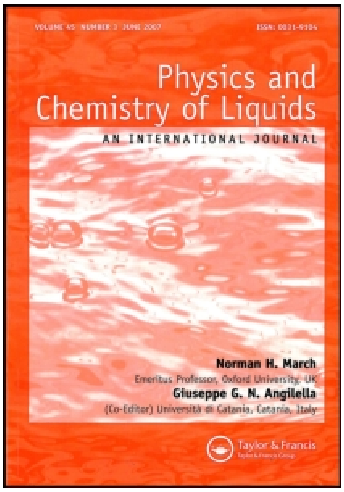

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Laura M. Sprunger[a], William E. Acree Jr[a]* and Michael H. Abraham[b]

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Gas-to-room temperature ionic liquid (RTIL) partition coefficients have been compiled from the published literature for solutes dissolved in 1-hexyloxymethyl-3-methylimidazolium bis(trifluoromethylsulphonyl)-imide, $\{[\mathrm{HxomMIm}]^+[(\mathrm{Tf})_2\mathrm{N}]^-\}$, and in 1,3-dihexyloxymethylimidazolium bis(trifluoromethylsulphonyl)imide, $\{[(\mathrm{Hxom})_2\mathrm{Im}]^+[(\mathrm{Tf})_2\mathrm{N}]^-\}$. These partition coefficients are converted into water-to-RTIL partition coefficients using the corresponding gas-to-water partition coefficients. Both sets of partition coefficients are analysed using the Abraham model with cation-specific and anion-specific equation coefficients. The equation coefficients are reported for the 1-hexyloxymethyl-3-methylimidazolium and 1,3-dihexyloxymethylimidazolium cations. The calculated cation coefficients can be combined with our previously determined nine sets of anion-specific equation coefficients to yield expressions capable of predicting the partition coefficients of solutes in 18 different RTILs.

Keywords: activity coefficients; room temperature ionic liquids; partition coefficients; linear free energy relationships

1. Introduction

This study continues our application of the Abraham general solvation model to describe the solubility of organic vapours and gases into room temperature ionic liquids (RTILs). The previous studies [1–5] have examined the feasibility of separating the various solute-RTIL interactions into the cation-specific and anion-specific interactions.

$$\log K = c_{\mathrm{cation}} + c_{\mathrm{anion}} + (e_{\mathrm{cation}} + e_{\mathrm{anion}}) \cdot E + (s_{\mathrm{cation}} + s_{\mathrm{anion}}) \cdot S + (a_{\mathrm{cation}} + a_{\mathrm{anion}}) \cdot A + (b_{\mathrm{cation}} + b_{\mathrm{anion}}) \cdot B + (l_{\mathrm{cation}} + l_{\mathrm{anion}}) \cdot L, \qquad (1)$$

where K is the solute's partition coefficient into the RTIL from the gas phase. The independent variables in Equation (1) are solute descriptors as follows: E and S refer to the excess molar refraction in units of $(\mathrm{cm}^3\,\mathrm{mol}^{-1})/10$ and

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dipolarity/polarisability descriptors of the solute, respectively, A and B are measures of the solute hydrogen-bond acidity and basicity and L is the logarithm of the gas-to-hexadecane partition coefficient at 298.15 K. The regression coefficients and constants (i.e. c_{cation}, c_{anion}, e_{cation}, etc.) are determined by regression analyses of the experimental data for a series of organic vapours and gases into a given RTIL. A similar correlation equation has been developed for describing solute partitioning into an RTIL from an aqueous phase, as $\log P$, where P is the water to RTIL partition coefficient

$$\log P = c_{\text{ation}} + c_{\text{anion}} + (e_{\text{cation}} + e_{\text{anion}}) \cdot E + (s_{\text{cation}} + s_{\text{anion}}) \cdot S \\ + (a_{\text{cation}} + a_{\text{anion}}) \cdot A + (b_{\text{cation}} + b_{\text{anion}}) \cdot B + (v_{\text{cation}} + v_{\text{anion}}) \cdot V, \qquad (2)$$

with the L solute descriptor being replaced by the McGowan volume, V in units of (cm^3 mol^{-1})/100. For any fully characterised RTIL (those with calculated values for the c_{cation}, c_{anion}, e_{cation}, etc. equation coefficients) further values of $\log K$ and $\log P$ can be estimated for the solutes with known values for the solute descriptors.

To date we have reported the Abraham model equation coefficients for 13 cations (4-methyl-N-butylpyridinium cation, $[\text{BMPy}]^+$; 1-methyl-3-ethylimidazolium cation, $[\text{MEIm}]^+$; 1,2-dimethyl-3-ethylimidazolium cation, $[\text{M}_2\text{EIm}]^+$; 1-methyl-3-butylimidazolium cation, $[\text{MBIm}]^+$; 1-methyl-3-hexylimidazolium cation, $[\text{MHIm}]^+$; trimethylbutylammonium cation, $[\text{M}_3\text{BAm}]^+$; 1-methyl-3-octylimidazolium cation, $[\text{MOIm}]^+$; N-ethylpyridinium cation, $[\text{NEPy}]^+$; 1-propyl-2,3-dimethyl-imidazolium cation, $[\text{PM}_2\text{Im}]^+$; trihexyl(tetradecyl)phosphonium cation, $[\text{H}_3\text{TdP}]^+$; trimethylhexylammonium $[\text{M}_3\text{HAm}]^+$; triethylsulphonium, $[\text{E}_3\text{S}]^+$; and 1-butyl-1-methylpyrrolidinium, $[\text{BMPyr}]^+$) and for nine anions (*bis*(trifluoromethylsulphonyl)imide anion, $[(\text{Tf})_2\text{N}]^-$; tetrafluoroborate anion, $[\text{BF}_4]^-$; hexafluorophosphate anion, $[\text{PF}_6]^-$; ethylsulphate anion, $[\text{EtSO}_4]^-$; trifluoromethanesulphonate anion, $[\text{Trif}]^-$; trifluoroacetate anion, $[\text{F}_3\text{Ac}]^-$; octylsulphate anion, $[\text{OtSO}_4]^-$; thiocyanate anion, $[\text{SCN}]^-$ and dicyanamide, $[\text{DCA}]^-$) [1–7]. Our calculated ion-specific equation coefficients were based on the 1221 $\log K$ and 1194 $\log P$ experimental values for solutes dissolved in only 33 RTILs. The major advantage of splitting the equation coefficients into the individual cation-specific and anion-specific contributions is that one can make predictions for more RTILs. The 13 sets of cation-specific equation coefficients and nine sets of anion-specific equation coefficients that we have already determined for the Abraham model can be combined to yield predictive $\log K$ and $\log P$ expressions for 117 different RTILs. That is more RTILs were used in regression analysis when the equation coefficients were determined. Past studies have shown [1,2] that very little loss in predictive ability results from splitting the equation coefficients into separate anion-specific and cation-specific terms.

At the time that we developed Equations (1) and (2) we suggested a computation methodology for calculating additional ion-specific equation coefficients as additional experimental data became available. In the present communication, we report equation coefficients for 1-hexyloxymethyl-3-methylimidazolium, $[\text{HxomMIm}]^+$, and 1,3-dihexyloxyimidazolium, $[(\text{Hxom})_2\text{Im}]^+$, cations based on the recently published infinite dilution activity coefficient data for the solutes dissolved in 1-hexyloxymethyl-3-methylimidazolium bis(trifluoromethylsulphonyl)imide, $\{[\text{HxomMIm}]^+ [(\text{Tf})_2\text{N}]^-\}$ [8], and in 1,3-dihexyloxymethylimidazolium *bis*(trifluoromethylsulphonyl)imide, $\{[(\text{Hxom})_2\text{Im}]^+[(\text{Tf})_2\text{N}]^-\}$ [8].

2. Database and computation methodology

All of the experimental data that we were able to retrieve from the published literature [8] for RTILs containing either $[\text{HxomMIm}]^+$ or $[(\text{Hxom})_2\text{Im}]^+$ cations pertained to the infinite dilution activity coefficient, $\gamma^{\infty}_{\text{solute}}$, for solutes dissolved in $\{[\text{HxomMIm}]^+[(\text{Tf})_2\text{N}]^-\}$ and $\{[(\text{Hxom})_2\text{Im}]^+[(\text{Tf})_2\text{N}]^-\}$. In order to apply the Abraham model the infinite dilution activity coefficients needed to be converted to log *K* values for gas-to-RTIL partition through Equation (3).

$$\log K = \log\left(\frac{RT}{\gamma^{\infty}_{\text{solute}} P^{\text{o}}_{\text{solute}} V_{\text{solvent}}}\right). \tag{3}$$

Here *R* is the universal gas constant, *T* is the system temperature, $P^{\text{o}}_{\text{solute}}$ is the vapour pressure of the solute at *T* and V_{solvent} is the molar volume of the solvent.

Predictive correlations can be developed for water-to-RTIL partition coefficients, log *P*. In the present case the values refer to a hypothetic partition in that the RTIL and aqueous phases are not in physical contact with each other. Even so the values are still quite useful. The values of the hypothetical partition coefficients can be used to calculate infinite dilution activity coefficients and the solubilities for solutes dissolved in RTILs. The calculation of log *P* values from log *K*

$$\log P = \log K - \log K_w \tag{4}$$

requires knowledge of the solute's gas phase partition coefficient into water, K_w, which is available for all of the solutes being studied. The experimental values of log *K* and log *P* for solutes dissolved in $\{[\text{HxomMIm}]^+[(\text{Tf})_2\text{N}]^-\}$ and $\{[(\text{Hxom})_2\text{Im}]^+[(\text{Tf})_2\text{N}]^-\}$ are given in Tables 1 and 2, along with the respective solute descriptors.

3. Results and discussion

In Table 1 we have assembled the log *P* and log *K* values for 34 solutes dissolved in 1-hexyloxymethyl-3-methylimidazolium, $[\text{HxomMIm}]^+$, covering a reasonably wide range of compound type and descriptor values. The analysis of the experimental water-to-RTIL and gas-to-RTIL partition data gave

$$\begin{aligned}\log K = &-0.462(0.050) - 0.397(0.096)E + 2.486(0.125)S\\ &+ 2.428(0.095)A + 0.333(0.100)B + 0.785(0.015)L\\ &(\text{with } N = 34,\ \text{SD} = 0.050,\ R^2 = 0.995,\ R^2_{\text{adj}} = 0.994,\ F = 1058.7)\end{aligned} \tag{5}$$

and

$$\begin{aligned}\log P = &-0.039(0.130) - 0.645(0.203)E + 1.184(0.266)S\\ &- 1.374(0.203)A - 4.779(0.219)B + 3.609(0.113)V\\ &(\text{with } N = 34,\ \text{SD} = 0.108,\ R^2 = 0.996,\ R^2_{\text{adj}} = 0.995,\ F = 1297.7),\end{aligned} \tag{6}$$

where *N* is the number of data points, that is the number of solutes, R^2 denotes the squared correlation coefficient, R^2_{adj} refers to the adjusted squared correlation coefficient, SD is the standard deviation and *F* corresponds to the Fisher *F* statistic. The errors in the coefficients are given in parenthesis. The statistics of the derived

Table 1. Logarithms of experimental gas-to-RTIL and water-to-RTIL partition data for solutes dissolved in 1-hexyloxymethyl-3-methylimidazolium *bis*(trifluoromethylsulphonyl) imide, $\{[\mathrm{HxomMIm}]^+[(\mathrm{Tf})_2\mathrm{N}]^-\}$, at 298.15 K.

Solute	E	S	A	B	L	V	$\log K$	$\log P$
Pentane	0.000	0.000	0.000	0.000	2.162	0.813	1.151	2.851
Hexane	0.000	0.000	0.000	0.000	2.668	0.954	1.622	3.442
Heptane	0.000	0.000	0.000	0.000	3.173	1.095	2.043	4.003
Octane	0.000	0.000	0.000	0.000	3.677	1.236	2.445	4.555
Nonane	0.000	0.000	0.000	0.000	4.182	1.377	2.837	4.987
Decane	0.000	0.000	0.000	0.000	4.686	1.518	3.222	5.482
Cyclopentane	0.263	0.100	0.000	0.000	2.477	0.705	1.602	2.482
Cyclohexane	0.305	0.100	0.000	0.000	2.964	0.845	2.000	2.900
Cycloheptane	0.350	0.100	0.000	0.000	3.704	0.986	2.573	3.153
Cyclooctane	0.413	0.100	0.000	0.000	4.329	1.127	3.065	3.685
1-Pentene	0.093	0.080	0.000	0.070	2.047	0.770	1.323	2.553
1-Hexene	0.078	0.080	0.000	0.070	2.572	0.911	1.770	2.930
1-Heptene	0.092	0.080	0.000	0.070	3.063	1.052	2.185	3.405
1-Octene	0.094	0.080	0.000	0.070	3.568	1.193	2.583	3.993
1-Pentyne	0.172	0.230	0.120	0.120	2.010	0.727	1.899	1.909
1-Hexyne	0.166	0.230	0.120	0.100	2.510	0.868	2.307	2.517
1-Heptyne	0.160	0.230	0.120	0.100	3.000	1.009	2.823	3.263
1-Octyne	0.155	0.230	0.120	0.100	3.521	1.150	3.118	3.638
Benzene	0.610	0.520	0.000	0.140	2.786	0.716	2.845	2.215
Toluene	0.601	0.520	0.000	0.140	3.325	0.857	3.249	2.599
Ethylbenzene	0.613	0.510	0.000	0.150	3.778	0.998	3.572	2.992
σ-Xylene	0.663	0.560	0.000	0.160	3.939	0.998	3.787	3.127
m-Xylene	0.623	0.520	0.000	0.160	3.839	0.998	3.650	3.040
p-Xylene	0.613	0.520	0.000	0.160	3.839	0.998	3.628	3.038
Methanol	0.278	0.440	0.430	0.470	0.970	0.308	2.491	−1.249
Ethanol	0.246	0.420	0.370	0.480	1.485	0.449	2.751	−0.919
1-Propanol	0.236	0.420	0.370	0.480	2.031	0.590	3.139	−0.421
1-Butanol	0.224	0.420	0.370	0.480	2.601	0.731	3.542	0.082
Thiophene	0.687	0.570	0.000	0.150	2.819	0.641	2.958	1.918
Tetrahydrofuran	0.289	0.520	0.000	0.480	2.636	0.622	2.891	0.341
Methyl *tert*-butyl ether	0.024	0.210	0.000	0.590	2.380	0.872	2.228	0.733
Diethyl ether	0.041	0.250	0.000	0.450	2.015	0.731	1.868	0.698
Dipropyl ether	0.008	0.250	0.000	0.450	2.954	1.013	2.465	1.575
Acetone	0.179	0.700	0.040	0.490	1.696	0.547	2.886	0.095

correlations are quite good given the limited number of data points. Figures 1 and 2 compare the calculated values of $\log K$ and $\log P$ based on Equations (5) and (6) against the experimental data.

Each equation coefficient represents the sum of the cation plus anion contribution, i.e. $e_{\mathrm{RTIL}} = e_{\mathrm{cation}} + e_{\mathrm{anion}}$, $s_{\mathrm{RTIL}} = s_{\mathrm{cation}} + s_{\mathrm{anion}}$, etc. In establishing the computation methodology, the equation coefficients for the *bis*(trifluoromethylsulphonyl)imide anion were set equal to zero to provide a convenient reference point from which all other equation coefficients would be calculated. The equation coefficients in Equations (5) and (6) thus correspond to the ion-specific equation coefficients for the 1-hexyloxymethyl-3-methylimidazolium cation.

Table 2. Logarithms of experimental gas-to-RTIL and water-to-RTIL partition coefficient data for solutes dissolved in 1,3-dihexyloxymethylimidazolium *bis*(trifluoromethyl-sulphonyl)imide, $\{[(\mathrm{Hxom})_2\mathrm{Im}]^+[(\mathrm{Tf})_2\mathrm{N}]^-\}$, at 298.15 K.

Solute	E	S	A	B	L	V	log K	log P
Pentane	0.000	0.000	0.000	0.000	2.162	0.813	1.454	3.154
Hexane	0.000	0.000	0.000	0.000	2.668	0.954	1.918	3.738
Heptane	0.000	0.000	0.000	0.000	3.173	1.095	2.355	4.315
Octane	0.000	0.000	0.000	0.000	3.677	1.236	2.780	4.890
Nonane	0.000	0.000	0.000	0.000	4.182	1.377	3.196	5.346
Decane	0.000	0.000	0.000	0.000	4.686	1.518	3.607	5.867
Cyclopentane	0.263	0.100	0.000	0.000	2.477	0.705	1.841	2.721
Cyclohexane	0.305	0.100	0.000	0.000	2.964	0.845	2.253	3.153
Cycloheptane	0.350	0.100	0.000	0.000	3.704	0.986	2.836	3.416
Cyclooctane	0.413	0.100	0.000	0.000	4.329	1.127	3.352	3.972
1-Pentene	0.093	0.080	0.000	0.070	2.047	0.770	1.524	2.754
1-Hexene	0.078	0.080	0.000	0.070	2.572	0.911	1.989	3.149
1-Heptene	0.092	0.080	0.000	0.070	3.063	1.052	2.426	3.646
1-Octene	0.094	0.080	0.000	0.070	3.568	1.193	2.850	4.260
1-Pentyne	0.172	0.230	0.120	0.120	2.010	0.727	1.973	1.983
1-Hexyne	0.166	0.230	0.120	0.100	2.510	0.868	2.408	2.618
1-Heptyne	0.160	0.230	0.120	0.100	3.000	1.009	2.956	3.396
1-Octyne	0.155	0.230	0.120	0.100	3.521	1.150	3.280	3.800
Benzene	0.610	0.520	0.000	0.140	2.786	0.716	2.847	2.217
Toluene	0.601	0.520	0.000	0.140	3.325	0.857	3.284	2.634
Ethylbenzene	0.613	0.510	0.000	0.150	3.778	0.998	3.641	3.061
σ-Xylene	0.663	0.560	0.000	0.160	3.939	0.998	3.837	3.177
m-Xylene	0.623	0.520	0.000	0.160	3.839	0.998	3.711	3.101
p-Xylene	0.613	0.520	0.000	0.160	3.839	0.998	3.691	3.101
Methanol	0.278	0.440	0.430	0.470	0.970	0.308	2.439	−1.301
Ethanol	0.246	0.420	0.370	0.480	1.485	0.449	2.737	−0.933
1-Propanol	0.236	0.420	0.370	0.480	2.031	0.590	3.167	−0.393
1-Butanol	0.224	0.420	0.370	0.480	2.601	0.731	3.630	0.170
Thiophene	0.687	0.570	0.000	0.150	2.819	0.641	2.949	1.909
Tetrahydrofuran	0.289	0.520	0.000	0.480	2.636	0.622	2.932	0.382
Methyl *tert*-butyl ether	0.024	0.210	0.000	0.590	2.380	0.872	2.330	0.835
Diethyl ether	0.041	0.250	0.000	0.450	2.015	0.731	1.971	0.801
Dipropyl ether	0.008	0.250	0.000	0.450	2.954	1.013	2.639	1.749
Acetone	0.179	0.700	0.040	0.490	1.696	0.547	2.827	0.037

Our search of the published chemical and engineering literature also found infinite dilution activity coefficient data for 34 organic solutes dissolved in 1,3-dihexyloxymethylimidazolium *bis*(trifluoromethylsulphonyl)imide, $\{[(\mathrm{Hxom})_2\mathrm{Im}]^+[(\mathrm{Tf})_2\mathrm{N}]^-\}$, covering a reasonably wide range of compound type and descriptor values. The log P and log K values calculated from the published activity coefficient data (Table 2) were analysed to give

$$\begin{aligned}\log K = {} & -0.314(0.050) - 0.479(0.098)E + 2.076(0.126)S \\ & + 2.376(0.095)A + 0.287(0.101)B + 0.835(0.015)L \qquad (7) \\ & (\text{with } N = 34,\ \mathrm{SD} = 0.050,\ R^2 = 0.994,\ R^2_{\mathrm{adj}} = 0.993,\ F = 936.1)\end{aligned}$$

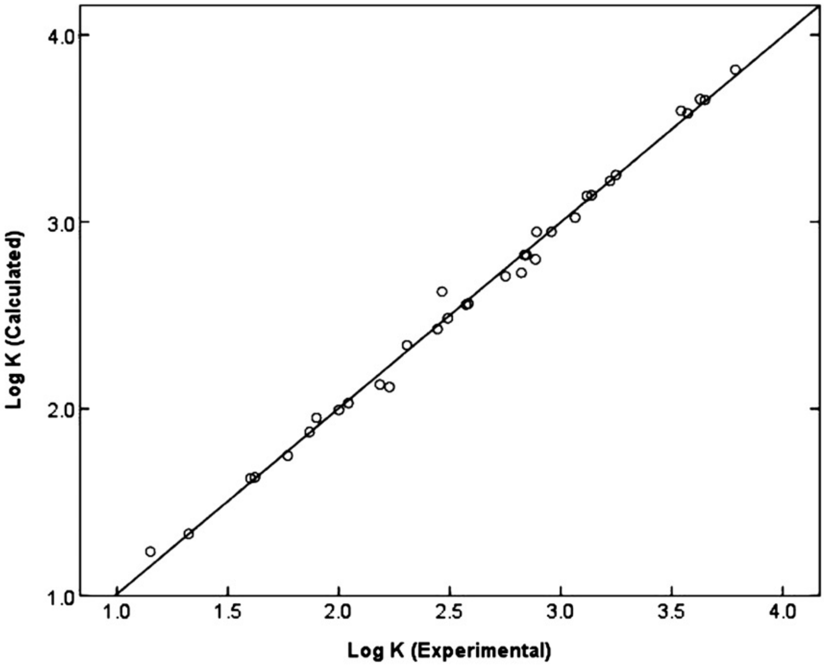

Figure 1. Comparison of experimental log *K versus* calculated log *K* values based on Equation (5) for solutes dissolved in $\{[\text{HxomMIm}]^+[(\text{Tf})_2\text{N}]^-\}$ at 298.15 K.

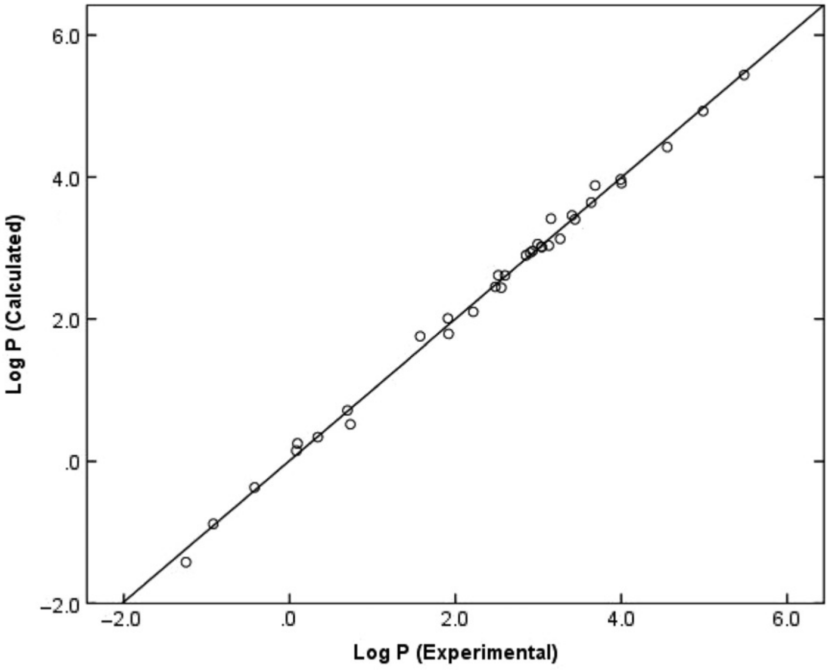

Figure 2. Comparison of experimental log *P versus* calculated log *P* values based on Equation (6) for solutes dissolved in $\{[\text{HxomMIm}]^+[(\text{Tf})_2\text{N}]^-\}$ at 298.15 K.

and

$$\log P = 0.107(0.125) - 0.628(0.196)E + 0.747(0.258)S - 1.441(0.197)A - 4.808(0.212)B + 3.750(0.110)V \quad (8)$$

$$(\text{with } N = 34, \text{SD} = 0.106, R^2 = 0.996, R^2_{\text{adj}} = 0.995, F = 1560.4).$$

The statistics of the derived correlations are quite good, given the limited number of data points. Figures 3 and 4 compare the calculated values of $\log K$ and $\log P$ based on Equations (7) and (8) against the experimental data. The anion is again *bis*(trifluoromethylsulphonyl)imide, and the calculated equation coefficients in Equations (7) and (8) thus correspond to the ion-specific equation coefficients for the 1,3-dihexyloxymethylimidazolium cation.

The present study increases by two the number of cation-specific equation coefficients for the Abraham model. The 15 sets of cation-specific equation coefficients and nine sets of anion-specific equation coefficients that we have now determined for both linear free energy relationship (LFER) models can be combined to yield predictive $\log K$ and $\log P$ expressions for 135 different RTILs. The 18 additional RTILs for which partition coefficient predictions are now possible are: 1-hexyloxymethyl-3-imidazolium bis(trifluoromethylsulphonyl)imide; 1-hexyloxymethyl-3-imidazolium tetrafluoroborate; 1-hexyloxymethyl-3-imidazolium hexafluorophosphate; 1-hexyloxymethyl-3-imidazolium ethylsulphate; 1-hexyloxymethyl-3-imidazolium trifluoromethanesulphonate; 1-hexyloxymethyl-3-imidazolium

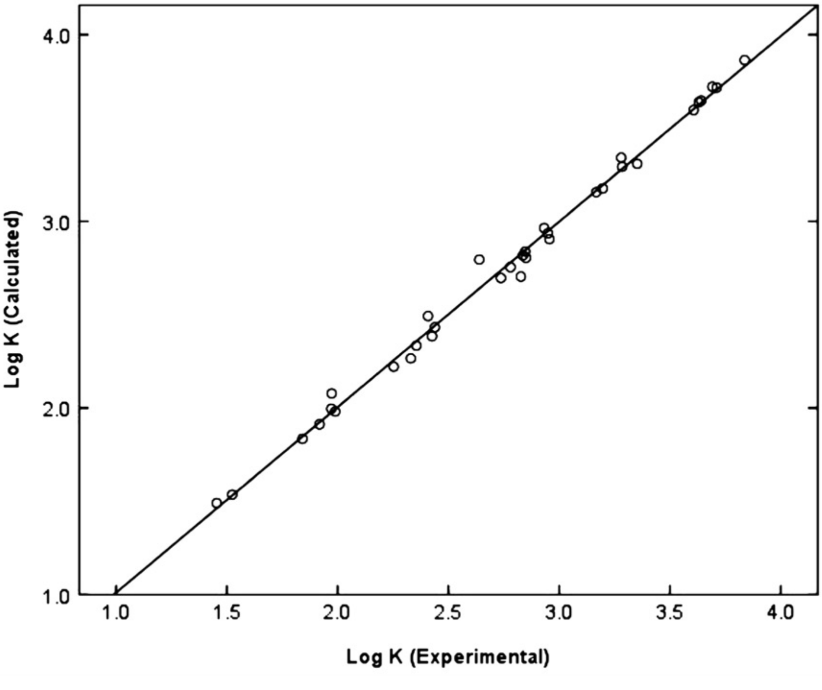

Figure 3. Comparison of experimental $\log K$ *versus* calculated $\log K$ values based on Equation (7) for solutes dissolved in $\{[(\mathrm{Hxom})_2\mathrm{Im}]^+[(\mathrm{Tf})_2\mathrm{N}]^-\}$ at 298.15 K.

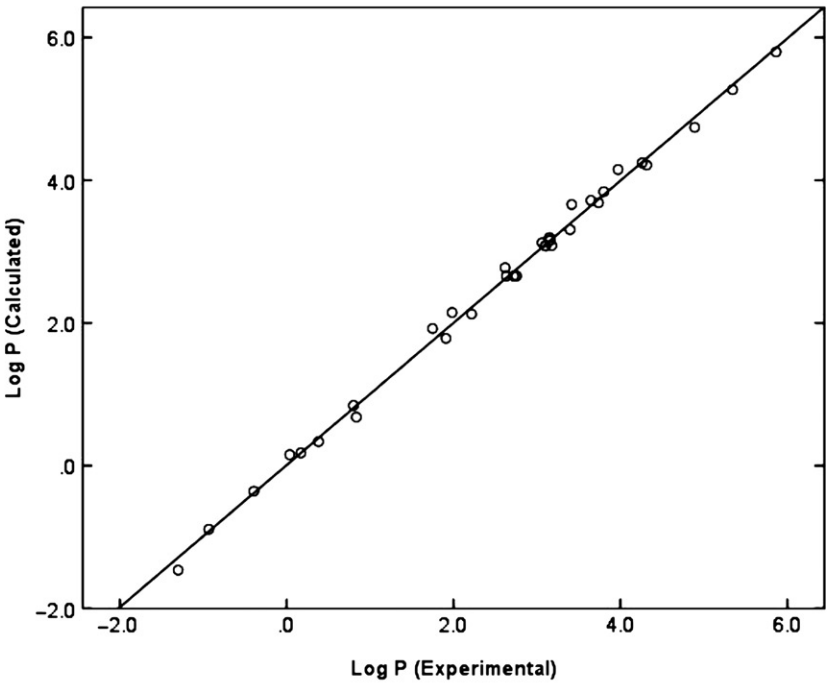

Figure 4. Comparison of experimental log P *versus* calculated log P values based on Equation (8) for solutes dissolved in $\{[(\mathrm{Hxom})_2\mathrm{Im}]^+[(\mathrm{Tf})_2\mathrm{N}]^-\}$ at 298.15 K.

trifluoroacetate; 1-hexyloxymethyl-3-imidazolium octylsulphate; 1-hexyloxymethyl-3-imidazolium thiocyanate; 1-hexyloxymethyl-3-imidazolium dicyanamide; 1,3-dihexyloxymethylimidazolium *bis*(trifluoromethylsulphonyl)imide; 1,3-dihexyloxymethylimidazolium tetrafluoroborate; 1,3-dihexyloxymethylimidazolium hexafluorophosphate; 1,3-dihexyloxymethylimidazolium ethylsulphate; 1,3-dihexyloxymethyl-imidazolium trifluoromethanesulphonate; 1,3-dihexyloxymethylimidazolium trifluoroacetate anion; 1,3-dihexyloxymethylimidazolium octylsulphate; 1,3-dihexyloxymethylimidazolium thiocyanate; and 1,3-dihexyloxymethylimidazolium dicyanamide. The anion-specific equation coefficients needed for these predictions are given elsewhere [3–7].

In using these predictive equations readers are reminded that the predictive area of chemical space is defined by the range of solute descriptors covered. Most of the experimental log K and log P data used in our regression analyses have come from gas solubilities and gas–liquid chromatographic retention measurements. The solutes studied have typically been inert gases, diatomic gas molecules, linear and cyclic alkanes and alkenes (up to dodecane), alkylbenzenes, linear and branched alcohols, linear and cyclic monoethers (plus 1,4-dioxane), chlorinated methanes and a few of the smaller aldehydes and ketones. The solute descriptor space defined by these compounds would be: $E = 0.000$ to $E = 0.850$; $S = 0.000$ to $S = 0.900$; $A = 0.000$ to $A = 0.430$; $B = 0.000$ to $B = 0.650$; $V = 0.109$ to $V = 1.800$; and $L = -1.200$ to $L = 5.700$. Unfortunately, in the present study we were unable to find experimental data for gaseous solutes, such as nitrogen gas, oxygen gas and carbon dioxide.

The predictive area of chemical space covered by the $[\mathrm{HxomMIm}]^+$ or $[(\mathrm{Hxom})_2\mathrm{Im}]^+$, equation coefficients is slightly smaller. The smallest solute contained in the two sets is methanol (with $V = 0.3083$ and $L = 0.970$). One should be able to make reasonably accurate partition coefficient predictions for most solutes having solute descriptors that fall within (or just slightly outside of) the aforementioned ranges.

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