2</sub>	131.58
31	M2,4,5I	2,4,5-trimethylimidazolium	C <sub>6</sub> H <sub>11</sub> N <sub>2</sub>	111.17
32	M1,2,3I	1,2,3-trimethylimidazolium	C <sub>6</sub> H <sub>11</sub> N <sub>2</sub>	111.17
319	DMNiI	1,3-dimethyl-nimtrimeimidazolium	C <sub>6</sub> H <sub>8</sub> N <sub>3</sub> S	154.22
33	M1,2E3I	1,2-dimethyl-3-ethylimidazolium	C <sub>7</sub> H <sub>13</sub> N <sub>2</sub>	125.19
34	E1M3,5I	1-ethyl-3,5-dimethylimidazolium	C <sub>7</sub> H <sub>13</sub> N <sub>2</sub>	125.19
35	EDMI	1-ethyl-2,3-dimethylimidazolium	C <sub>7</sub> H <sub>13</sub> N <sub>2</sub>	125.19
36	E1,3M4I	1,3-dimethyl-4-methylimidazolium	C <sub>8</sub> H <sub>15</sub> N <sub>2</sub>	139.22
37	DMPI	1,2-methyl-3-propylimidazolium	C <sub>8</sub> H <sub>15</sub> N <sub>2</sub>	139.22
38	E1,2M3I	1,2-ethyl-3-methylimidazolium	C <sub>8</sub> H <sub>15</sub> N <sub>2</sub>	139.22
39	P1M2,3I	1-propyl-2,3-dimethylimidazolium	C <sub>8</sub> H <sub>15</sub> N <sub>2</sub>	139.22
310	BDMI	1-butyl-2,3-dimethylimidazolium	C <sub>9</sub> H <sub>17</sub> N <sub>2</sub>	153.25

TABLE I. Cations and Anions—Continued

ID	Abbreviation	Name	Formula	M/g mol <sup>-1</sup>
322	B3M1,5I	3-butyl-1,5-dimethylimidazolium	C <sub>9</sub> H <sub>17</sub> N <sub>2</sub>	153.25
320	DMPHl	1,3-dimethyl-2-phenylimidazolium	C <sub>11</sub> H <sub>13</sub> N <sub>2</sub>	173.24
313	BzMPI	1-benzyl-2-methyl-3-propyl	C <sub>13</sub> H <sub>19</sub> N <sub>2</sub>	203.31
312	ODMI	1-octyl-2,3-dimethylimidazolium	C <sub>13</sub> H <sub>25</sub> N <sub>2</sub>	209.35
323	DPB'I	1,3-dipropyl-2-isobutylimidazolium	C <sub>13</sub> H <sub>25</sub> N <sub>2</sub>	209.35
353	MPOEMOI	1-methyl-3-(2-phenyl-2-oxoethyl)-5-methoxyimidazolium	C <sub>13</sub> H <sub>15</sub> N <sub>2</sub> O <sub>2</sub>	231.27
321	PCIDMI	1,2-dimethyl-3-phenylethanol(p-Cl) imidazolium	C <sub>13</sub> H <sub>14</sub> ClN <sub>2</sub> O	249.72
339	HyEPOEI	1-hydroxy-2-ethyl-3-[2-(4-chloro phenyl)-2-oxoethyl]imidazolium	C <sub>13</sub> H <sub>14</sub> ClN <sub>2</sub> O <sub>2</sub>	265.72
314	BzMBI	1-benzyl-2-methyl-3-butylimidazolium	C <sub>14</sub> H <sub>21</sub> N <sub>2</sub>	217.33
315	BzMB'I	1-benzyl-2-methyl-3-(3-methyl) propylimidazolium	C <sub>14</sub> H <sub>21</sub> N <sub>2</sub>	217.33
316	BzMAI	1-benzyl-2-methyl-3-amyylimidazolium	C <sub>15</sub> H <sub>23</sub> N <sub>2</sub>	231.36
317	DDMI	1-decyl-2,3-dimethylimidazolium	C <sub>15</sub> H <sub>29</sub> N <sub>2</sub>	237.41
325	HBeMI	1-methyl-2-n-heptyl-3-benzyl imidazolium	C <sub>18</sub> H <sub>27</sub> N <sub>2</sub>	271.43
328	DMPPOEMI	1-methyl-2-(2,2-Dimethyl-1-methylene-propyl)-3-(2-phenyl-2-oxyethyl) imidazolium	C <sub>18</sub> H <sub>23</sub> N <sub>2</sub> O	283.39
338	POCPOEI	1-(2,2-dimethylpropionyloxy)-2-ethyl-3-[2-(4-chlorophenyl)-2-oxoethyl]imidazolium	C <sub>18</sub> H <sub>22</sub> ClN <sub>2</sub> O <sub>3</sub>	349.84
332	DNBOMI	1,3-di-[4-nitrobenzyloxy]-2-methyl imidazolium	C <sub>18</sub> H <sub>17</sub> N <sub>4</sub> O <sub>6</sub>	385.36
335	DBBOMI	1,3-di-[4-bromobenzyloxy]-2-methyl imidazolium	C <sub>18</sub> H <sub>17</sub> Br <sub>2</sub> N <sub>2</sub> O <sub>2</sub>	453.15
348	PMOPOEI	1-phenyl-2-methyl-3-[2-(4-methoxy phenyl)-2-oxoethyl]imidazolium	C <sub>19</sub> H <sub>19</sub> N <sub>2</sub> O	291.37
352	BPOEMI	1-benzyl-2-(2-phenyl-2-oxoethyl)-3-methylimidazolium	C <sub>19</sub> H <sub>19</sub> N <sub>2</sub> O	291.37
344	DBHOEI	1,3-dibenzyl-4-(2-hydroxyethyl) imidazolium	C <sub>19</sub> H <sub>21</sub> N <sub>2</sub> O	293.39
351	BMPOEI	1-benzyl-2-methyl-3-3-[2-(4-chloro phenyl)-2-oxoethyl]imidazolium	C <sub>19</sub> H <sub>18</sub> ClN <sub>2</sub> O	325.82
334	PCPOEI	1-phenyloxy-2-ethyl-3-[2-(4-chloro phenyl)-cf2-oxoethyl]imidazolium	C <sub>19</sub> H <sub>18</sub> ClN <sub>2</sub> O <sub>2</sub>	341.82
329	DMNBAl	1,2-dimethyl-3-[2-(4-Nitro-benzoic acid)-benzyl]imidazolium	C <sub>19</sub> H <sub>18</sub> N <sub>3</sub> O <sub>4</sub>	352.37
330	DCBEI	1,3-di-(2,6-dichlorobenzyloxy)-2-ethylimidazolium	C <sub>19</sub> H <sub>17</sub> Cl <sub>4</sub> N <sub>2</sub> O <sub>2</sub>	447.17
336	DDCBEI	1,3-di-(2,4-dichlorobenzyloxy)-2-ethylimidazolium	C <sub>19</sub> H <sub>17</sub> Cl <sub>4</sub> N <sub>2</sub> O <sub>2</sub>	447.17
333	DBBOEI	1,3-di-[4-bromobenzyloxy]-2-ethyl imidazolium	C <sub>19</sub> H <sub>19</sub> Br <sub>2</sub> N <sub>2</sub> O <sub>2</sub>	467.18
326	NBeMI	1-methyl-2-n-nonyl-3-benzylimidazolium	C <sub>20</sub> H <sub>31</sub> N <sub>2</sub>	299.48
324	PvPEMI	1-methyl-2-phenylvinyl-3-[2-phenyl-2-oxyethyl]imidazolium	C <sub>20</sub> H <sub>19</sub> N <sub>2</sub> O	303.38
318	PEStMI	1-phenylethanol-2-styrene-3-methylimidazolium	C <sub>20</sub> H <sub>20</sub> N <sub>2</sub> O	304.39
346	PMCPoEI	1-phenemyl-2-methyl-3-[2-(4-chlorophenyl)-2-oxoethyl]imidazolium	C <sub>20</sub> H <sub>20</sub> N <sub>2</sub> O	304.39
341	BMDI	1-benzyl-2-methyl-3-n-decylimidazolium	C <sub>21</sub> H <sub>33</sub> N <sub>2</sub>	313.51
350	MOBPOEI	1-(4-methoxy-benzyl)-2-methyl-3-[2-(4-methoxyphenyl)-2-oxoethyl]imidazolium	C <sub>21</sub> H <sub>23</sub> N <sub>2</sub> O <sub>2</sub>	335.43
345	BUMI	1-benzyl-2-n-undecyl-3-methylimidazolium	C <sub>22</sub> H <sub>35</sub> N <sub>2</sub>	327.53
331	BOTMOBI	1-benzyloxy-2-ethyl-3-(3,4,5-tri methyloxybenzyl)imidazolium	C <sub>22</sub> H <sub>27</sub> N <sub>2</sub> O <sub>4</sub>	383.47
342	BMTDI	1-benzyl-2-methyl-3-n-tetradecyl imidazolium	C <sub>25</sub> H <sub>41</sub> N <sub>2</sub>	369.61
343	BUAI	1-benzyl-2-n-undecyl-3-amyylimidazolium	C <sub>26</sub> H <sub>43</sub> N <sub>2</sub>	383.64
42	DHMBrl	1,3-dihydroxy-2-methyl-4-bromo imidazolium	C <sub>4</sub> H <sub>6</sub> BrN <sub>2</sub> O <sub>2</sub>	194.01
43	DHPBrI	1,3-dihydroxy-2-phenyl-4-bromo imidazolium	C <sub>9</sub> H <sub>8</sub> BrN <sub>2</sub> O <sub>2</sub>	256.08
41	DEDPhI	1,3-diethyl-4,5-diphenylimidazolium	C <sub>19</sub> H <sub>21</sub> N <sub>2</sub>	277.39
53	DHBrDMI	1,3-dihydroxy-2-bromo-4,5-dimethylimidazolium	C <sub>5</sub> H <sub>8</sub> BrN <sub>2</sub> O <sub>2</sub>	208.03
52	DMBBr <sub>3</sub> I	1,3-dimethyl-2,4,5-tri-bromo imidazolium	C <sub>5</sub> H <sub>6</sub> Br <sub>3</sub> N <sub>2</sub>	333.83
51	M <sub>5</sub> I	1,2,3,4,5-□-methylimidazolium	C <sub>8</sub> H <sub>15</sub> N <sub>2</sub>	139.22
61	C <sub>2</sub> (IBr) <sub>2</sub>	a,ω-dimethyl bromide	C <sub>10</sub> H <sub>18</sub> N <sub>4</sub> Br <sub>2</sub>	354.09
62	C <sub>3</sub> (IBr) <sub>2</sub>	a,ω-dipropyl bromide	C <sub>11</sub> H <sub>20</sub> N <sub>4</sub> Br <sub>2</sub>	368.11
63	C <sub>4</sub> (IBr) <sub>2</sub>	a,ω-dibutyl bromide	C <sub>12</sub> H <sub>22</sub> N <sub>4</sub> Br <sub>2</sub>	382.14
64	C <sub>6</sub> (IBr) <sub>2</sub>	a,ω-dihexyl bromide	C <sub>14</sub> H <sub>26</sub> N <sub>4</sub> Br <sub>2</sub>	410.20
65	C <sub>2</sub> (ITf) <sub>2</sub>	a,ω-dimethylbis((trifluoro methyl)sulfonyl)imides	C <sub>14</sub> H <sub>18</sub> F <sub>12</sub> S <sub>4</sub> O <sub>8</sub> N <sub>6</sub>	754.58
66	C <sub>3</sub> (ITf) <sub>2</sub>	a,ω-diimpropyl bis((trifluoro methyl)sulfonyl)imides	C <sub>15</sub> H <sub>20</sub> F <sub>12</sub> S <sub>4</sub> O <sub>8</sub> N <sub>6</sub>	768.60
67	C <sub>4</sub> (ITf) <sub>2</sub>	a,ω-diimbutyl bis((trifluoro methyl)sulfonyl)imides	C <sub>16</sub> H <sub>22</sub> F <sub>12</sub> S <sub>4</sub> O <sub>8</sub> N <sub>6</sub>	782.63
71	Bt <sub>14</sub>	1-butyl-3-methylbenzotriazolium	C <sub>11</sub> H <sub>16</sub> N <sub>3</sub>	190.27
72	Bt <sub>1 Bn</sub>	1-benzyl-3-methylbenzotriazolium	C <sub>14</sub> H <sub>14</sub> N <sub>3</sub>	224.29
81	P11	N,N-dimethylpyrrolidinium	C <sub>6</sub> H <sub>14</sub> N	100.18

TABLE I. Cations and Anions—Continued

ID	Abbreviation	Name	Formula	M/g mol <sup>-1</sup>
82	P12	N-methyl-N-ethyl-pyrrolidinium	C <sub>7</sub> H <sub>16</sub> N	114.21
83	P13	N-methyl-N-propyl-pyrrolidinium	C <sub>8</sub> H <sub>18</sub> N	128.24
84	P14	N-methyl-N-butyl-pyrrolidinium	C <sub>9</sub> H <sub>20</sub> N	142.26
85	P16	N-methyl-N-hexyl-pyrrolidinium	C <sub>11</sub> H <sub>24</sub> N	170.32
9	PP13	N-methyl-N-propylpiperidinium	C <sub>9</sub> H <sub>20</sub> N	142.26
1001	MP2	1-ethyl-2-methylpyrroliminium	C <sub>7</sub> H <sub>14</sub> N	112.19
1002	MP3	1-propyl-2-methylpyrroliminium	C <sub>8</sub> H <sub>16</sub> N	126.22
1003	MP4	1-butyl-2-methylpyrroliminium	C <sub>9</sub> H <sub>18</sub> N	140.25
1101	C <sub>4</sub> -py	n-butyl pyridinium	C <sub>9</sub> H <sub>14</sub> N	136.22
1109	M <sub>4</sub> B-py	4-methyl-N-butylpyridinium	C <sub>10</sub> H <sub>16</sub> N	150.24
1102	C <sub>6</sub> -py	n-hexyl pyridinium	C <sub>11</sub> H <sub>18</sub> N	164.27
1103	C <sub>8</sub> -py	n-octyl pyridinium	C <sub>13</sub> H <sub>22</sub> N	192.32
1104	C <sub>10</sub> -py	n-decyl pyridinium	C <sub>15</sub> H <sub>26</sub> N	220.38
1105	C <sub>12</sub> -py	n-dodecyl pyridinium	C <sub>17</sub> H <sub>30</sub> N	248.43
1110	C <sub>12</sub> Mpy	1-dodecyl-3-methylpyridinium	C <sub>18</sub> H <sub>32</sub> N	262.46
1111	C <sub>12</sub> M'py	1-dodecyl-4-methylpyridinium	C <sub>18</sub> H <sub>32</sub> N	262.46
1106	C <sub>14</sub> -py	n-tetradecyl pyridinium	C <sub>19</sub> H <sub>34</sub> N	276.49
1112	C <sub>14</sub> Mpy	1-tetradecyl-3-methylpyridinium	C <sub>20</sub> H <sub>36</sub> N	290.51
1113	C <sub>14</sub> M'py	1-tetradecyl-4-methylpyridinium	C <sub>20</sub> H <sub>36</sub> N	290.51
1107	C <sub>16</sub> -py	n-hexadecyl pyridinium	C <sub>21</sub> H <sub>38</sub> N	304.54
1114	C <sub>16</sub> Mpy	1-hexadecyl-3-methylpyridinium	C <sub>22</sub> H <sub>40</sub> N	318.57
1115	C <sub>16</sub> M'py	1-hexadecyl-4-methylpyridinium	C <sub>22</sub> H <sub>40</sub> N	318.57
1108	C <sub>18</sub> -py	n-octadecyl pyridinium	C <sub>23</sub> H <sub>42</sub> N	332.59
1116	C <sub>18</sub> Mpy	1-octadecyl-3-methylpyridinium	C <sub>24</sub> H <sub>44</sub> N <sub>2</sub>	360.63
1117	C <sub>18</sub> M'py	1-octadecyl-4-methylpyridinium	C <sub>24</sub> H <sub>44</sub> N <sub>2</sub>	360.63
1201	C <sub>4</sub> isoq	N-butyl-isoquinolinium	C <sub>13</sub> H <sub>16</sub> N	186.28
1202	C <sub>6</sub> isoq	N-hexyl-isoquinolinium	C <sub>15</sub> H <sub>20</sub> N	214.33
1203	C <sub>8</sub> isoq	N-octyl-isoquinolinium	C <sub>17</sub> H <sub>24</sub> N	242.38
1204	C <sub>10</sub> isoq	N-decyl-isoquinolinium	C <sub>19</sub> H <sub>28</sub> N	270.44
1205	C <sub>12</sub> isoq	N-dodecyl-isoquinolinium	C <sub>21</sub> H <sub>32</sub> N	298.49
1206	C <sub>14</sub> isoq	N-tetradecyl-isoquinolinium	C <sub>23</sub> H <sub>36</sub> N	326.55
1207	C <sub>16</sub> isoq	N-hexadecyl-isoquinolinium	C <sub>25</sub> H <sub>40</sub> N	354.60
1208	C <sub>18</sub> isoq	N-octadecyl-isoquinolinium	C <sub>27</sub> H <sub>44</sub> N	382.65
1301	thia(1)	4-ethyl-2-isopropyl-3-butyl-4,5-dihydro-thiazolium	C <sub>12</sub> H <sub>24</sub> NS	214.40
1302	thia(2)	4-ethyl-2-isopropyl-3-dodecyl-4,5-dihydro-thiazolium	C <sub>20</sub> H <sub>40</sub> NS	326.61
1401	S111	tri-methylsulfonium	C <sub>3</sub> H <sub>9</sub> S	77.17
1402	S222	tri-ethylsulfonium	C <sub>6</sub> H <sub>15</sub> S	119.25
1404	S2222	tetra-methylsulfonium	C <sub>8</sub> H <sub>20</sub> S	148.31
1403	S444	tri-butylsulfonium	C <sub>12</sub> H <sub>27</sub> S	203.41
1501	N1111	tetrammoniummethylammonium	C <sub>4</sub> H <sub>12</sub> N	74.15
1503	N111C <sub>2</sub> H	trimethyl-ethynyl ammonium	C <sub>5</sub> H <sub>10</sub> N	84.14
1502	N1112	trimethylethylammonium	C <sub>5</sub> H <sub>14</sub> N	88.17
1504	N111C <sub>2</sub> O	trimethyl-methoxymethylammonium	C <sub>5</sub> H <sub>14</sub> NO	104.17
1509	N111C <sub>3</sub> '	trimethyl-propargyl ammonium	C <sub>6</sub> H <sub>12</sub> N	98.17
1508	N111C <sub>3</sub>	trimethyl-allylammonium	C <sub>6</sub> H <sub>14</sub> N	100.18
1505	TMPA	trimethylpropylammonium	C <sub>6</sub> H <sub>16</sub> N	102.20
1506	N1113'	trimethyl-isopropylammonium	C <sub>6</sub> H <sub>16</sub> N	102.20
1507	N1122	dimethyl-diethylammonium	C <sub>6</sub> H <sub>16</sub> N	102.20
1510	N112C <sub>2</sub> O	dimethylethylmethoxymethylammonium	C <sub>6</sub> H <sub>16</sub> NO	118.20
1511	MONM <sub>2</sub> E	methoxymethylenedimethylethylammonium	C <sub>6</sub> H <sub>16</sub> NO	118.20
1512	N1123	dimethyl-ethyl-propylammonium	C <sub>7</sub> H <sub>18</sub> N	116.23
1513	N1114	trimethyl-butylammonium	C <sub>7</sub> H <sub>18</sub> N	116.23
1514	N1222	triethyl-methylammonium	C <sub>7</sub> H <sub>18</sub> N	116.23
1515	EOMNM <sub>2</sub> E	ethoxymethylene-dimethyl-ethyl ammonium	C <sub>7</sub> H <sub>18</sub> NO	132.23
1516	MOENM <sub>2</sub> E	methoxyethyl-dimethyl-ethylammonium	C <sub>7</sub> H <sub>18</sub> NO	132.23
1518	TEA	tetraethylammonium	C <sub>8</sub> H <sub>20</sub> N	130.25
1519	BNM <sub>2</sub> E	dimethyl-ethyl-butylammonium	C <sub>8</sub> H <sub>20</sub> N	130.25
1517	EOENM <sub>2</sub> E	ethoxyethyl-dimethyl-ethylammonium	C <sub>8</sub> H <sub>20</sub> NO	146.25
1520	N1134	dimethyl-propyl-butylammonium	C <sub>9</sub> H <sub>22</sub> N	144.28
1521	N6111	trimethyl-hexylammonium	C <sub>9</sub> H <sub>22</sub> N	144.28

TABLE I. Cations and Anions—Continued

ID	Abbreviation	Name	Formula	M/g mol <sup>-1</sup>
1522	N123'3'	methyl-ethyl-dipropylammonium	C <sub>9</sub> H <sub>22</sub> N	144.28
1523	N223'3'	diethyl-di(iso)propylammonium	C <sub>10</sub> H <sub>24</sub> N	158.31
1524	N7111	trimethyl-heptylammonium	C <sub>10</sub> H <sub>24</sub> N	158.31
1525	N8111	trimethyl-octylammonium	C <sub>11</sub> H <sub>26</sub> N	172.33
1526	N2225'	triethyl-(2-methylbutyl)ammonium	C <sub>11</sub> H <sub>26</sub> N	172.33
1527	N3333	tetrapropylammonium	C <sub>12</sub> H <sub>28</sub> N	186.36
1528	N6222	triethyl-hexylammonium	C <sub>12</sub> H <sub>28</sub> N	186.36
1529	N7222	triethyl-heptylammonium	C <sub>13</sub> H <sub>30</sub> N	200.39
1530	N8222	triethyl-octylammonium	C <sub>14</sub> H <sub>32</sub> N	214.41
1531	N723'3'	di(iso)propylethylheptylammonium	C <sub>15</sub> H <sub>34</sub> N	228.44
1532	TBA	tetrabutylammonium	C <sub>16</sub> H <sub>36</sub> N	242.47
1533	N6444	tributyl-hexylammonium	C <sub>18</sub> H <sub>40</sub> N	270.52
1534	N7444	tributyl-heptylammonium	C <sub>19</sub> H <sub>42</sub> N	284.55
1535	N8444	tributyl-octyl ammonium	C <sub>20</sub> H <sub>44</sub> N	298.58
1536	TPA	tetramyl ammonium	C <sub>20</sub> H <sub>44</sub> N	298.58
1537	THA	tetrahexyl ammonium	C <sub>24</sub> H <sub>52</sub> N	354.68
1538	N3888	trioctyl-propyl ammonium	C <sub>27</sub> H <sub>58</sub> N	396.76
1539	ThpA	tetraheptyl ammonium	C <sub>28</sub> H <sub>60</sub> N	410.79
1540	N5 <sub>3</sub> 14	triy-tetradecyl ammonium	C <sub>29</sub> H <sub>62</sub> N	424.82
1541	TOA	tetraoctyl ammonium	C <sub>32</sub> H <sub>68</sub> N	466.90
1542	N6 <sub>3</sub> 14	trihexyl-tetradecyl ammonium	C <sub>32</sub> H <sub>68</sub> N	466.90
1543	N1,12 <sub>3</sub>	tridodecyl-methyl ammonium	C <sub>37</sub> H <sub>78</sub> N	537.03
1544	TDA	tetradecyl ammonium	C <sub>40</sub> H <sub>84</sub> N	579.11
1601	C <sub>13</sub> guan	[bis(butyl-methyl-amino)-methylene] dimethylammonium	C <sub>13</sub> H <sub>30</sub> N <sub>3</sub>	228.40
1602	C <sub>15</sub> guan	[bis(butyl-ethyl-amino)-methylene] dimethyl-ammonium	C <sub>15</sub> H <sub>34</sub> N <sub>3</sub>	256.46
1603	C <sub>19</sub> guan	[bis(bis-butyl-amino)-methylene] dimethyl-ammonium	C <sub>19</sub> H <sub>42</sub> N <sub>3</sub>	312.56
1604	C <sub>23</sub> guan	[bis(bis-hexyl-amino)-methylene] dimethyl-ammonium	C <sub>23</sub> H <sub>50</sub> N <sub>3</sub>	368.67
1605	C <sub>27</sub> guan	[bis(bis-octyl-amino)-methylene] dimethyl-ammonium	C <sub>27</sub> H <sub>58</sub> N <sub>3</sub>	424.78
1701	P1111	tetraphosphonium	C <sub>4</sub> H <sub>12</sub> P	91.11
1702	P2222	tetraethylphosphoniumimethylene-1,4,10,13-tetrakisazacycloheptadecane	C <sub>8</sub> H <sub>20</sub> P	147.22
1703	P1,10 <sub>3</sub>	Tridecylmethylphosphonium	C <sub>31</sub> H <sub>66</sub> P	469.84
1704	P6 <sub>3</sub> 14	trihexyl-tetradecylphosphonium	C <sub>32</sub> H <sub>68</sub> P	483.87
1800	As1111	tetra-methyl arsenic	C <sub>4</sub> H <sub>12</sub> As	135.06
1902	Com2	1,1,6,6-tetramethyl-3-yn-1,6-diazecanediaminium	C <sub>12</sub> H <sub>24</sub> N <sub>2</sub>	196.34
1901	Com1	(z)-1,1,6,6-tetramethyl-3-en-1,6-diazecanediaminium	C <sub>12</sub> H <sub>26</sub> N <sub>2</sub>	198.35
1903	Com3	1,1,6,6-tetramethyl-1,6-diazecanediaminium	C <sub>12</sub> H <sub>28</sub> N <sub>2</sub>	200.37
1904	Com4	N-(2-(((3-hydroxypropyl)dimethylammonio)methyl)benzyl)-3-hydroxy-N,N-dimethylpropyl-1-aminium	C <sub>18</sub> H <sub>34</sub> O <sub>2</sub>	282.47
1905	Com5	(1,4),(1,4),(9,12),(9,12)-tetradimethylene-6-en-1,4,9,12-tetrakisazacyclohexadecane tetraminium	C <sub>20</sub> H <sub>38</sub> N <sub>4</sub>	334.55
1906	Com6	6,8-(1',3'-phenylene)-(1,4),(1,4),(10,13),(10,13)-tetradimethylene-1,4,10,13-tetrakisazacycloheptadecanetetraminium	C <sub>24</sub> H <sub>36</sub> N <sub>4</sub>	380.58
1907	Com7	6,8-(1',3'-phenylene)-(1,4),(1,4),(10,13),(10,13)-tetradimethylene-1,4,10,13-tetrakisazacycloheptadecanetetraminium	C <sub>28</sub> H <sub>48</sub> N <sub>4</sub>	440.72
1908	Com8	6,8-(1',3'-phenylene)-(1,4),(1,4),(10,13),(10,13)-tetradimethylene-1,4,10,13-tetrakisazacyclotricosanetetraminium	C <sub>30</sub> H <sub>52</sub> N <sub>4</sub>	468.77
<b>Zwitterionic-type ionic liquids</b>				
215	ZT1	1-propylsulphonate-3-ethylimidazolium	C <sub>8</sub> H <sub>14</sub> N <sub>2</sub> O <sub>3</sub> S	218.28
223	ZT2	1-trifluoroethylsulfinamidepropyl-3-ethylimidazolium	C <sub>10</sub> H <sub>16</sub> F <sub>3</sub> N <sub>3</sub> O <sub>2</sub> S	299.32
311	ZT3	1-trifluoroethylsulfinamidepropyl-2,3-diethylimidazolium	C <sub>12</sub> H <sub>21</sub> F <sub>3</sub> N <sub>3</sub> O <sub>2</sub> S	328.38
<b>Anions</b>				
011	Cl	chloride	Cl	35.45
014	ClO <sub>4</sub>	perchloric acid	ClO <sub>4</sub>	99.45
012	Br	bromide	Br	79.90

TABLE I. Cations and Anions—Continued

ID	Abbreviation	Name	Formula	M/g mol <sup>-1</sup>
013	I	iodine	I	126.90
021	BF <sub>4</sub>	tetrafluoroborate	BF <sub>4</sub>	86.80
022	CB <sub>11</sub>	1-carbon icosahedral	CB <sub>11</sub> H <sub>12</sub>	143.03
025	MeCB <sub>11</sub>	methylcarbonicosahedral	C <sub>2</sub> B <sub>11</sub> H <sub>14</sub>	157.05
026	EtCB <sub>11</sub>	ethylcarbonicosahedral	C <sub>3</sub> B <sub>11</sub> H <sub>16</sub>	171.08
027	ProCB <sub>11</sub>	propylcarbonicosahedral	C <sub>4</sub> B <sub>11</sub> H <sub>18</sub>	185.11
028	ButCB <sub>11</sub>	butylcarbonicosahedral	C <sub>5</sub> B <sub>11</sub> H <sub>20</sub>	199.13
023	CB <sub>11</sub> Cl	hexachloride-1-carbon icosahedral	CB <sub>11</sub> H <sub>6</sub> Cl <sub>6</sub>	349.70
024	CB <sub>11</sub> Br	hexabromide-1-carbon icosahedral	CB <sub>11</sub> H <sub>6</sub> Br <sub>6</sub>	616.40
0211	BMLB	bis(2-methylactato)borate	C <sub>4</sub> H <sub>12</sub> O <sub>6</sub> B	166.95
0210	0210	bis(oxalato)borate	C <sub>4</sub> O <sub>8</sub> B	186.85
0212	BMB	bis(malonato)borate	C <sub>6</sub> H <sub>4</sub> O <sub>8</sub> B	214.90
0213	BScB	bis(salicylato)borate	C <sub>14</sub> H <sub>8</sub> O <sub>6</sub> B	283.02
0214	BPh <sub>4</sub>	tetraphenylborate	C <sub>24</sub> H <sub>20</sub> B	319.23
0215	BPM	tetrakis-((4-methyl)phenyl)borate	C <sub>28</sub> H <sub>28</sub> B	375.34
0216	BPMF	tetrakis-((4-trifluoromethyl)phenyl)borate	C <sub>28</sub> H <sub>16</sub> F <sub>12</sub> B	591.23
0218	BPSi	tetrakis-((4-trimethylsilyl)phenyl)borate	C <sub>36</sub> H <sub>52</sub> Si <sub>4</sub> B	607.96
0217	BPDMF	tetrakis-(3,5-bis(trifluoromethyl)phenyl) borate	C <sub>32</sub> F <sub>24</sub> H <sub>12</sub> B	863.22
0219	BPSiF	tetrakis-((4-dimethyl-(3,3,3-trifluoro propyl)-silane)phenyl)borate	C <sub>44</sub> H <sub>56</sub> F <sub>12</sub> Si <sub>4</sub> B	936.06
0221	BPSiM	tetrakis-((4-dimeth-heptylsilane)phenyl) borate	C <sub>64</sub> H <sub>108</sub> Si <sub>4</sub> B	1000.71
0220	BPF	tetrakis-((4-perfluorohexyl)phenyl)borate	C <sub>48</sub> H <sub>16</sub> F <sub>52</sub> B	1591.38
029	BARF	tetrakis-(3,5-bis(trifluoromethyl)phenyl) borate	C <sub>72</sub> H <sub>39</sub> B <sub>2</sub> F <sub>48</sub> N <sub>2</sub>	1865.66
0222	BPSiMF	tetrakis-((4-dimeth-perfluoroheptylsilane) phenyl)borate	C <sub>64</sub> H <sub>56</sub> F <sub>52</sub> Si <sub>4</sub> B	1936.22
038	NO <sub>2</sub>	nitrite	NO <sub>2</sub>	46.01
034	N(CN) <sub>2</sub>	dicyanoamides	CN <sub>3</sub>	54.03
039	NO <sub>3</sub>	nitrate	NO <sub>3</sub>	62.00
037	MSI	bis(methylsulfonyl)imides	C <sub>2</sub> H <sub>6</sub> NO <sub>4</sub> S <sub>2</sub>	172.21
035	TSAC	2,2,2-(trifluoromethylsulfonyl)acetamide	C <sub>3</sub> F <sub>6</sub> NO <sub>3</sub> S	244.09
036	PFI	perfluoroethylimide	C <sub>4</sub> F <sub>10</sub> N	252.03
031	TFSI	bis((trifluoromethyl)sulfonyl)imides	C <sub>2</sub> F <sub>6</sub> NO <sub>4</sub> S <sub>2</sub>	280.15
032	TFS'I	bis((trifluoromethyl)sulfonyloxyl) imides	C <sub>2</sub> F <sub>6</sub> NO <sub>6</sub> S <sub>2</sub>	312.15
033	BETI	bis((perfluoroethane)sulfonyl)imides	C <sub>4</sub> F <sub>10</sub> NO <sub>4</sub> S <sub>2</sub>	380.16
042	mesy	mesylate	CH <sub>3</sub> SO <sub>3</sub>	95.10
041	SO <sub>4</sub>	sulfate	SO <sub>4</sub>	96.06
044	TfO'	trifluoromethanesulfonates	CF <sub>3</sub> SO <sub>2</sub>	133.07
043	TfO	trifluoromethanesulfonates	CF <sub>3</sub> SO <sub>3</sub>	149.07
047	Tos	tosylate	C <sub>7</sub> H <sub>7</sub> SO <sub>3</sub>	171.20
048	C <sub>8</sub> S	octylsulfate	C <sub>8</sub> H <sub>17</sub> O <sub>4</sub> S	209.29
046	NfO'	perfluorobutylsulfinate	C <sub>4</sub> F <sub>9</sub> SO <sub>2</sub>	283.09
045	NfO	perfluorobutylsulfonate	C <sub>4</sub> F <sub>9</sub> SO <sub>3</sub>	299.09
052	PO <sub>4</sub>	phosphate	PO <sub>4</sub>	94.97
051	PF <sub>6</sub>	hexafluorophosphate	PF <sub>6</sub>	144.96
063	AcO	acetate	C <sub>2</sub> H <sub>3</sub> O <sub>2</sub>	59.04
061	TA	trifluoroacetates	C <sub>2</sub> F <sub>3</sub> O <sub>2</sub>	113.02
062	HB	heptafluorobutanoates	C <sub>4</sub> F <sub>7</sub> O <sub>2</sub>	213.03
07	Me	tri(trifluoromethylsulfonyl)methyl	C <sub>4</sub> F <sub>9</sub> O <sub>6</sub> S <sub>3</sub>	411.22
082	F(HF) <sub>2,3</sub>	hydrofluoride anions (H <sub>2</sub> F <sub>3</sub> <sup>-</sup> : H <sub>3</sub> F <sub>4</sub> <sup>-</sup> =7:3)	H <sub>2,3</sub> F <sub>3,3</sub>	65.01
081	AlCl <sub>4</sub>	tetrachloroaluminate	AlCl <sub>4</sub>	168.79
085	AsF <sub>6</sub>	hexafluoroarsenic	AsF <sub>6</sub>	188.91
083	NbF <sub>6</sub>	hexafluoroniobium	NbF <sub>6</sub>	206.90
086	SbF <sub>6</sub>	hexafluoroantimony	SbF <sub>6</sub>	235.75
084	TaF <sub>6</sub>	hexafluorotantalum	TaF <sub>6</sub>	294.94

induces weaker electrostatic interaction with imidazolium cation. However, ILs with anions of PF<sub>6</sub> have strong hydrogen bonds for the sake of an F atom and their melting points are comparatively higher. Methylation at C(2) increases the melting point; for example, the melting point of 1-ethyl-2-

methyl imidazolium chloride is 454.15 K, which is much higher than that of 1-ethyl-3-methylimidazolium chloride (360.15 K), this implies that the effect of the van der Waals interaction via a methyl group dominates over the electrostatic interaction via proton on C(2).<sup>97</sup>



TABLE 2. Melting point ( $T_m$ ) and glass transition point ( $T_g$ )

ID	Cation	ID	Anion	$T_g$ (K)	Reference	$T_m$ (K)	Reference		
11	C1HI	011	Cl			345.15	97		
		012	Br	213.15	97	314.15	97		
		014	ClO <sub>4</sub>			430.15	97		
		021	BF <sub>4</sub>			310.15	97		
						325.55	37		
		031	TFSI	189.15	97	282.15	97		
		033	BETI	200.15	97	284.15	97		
		039	NO <sub>3</sub>			343.15	97		
		043	TfO			357.15	97		
		051	PF <sub>6</sub>	269.15	97	389.15	97		
		12	C2HI	011	Cl	216.15	97	331.15	97
012	Br					333.15	97		
014	ClO <sub>4</sub>			192.15	97	294.15	97		
021	BF <sub>4</sub>			186.15	97				
031	TFSI			184.15	97				
033	BETI			187.15	97				
039	NO <sub>3</sub>					343.15	97		
043	TfO					281.15	97		
051	PF <sub>6</sub>			211.15	97				
201	C1MI			011	Cl			398.15	71
								398.15	3
		012	Br			382.65	91		
		021	BF <sub>4</sub>			376.55	37		
		031	TFSI			295.15	18		
		043	TfO			312.15	18		
		047	Tos			372.6	102		
		061	TA			325.15	18		
		202	DMI	011	Cl	187.15	97	454.15	97
				012	Br			449.15	97
				014	ClO <sub>4</sub>	270.15	97	337.15	97
021	BF <sub>4</sub>			176.15	97				
031	TFSI			194.15	97	295.15	97		
033	BETI					288.15	97		
039	NO <sub>3</sub>					357.15	97		
043	TfO					392.15	97		
051	PF <sub>6</sub>					388.15	97		
203	EMI			011	Cl			362.15	52
								360.15	71
						357.15	3		
		012	Br			352.15	52		
						338.05	91		
		013	I			352.15	52		
		021	BF <sub>4</sub>	178	39	288.15	12, 22, 45, and 69		
				181.15	118	279.15	71		
				183.75	96	284.15	52 and 39		
				184	69	285.3	24		
						287.75	96		
						286.15	118		
		022	CB <sub>11</sub>			395.15	48		
		023	CB <sub>11</sub> Cl			387.15	48		
		024	CB <sub>11</sub> Br			412.15	48		
		025	MeCB <sub>11</sub>			332.15	48		
		026	EtCB <sub>11</sub>			337.15	48		
		027	ProCB <sub>11</sub>			318.15	48		
						318.15	98		
		028	ButCB <sub>11</sub>			322.15	48		
		031	TFSI	175.15	84	258.15	39, 24, and 52		

TABLE 2. Melting point ( $T_m$ ) and glass transition point ( $T_g$ )—Continued

ID	Cation	ID	Anion	$T_g$ (K)	Reference	$T_m$ (K)	Reference
				195.15	83	270	18
				186	69	261.15	50 and 95
				175.15	39	252.15	83
						257	69
						270.15	95
						269.15	73
		032	TFS'I			270.15	71
		033	BETI	188	39	272.15	39
						272.15	52
		034	dca	169.15±2	62	252.15±2	62
		035	TSAC			275.75	95
		036	PFI	188.15	84		
		037	MSI			223.15	119
		038	NO <sub>2</sub>			328.15	12 and 73
		039	NO <sub>3</sub>			311.15	71, 12, and 73
203	EMI	041	SO <sub>4</sub>			343.15	73
		043	TfO			263	9
						264	18 and 71
		044	TfO'			264.15	73
		045	NfO			301.15	18
		046	NfO'			301.15	73
		051	PF <sub>6</sub>	193	39	332.15±1	12 and 73
						335.15	39 and 52
						331.15	45 and 83
						332.8	110
		061	TA			259	18
						259.15	37
		063	AcO			259.15	71
						228.15	12 and 73
		007	Me			312.15	52
		081	AlCl <sub>4</sub>			280.15	71
		083	NbF <sub>6</sub>	181	94	272	94
		084	TaF <sub>6</sub>			275	94
		085	AsF <sub>6</sub>			326.15	39
						326.15	52
204	E'MI	011	Cl			451.15	97
		012	Br			417.15	97
		014	ClO <sub>4</sub>	197.15	97	280.15	97
		021	BF <sub>4</sub>	185.15	97		
		031	TFSI	189.15	97		
		033	BETI			254.15	97
		039	NO <sub>3</sub>			348.15	97
		043	TfO			306.15	97
		051	PF <sub>6</sub>	231.15	97		
205	C2OMI	011	Cl	162.15	79		
		012	Br			370.5	91
		021	BF <sub>4</sub>	189.15	79		
		031	TFSI	194.15	84		
		051	PF <sub>6</sub>	201.15	79		
		061	TA	184.15	79		
206	C2F3MI	031	TFSI			233±10	18
206	C2F3MI	043	TfO			318.15	18
207	DEI	031	TFSI			287	18
		043	TfO			296.15	18
		061	TA	233.15	18		
208	C3MI	011	Cl			333.15	4
		021	BF <sub>4</sub>	185.15	118	256.15	118

TABLE 2. Melting point ( $T_m$ ) and glass transition point ( $T_g$ )—Continued

ID	Cation	ID	Anion	$T_g$ (K)	Reference	$T_m$ (K)	Reference
				259.25	37		
		031	TFSI	186.15	118, 83, and 84		
				183.15	52		
		051	PF <sub>6</sub>	199.15	83	313.15	12
						313.15	52
						294.15	83
209	i-C3MI	013	I			387.15	52
		031	TFSI			289.15	52
209	i-C3MI	051	PF <sub>6</sub>			375.15	12
						375.15	52
285	VMI	012	Br			372.65	91
210	C3OMI	011	Cl	213.15	79		
		021	BF <sub>4</sub>	185.15	79		
		031	TFSI	192.15	84	233±1	18
		043	TfO			300.15	18
		051	PF <sub>6</sub>			247.15	79
289	VPI	012	Br			428.15	91
211	C4MI	011	Cl			314.15	63 and 100
						338.15	71 and 4
211	C4MI	011	Cl	197.35	108	341.95	108
		013	I			201.15	63
		021	BF <sub>4</sub>	188.15	118	190.65±0.5	98
				176.15	63 and 100	191	27
				187.85	123	192.15	63, 32, 98, 97, and 118
				192	23	198.15	73
211	C4MI	021	BF <sub>4</sub>	202.15	37		
		029	BARF			378.15±2	113
		0211	BMLB	233.75	123		
		0212	BMB	240.05	123		
		0213	BScB	294.65	123		
		0214	BPh4			399.15	105
		0216	BPMF			425.15	105
		0217	BPD MF			382.15	105
		0219	BPSiF			377.15	105
		0220	BPF			363.15	105
		0221	BPSI	253.15	105		
		0222	BPSIF	263.15	105		
		031	TFSI	169.15	63	269.15	18 and 98
				186.15	83	268.25	123
				187.25	123	267.15	83
				184.15	73		
			TFSI w	171.15	63	248.15	63
		043	TfO	191.55	123	289.15	18
						289.15	98 and 71
						289.55	123
		045	NfO			293	18
		048	C8S			307.5±0.5	102
		051	PF <sub>6</sub>	193.15	63		
211	C4MI	051	PF <sub>6</sub>	196.15	83	283.15	63
				212	23	276.43	110
				196.15	60	277.15	73
				212 g	32	265.15	106
						212.15	98 and 65
			PF <sub>6</sub> w	190.15	63	277.15	63 and 100
				187.15	100		
		061	TA	233.15±10	80	233.15±10	18
							98

TABLE 2. Melting point ( $T_m$ ) and glass transition point ( $T_g$ )—Continued

ID	Cation	ID	Anion	$T_g$ (K)	Reference	$T_m$ (K)	Reference
		062	HB	233.15±10	18		
212	i-C4MI	031	TFSI			233.151	18
214	C4OMI	012	Br	190.15	79		
215	ZT1					423.15	98
216	C5MI	021	BF <sub>4</sub>	185.65 h	37		
				185.15 c	37		
216	C5MI	031	TFSI	188.15	83	264.15	83
		051	PF <sub>6</sub>	193.15	83		
				193.15	60		
217	C4C2I	031	Tf2N			233.15±10	18
		043	TfO			275	18
		045	NfO			294.15	18
		061	TA			233.15±10	18
218	VBI	012	Br			356.15	91
219	MOBMI	011	Cl	187.15	97	444.15	97
		012	Br	243.15	97	396.15	97
		014	ClO <sub>4</sub>	242.15	97		
		021	BF <sub>4</sub>	230.15	97		
		031	TFSI	216.15	97		
		033	BETI	219.15	97		
219	MOBMI	039	NO <sub>3</sub>	242.15	97	325.15	97
		043	TFO	225.15	97		
		005	PF <sub>6</sub>	249.15	97		
220	C5O2MI	011	Cl	188.15	79		
220	C <sub>5</sub> O <sub>2</sub> MI	011	Cl	188.6	120		
		021	BF <sub>4</sub>	187.15	79		
		051	PF <sub>6</sub>	206.3	120		
				204.15	79		
283	ACyI	012	Br			361.65	91
221	C6MI	011	Cl	198.15	63 and 100		
		021	BF <sub>4</sub>	190.75	37		
		031	TFSI	189.15	83		
221	C6MI	051	PF <sub>6</sub>	195.15	63	212.15	32
				193.15	83		
			PF <sub>6</sub> w	198.15	63 and 100		
222	PEMI	012	Br			322.15	91
276	CPCEI	012	Br			423.95	91
227	MAI	012	Br			436.15	91
223	ZT2			212.15	98		
224	C7MI	021	BF <sub>4</sub>	192.75 h	37		
				191.25 c	37		
		031	TFSI	188.15	83	280.15	83
		051	PF <sub>6</sub>	189.15	107		
226	C4C4I	011	Cl			328.15	4
2100	BenMI	012	Br			399.15	91
		031	TFSI	217.15	84 and 83		
		043	TfO			300.15	103
		051	PF <sub>6</sub>			403.15	83
228	MPMI	043	TfO			318.15	103
229	C8MI	011	Cl	186.15	63 and 100	191.15	65
				210.85	108	285.41	108
229	C8MI	011	Cl	224.45	65		
		021	BF <sub>4</sub>	194.65 h	37	193.15	65
				192.65 c	37		
		022	CB11			343.15	48
		023	CB11Cl			340.15	48
		031	TFSI	189.15	83		

TABLE 2. Melting point ( $T_m$ ) and glass transition point ( $T_g$ )—Continued

ID	Cation	ID	Anion	$T_g$ (K)	Reference	$T_m$ (K)	Reference
		051	PF <sub>6</sub>	191.15	63	203.15	65
				202.15	83	198.15	73
			PF <sub>6</sub> w	198.15	63 and 100		
		031	TFSI	189.15	83		
230	C8MI	031	TFSI	214.15	83	310.15	83
		051	PF <sub>6</sub>			376.15	83
231	C8OMI	051	PF <sub>6</sub>			310.65±0.5	70
232	C8OPI	012	Br			422.15	116
233	PBOMI	051	PF <sub>6</sub>			321.15±1	70
286	M3BzMI	012	Br			388.15	114
287	M2BzMI	012	Br			388.15	91
295	EtODBeI	012	Br			390.15	91
293	EONiBeI	012	Br			393.15	91
294	EODBeI	012	Br			407.15	91
2103	EBPOEI	012	Br			471.15	91
234	C9MI	021	BF <sub>4</sub>	195.95 h	37		
				193.15 c	37		
		031	TFSI	190.15	83		
		051	PF <sub>6</sub>	207.15	83	287.15	83
						321.15±1	83
235	C2C8I	047	Tos			343.15±2	102
236	C9'MI	031	TFSI			321.15	83
		051	PF <sub>6</sub>			325.15	83
237	DBOMI	051	PF <sub>6</sub>			330.15±1	70
298	EOPOEI	012	Br			403.15	91
239	C10MI	011	Cl			311.17	108
		021	BF <sub>4</sub>			268.95	37
						195.65	73
		051	PF <sub>6</sub>	202.15	83	305.15	83
						307.15	73
		031	TFSI	190.15	83 and 84	244.15	83
240	MDI	031	TFSI	217.15	83 and 84		
		043	TfO			300.15	103
242	ABOMI	051	PF <sub>6</sub>			311.15±2	70
243	C11MI	021	BF <sub>4</sub>			294.55	37
244	DOMMI	021	BF <sub>4</sub>			329.5±1	70
244	DOMMI	051	PF <sub>6</sub>			319.5±1	70
245	HxBOMI	051	PF <sub>6</sub>			323.15±1	70
288	ABMI	012	Br			389.65	91
246	C12MI	011	Cl			369.78	109
						270.35	78
						369.78	108
			Cl w			317.65	78
		012	Br			267.85	78
			Br w			306.45	78
		021	BF <sub>4</sub>			312.15	65
						299.55	37
						307.15	124
		051	PF <sub>6</sub>			323.15	65
						333.15	31 and 124
		031	TFSI			289.85	78
			TFSI w			289.75	78
		043	TfO			312.85	78
			TfO w			312.05	78
247	UOMMI	021	BF <sub>4</sub>			334.15±1	70
		051	PF <sub>6</sub>			325.5±1	70
248	HpBOMI	051	PF <sub>6</sub>			330.15±1	70

TABLE 2. Melting point ( $T_m$ ) and glass transition point ( $T_g$ )—Continued

ID	Cation	ID	Anion	$T_g$ (K)	Reference	$T_m$ (K)	Reference
277	POCPOEI	012	Br			413.15	91
2104	BODCBI	012	Br			417.15	91
249	C13MI	021	BF <sub>4</sub>			322.25	5
251	C14MI	011	Cl			292.55	78
251	C14MI	011	Cl w			322.25	78
		012	Br			293.95	78
			Br w			319.25	78
251	C14MI	021	BF <sub>4</sub>			315.55	37
						311.15	124
		031	TFSI			307.45	78
			TFSI w			307.85	78
		043	TfO			323.15	78
			TfO w			327.15	78
		051	PF <sub>6</sub>			347.15	31
						346.15	124
252	NBOMI	051	PF <sub>6</sub>			323.15±1	70
2105	PEODCBI	012	Br			411.15	91
253	C15MI	021	BF <sub>4</sub>			328.35	37
2106	PDAOI	012	Br			414.15	91
256	DBOMI	021	BF <sub>4</sub>			289.15±1	70
		051	PF <sub>6</sub>			327.15±1	70
255	C16MI	011	Cl			315.15	78
			Cl w			339.85	78
		012	Br			313.35	78
		012	Br w			339.15	78
		021	BF <sub>4</sub>			322.75	37
						319.15	124
		031	TFSI			315.25	78
			TFSI w			316.25	78
		043	TfO			331.25	78
			TfO w			332.75	78
		051	PF <sub>6</sub>			348.15	31 and 107
						356.15	124
254	DOMHI	021	BF <sub>4</sub>			311.15±1	70
257	UBOMI	021	BF <sub>4</sub>			295.15±1	70
		051	PF <sub>6</sub>			333.15±1	70
258	UOMHI	051	PF <sub>6</sub>			303.15±1	70
259	C18MI	011	Cl			326.35	78
		011	Cl w			344.85	78
		021	BF <sub>4</sub>			339.95	37
		031	TFSI			317.95	78
			TFSI w			317.95	78
		043	TfO			339.15	78
			TfO w			336.95	78
		051	PF <sub>6</sub>			353.15	31
260	C20MI	012	Br			333.35	78
			Br w			349.65	78
261	PEOI-I	011	Cl	199.15	41		
		031	TFSI	201.15	41		
262	PEOII-I	011	Cl	211.15	41		
		031	TFSI	209.15	41		
275	DBI	012	Br			335.65	91
292	FOEMI	012	Br			420.15	91
263	PE(o-F)MI	012	Br			452.15	91
264	CPOEMI	012	Br			449.15	91
265	C'POEMI	012	Br			421.65	91
266	PE(Cl)2MI	012	Br			456.65	91

TABLE 2. Melting point ( $T_m$ ) and glass transition point ( $T_g$ )—Continued

ID	Cation	ID	Anion	$T_g$ (K)	Reference	$T_m$ (K)	Reference
290	MOPOEI	012	Br			429.15	91
267	NPOEMI	012	Br			460.65	91
297	NPEMI	012	Br			458.15	91
268	MOTEI	012	Br			426.15	91
269	MOPOMI	012	Br			430.65	91
270	M'OPOMI	012	Br			439.15	91
2102	HyTMOBI	012	Br			463.15	91
271	PE(Me) <sub>2</sub> MI	012	Br			453.15	91
296	DMPEMI	012	Br			411.65	91
272	PE(Me) <sub>2</sub> MI	012	Br			437.15	91
273	PE(OEt)MI	012	Br			410.65	91
274	POEMI	012	Br			417.65	91
279	PPOMI	012	Br			358.15	91
280	MOOPI	012	Br			451.15	91
2101	MOPOPI	012	Br			420.15	91
298	POPOEI	012	Br			378.15	91
299	HyDBeI	012	Br			388.15	91
337	DHBrI	012	Br			454.15	91
327	DMCII	012	Br			468.65	91
31	M2,4,5I	011	Cl			467.15	52
32	M1,2,3I	011	Cl			462.15	4
33	M1,2E3I	011	Cl			461.15	52
		012	Br			414.15	52
		031	TFSI			293	18
						300.15	52
		033	BETI			298.15	52
		043	TfO			382.15	18
		051	PF <sub>6</sub>			469.15	52
		061	TA			332.15	18
34	E1M3,5I	031	TFSI			270	18
		043	TfO			279	18
35	EDMI	022	CB11			429.15	48
35	EDMI	023	CB11Cl			410.15	48
36	E1,3M4I	043	TfO			308.15	18
		031	TFSI			251	18
37	DMPI	011	Cl			411.15	52
		031	TFSI	192	39	192.15	39
				191.15	52	288.15	52
		033	BETI			307.15	52
		051	PF <sub>6</sub>			351.15	39 and 52
38	E1,2M3I	031	TfSI			301.15	18
		043	TfO			386.15	18
310	BDMI	022	CB11			402.15	48
		023	CB11Cl			374.15	48
322	B3M1,5I	012	Br			383.65	91
311	ZW3			250.15	98		
353	MOEMOI	012	Br			469.15	91
323	DPB'I	012	Br			435.65	91
317	DEMI	012	Br			357.65	91
324	PvPEMI	012	Br			458.15	91
339	HyEPOEI	021	Br			472.15	91
325	HBeMI	012	Br			459.65	91
338	POCPOEI	012	Br			457.15	91
329	DMNBAI	012	Br			496.65	91
330	DCBEI	012	Br			429.15	91
336	DDCBEI	012	Br			449.15	91
326	NBeMI	012	Br			467.15	91

TABLE 2. Melting point ( $T_m$ ) and glass transition point ( $T_g$ )—Continued

ID	Cation	ID	Anion	$T_g$ (K)	Reference	$T_m$ (K)	Reference
332	DNBOMI	012	Br			441.15	91
335	DBBOMI	012	Br			447.15	91
344	DBHOEI	012	Br			408.15	91
348	PMOPOEI	012	Br			478.65	91
334	PCPOEI	012	Br			444.15	91
351	BMPOEI	012	Br			501.65	91
352	BPOEMI	012	Br			512.15	91
333	DBBOEI	012	Br			443.15	91
346	PMCPOEI	012	Br			466.15	91
341	BMDI	012	Br			360.65	91
350	MOBPOEI	012	Br			497.65	91
331	BOTMOBI	012	Br			432.15	91
345	BUMI	012	Br			459.65	91
342	BMTDI	012	Br			376.15	91
343	BUAI	012	Br			389.65	91
349	TPPOEMI	012	Br			478.65	91
41	DEDPhI	021	Br			426.65	91
42	DHMBrI	021	Br			427.15	91
43	DHPBrI	021	Br			431.15	91
51	MSI	013	I			486.15	52
		031	TFSI			391.15	52
		051	PF <sub>6</sub>			439.15	52
53	DHBrDMI	021	Br			425.15	91
61	C2(Im)2	021	Br			500.85	46
		031	TFSI			360.35	46
62	C3(Im)2	021	Br			456.95	46
		031	TFSI			329.55	46
63	C4(Im)2	021	Br			406.75	46
		031	TFSI			324.85	46
64	C6(Im)2	021	Br			450.15	46
71	Bt14	013	I			373.15	114
71	Bt14	031	TFSI	213.15	116	302.15	114
		034	N(CN)2	208.15	114		
		042	mesy	235.15	114	330.15	114
		047	Tos			393.15	114
72	Bt1	012	Br			446.15	114
	Bn	031	TFSI	246.15	114	342.15	114
		034	N(CN)2	239.15	114		
		042	mesy	261.15	114	365.15	114
		047	Tos			416.15	114
81	P11	031	TFSI			405.15±1	38 and 44
						378.15	95
		034	dca			388.15±2	62
		035	TSAC			287.15	95
		037	MSI			215.15	119
		042	mesy			473.15±2	86
		047	Tos			440.15±2	86
82	P12	031	TFSI	171.15	38	359.15±1	38 and 44
						382.15	122
		034	dca			263.15±2	62
		037	MSI			209.15	119
		042	mesy	167.15±2	86	313.15±2	86
		047	Tos			393.15±2	86
83	P13	031	TFSI	183.15±2	38 and 44	285.15±1	38 and 44
				182.15±2	122	279.15	122
		034	dca			238.15±2	62



TABLE 2. Melting point ( $T_m$ ) and glass transition point ( $T_g$ )—Continued

ID	Cation	ID	Anion	$T_g$ (K)	Reference	$T_m$ (K)	Reference
		037	MSI			210.15	119
		042	mesy	201.15±2	86	353.15±2	86
		047	Tos			353.15±2	86
84	P14	0210	BOB	235.35	123		
		031	TFSI	186.15±2	38 and 44	255.15±1	38 and 44
				185.15	122	251.5	122
		034	dca	167.15±2	62	218.15	62
		037	MSI			215.15	119
		042	mesy	205.15±2	86	336.15±2	86
		047	Tos			388.15±2	86
85	P16	034	dca	173.15±2	62	262.15±2	62
		037	MSI			218.15	119
		042	mesy			359.15±2	86
		047	Tos			410.15±2	86
9	PP13	031	TFSI			281.85	121
1001	MP2	031	TFSI			318.15±1	122
1002	MP3	013	I			358.15±1	122
1002	MP3	031	TFSI	201.15±2	122	292.15±1	122
1003	MP4	013	I			384.15±1	122
		031	TFSI	209.15±2	122	309.15±1	122
1101	C4-py	021	BF <sub>4</sub>	206.45	96	288.45	96
				202	69	272	69
		031	TFSI			299	69
		0210	BOB	252.65	123		
1105	C12-py	051	PF <sub>6</sub>			379.15	31
1106	C14-py	051	PF <sub>6</sub>			397.15	31
1107	C16-py	051	PF <sub>6</sub>			399.15	31
1108	C18-py	051	PF <sub>6</sub>			399.15	31
1110	C12Mpy	051	PF <sub>6</sub>			328.15	31
1111	C12M'py	051	PF <sub>6</sub>			329.15	31
1112	C14Mpy	051	PF <sub>6</sub>			341.15	31
1113	C14M'py	051	PF <sub>6</sub>			344.15	31
1114	C16Mpy	051	PF <sub>6</sub>			347.15	31
1115	C16M'py	051	PF <sub>6</sub>			348.15	31
1116	C18Mpy	051	PF <sub>6</sub>			360.15	31
1117	C18M'py	051	PF <sub>6</sub>			361.15	31
1201	C4isoq	033	BETI w	187.95	72	211.15	72
1202	C6isoq	033	BETI w	189.15	72	195.85	72
1203	C8isoq	033	BETI w	193.75	72	205.05	72
1203	C8isoq	033	PF <sub>6</sub> w	218.15	101	281.35	101
1204	C10isoq	033	BETI w	195.35	72	213.85	72
1205	C12isoq	033	BETI w	197.75	72	222.15	72
1206	C14isoq	033	BETI w	206.45	72	223.45	72
1207	C16isoq	033	BETI w	211.35	72	224.55	72
1208	C18isoq	033	BETI w	213.85	72	225.95	72
1301	thia(1)	013	I			410.15	115
		021	BF <sub>4</sub>			384.15	115
		031	TFSI	205.15	115		
		051	PF <sub>6</sub>			439.15	115
1302	thia(2)	051	PF <sub>6</sub>			315.15	115
1401	S111	031	TFSI			317.65	95
						317.65	49
		035	TSAC			305.15	95
		021	BF <sub>4</sub>			490.15	95
1402	S222	031	TFSI			238.15	98
			TFSI			237.65	95 and 49
		035	TSAC			305.15	95

TABLE 2. Melting point ( $T_m$ ) and glass transition point ( $T_g$ )—Continued

ID	Cation	ID	Anion	$T_g$ (K)	Reference	$T_m$ (K)	Reference
1403	S444	031	TFSI			265.65	49
1404	S2222	031	TFSI			391.15	95
		035	TSAC			292.15	95
1501	N1111	031	TFSI			406.15±1	33 and 44
						403.15	95
						409.5±1	76
		035	TSAC			337.15	95
1502	N1112	031	TFSI			382.15±1	44
						378.15	95
		035	TSAC			263.15	95
1504	N111C2O	031	TFSI			277.65	50
		021	BF <sub>4</sub>			319.15	6
1505	TMPA	031	TFSI			295.15	51
						290.15	50
						292.15	95
		035	TSAC			283.15	95
1506	N1113'	031	TFSI			402.15	95
		035	TSAC			302.15	95
1507	N1122	031	TFSI			269.15±1	44
1508	N111C3	031	TFSI			314.15	95
1508	N111C3	035	TSAC			270.25	95
1509	N111C3'	031	TFSI			318.15	95
1510	N112C2H5O	021	BF <sub>4</sub>			257.15	6
1511	MOMNM2E	0210	BOB	240.75	123	323.95	123
1512	N1123	031	TFSI	178.15±2	44	259.15±1	44
1513	N1114	031	TFSI	192.15±2	44	280.15±1	44
1514	N1222	031	TFSI			402.15	95
		035	TSAC			293.15	95
1515	EOMNM2E	0210	BOB	232.95	123	319.85	123
1516	MOENM2E	0210	BOB	237.25	123	321.45	123
1517	EOENM2E	0210	BOB	228.35	123		
1518	TEA	021	BF <sub>4</sub>			345.15	52
		051	PF <sub>6</sub>			343.15	52
		031	TFSI			377.15	52
1512	N1123	031	TFSI	178.15±2	44	259.15±1	44
1513	N1114	031	TFSI	192.15±2	44	280.15±1	44
						378.15	
						382.15±1	
						383.15	
		035	TSAC			296.15	
						293.15	
		033	BETI			356.15	
		007	Me			319.15	
1519	BNM2E	031	TFSI	181.15±2	44	265.15±1	
		021	BF <sub>4</sub>			431.15	
		0210	BOB	228.75	123		
1520	N1134	031	TFSI	190.15±2	44	288.15±1	
						378.15	
1521	N6111	031	TFSI	199.15±2	33 and 44	300.15	
		021	BF <sub>4</sub>			399.15	
1522	N123'3'	031	TFSI			413.15±1	
						413.15±1	44
1523	N223'3'	031	TFSI			421.15±1	33 and 44
1524	N7111	031	TFSI	200.15±2	33 and 44		
1525	N8111	031	TFSI	200.15±2	33 and 44	278.15	95
1526	N2225'	012	Br			373.15	111
		035	TSAC				

TABLE 2. Melting point ( $T_m$ ) and glass transition point ( $T_g$ )—Continued

ID	Cation	ID	Anion	$T_g$ (K)	Reference	$T_m$ (K)	Reference
1527	N3333	031	TFSI			378.15±1	33 and 44
1528	N6222	031	TFSI	192.15±2	33 and 44	293.15±1	33 and 44
1528	N6222	034	dca	191.15±2	62		
		037	MSI			219.15	119
		047	Tos			382.15±2	86
		042	mesy			335.15±2	86
1529	N7222	031	TFSI	194.15±2	33 and 44		
1530	N8222	031	TFSI	199.15±2	33 and 44		
1531	N723'3'	031	TFSI	191.15±2	33 and 44		
1532	TBA	031	TFSI			363.15	52
						364.15	66
						369.15±1	33 and 44
		007	Me			332.15	52
1533	N6444	031	TFSI	205.15±2	33 and 44	299.15±1	33 and 44
		034	dca			230.15	62
		037	MSI			231.15	119
		047	Tos	233.15±2	86	323.15±2	86
1534	N7444	031	TFSI	206.15±2	33 and 44		
		043	TfO	218.15±2	33 and 44		
1535	N8444	031	TFSI	210.15±2	33 and 44		
		043	TfO	216.15±2	33 and 44		
1536	TPA	031	TFSI			298.35	66
1537	THA	021	BF4			360.15	6
		031	TFSI			266.35	66
1538	N3888	012	Br			347.15	111
1539	THpA	031	TFSI			284.35	66
1540	N5314	012	Br			336.15	111
1541	TOA	031	TFSI			304.35	66
1543	N1,123	012	Br			348.15	111
1544	TDA	031	TFSI			303.95	66
1602	C15guan	011	Cl	194.15	117		
		031	TFSI	198.05	117		
		051	PF <sub>6</sub>	205.35	117		
1603	C19guan	011	Cl	217.85	117		
		021	BF4	215.45	117		
1604	C23guan	011	Cl	210.15	117		
		021	BF4	197.55	117		
		031	TFSI	201.75	117		
1604	C23guan	051	PF <sub>6</sub>	212.65	117		
1605	C27guan	011	Cl	197.15	117		
		021	BF4	197.85	117		
		051	PF <sub>6</sub>	195.15	117		
1701	P1111	031	TFSI			423±1	76
1702	P2222	031	TFSI			391.15	95
		035	TSAC			292.15	95
1703	P1,10 <sub>3</sub>	011	Cl			372.05	80
			Cl w			280.75	80
		012	Br			368.35	80
			Br w			269.35	80
		039	NO <sub>3</sub>			332.85	80
1800	As1111	031	TFSI			413.5±2	76
		051	PF <sub>6</sub>	195.15	117		

The melting point is a fundamental physical property of compounds, which has been found to have a wide use in chemical identification.<sup>64</sup> For ILs, melting points have an especially significant meaning because ILs have a large li-

quidus range determined by their low melting points as well as high decomposition points, and the solubility of ILs in water or organic solvents is strongly correlated with their melting points.<sup>8</sup> An estimate of the melting point and solu-

TABLE 3. Freezing points ( $T_f$ )<sup>a</sup>

ID	Cation	ID	Anion	$T_f$ (K)	Reference
201	C1MI	021	BF <sub>4</sub>	346.75	37
203	EMI	011	Cl	306.15	52
		012	Br	303.15	52
		013	I	312.15	52
		021	BF <sub>4</sub>	215.15	118
				222	69
				210.15	52
				222.65	96
		022	CB <sub>11</sub>	392.15	48
		023	CB <sub>11</sub> Cl	382.15	48
		024	CB <sub>11</sub> Br	372.15	48
		031	TFSI	181	69
				223.15	39 and 52
		033	BETI	261.15	39 and 52
		051	PF <sub>6</sub>	278.15	39 and 52
		007	Me	239.15	52
		082	F(HF) <sub>2,3</sub>	183	35
		085	AsF <sub>6</sub>	258.15	39
				240.15	52
208	C3MI	011	Cl	133.15	52
				192.15	52
209	i-C3MI	005	PF <sub>6</sub>	308.15	52
211	C4MI	031	TFSI	257.15	123
		043	TfO	276.05	123
239	C10MI	021	BF <sub>4</sub>	248.45	37
243	C11MI	021	BF <sub>4</sub>	270.65	37
246	C12MI	021	BF <sub>4</sub>	310.15 I-SA	37
				280.55 SA-C	37
249	C13MI	021	BF <sub>4</sub>	290.45 SA-C	37
				364.85 I-SA	37
251	C14MI	021	BF <sub>4</sub>	302.45 SA-C	37
				403.15 I-SA	37
253	C15MI	021	BF <sub>4</sub>	308.15 SA-C	37
				420.65 I-SA	37
255	C16MI	021	BF <sub>4</sub>	445.35 I-SA	37
255	C16MI	021	BF <sub>4</sub>	318.25 SA-C	37
259	C18MI	021	BF <sub>4</sub>	486.55 I-SA	37
				337.65 SA-C	37
				364.85 I-SA	37
31	M2, 4, 5I	011	Cl	441.15	52
33	M1, 2E3I	011	Cl	376.15	52
		012	Br	365.15	52
		031	TFSI	255.15	52
		033	BETI	248.15	52
33	M1, 2E3I	051	PF <sub>6</sub>	466.15	52
35	EDMI	022	CB <sub>11</sub>	428.15	48
		023	CB <sub>11</sub> Cl	399.15	48
37	DMPI	011	Cl	316.15	52
		031	TFSI	143.15	39
		033	BETI	247.15	52
		051	PF <sub>6</sub>	291.15	39 and 52
310	BDMI	022	CB <sub>11</sub>	390.15	48
51	M5I	013	I	396.15	52
		031	TFSI	381.15	52
		051	PF <sub>6</sub>	389.15	52
1101	C4-py	021	BF <sub>4</sub>	261.25	96
				251	69
		031	TFSI	224	69

TABLE 3. Freezing points ( $T_f$ )<sup>a</sup>—Continued

ID	Cation	ID	Anion	$T_f$ (K)	Reference
1114	C16Mpy	051	PF <sub>6</sub>	334.15	31
				331.15	31
1115	C16M'py	051	PF <sub>6</sub>	333.15	31
				328.15	31
				357.15	31
1117	C18M'py	051	PF <sub>6</sub>	350.15	31
				357.15	31
1518	TEA	011	Cl	364.15 ± 1	57
		021	BF <sub>4</sub>	318.15	52
		051	PF <sub>6</sub>	215.15	52
		031	TFSI	371.15	52
		033	BETI	348.15	52
		07	Me	302.15	52
1532	TBA	031	TFSI	341.15	52
		007	Me	307.15	52
1703	P1,10 <sub>3</sub>	011	Cl	374.15	80
			Cl·H <sub>2</sub> O	374.95	80
		012	Br	369.85	80
			Br·H <sub>2</sub> O	369.95	80
		039	NO <sub>3</sub>	335.25	80
			356.95	80	

<sup>a</sup>I-SA, from isotropic liquid to smectic A mesophase and SA-C, from smectic A mesophase to crystal.

bility of an ionic liquid would be most useful before synthesis, or available in sufficient purity for analytical measurements. Researchers have used the QSPR to predict the melting points for different kinds of ILs.<sup>91,92,111,129</sup> The results are listed in Table 6.<sup>130</sup> Due to more available data on bromide systems the research is focused on them. In our work, we attempt to use QSPR models for correlating the melting points of two kinds of (A) disubstituted imidazolium tetrafluoroborates room temperature ionic liquids, and (B) hexafluorophosphates. In our database, there are several entries of melting points for the same compounds. The values which explicitly indicated impurities were discarded and the most recent data entry was used. The same selection policy is applied when we draw other figures. The three-dimensional-optimized structures of cations were obtained using semi-empirical quantum chemical method AM1 programs. Then, the molecular descriptors were calculated using the CODESSA program. The set of molecular descriptors is further treated using the heuristic method to preselect descriptors and the set of best multilinear correlations were found by the best multilinear regression method. Set A was correlated using a three-parameter equation whereas for set B a six-parameter equation was obtained (see Table 7). The melting points of the seven compounds in the test set, which are listed in Table 8, can be predicted by using the two models. Compound Nos. 1–3 are imidazolium tetrafluoroborates, which are predicted by using the three-parameter model and Nos. 4–7 are imidazolium hexafluorophosphates, which are predicted by using the six-parameter model. The two correlations are expected to perform well due to the satisfactory results.

Theoretically, the freezing point occurs at the same temperature as the melting point. Some ILs display substantial

supercooling while being cooled from relatively high temperature. The effect of supercooling for [emim] X<sup>-</sup> is shown in Fig. 3.

Thermal decomposition is strongly dependent on the structure of ILs. With certain ions it is also dependent on the sample pan composition.<sup>52</sup> Different from organic solvents, many kinds of ILs can be kept in the liquid state above 400 °C (with  $T_d$  ranging from 600 to 700 K), which make them have good dynamic properties and excellent catalytic activity. Generally, the imidazolium cations tend to be thermally more stable than the tetra-alkyl ammonium cations. High thermal stability is provided by certain kinds of anions such as TFSI<sup>-</sup>(a31,[(CF<sub>3</sub>SO<sub>2</sub>)<sub>2</sub>N]) and BETI<sup>-</sup>(a33, [C<sub>2</sub>F<sub>5</sub>SO<sub>2</sub>]<sub>2</sub>N]). The relative anion stabilities are PF<sub>6</sub> > BETI > TFSI > CF<sub>3</sub>SO<sub>3</sub> > BF<sub>4</sub> > Me[(CF<sub>3</sub>SO<sub>2</sub>)<sub>3</sub>C]<sup>-</sup> ≫ I, Br, Cl.

#### 4. Density ( $\rho$ ), Viscosity ( $\eta$ ), and Surface Tension ( $\sigma_s$ )

Data on density, viscosity, and surface tension are tabulated in Tables 6–8, respectively. The densities of most of the ILs are bigger than water except for pyrrolidinium dicyanodiamide and guanidinium with density ranging from 0.9 to 0.97 g/cm<sup>3</sup>. In Fig. 4 the density for the three series of ILs decreases as the number of carbon atoms in the alkyl group and sum carbon number for quaternary ammonium ILs increases. It is interesting to note that the density of 1-methylimidazolium ionic liquids decreases linearly with increasing temperature but at a rate less than that for molecular organic solvents.<sup>37</sup>

The trends are reversed for viscosity in Fig. 5. Compared to the conventional organic solution, ILs are viscous liquids

TABLE 4. Decomposition point ( $T_d$ )-w, water equilibrated

ID	Cation	ID	Anion	$T_d$ (K)	Method	Reference
12	C2HI	021	BF <sub>4</sub>	582.15	TGA	97
		031	TFSI	686.15	TGA	97
		033	BETI	675.15	TGA	97
		043	TfO	643.15	TGA	97
203	EMI	011	Cl	558.15	pan:Al	52
				554.15	pan:Al <sub>2</sub> O <sub>3</sub>	52
		012	Br	584.15	pan:Al <sub>2</sub> O <sub>3</sub>	52
		013	I	576.15	pan:Al	52
				583.15	pan:Al <sub>2</sub> O <sub>3</sub>	52
		021	BF <sub>4</sub>	720.15	TGA	118
				685.15		65
				664	TGA	69
				723.15	pan:Al <sub>2</sub> O <sub>3</sub>	52
		031	TFSI	728.15	pan:Al	52
				726.15	pan:Al <sub>2</sub> O <sub>3</sub>	52
				713.15		18
				690	TGA	69
		033	BETI	696.15	pan:Al	52
				735.15	pan:Al <sub>2</sub> O <sub>3</sub>	52
		043	TfO	713.15		18
		051	PF <sub>6</sub>	648.15	pan:Al	52
				754.15	pan:Al <sub>2</sub> O <sub>3</sub>	52
		061	TA	423.15		18
		07	Me	723.15	pan:Al	52
		703.15	pan:Al <sub>2</sub> O <sub>3</sub>	52		
085	AsF <sub>6</sub>	689.15	pan:Al	52		
		703.15	pan:Al <sub>2</sub> O <sub>3</sub>	52		
208	C3MI	011	Cl	555.15	pan:Al	52
				554.15	pan:Al <sub>2</sub> O <sub>3</sub>	52
		021	BF <sub>4</sub>	708.15	TGA	118
		031	TFSI	725.15	pan:Al	52
				726.15	pan:Al <sub>2</sub> O <sub>3</sub>	52
		051	PF <sub>6</sub>	708.15	pan:Al	52
		713.15	pan:Al <sub>2</sub> O <sub>3</sub>	52		
209	i-C3MI	013	I	569.15	pan:Al <sub>2</sub> O <sub>3</sub>	52
209	i-C3MI	031	TFSI	705.15	pan:Al	52
				682.15	pan:Al <sub>2</sub> O <sub>3</sub>	52
		051	PF <sub>6</sub>	705.15	pan:Al	52
				656.15	pan:Al <sub>2</sub> O <sub>3</sub>	52
211	C4MI	011	Cl	527.15	TGA	63 and 100
		013	I	538.15	TGA	63 and 100
		021	BF <sub>4</sub>	676.15	TGA	63 and 100
				633.15	TGA	63
				708.15	TGA	118
				680.15	TGA	73
		0214	BPh4	458.15	TGA	105
		0215	BPM	446.15	TGA	105
		0216	BPMF	548.15	TGA	105
		0217	BPDMF	518.15	TGA	105
		0218	BPSi	523.15	TGA	105
		0219	BPSiF	448.15	TGA	105
		0220	BPF	498.15	TGA	105
		0221	BPSI	443.15	TGA	105
		0222	BPSiF	463.15	TGA	105
		031	TFSI	712.15	TGA	63
				675.15	TGA	73
			TFSI w	667.15	TGA	63
		048	C8S	614.15	TGA	102
		051	PF <sub>6</sub>	622.15	TGA	63

TABLE 4. Decomposition point ( $T_d$ )-w, water equilibrated—Continued

ID	Cation	ID	Anion	$T_d$ (K)	Method	Reference
				663.15	TGA	73
			PF <sub>6</sub> w	633.15	TGA	63 and 100
221	C6MI	011	Cl	526.15	TGA	63 and 100
		051	PF <sub>6</sub>	690.15	TGA	63
			PF <sub>6</sub> w	663.15	TGA	63 and 100
229	C8MI	011	Cl	516.15	TGA	63 and 100
		021	BF <sub>4</sub>	633.15		37
		051	PF <sub>6</sub>	649.15	TGA	63
				689.15	TGA	73
				663.15	TGA	73
229	C8MI	051	PF <sub>6</sub> w	647.15	TGA	63 and 100
31	M2,4,5I	011	Cl	526.15	pan: Al <sub>2</sub> O <sub>3</sub>	52
33	M1,2E3I	011	Cl	560.15	pan: Al	52
				563.15	pan: Al <sub>2</sub> O <sub>3</sub>	52
		012	Br	595.15	pan: Al <sub>2</sub> O <sub>3</sub>	52
		031	TFSI	729.15	pan: Al <sub>2</sub> O <sub>3</sub>	52
		033	BETI	693.15	pan: Al <sub>2</sub> O <sub>3</sub>	52
		051	PF <sub>6</sub>	773.15	pan: Al <sub>2</sub> O <sub>3</sub>	52
37	DMPI	011	Cl	559.15	pan: Al	52
				557.15	pan: Al <sub>2</sub> O <sub>3</sub>	52
		031	TFSI	735.15	pan: Al	52
				735.15	pan: Al <sub>2</sub> O <sub>3</sub>	52
		051	PF <sub>6</sub>	672.15	pan: Al	52
51	M5I	013	I	576.15	pan: Al	52
				606.15	pan: Al <sub>2</sub> O <sub>3</sub>	52
		031	TFSI	743.15	pan: Al	52
				739.15	pan: Al <sub>2</sub> O <sub>3</sub>	52
		051	PF <sub>6</sub>	674.15	pan: Al	52
				760.15	pan: Al <sub>2</sub> O <sub>3</sub>	52
		31	TFSI	729.15	pan: Al <sub>2</sub> O <sub>3</sub>	52
71	Bt14	013	I	438.15	pan: Al	114
		031	TFSI	588.15	pan: Al	114
		034	N(CN) <sub>2</sub>	458.15	pan: Al	114
		042	mesy	473.15	pan: Al	114
		047	Tos	498.15	pan: Al	114
72	Bt1 Bn	012	Br	443.15	pan: Al	114
		031	TFSI	553.15	pan: Al	114
		034	N(CN) <sub>2</sub>	428.15	pan: Al	114
		042	mesy	453.15	pan: Al	114
		047	Tos	478.15	pan: Al	114
1101	C4-py	021	BF <sub>4</sub>	615	TGA	69
		031	TFSI	677	TGA	69
1203	C8isoq	033	PF <sub>6</sub> w	638.15		101
1501	N1111	031	TFSI	653.15		76
1518	TEA	011	Cl	537.15	pan: Al <sub>2</sub> O <sub>3</sub>	52
		051	PF <sub>6</sub>	661.15	pan: Al <sub>2</sub> O <sub>3</sub>	52
				672.15	pan: Al <sub>2</sub> O <sub>3</sub>	52
		033	BETI	696.15	pan: Al	52
				670.15	pan: Al <sub>2</sub> O <sub>3</sub>	52
		07	Me	684.15	pan: Al	52
				670.15	pan: Al <sub>2</sub> O <sub>3</sub>	52
1532	TBA	031	TFSI	676.15	pan: Al	52
				661.15	pan: Al <sub>2</sub> O <sub>3</sub>	52
		07	Me	676.15	pan: Al	52
				671.15	pan: Al <sub>2</sub> O <sub>3</sub>	52
1701	P1111	031	TFSI	693.15		58
1800	As1111	031	TFSI	633.15		58

TABLE 5. Clearing point ( $T_c$ )-w, water equilibrated

ID	Cation	ID	Anion	$T_c$ (K)	Reference				
246	C12MI	011	Cl	377.55	78				
			Cl w	424.85	78				
		012	Br	355.12	78				
			Br w	388.65	78				
			BF <sub>4</sub>	311.65	37				
249	C13MI	021	BF <sub>4</sub>	365.85	37				
		011	Cl	435.65	78				
251	C14MI	012	Cl w	460.85	78				
			Br	436.05	78				
			Br w	449.15	78				
		021	BF <sub>4</sub>	402.65	37				
			PF <sub>6</sub>	350.15	31				
		253	C15MI	021	BF <sub>4</sub>	421.25	37		
				011	Cl	477.15	78		
					Cl w	495.35	78		
		255	C16MI	012	Br	480.65	78		
					Br w	492.85	78		
					BF <sub>4</sub>	455.15	37		
				021	TfO	343.35	78		
					TfO w	344.75	78		
				259	C18MI	051	PF <sub>6</sub>	398.15	31 and 107
						011	Cl w	495.05	78
BF <sub>4</sub>	487.95						37		
043	TfO			380.65	78				
	TfO w			380.55	78				
	PF <sub>6</sub>	438.15	31						
260	C20MI	012	Br w	513.05	78				
1107	C16-py	051	PF <sub>6</sub>	411.15	31				
1108	C18-py	051	PF <sub>6</sub>	449.15	31				
1116	C18Mpy	051	PF <sub>6</sub>	367.15	31				
1703	P1, 10 <sub>3</sub>	011	Cl·H <sub>2</sub> O	375.85	80				
			Br·H <sub>2</sub> O	367.95	80				
		039	NO <sub>3</sub>	355.05	80				

being 1–3 orders of magnitude higher.<sup>34</sup> This high viscosity will negatively affect the operating process. The viscosities of ILs are governed essentially by van der Waals interactions and H bonding. Alkyl chain lengthening or fluorination makes the salt more viscous, due to an increase in van der Waals interactions and hydrogen bonds.<sup>18</sup> Alkyl chain ramification increases the viscosity due to reduced rotation freedom. For example, the viscosity of 1-isobutyl-3-methylimidazolium bis((trifluoromethyl)sulfonyl)imide (212-031, 83cp) is more than three times of the viscosity of 1-butyl-3-methylimidazolium bis((trifluoromethyl)sulfonyl)imide (211-031, 27cp). It is obvious that for certain cations, such as [emim]<sup>+</sup> (c23), the ionic liquids with larger anions show higher viscosities, from trifluoroacetates (a061): 35cp to heptafluorobutanoates (a062):105cp. Although such phenomena or rules cannot be applied to all kinds of ILs, it has been pointed out that for ILs with a cation of 1-ethyl-2-methylimidazolium (c24), the size of component ions has little relation with the viscosity.<sup>22</sup> Methylation at C(2), but not at C(3), increases the viscosity as it does for the melting point, for example, 1-ethyl-3-methylimidazolium tetrafluoroborate (23-021,43cp) compared to 1-ethyl-2-methyl imidazolium tetrafluoroborate (24-021, 67cp). The empirical equa-

tion is also applicable in ionic liquid systems to describe the temperature dependence of the dynamic viscosity for unassociated liquid electrolytes<sup>18</sup>:

$$\eta = Ae^{E/RT}. \quad (1)$$

Temperature and additive are also important factors to influence the viscosity of ILs. The viscosity will decrease obviously when the temperature is subtly improved<sup>3,17,21</sup> or little organic solvent<sup>17,21</sup> is added to ILs.

Available data on the surface tension of ILs are very limited. In general these liquid/air surface tension values are somewhat higher than conventional solvents (e.g., hexane: 1.8 Pa cm), but not so high as water (7.3 Pa cm).<sup>63</sup> Dzyuba and Bartsch reported the influence of the 1-alkyl group on the surface tension of [C<sub>n</sub>MIM]PF<sub>6</sub> and [C<sub>n</sub>MIM]TFSI and pointed surface tension decreases with the increase of the carbon number, and a lower surface tension is found for TFSI<sup>-</sup> salt than the corresponding PF<sub>6</sub><sup>-</sup>.<sup>83</sup> See Figs. 6 and 7.

## 5. Conductivity ( $\sigma$ ), Polarity ( $E_T[30]$ , $E_{NR}$ ), and the Electrochemical Window

Data on conductivity ( $\sigma$ ), polarity [ $E_T(30)$ ,  $E_{NR}$ , and  $E_T^N$ ], and the electrochemical window are tabulated in Tables



TABLE 6. Density ( $\rho$ )—w, water equilibrated<sup>a</sup>

ID	Cation	ID	Anion	$\rho$ [g/cm <sup>3</sup> ]	$t$ (°C)	Method	Reference
11	C1HI	051	PF <sub>6</sub>	1.0316(0.0061)	25		87
201	C1MI	011	Cl	1.1399(0.0074)		DT	4
		031	TFSI	1.559	22		18
203	EMI	011	Cl	1.1362(0.0243)		DT	4
		021	BF <sub>4</sub>	1.28	25	DMR	118
				1.24	22		24
				1.240	22		81
				1.279	25	GM	69
				1.283	20	GM	69
		022	CB <sub>11</sub>	1.067			48
		023	CB <sub>11</sub> Cl	1.431			48
		024	CB <sub>11</sub> Br	2.151			48
		025	MeCB <sub>11</sub>	1.036			48
		026	EtCB <sub>11</sub>	1.05			48
		031	TFSI	1.52	22		18 and 95
				1.519	25	AP	83
				1.51	25		50
				1.518	25	GM	69
				1.523	20	GM	69
		034	dca	1.06(±5%)	25		62
		035	TSAC	1.46	25		95
		037	MSI	1.343		MS	119
		043	TfO	1.38(3)	25		9
		052	PO4	1.98			47
		061	TA	1.285	22		18
		062	HB	1.45	22		18
203	EMI	081	AlCl <sub>4</sub>	1.302	25		81
203	EMI	082	F(HF) <sub>2,3</sub>	1.13	25		88
		083	NbF <sub>6</sub>	1.67	25		94
		084	TaF <sub>6</sub>	2.17	25		94
205	C2OMI	021	BF <sub>4</sub>	1.33	25		79
			TFSI w	1.572	25	AP	84
		051	PF <sub>6</sub>	1.48	25	PM	79
206	C2F3MI	031	TFSI	1.656	20		18
207	DEI	031	TFSI	1.452	21		13
		043	TfO	1.33	22		18
		061	TA	1.25	22		18
208	C3MI	011	Cl	1.1014(0.0265)	DT		4
		021	BF <sub>4</sub>	1.24	25	DMR	118
		031	TFSI	1.475	25	AP	83
			TFSI w	1.473	25	AP	84
210	C3OMI	021	BF <sub>4</sub>	1.26	25	PM	79
		031	TFSI	1.496	22		18
		031	TFSI w	1.509	25	AP	84
		051	PF <sub>6</sub>	1.4	25	PM	79
211	C4MI	011	Cl	1.08	25	GA	63 and 100
				1.1044(0.0218)		DT	4
				1.1			106
		013	I	1.44	25	GA	63 and 100
		021	BF <sub>4</sub>	1.12	25	GA	63 and 100
				1.19	25		73
				1.21	25	DMR	118
211	C4MI	021	BF <sub>4</sub>	1.26	25	PM	79
				1.17			106
				1.17	30		81
		029	BARF	1.544			113
		031	TFSI	1.429	19		98
				1.429	22		1
				1.43	25	GA	63 and 106
				1.436	25	AP	83

TABLE 6. Density ( $\rho$ )—w, water equilibrated<sup>a</sup>—Continued

ID	Cation	ID	Anion	$\rho$ [g/cm <sup>3</sup> ]	$t$ (°C)	Method	Reference
			TFSIw	1.39	25	GA	63
		043	TfO	1.2908	20		18
				1.29	20		98
		045	NfO	1.473	22		11
		051	PF <sub>6</sub>	1.35	25	GA	63 and 100
				1.3669			125
				1.363			60
				1.368	25	AP	83
				1.3603 (0.008)	25		87
				1.37		MS	116
				1.31	25	PM	79
				1.36			106
		061	TA	1.209	21		98
				1.209	22		13
		062	HB	1.333	22		18
		081	AlCl <sub>4</sub>	1.238	25		81
212	i-C4MI	031	TFSI	1.428	20		18
216	C5MI	031	TFSI	1.403	25	AP	83
		051	PF <sub>6</sub>	1.326	25	AP	83
216	C5MI	051	PF <sub>6</sub>	1.333			60
217	C4C2I	031	Tf <sub>2</sub> N	1.404	22		1
		043	TfO	1.27(1)			9
217	C4C2I	045	NfO	1.427	22		11
		061	TA	1.183	22		14
220	C5O2MI	011	Cl	1.14	25	PM	79
		021	BF <sub>4</sub>	1.22	25	PM	79
220	C5O2MI	051	PF <sub>6</sub>	1.32	25	PM	79
221	C6MI	011	Cl	1.03	25	GA	63 and 100
		031	TFSI	1.372	25	AP	83
		051	PF <sub>6</sub>	1.29	25	GA	63
				1.24	25	GA	100
				1.292	25	AP	83
				1.2928			125
				1.3		MS	116
				1.307			60
			PF <sub>6</sub> w	1.24	25	GA	63 and 100
224	C7MI	031	TFSI	1.344	25	AP	83
		051	PF <sub>6</sub>	1.262	25	AP	83
				1.274	25		60
225	C2C6I	051	PF <sub>6</sub>	1.2622			125
226	C4C4I	011	Cl	1.0082(0.0219)		DT	4
		031	TFSI	1.491	25	AP	83
			TFSIw	1.491	25	AP	84
		043	TfO	1.3	30		103
228	MPMI	043	TfO	1.32	50		103
229	C8MI	011	Cl	1	25	GA	63 and 100
229	C8MI	011	Cl	1.0104	25	AP	93
		021	BF <sub>4</sub>	1.08	25	PM	79
		023	CB <sub>11</sub> Cl	1.341			48
		031	TFSI	1.32	25	AP	83
		051	PF <sub>6</sub>	1.22	25	GA	63
				1.2367			125
229	C8MI	051	PF <sub>6</sub>	1.237	25	AP	60 and 83
				1.4	25	AP	73
				1.2245(0.0072)	25		87
				1.2		MS	116
				1.19	25	PM	79
			PF <sub>6</sub> w	1.16	25	GA	63 and 100
230	C8MI	031	TFSI	1.47	25	GA	83
234	C9MI	031	TFSI	1.299	25	AP	83

TABLE 6. Density ( $\rho$ )—w, water equilibrated<sup>a</sup>—Continued

ID	Cation	ID	Anion	$\rho$ [g/cm <sup>3</sup> ]	$t$ (°C)	Method	Reference
		051	PF <sub>6</sub>	1.212	25	AP	83
				1.202			60
235	C2C8I	051	PF <sub>6</sub>	1.2118			125
236	C9'MI	031	TFSI	1.455	25	AP	83
236	C9'MI	051	PF <sub>6</sub>	1.407	25	AP	83
238	C3C8I	051	PF <sub>6</sub>	1.1182			125
239	C10MI	021	BF <sub>4</sub>	1.04	25	PM	79
239	C10MI	031	TFSI	1.271	25	AP	83
			TFSI w	1.271	25	AP	84
33	M1,2E3I	031	TFSI	1.495	22		13
34	E1M3,5I	031	TFSI	1.47	22		18
		043	TfO	1.334	22		5
35	EDMI	022	CB <sub>11</sub>	1.072			48
36	E1,3M4I	031	TFSI	1.432	22		14
310	BDMI	023	CB <sub>11</sub> Cl	1.367			48
83	P13	031	TFSI	1.45 9(±5 %)	20	WV	38, 122, and 44
		034	N(CN) <sub>2</sub>	0.92(±5 %)	25		62
84	P14	031	TFSI	1.41(±5 %)	20	WV	38
							44
		034	N(CN) <sub>2</sub>	0.95(±5 %)	25		62
		037	MSI	1.28		MS	119
85	P16	034	N(CN) <sub>2</sub>	0.92(±5 %)	25		62
1002	MP3	031	TFSI	1.46(±5 %)	20	WV	122
1003	MP4	031	TFSI	1.43(±5 %)	20	WV	122
1101	C4-py	021	BF <sub>4</sub>	1.224	20	GM	69
				1.22	25	GM	69
				1.208	30	GM	69
				1.216	30	GM	69
1101	C4-py	021	BF <sub>4</sub>	1.212	35	GM	69
		031	TFSI	1.453	20	GM	69
				1.449	25	GM	69
				1.444	30	GM	69
		031	TFSI	1.44	35	GM	69
				1.436	40	GM	69
		051	PF <sub>6</sub>	1.2144(0.0072)	25		87
				1.2118(0.0072)	30		87
				1.2053(0.0072)	40		87
				1.1988(0.0072)	50		87
1101	C4-py	051	PF <sub>6</sub>	1.1922(0.0072)	60		87
				1.1856(0.0072)	70		87
1109	M4B-py	021	BF <sub>4</sub>	1.1811	25	AP	90
				1.17194	40	AP	90
1201	C4isoq	033	BETIw	1.23			72
1202	C6isoq	033	BETIw	1.2			72
1203	C8isoq	033	BETIw	1.17			72
1203	C8isoq	051	PF <sub>6</sub> w	1.19			101
1204	C10isoq	033	BETIw	1.09			72
1205	C12isoq	033	BETIw	1.08			72
1206	C14isoq	033	BETIw	1.07			72
1207	C16isoq	033	BETIw	1.05			72
1208	C18isoq	033	BETIw	1.05			72
401	S111	031	TFSI	1.58	45		49
1402	S222	031	TFSI	1.46	25		49
1403	S444	031	TFSI	1.29	25		49
1504	N111C2O	031	TFSI	1.51	25		50
1505	TMPA	031	TFSI	1.44	20,25		51 and 50
		035	TSAC	1.38	25		95
1512	N1123	031	TFSI	1.41	20		44
1513	N1114	031	TFSI	1.41	20		44
1519	BNM2E	031	TFSI	1.37	20		44

TABLE 6. Density ( $\rho$ )—w, water equilibrated<sup>a</sup>—Continued

ID	Cation	ID	Anion	$\rho$ [g/cm <sup>3</sup> ]	$t$ (°C)	Method	Reference
1520	N1134	031	TFSI	1.34	20		44
1521	N6111	031	TFSI	1.33	20	WV	33 and 44
1524	N7111	031	TFSI	1.28	20	WV	33 and 44
1525	N8111	031	TFSI	1.27	20	WV	33 and 44
1528	N6222	031	TFSI	1.27	20	WV	33 and 44
1529	N7222	031	TFSI	1.26	20	WV	33 and 44
1530	N8222	031	TFSI	1.25	20	WV	33 and 44
1531	N723'3'	031	TFSI	1.27	20	WV	33 and 44
1533	N6444	031	TFSI	1.15	20	WV	33 and 44
1534	N7444	031	TFSI	1.17	20	WV	33 and 44
1535	N8444	031	TFSI	1.12	20	WV	33 and 44
		043	TfO	1.02	20	WV	33 and 44
1536	TPA	031	TFSI	1.16	25		66
1537	THA	031	TFSI	1.11	25		66
1539	THpA	031	TFSI	1.1	25		66
1541	TOA	031	TFSI	1.06	25		66
1544	TDA	031	TFSI	1.04	25		66
1602	C15guan	021	BF <sub>4</sub>	1.05	25	PM	117
		031	TFSI	1.36	25	PM	117
1604	C23guan	011	Cl	0.9	25	PM	117
		021	BF <sub>4</sub>	0.97	25	PM	117
		031	TFSI	1.2	25	PM	117
1605	C27guan	011	Cl	0.96	25	PM	117
1903	Com3	052	(PO <sub>4</sub> ) <sub>2</sub>	1.82			47
1904	Com4	052	(PO <sub>4</sub> ) <sub>2</sub>	1.9			47
1905	Com5	052	(PO <sub>4</sub> ) <sub>4</sub>	1.58			47
1906	Com6	052	(PO <sub>4</sub> ) <sub>4</sub>	1.96			47
1907	Com7	052	(PO <sub>4</sub> ) <sub>4</sub>	1.78			47
1908	Com8	052	(PO <sub>4</sub> ) <sub>4</sub>	1.86			47

<sup>a</sup>The number in parenthesis is the standard deviation.

9–11, respectively. The electrochemical window is defined by the reduction of the organic cation and the oxidation of the anion. The polarity of ILs can be measured with solvatochromic dyes, Reichardt's dye, and Nile Red.<sup>84</sup>  $E_T(30)$  are calculated from the absorbance maximum,  $\lambda_{\max}$ , of the CT band of Reichardt's dye 30<sup>74</sup>:

$$E_T(30)/\text{kcal mol}^{-1} = 28591/\lambda_{\max} (\text{nm}). \quad (2)$$

For convenience,  $E_T(30)$  values are often normalized to give a parameter  $E_T^N$ , where  $E_T^N=0.0$  for tetramethylsilane, and 1.0 for water. The  $E_{NR}$  values based on Nile Red.<sup>68</sup>

A wide electrochemical window makes ILs a promising electrolyte for electrochemical power applications.<sup>40</sup> Most ILs have a wide electrochemical window above 4 V. It has been found for some ionic liquids the potential of anode limit proportionally decreases with increasing highest occupied molecular orbit energy calculated for the anion.<sup>20</sup>

Higher conductivity is generally associated with lower viscosity and the order of conductivity values (from high to low) for the imide salts is concordant with the order of the  $T_g$  data (from low to high).<sup>33,122</sup> Bonhôte *et al.*<sup>18</sup> has derived the relation between specific conductivity and anion, cation hydrodynamic radii as well as other physical parameters:

$$\sigma = yF^2 d / (6\pi N_A F W \eta) [(\zeta_a r_a)^{-1} + (\zeta_c r_c)^{-1}]. \quad (3)$$

This includes the "correction" factor  $\zeta$  taking into account the specific interactions between the mobile ions in the melt, their viscosities ( $\eta$ ), formula weight (FW), densities ( $d$ ), and the radii of their ions ( $r_a$  and  $r_c$ ). Furthermore, Vogel-Tammann-Fulcher equation provides a good description of molten salt electrolyte behavior change with temperature:

$$\sigma(T) = \frac{A}{\sqrt{T}} \exp\left(\frac{-B}{T-T_0}\right), \quad (4)$$

where  $A$ ,  $B$ , and  $T_0$  are the frequency factors related to the activation energy, and ideal glass transition temperature, respectively.<sup>44,97</sup>

## 6. Concluding Remarks

The data of physical chemical properties on ionic liquids are essential for both theoretical research and industrial application. The establishment of the database will definitely promote the research and development of ionic liquids. By analyzing the available data in our database, we found that there is a demonstrable lack of data of physical chemical properties and some entries listed several data entries reported from different sources with great deviations. So, more

TABLE 7. Viscosity ( $\eta$ )-w, water equilibrated

ID	Cation	ID	Anion	$\eta$ /cp	$t$ (°C)	Method	Reference
11	C1HI	013	I	1800			22
		031	TFSI	81	25	dv	97
		033	BETI	218	25	dv	97
12	C2HI	014	ClO <sub>4</sub>	112	25	dv	97
		021	BF <sub>4</sub>	41	25	dv	97
		031	TFSI	54	25	dv	97
		033	BETI	133	25	dv	97
		043	TfO	58	25	dv	97
		051	PF <sub>6</sub>	550	25	dv	97
201	C1MI	021	BF <sub>4</sub>	67	25	dv	97
		031	TFSI	44	20	dv	18
				100	25	dv	97
		033	BETI	186	25	dv	97
202	DMI	021	BF <sub>4</sub>	100	25	dv	97
				154	25		55
				91.4	28		55
		031	TFSI	100	25	dv	97
		021	BF <sub>4</sub>	43	26±1	dv	39
203	EMI			37	25	ov	118
				66.5	25		55
				37.7	22		24
				43	28		55
		031	TFSI	34	20	dv	18
					20		98
					25	vc	95
							50 and 67
				32.1	20	pv	112
				28	26±1	pv	39
203	EMI	033	BETI	61	26±1	pv	39
		034	N(CN) <sub>2</sub>	21(±5%)	25		62
		035	TSAC	24	25	vc	95
		037	MSI	787	20	vc	119
		043	TfO	42.7	25		9
				15	80	pv	39
		061	TA	35	20	dv	18
		062	HB	105	20	dv	18
		063	AcO	162	20	dv	18
203	EMI	082	F(HF) <sub>2,3</sub>	4.9	25		88
				4.8	25		67
		083	NbF <sub>6</sub>	49	25	vc	94
		084	TaF <sub>6</sub>	51	25	vc	94
205	C2OMI	021	BF <sub>4</sub>	90.9	20	dv	79
				70.9	30	dv	79
				157.6	10	dv	79
205	C2OMI	051	PF <sub>6</sub>	148.8	20	dv	79
				82.7	30	dv	79
				279.5	10	dv	79
206	C2F3MI	031	TFSI	248	20	dv	18
207	DEI	031	TFSI	35	20	dv	18
		043	TfO	53	20	dv	18
		061	TA	43	20	dv	18
208	C3MI	021	BF <sub>4</sub>	103	25	ov	118
		051	PF <sub>6</sub>	312	25		32
				450	25		104
				371	25		39

TABLE 7. Viscosity ( $\eta$ )-w, water equilibrated—Continued

ID	Cation	ID	Anion	$\eta$ /cp	$t$ (°C)	Method	Reference		
				204	28		39		
210	C3OMI	021	BF <sub>4</sub>	262.8	20	dv	79		
				138	30	dv	79		
				374.3	10	vc	79		
				54	20	dv	18		
			043	TfO	74	20	dv	18	
			051	PF <sub>6</sub>	148.1	30	dv	79	
					607.5	10	dv	79	
					283.6	20	dv	79	
211	C4MI	013	I	1110	25	vc	63 and 100		
		021	BF <sub>4</sub>	219	25	vc	63 and 100		
				180	25	ov	118		
				219	25		73		
				185.9	10	dv	79		
				233	30		98 and 28		
				233	20		106		
				65.2	30		79		
				91.4	30		55		
				104.9	20		79		
				154.0	20		55		
		031	TFSI	52	20	dv	18 and 98		
				54.5	25		73		
				69	25	vc	63		
				57.6	20	pv	112		
		031	TFSIw	27	25	vc	63		
043	TfO	90	20	dv	18				
		90	20		98				
211	C4MI	045	NfO	373	20	dv	18		
		048	C8S	874.5	20	vc	102		
				207	45	vc	102		
				152.3	50	vc	102		
				051	PF <sub>6</sub>	450	25	vc	63
						312	25		73
						393	25		116
						308.3	20	dv	79
						312	30		32 and 98
						172.8	30	dv	79
						615.0	10	dv	79
						285.83±6.08	20	dv	59
				207±11.12	25	dv	59		
				152.67±0.82	31	dv	59		
				116.33±5.5	35	dv	59		
				94.32±0.29	40	dv	59		
				73.35±0.64	45	dv	59		
58.02±1.42	50	dv	59						
45.93±0.72	55	dv	59						
40.4±0.89	60	dv	59						
34.6±0.17	65	dv	59						
28.53±0.81	70	dv	59						
		PF <sub>6</sub> w	397	25	vc	63 and 100			
	061	TA	73	20	dv	18 and 98			
	062	HB	182	20	dv	18			
212	i-C4MI	031	TFSI	83	20	dv	18		
217	C4C2I	031	TFSI	48	20	dv	18		
				045	NfO	323	20	dv	18

TABLE 7. Viscosity ( $\eta$ )-w, water equilibrated—Continued

ID	Cation	ID	Anion	$\eta$ /cp	$t$ (°C)	Method	Reference		
219	MOBMI	031	TFSI	252	25	dv	97		
		033	BETI	552	25	dv	97		
220	C5O2MI	011	Cl	613.4	20	vc	79		
				283.7	30	vc	79		
				1515.8	10	vc	79		
		021	BF <sub>4</sub>	377	20	vc	79		
				189.2	30	vc	79		
				860.4	10	vc	79		
		051	PF <sub>6</sub>	425.8	20	vc	79		
				212.3	30	vc	79		
		220	C5O2MI	051	PF <sub>6</sub>	1034.9	10	vc	79
		221	C6MI	011	Cl	716	25	vc	63 and 100
021	BF <sub>4</sub>					314	25		55
						314	20		89
						177	28		55
031	TFSI					22.6	80		89
				87.3	20		89		
051	PF <sub>6</sub>			10.5	80		89		
				560	25		116		
				585	25	vc	63		
				690	20		89		
				363	28		55		
				37.6	80		89		
229	C8MI			011	Cl	PF <sub>6</sub> w	45225	vc	63 and 100
		337	25			vc	63 and 100		
		337	20			dv	79		
		135	20			dv	79		
		119.3	20			pv	112		
		051	PF <sub>6</sub>	682	25	vc	63		
				710	25		116		
				425.2	30	vc	79		
				452.0	28		55		
				294.3	10	vc	79		
239	C10MI	031	TFSI	866			55		
				857.4	20	vc	79		
				866.0	20		55		
				1922.4	10	vc	79		
				506	25	vc	63 and 100		
		021	BF <sub>4</sub>	416.6	20	dv	79		
				223.1	30	dv	79		
				846.3	10	dv	79		
				152.8	20	pv	112		
				88	20	dv	18		
34	E1M3,5I	031	TFSI	37	20	dv	18		
043		TfO	51	20	dv	18			
36	E1,3M4I	031	TFSI	36	20	dv	18		
37	DMPI	031	TFSI	60	26±1	pv	39		
		051	PF <sub>6</sub>	34	100	pv	39		
38	E1,2M3I	031	TfSI	88	20	dv	18		
42	E1,3M3,5I	043	TfO	51	20	mv	18		
81	P11	031	TFSI	63(±5%)	25	vc	38 and 44		
		035	TSAC	80	25	vc	95		
83	P13	034	dca	45(±5%)	25		62		
84	P14	031	TFSI	85(±5%)	25	vc	38 and 44		
				85(±5%)	25	vc	122		

TABLE 7. Viscosity ( $\eta$ )-w, water equilibrated—Continued

ID	Cation	ID	Anion	$\eta$ /cp	$t$ (°C)	Method	Reference
				70	25		50
84	P14	034	N(CN) <sub>2</sub>	509(±5%)	25		62
		037	MSI	1680	20	vc	119
85	P16	034	dca	45(±5%)	25		62
9	PP13	031	TFSI	117	25		121
1001	MP2	031	TFSI	57(±5%)	25	vc	122
		031	TFSI	58(±5%)	25	vc	122
1101	C4-py	031	TFSI	9.9	80		89
1102	C6-py	021	BF <sub>4</sub>	240.9	20		89
				15.7	80		89
1102	C6-py	031	TFSI	53.8	20		89
				5.9	80		89
1103	C8-py	031	TFSI	134.4	20		89
				13.5	80		89
1104	C10-py	031	TFSI	160.1	20		89
				15	80		89
1107	C16-py	031	TFSI	29.4	80		89
1109	M4C4-py	021	BF <sub>4</sub>	80.85	40	vc	90
				50.22	50	vc	90
1401	S111	031	TFSI	44	45	vc	49
1402	S222	031	TFSI	30	25	vc	98 and 49
		035	TSAC	80	25	vc	95
1403	S444	031	TFSI	75	25		49
1404	S2222	035	TSAC	50	25	vc	95
1502	N1112	035	TSAC	51	25	vc	95
1504	N111C2O	031	TFSI	50	25		50
1505	TMPA	031	TFSI	72	25		51 and 50
				72.69	25	vc	95
1505	TMPA	035	TSAC	45	25	vc	95
1506	N1113'	035	TSAC	108	25	vc	95
1508	N111C3	035	TSAC	42	25	vc	48
1509	N111C3'	035	TSAC	65	25	vc	95
1512	N1123	031	TFSI	83(±5%)	25	vc	44
1513	N1114	031	TFSI	116(±5%)	25	vc	44
1514	N1222	035	TSAC	61	25	vc	95
1519	BNM2E	031	TFSI	110(±5%)	25	vc	44
1520	N1134	031	TFSI	170(±5%)	25	vc	44
1521	N6111	031	TFSI	153(±5%)	25	vc	33 and 44
				132	25	vc	95
1521	N6111	035	TSAC	119	25	vc	95
1524	N7111	031	TFSI	153(±5%)	25	vc	33 and 44
1525	N8111	031	TFSI	181(±5%)	25	vc	33 and 44
				156	25	vc	95
			TSAC	151	25	vc	95
1526	N2225'	035	TSAC	80	25	vc	95
1528	N6222	031	TFSI	167(±5%)	25	vc	33 and 44
1528	N6222	031	TFSI	220	20	pv	112
1529	N7222	031	TFSI	75.5(±5%)	25	vc	33 and 44
1530	N8222	031	TFSI	202(±5%)	25	vc	33 and 44
1531	N723'3'	031	TFSI	362(±5%)	25	vc	33 and 44
1533	N6444	031	TFSI	595(±5%)	25	vc	33 and 44
1534	N7444	031	TFSI	606(±5%)	25	vc	33 and 44
1535	N8444	031	TFSI	574(±5%)	25	vc	33 and 44
		043	TfO	2030(±5%)	25	vc	33 and 44
1536	TPA	031	TFSI	430	25		66



TABLE 7. Viscosity ( $\eta$ )-w, water equilibrated—Continued

ID	Cation	ID	Anion	$\eta$ /cp	$t$ (°C)	Method	Reference
1537	THA	031	TFSI	435	25		66
1537	THA	031	TFSI	453	25		66
1541	TOA	031	TFSI	>500	25		66
1542	N <sub>6</sub> 14	011	Cl	24.69	20		77
				1288	-20		77
				414.8	-10		77
				144	0		77
				56.03	10		77
				11.84	30		77
				6.09	40		77
				3.37	50		77
				2.08	60		77
				1.25	70		77
				0.85	80		77
				0.58	90		77
				0.41	100		77
1544	TDA	031	TFSI	>500	25		66
		031	TFSI	346	25	vc	117
1604	C23gua	031	TFSI	335	30	vc	117
				296	35	vc	117
				269	40	vc	117
				182	50	vc	117
				124	60	vc	117
1704	P <sub>6</sub> 14	031	TFSI	165	20		88
				14.1	80		88

TABLE 8. Surface tension ( $\sigma_s$ )-w, water equilibrated

ID	Cation	ID	Anion	$\sigma_s$ (Pa cm)	at. %	Method	Reference
202	DMI	021	BF <sub>4</sub>	4.66	25	TM	63
211	C4MI	013	I	5.47	25	TM	63 and 100
		021	BF <sub>4</sub>	4.66	25	TM	63 and 100
				3.84	63	TM	65
		031	TFSI	3.75	25	TM	63
			TFSIw	3.68	25	TM	63
		051	PF <sub>6</sub>	4.88	25	TM	63
				4.98	25	TM	100
				4.29	63	TM	65
			PF <sub>6</sub> w	4.98	25	TM	63
221	C6MI	11	Cl	4.25	25	TM	63 and 100
		51	PF <sub>6</sub>	4.34	25	TM	63
			PF <sub>6</sub> w	3.68	25	TM	63
227	BenMI	031	TFSI	4.08	25	CRM	85
229	C8MI	011	Cl	3.38	25	TM	63 and 100
				3.05	63	TM	65
		012	Br	3.2	63	TM	65
		021	BF <sub>4</sub>	2.98	63	TM	65
		051	PF <sub>6</sub>	3.65	25	TM	63
				3.28	63	TM	65
			PF <sub>6</sub> w	3.42	25	TM	63 and 100
230	C8pMI	031	TFSI	4.21	25	CRM	83
236	C9'MI	031	TFSI	4.35	25	CRM	83
		051	PF <sub>6</sub>	3.3	25	CRM	83
246	C12MI	021	BF <sub>4</sub>	2.52	63	TM	65
		051	PF <sub>6</sub>	2.36	63	TM	65

TABLE 9. Conductivity

ID	Cation	ID	Anion	$\sigma_c$ (S/m)	$t$ ( $^{\circ}\text{C}$ )	Reference
201	C1MI	011	Cl	$11.874^{\pm 1.017}$	25	4
		031	TFSI	0.84	20	18
204	EMI	011	Cl	0.343–3.709	25	4
			BF <sub>4</sub>	1.16a	20	24
				1.22b	20	24
				1.3	22	25
				1.31	25	24
				1.38	25	24
				1.4	25	118
				1.58	25	40
				1.3	26 $\pm$ 1	32
				1.44a	30	24
				1.54b	30	24
				1.63a	35	24
				1.74b	35	24
				1.8a	40	24
				1.99b	40	24
				2.29a	50	24
				2.55b	50	24
				2.6a	60	24
				2.95b	60	24
				3.05a	70	24
	3.65b	70	24			
	3.65a	80	24			
	4.35b	80	24			
	4.05a	90	24			
	5.2b	90	24			
204	EMI	021	BF <sub>4</sub>	4.55a	100	24
				5.9b	100	24
		031	TFSI	0.86	22	25
				0.84	26 $\pm$ 1	39
				0.88	20	18
				0.108	25	24
				0.92	25	50
				0.921	25	95
		033	BETI	0.34	26 $\pm$ 1	39
		035	TSAC	0.978	25	95
		037	MSI	0.017	25	119
		043	TfO	1.1	22	25
				0.92(9)	25	9
				0.86	20	18
051	PF <sub>6</sub>	0.13	22	25		
		0.52	26 $\pm$ 1	39		
204	EMI	052	PO <sub>4</sub>	2.2	25	47
		052	PO <sub>4</sub>	3	40	47
				3.7	60	47
				0.96	20	18
		061	TA	0.96	20	18
		062	HB	0.27	20	18
		063	AcO	0.28	20	18
		007	Me	0.13	22	25
		082	F(HF) <sub>2,3</sub>	12	25	35
		083	NbF <sub>6</sub>	0.85	25	94
084	TaF <sub>6</sub>	0.71	25	94		

TABLE 9. Conductivity—Continued

ID	Cation	ID	Anion	$\sigma_c$ (S/m)	$t$ (°C)	Reference
206	C2F3MI	031	TFSI	0.098	20	18
207	DEI	031	TFSI	0.85	20	18
		043	TfO	0.75	20	18
		061	TA	0.74	20	18
208	C3MI	011	Cl	0.332– 4.969	25	4
		021	BF <sub>4</sub>	0.59	25	118
		031	TFSI	0.252	25	16
210	C3OMI	031	TFSI	0.42	20	18
		043	TfO	0.36	20	18
		011	Cl	0.218– 1.002	25	4
		021	BF <sub>4</sub>	0.173	25	32 and 98
				0.35	25	118
211	C4MI	031	TFSI	0.39	20	18 and 98
		043	TfO	0.37	20	18
					20	98
		045	NfO	0.045	20	18
		051	PF <sub>6</sub>	0.1	25	32
				0.146	25	32 and 98
		061	TA	0.32	20	18
					20	98
		062	HB	0.1	20	18
212	i-C4MI	031	TFSI	0.26	20	18
217	C4C2I	031	TFSI	0.41	20	18
		043	TfO	0.27	20	18
				0.27	25	94
		045	NfO	0.053	20	18
		061	TA	0.25	20	18
226	C4C4I	011	Cl	0.221–0.297	25	4
255	C16MI <sub>m</sub>	051	PF <sub>6</sub>	0.002	65	107
				0.063	79	107
				0.26	100	107
				0.25	120	107
261	PEOI-I	031	TFSI	0.0551	30	41
262	PEOII-I	031	TFSI	0.012	30	41
33	M1,2E3I	031	TFSI	0.32	20	18
34	E1M3,5I	031	TFSI	0.66	20	18
		043	TfO	0.64	20	18
	E1,3M4I	031	TFSI	0.62	20	18
37	DMPI	021	BF <sub>4</sub>	0.522	22	99
		031	TFSI	0.3	26±1	39
				0.252	25	16
		051	PF <sub>6</sub>	0.05	35	39
		007	Me	0.046	25	16
		081	AlCl <sub>4</sub>	0.71		16
39	P1M2,3I	031	TfSI	0.252	25	16
		07	Me	0.046	25	16
313	BzMPI	031	TFSI	0.0059	20	30
314	BzMBI	031	TFSI	0.0027	20	30
315	BzMB'I	031	TFSI	0.0037	20	30
316	BzMAI	031	TFSI	0.0029	20	30
83	P13	031	TFSI	0.14	25	38 and 44

TABLE 9. Conductivity—Continued

ID	Cation	ID	Anion	$\sigma_c$ (S/m)	$t$ (°C)	Reference
84	P14	031	TFSI	0.22	25	38 and 44
				0.29	25	50
				0.007	25	119
9	PP13	031	TFSI	0.151	25	121
1401	S111	031	TFSI	0.82	45	49
1402	S222	031	TFSI	0.71	25	49
1403	S444	031	TFSI	0.14	25	49
1504	N111C2O	031	TFSI	0.47	25	50
1505	TMPA	031	TFSI	0.327	25	51
				0.33	25	50 and 95
		035	TSAC	0.434	25	95
1512	N1123	031	TFSI	0.12 $\pm$ 5%	25	44
1513	N1114	031	TFSI	0.14 $\pm$ 5%	25	44
1519	BNM2E	031	TFSI	0.12 $\pm$ 5%	25	44
1520	N1134	031	TFSI	0.082 $\pm$ 5%	25	44
1521	N6111	031	TFSI	0.043 $\pm$ 5%	25	33 and 44
1524	N7111	031	TFSI	0.04 $\pm$ 5%	25	33 and 44
1525	N8111	031	TFSI	0.035 $\pm$ 5%	25	33 and 44
1528	N6222	031	TFSI	0.067 $\pm$ 5%	25	33 and 44
1529	N7222	031	TFSI	0.051 $\pm$ 5%	25	33 and 44
1530	N8222	031	TFSI	0.033 $\pm$ 5%	25	33 and 44
1531	N723'3'	031	TFSI	0.031 $\pm$ 5%	25	33 and 44
1533	N6444	031	TFSI	0.016 $\pm$ 5%	25	33 and 44
				0.005	25	119
1534	N7444	031	TFSI	0.016 $\pm$ 5%	25	33 and 44
1535	N8444	031	TFSI	0.013 $\pm$ 5%	25	33 and 44
				0.0017 $\pm$ 5%	25	33 and 44
1525	N8111	031	TFSI	0.035 $\pm$ 5%	25	33 and 44
1901	Com1	052	PO <sub>4</sub>	5.3	25	47
				5.6	40	47
				7.1	60	47
1902	Com2	052	PO <sub>4</sub>	3.8	25	47
				5.2	40	47
				5	60	47
1903	Com3	052	PO <sub>4</sub>	6.3	25	47
				6	40	47
				7.1	60	47
1904	Com4	052	PO <sub>4</sub>	4.2	25	47
				5.3	40	47
				6.7	60	47
1905	Com5	052	PO <sub>4</sub>	6.4	25	47
				8.1	40	47
				8.7	60	47
1906	Com6	052	PO <sub>4</sub>	2.6	25	47
				2.7	40	47
				4.2	60	47
1907	Com7	052	PO <sub>4</sub>	5.7	25	47
				6.3	40	47
				6.1	60	47
1908	Com8	052	PO <sub>4</sub>	6.3	25	47
				5.2	40	47
				8.2	60	47

TABLE 10. Polarity [ $E_T(30)$ ]-w, water equilibrated

ID	Cation	ID	Anion	[ $E_T(30)$ ] (kcal/mol)	$t$ (°C)	Reference
203	EMI	031	TFSI	52.6		85
205	C2OMI	031	TFSI	60.8		84
			TFSI w	61.4		84
208	C3MI	031	TFSI	51.9		84
			TFSI w	52		84
210	C3OMI	031	TFSI w	54.1		84
211	C4MI	021	BF <sub>4</sub>	52.5		68
		0221	BPSiM			
		0222	BPSiMF			
		031	TFSI	51.5		68
				50		85
		043	TfO	52.3		68
		051	PF <sub>6</sub>	52.3		68
				52.5		61
				53.2	10	75
				52.9	20	75
				52.6	30	75
				52.4	40	75
				52.1	50	75
				51.9	60	75
				51.6	70	75
			PF <sub>6</sub> w	55.7	10	75
				55.2	20	75
				54.8	30	75
				54.3	40	75
				53.9	50	75
				53.5	60	75
				53.1	70	75
227	BenMI	031	TFSI	52.4		84
229	C8MI	031	Tf2N	51.1		68
		051	PF <sub>6</sub>	51.2		68
239	C10MI	021	BF <sub>4</sub>			
		031	TFSI w	51		84
310	BDMI	031	TFSI	48.6		68
312	ODMI	021	BF <sub>4</sub>	48.3		68
		031	TFSI	47.7		68

TABLE 11. Electrochemical window

ID	Cation	ID	Anion	Elec. win (V)	Cathode limit (V)	Anode limit (V)	<i>t</i> (°C)	Method	Reference				
204	EMI	011	Cl	5	-3	2			19				
		021	BF <sub>4</sub>	4.3	-2.1	2.2		P/G	24				
						2.33		P/G	25				
		031	TFSI	4.3	-1.8	2.5		CV	18				
						2.49		P/G	25				
						2.54		CV	112				
				4.78	-2.24	2.1		CV	39				
				4.1	-2	2.1		CV	39				
				033	BETI	4.1	-2	2.1		CV	39		
				037	MSI	2.5	-1.5	1		CV	119		
				043	TfO	4.1	-2.2	1.9		CV	9		
		4.1	-1.8			2.3		CV	18				
		061	TA	3.4	-1.8	1.6		CV	18				
				07	Me			2.77		P/G	25		
082	F(HF)2.3			3.3	-0.8	2.5		CV	35				
						1.7			66				
				3.2	-1.5	1.7							
						4.5							
211	C4MI	021	BF <sub>4</sub>	6.1	-1.6	4.5		LV	27				
				5.45	-1.8	3.65		LV	27				
211	C4MI	021	BF <sub>4</sub>	4.2	-1.85	2.35		LV	27				
				4.6	-1.6	3		LV	27				
				4	-1.5	2.5		LV	27				
				4.1	-1.6	2.5	22±2	CV	54				
				1.95	1.02	-0.93	22±2	CV	54				
				031	TFSI	4.76	-2.04	2.72		CV	112		
				051	PF <sub>6</sub>	4.76	-2.1	>5.00		LV	27		
						6.35	-2.5	3.85		LV	27		
						5.95	-2.5	3.45		LV	27		
						5	-2	3		LV	27		
						4.15	-1.12	1	22±2	CV	54		
						5.7	-2.3	3.4		LV	27		
				211	C4MI	061	TA	5.7	-2.3	3.4		LV	27
				229	C8MI	031	TFSI	4.83	-2.27	2.56		CV	112
239	C10MI	031	TFSI	4.89	-2.24	2.65		CV	112				
240	MDI	021	BF <sub>4</sub>	3.8	-2.4	1.4	22±2	CV	54				
				4.15	-1.12	1	22±2	CV	54				
				061	TA	5.7	-2.3	3.4		LV	27		
						4.6	-1.6	3		LV	27		
						4	-1.5	2.5		LV	27		
						4.1	-1.6	2.5	22±2	CV	54		
						1.95	1.02	-0.93	22±2	CV	54		
						031	TFSI	4.76	-2.04	2.72		CV	112
				051	PF <sub>6</sub>	4.76	-2.1	>5.00		LV	27		
						6.35	-2.5	3.85		LV	27		
						5.95	-2.5	3.45		LV	27		
						5	-2	3		LV	27		
						4.15	-1.12	1	22±2	CV	54		
						5.7	-2.3	3.4		LV	27		
229	C8MI	031	TFSI	4.83	-2.27	2.56		CV	112				
239	C10MI	031	TFSI	4.89	-2.24	2.65		CV	112				
240	MDI	021	BF <sub>4</sub>	3.8	-2.4	1.4	22±2	CV	54				
				2	-1.05	0.95	22±2	CV	54				
33	M1,2E3I	031	TFSI	4.4	-2	2.4		CV	18				
37	DMPI	031	TFSI	5.2			22		106				
				5.2±0.04	0.2±0.02	5.4±0.02	22	LV	20				
				4.55			80		106				
				5.37	0.28	5.65	22	LV	20				
				5.37±0.04			22		106				
				4.9±0.04			80		106				
83	P13	037	MSI	4.25	-2.25	2		CV	119				
				6	-3	3		CV	38				
				4	-2	2		CV	119				
				2.97			240		106				
84	P14	031	TFSI	6	-3	3		CV	38				
		037	MSI	4	-2	2		CV	119				
1501	N1111	031	TFSI	5.6	-2.9	2.7		CV	76				
1528	N6222	031	TFSI	5.99	-3.13	2.86		CV	112				

TABLE 11. Electrochemical window—Continued

ID	Cation	ID	Anion	Elec. win (V)	Cathode limit (V)	Anode limit (V)	<i>t</i> (°C)	Method	Reference
1533	N6444	037	MSI	6	−3	3		CV	119
				5	−3	2		CV	119
1701	P1111	031	TFSI	5.8	−3.2	2.6		CV	76
1800	As1111	031	TFSI	6	−3.4	2.6		CV	76

TABLE 12. The QSPR models for melting points of ILs from different references<sup>a</sup>

Structures	<i>n</i>	<i>R</i> <sup>2</sup>	<i>F</i>	<i>N</i> <sub><i>p</i></sub>	Reference
1-substituted 4-amino-1,2,4-triazolium bromide	13	0.914	31.9	3	40
1-substituted 4-amino-1,2,4-triazolium nitrate	13	0.933	41.5	3	40
Pyridinium Bromide	126	0.7883	73.24	6	28
Imidazolium Bromide	57	0.7442	29.67	5	51
Imidazolium Bromide	29	0.7517	13.93	5	51
Imidazolium Bromide	18	0.9432	77.53	3	51
Benzimidazolium Bromide	45	0.6899	16.91	5	51
Tetraalkyl-ammonium Bromide	75	0.775		5	100
( <i>n</i> -Hydroxyalkyl)-trialkyl-ammonium Bromide	34	0.716		5	100
Disubstituted imidazolium tetrafluoroborate	16	0.9047	37.99	3	This work
Disubstituted imidazolium hexafluorophosphate	25	0.9207	34.85	6	This work

<sup>a</sup>*n* is the number of structures, *R*<sup>2</sup> is the squared correlation coefficient, *F* is the F-criterion value, and *N*<sub>*p*</sub> is the number of parameters.

TABLE 13. Correlation models of melting points for two systems<sup>a</sup>

<i>N</i> <sub><i>p</i></sub>	<i>R</i> <sup>2</sup>	<i>R</i> <sub>cv</sub> <sup>2</sup>	<i>F</i>	X+DX	t-test	Name of the descriptor	
				0	−(1704±367.88)	−4.632	Intercept
				1	4.5854±0.79641	5.7576	H-donors surface area
3	0.9047	0.7763	37.99	2	16.146±2.9269	5.5163	minimum electron-electron repulsion for a C–C bond
				3	−(2641.2±553.5)	−4.7719	image of the Onsager-Kirkwood solvation energy
				0	−(13936±1313.9)	−10.6072	Intercept
				1	22.418±2.0345	11.0191	minimum electron-electron repulsion for a C–C bond
				2	819.81±74.561	10.9952	maximum resonance energy for a C–H bond
6	0.9207	0.8423	34.85	3	8861.6±1227.5	7.2193	minimum partial charge for a H atom
				4	−(11.4±3.2791)	−3.4765	relative negative charged surface area
				5	(2410.8±598.43)	4.0286	maximum bond order of a N atom
				6	−(299.01±181.43)	−1.648	maximum bonding contribution of a molecular orbit

<sup>a</sup>*N*<sub>*p*</sub> is the number of parameters, *R*<sup>2</sup> is the squared correlation coefficient, *R*<sub>cv</sub><sup>2</sup> is the cross validated squared correlation coefficient, and *F* is the F-criterion value.

TABLE 14. Compounds studied in test set with calculated and experimental *T*<sub>*m*</sub> (K) values<sup>a</sup>

ID	3-substituent	1-substituent	Cal. <sup>*</sup> (K)	Expt. <sup>**</sup> (K)	Deviation (K)	
1	a	−CH <sub>3</sub>	−C <sub>12</sub> H <sub>25</sub>	315.2459	307.15	8.0959
2	a	−CH <sub>3</sub>	−CH <sub>2</sub> OC <sub>12</sub> H <sub>25</sub>	330.6841	336.15	−5.4659
3	a	−CH <sub>2</sub> OC <sub>4</sub> H <sub>9</sub>	−CH <sub>2</sub> OC <sub>10</sub> H <sub>21</sub>	309.8277	289.15	20.6777
4	b	−CH <sub>3</sub>	−CH <sub>2</sub> OC <sub>7</sub> H <sub>15</sub>	272.7229	310.65	−37.9271
5	b	−CH <sub>3</sub>	−CH <sub>2</sub> OC <sub>12</sub> H <sub>25</sub>	299.2789	335.15	−35.8711
6	b	−CH <sub>3</sub>	−C <sub>16</sub> H <sub>33</sub>	339.0689	348.15	−9.0811
7	b	−CH <sub>3</sub>	−C <sub>18</sub> H <sub>37</sub>	377.319	353.15	24.169

<sup>a</sup>a, tetrafluoroborates and b, hexafluorophosphates.

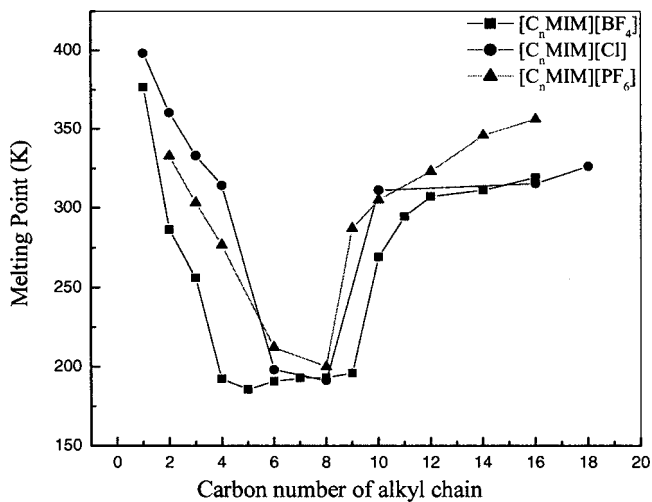


FIG. 1. Melting point variation with carbon number in alkyl chain for  $C_n$ MIX.

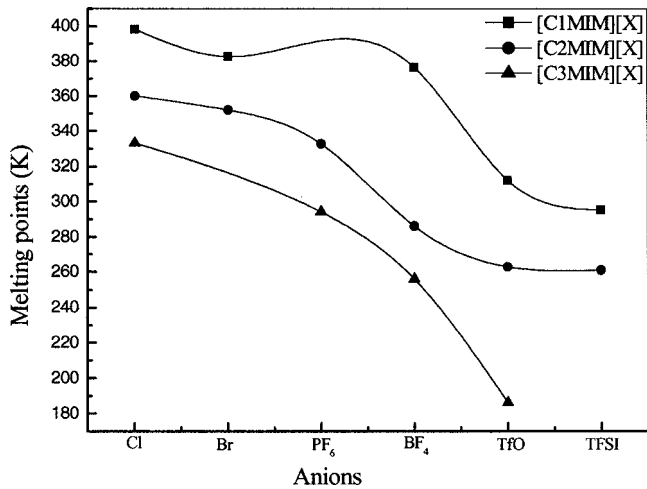


FIG. 2. Melting point variation with anions.

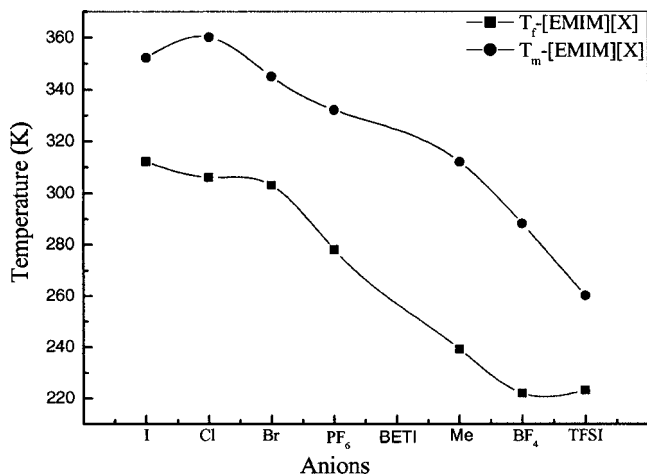


FIG. 3. Melting points and freezing points of EMIX.

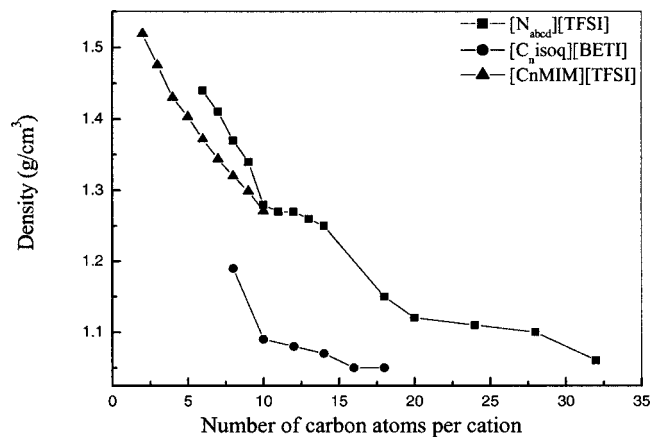


FIG. 4. Density variation of several systems with number of carbon atoms.

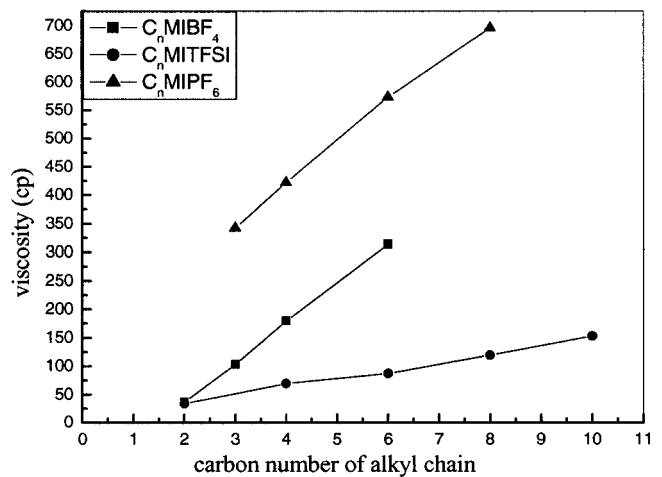


FIG. 5. Viscosity variation of several systems with number of carbon atoms.

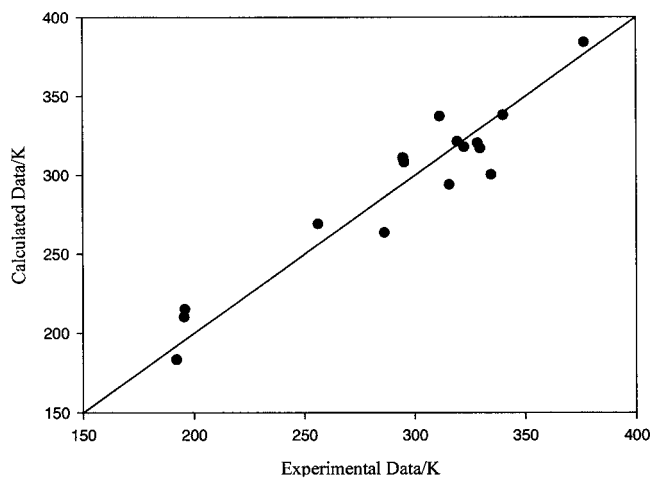


FIG. 6. Plot of experimental and calculated melting points for disubstituted imidazolium tetrafluoroborates.



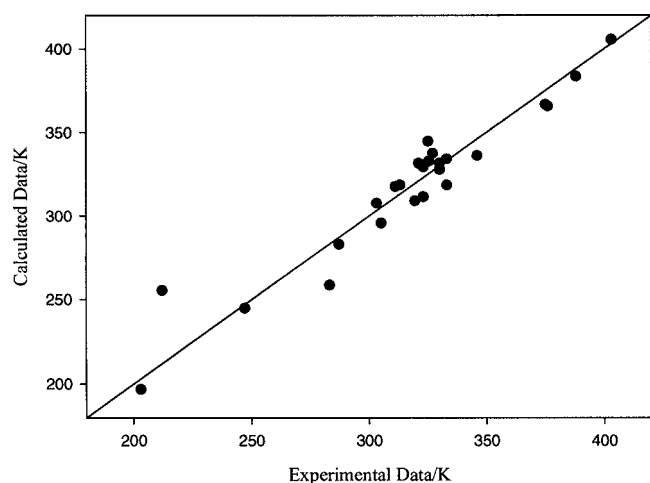


FIG. 7. Plot of experimental and calculated melting points for disubstituted imidazolium hexafluorophosphates.

attention should be paid on the measurement of physical chemical properties of ionic liquids. Further, with the rapid growth of the number of ionic liquids it is necessary to develop prediction methods. The study of structure-property relationship may provide both the direction for the design of the potential ionic liquids and the reference to evaluate the reported data. Our studies showed that the QSPR models could give a reasonable prediction of unknown or unavailable compounds of the same class. See Tables 12–14.

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## 8. Appendix: Explanation of Measuring Methods

Melting point	
DSC	Differential scanning calorimeter
Density	
DT	Dilatometric tubes
GM	Gravity meter
AP	Anton-Paar density measurement system
MS	Microsyringe
PM	Picnometer
GA	Gravimetric analysis
WV	Weighing a measured volume
Molar volume	
Cacu	Calculate
Mcs	Monte Carlo simulation
Ex	Experiment
Viscosity	

Dv	DV-I(II) viscometer (Brookfield)
Ov	Oscillating type viscosity meter
Pv	Plate viscometer
Mv	Microviscosimeter
Surface tension	
CRM	Capillary rise method
TM	Tensiometer
Conductivity	
CM	Measured using conductivity cell
CM-a	Conductivity bridge operated at 60 Hz
CM-b	Conductivity bridge operated at 1 kHz
Electrochemical window	
LV	Linear sweep voltammetry
CV	Cyclic voltammograms
P/G	Potentiostat/galvanostat

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