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Solubilities of Solutes in Ionic Liquids from a Simple Perturbed-Hard-Sphere Theory

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Abstract

In recent years, several publications have provided solubilities of ordinary gases and liquids in ionic liquids. This work reports an initial attempt to correlate the experimental data using a perturbed-hard-sphere theory; the perturbation is based on well-known molecular physics when the solution is considered as a dielectric continuum. For this correlation, the most important input parameters are hard-sphere diameters of the solute and of the cation and anion that constitute the ionic liquid. In addition, the correlation uses the solvent density and the solute's polarizability and dipole and quadrupole moments, if any. Dispersion-energy parameters are obtained from global correlation of solubility data. Results are given for twenty solutes in several ionic liquids at normal temperatures; in addition, some results are given for gases in two molten salts at very high temperatures. Because the theory used here is much simplified, and because experimental uncertainties (especially for gaseous solutes) are often large, the accuracy of the correlation presented here is not high; in general, predicted solubilities (Henry's constants) agree with experiment to within roughly $\pm 70\%$. As more reliable experimental data become available, modifications in the charactering parameters are likely to improve accuracy. Nevertheless, even in its present form, the correlation may be useful for solvent screening in engineering design.

Introduction

Although ionic liquids have been known for a long time, they have attracted significant attention only during the last 5 to 10 years. For most practical purposes, ionic liquids are electrolytes with melting points near or below 25 °C. At normal temperatures, these liquids have high dielectric constants, densities somewhat larger than that of water and, most important, negligible vapor pressure. Because they are nonvolatile at normal temperatures, ionic liquids may be useful as “green” solvents that do not pollute the atmosphere [1,2]. Numerous reviews of ionic-liquid properties are now available, notably those by Heintz [3] and by Poole [4].

An increasing number of authors has reported experimental data for Henry’s constants of gases and for infinite-dilution activity coefficients of non-electrolytes in ionic liquids[5-17]. Toward interpretation and correlation of solubility data, in addition to molecular simulations [18,19], Eike *et al.* [22] have used quantitative structure-property relationship (QSPR) and Diedenhofen *et al.* [23] have used quantum-mechanical calculations (COSMO-RS) to correlate such data. In this work, we report an initial correlation of Henry’s constants for ordinary solutes in ionic liquids based on a perturbed-hard-sphere theory. A main advantage of our theory is its simplicity. Because it is based on several simplifying assumptions, it provides only approximate results. Nevertheless, these approximate results may be useful for engineering calculations, in particular, for screening possible ionic-liquid solvents for a specific application. As more reliable experimental solubility data become available, it is likely that modifications in our theory will improve its accuracy.

Theoretical Framework

Numerous authors, notably Pierotti [26], have used perturbed-hard-sphere theory for correlating solubilities in nonelectrolyte systems. Consistent with these earlier studies, we postulate that introducing a solute molecule into an ionic-liquid solvent consists of two steps: 1. Creation of a cavity of solute size in the solvent; 2. Charging the cavity to the appropriate

potential. As discussed elsewhere [26], Henry's constant H can be expressed as

$$\ln(HV_m / RT) = G_{hs} / RT + G_i / RT \quad (1)$$

where R is the gas constant, T is temperature, V_m is the molar volume of the solvent, G_{hs} is the molar hard-sphere cavity-formation energy, and G_i is the molar solute-solvent interaction energy.

The ionic liquid consists of cation c and anion a . The hard-sphere diameters of the cation, anion and the solute are σ_c , σ_a and σ_s , respectively. G_{hs} is given by scaled-particle theory [25]:

$$\frac{G_{hs}}{RT} = -\ln(1-\xi_3) + \frac{3\xi_2}{1-\xi_3}\sigma_s + \left[\frac{3\xi_1}{1-\xi_3} + \frac{9}{2}\left(\frac{\xi_2}{1-\xi_3}\right)^2 \right] \sigma_s^2 + \frac{P}{k_B T} \frac{\pi\sigma_s^3}{6} \quad (2)$$

where ξ_0 , ξ_1 , ξ_2 and ξ_3 are given by

$$\xi_0 = \frac{\pi}{6}(\rho_c + \rho_a) \quad (3a)$$

$$\xi_1 = \frac{\pi}{6}(\rho_c\sigma_c + \rho_a\sigma_a) \quad (3b)$$

$$\xi_2 = \frac{\pi}{6}(\rho_c\sigma_c^2 + \rho_a\sigma_a^2) \quad (3c)$$

$$\xi_3 = \frac{\pi}{6}(\rho_c\sigma_c^3 + \rho_a\sigma_a^3). \quad (3d)$$

Here ρ_c is the number density of the cation, ρ_a is the number density of the anion, k_B is the Boltzmann constant, and P is the hard-sphere pressure of the ionic liquid [25]

$$P = \frac{6k_B T}{\pi} \left[\frac{\xi_0}{1-\xi_3} + \frac{3\xi_1\xi_2}{(1-\xi_3)^2} + \frac{3\xi_2^3}{(1-\xi_3)^3} \right] \quad (4)$$

In the original scaled-particle theory, Pierotti [26] assumed that P is the experimental pressure of the solvent; that assumption makes the last term in Eq. (2) negligible. However, based on molecular simulations, Hu *et al.* [27] reported that when Eq. (4) is used and a more reasonable radial distribution function for solvent is used, Eq. (2) gives better results. In this work, we use Eqs. (2) and (4).

The solvent molecule is polarizable and may have a dipole and/or quadrupole moment. Therefore G_i consists of four parts, reflecting contributions from dispersion, induction, dipole-charge interaction and quadrupole-charge interactions:

$$G_i = G^{\text{dispision}} + G^{\text{induction}} + G^{\text{dipole}} + G^{\text{quadrupole}} . \quad (5)$$

The dispersion interaction between solute and solvent is given by

$$G^{\text{dispersion}} = \sum_{j=c,a} N_A \int_{\sigma_{js}}^{+\infty} \Gamma_{js}^{\text{dis}}(r) g_{js}(r) \rho_j 4\pi r^2 dr \quad (6)$$

where r is the molecular center-to-center distance, $\Gamma_{js}^{\text{dis}}(r)$ is the potential between ion and solute; $g_{js}(r)$ is the radial distribution function of ions j around the solute; $\sigma_{js} = (\sigma_j + \sigma_s)/2$ is the collision diameter of ion j and solute s , and N_A is Avogadro's constant. For our approximate data-correlation purposes, we use the van der Waals simplification $g_{js}(r)=1$ for $r > \sigma_{js}$. For the dispersion potential between ion and solute, we assume

$$\Gamma_{js}^{\text{dis}}(r) = 4\sqrt{\varepsilon_j \varepsilon_s} \left[\left(\frac{\sigma_{js}}{r} \right)^{12} - \left(\frac{\sigma_{js}}{r} \right)^6 \right] \quad r > \sigma_{js} \quad (7)$$

where ε_j and ε_s are dispersion-energy parameters of ion j and solute s , respectively.

To calculate the electrostatic contribution, we consider the solvent as a dielectric continuum with dielectric constant D , and the solute as a cavity with diameter a in the dielectric continuum [28,29]. Diameter a is not necessarily the same as the diameter of the solute. Following Onsager's [28,29] suggestion for a cavity in a pure fluid, we use

$$a = \frac{\sigma_s}{\xi_3^{1/3}} \quad (8)$$

where ξ_3 , given by Eq. (3d), is the packing fraction of the solvent.

Embedded in the dielectric continuum, the solute experiences a fluctuating electrical field

e [29] given by

$$\langle e^2 \rangle = \frac{6(D-1)}{(2D+1)(a/2)^3} k_B T. \quad (8)$$

The induction energy is given by

$$G^{\text{induction}} = -\frac{1}{2} N_A \alpha_s \langle e^2 \rangle \quad (9)$$

where α_s is the polarizability of the solute.

The solute molecule may have a dipole moment μ and/or a quadrupole moment Q . When a dipole or quadrupole is placed into a continuum dielectric, the potentials are [28,29]

$$\varphi^{\text{dipole}} = -\frac{2(D-1)}{(2D+1)(a/2)^3} \mu \quad (10)$$

$$\varphi^{\text{quadrupole}} = -\frac{(D-1)}{(3D+2)(a/2)^5} Q. \quad (11)$$

Contributions of the dipole-charge and quadrupole-charge interactions to G_i are given by

$$\begin{aligned} G^{\text{dipole}} &= N_A \varphi^{\text{dipole}} \mu \\ &= -N_A \frac{2(D-1)}{(2D+1)(a/2)^3} \mu^2 \end{aligned} \quad (12)$$

$$\begin{aligned} G^{\text{quadrupole}} &= N_A \varphi^{\text{quadrupole}} Q \\ &= -N_A \frac{(D-1)}{(3D+2)(a/2)^5} Q^2. \end{aligned} \quad (13)$$

Substituting Eqs. (2), (5), (9), (13), (13) into Eq. (1) and noting that for ionic liquids, $D \gg 1$, we obtain an expression for Henry's constant:

$$\begin{aligned}
\ln(HV_m / RT) = & -\ln(1-\xi_3) + \frac{3\xi_2}{1-\xi_3} \sigma_s + \left[\frac{3\xi_1}{1-\xi_3} + \frac{9}{2} \left(\frac{\xi_2}{1-\xi_3} \right)^2 \right] \sigma_s^2 \\
& + \left[\frac{\xi_0}{1-\xi_3} + \frac{3\xi_1\xi_2}{(1-\xi_3)^2} + \frac{3\xi_2^3}{(1-\xi_3)^3} \right] \sigma_s^3 - \frac{32\pi}{9k_B T} \sum_{j=c,a} \rho_j \sigma_{js}^3 \sqrt{\varepsilon_j \varepsilon_s} \\
& - \frac{1}{k_B T} \left(\frac{3k_B T \alpha_s \xi_3}{2(\sigma_s/2)^3} + \frac{\mu^2 \xi_3}{(\sigma_s/2)^3} + \frac{Q^2 \xi_3^{5/3}}{3(\sigma_s/2)^5} \right). \tag{14}
\end{aligned}$$

Data Correlation

In Eq. (12), Henry's constant depends on temperature T and on solvent molar volume V_m . The solvent is characterized by two ionic diameters, σ_c and σ_a , and two dispersion-energy parameters, ε_c and ε_a . The solute is characterized by diameter σ_s , dispersion-energy parameter ε_s and polarizability α_s . For polar solute molecules, we also need dipole moment μ and quadrupole moment Q .

For high-temperature molten salts, we use ion diameters that are slight modifications of those given by Pauling [30]. For ionic liquids, each ion diameter is estimated according to the ion's structure [1] and then slightly adjusted as dictated by an overall examination of the solubility data. The densities of ionic liquids are from [16, 17, 20, 21,22], and those of molten salts are from the CRC handbook [33]. Solute polarizabilities, dipole moments and some of the quadrupole moments are from Gray and Gubbins [31] and the CRC handbook [33]. The quadrupole moments of relatively complex molecules are estimated from molecular structure. Because quadrupole data are not available for 1-pentene, 1-hexene, 1-heptene and toluene, we assume that these liquids have the same quadrupole moment as that of ethylene, and that toluene has the same quadrupole moment as that of benzene. The diameter of the solute, the dispersion-energy parameter of the solute and the dispersion-energy parameters of the ions are used as adjustable parameters to correlate Henry's constants.

For solutes that are liquids at ordinary temperatures, we obtain experimental Henry's

constants from experimental data for γ^∞ , the activity coefficient at infinite dilution:

$$H = P^s \varphi^s \gamma^\infty \quad (3)$$

where P^s and φ^s are the saturation pressure and saturation fugacity coefficient of the pure solute, respectively. P^s and φ^s of the solutes are given by Krummen *et al.* [16].

We correlate Henry's constants of gases at high temperatures in two molten salts, NaCl and RbCl, and at ordinary temperatures in two ionic liquids, [BMIM][PF₆] and [BMIM][BF₄]. We also correlate Henry's constants of organic solutes in 10 ionic liquids; results are given in the Appendix. Tables 1 and 2 give parameters for ions and for solutes. Table 3 gives sources for experimental solubility data. Figs. 1-4 compare some calculated and observed Henry's constants.

In many cases, experimental Henry's constants for gases are subject to considerable uncertainty, especially for those gases whose solubility is very small. In some cases, for the same system, different laboratories report appreciably different experimental results. Nevertheless, calculated Henry's constants are in reasonable agreement with experiment. While our results for hydrogen do not show the reported minimum near 314K, we do not know if the experimentally observed weak minimum is real.

The results shown in Figures 1-4 and in the Appendix suggest that calculated Henry's constants agree with experiment within about $\pm 70\%$. This uncertainty is similar to that when Henry's constants for ordinary systems are correlated with perturbed-hard-sphere theory.

Conclusion

The correlation presented here is necessarily preliminary because, as yet, the experimental data base is small. Further, there is considerable uncertainty in the measured Henry's constants for gases. As more reliable experimental data become available, some of the parameters reported in Tables 1 and 2 will require revision. Nevertheless, the promising initial correlation results reported here suggest that our simple perturbed-hard-sphere theory may be useful for estimating solubilities of volatile nonelectrolytes in ionic liquids.

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Table 1. Parameters for ions

	$10^8 \sigma_c$ (cm)	ε_c / k_B (K)		$10^8 \sigma_a$ (cm)	ε_a / k_B (K)
Na^+	1.71	250	Cl^-	3.35	250
Rb^+	3.11	230	$[\text{BF}_4]^-$	4.40	250
$[\text{MMIM}]^+$	5.00	380	$[\text{PF}_6]^-$	4.76	205
$[\text{EMIM}]^+$	5.25	380	$[(\text{CF}_3\text{SO}_2)_2\text{N}]^-$	6.05	500
$[\text{BMIM}]^+$	5.70	380	$[(\text{CH}_3)_2\text{PO}_4]^-$	5.03	455
$[\text{PY}]^+$	4.80	458	$[\text{CH}_3\text{SO}_4]^-$	4.70	565
$[\text{EPY}]^+$	5.18	350	$[\text{C}_2\text{H}_5\text{SO}_4]^-$	5.05	450
$[\text{BMPY}]^+$	5.81	525	$[\text{CH}_3\text{OC}_2\text{H}_4\text{SO}_4]^-$	5.34	440
			$[\text{C}_2\text{H}_5\text{OC}_2\text{H}_4\text{SO}_4]^-$	5.50	430

k_B is Boltzmann's constant

$[\text{MMIM}]^+$ 1-methyl-3-methylimidazolium

$[\text{EMIM}]^+$ 1-ethyl-3-methylimidazolium

$[\text{BMIM}]^+$ 1-butyl-3-methylimidazolium

$[\text{PY}]^+$ pyridinium

$[\text{EPY}]^+$ N-ethyl-pyridinium

$[\text{BMPY}]^+$ 4-methyl-N-butyl-pyridinium

Table 2. Parameters for solutes

	$10^8 \sigma_s$ (cm)	ε_s / k_B (K)	$10^{24} \alpha_s$ (cm ³)	$10^{18} \mu$ (esu · cm)	$10^{26} Q$ (esu · cm ²)
Argon	3.60	120	1.64	0	0
Hydrogen	3.00	25	0.806	0	0.637
Oxygen	3.80	130	1.58	0	0.4
Nitrogen	3.90	130	1.74	0	1.4
Carbon dioxide	3.81	280	2.64	0	4.30
Hydrogen chloride	3.50	335	2.63	1.11	0
Methane	3.95	180	2.60	0	0
Ethane	4.32	300	4.50	0	0.65
Ethylene	4.28	350	4.25	0	1.50
n-Pentane	5.10	450	9.99	0	0
n-Hexane	5.31	505	11.9	0	0
n-Heptane	5.54	550	13.6	0	0
Cyclopentane	4.90	510	9.15	0	0
Cyclohexane	5.10	570	11.0	0	0
1-Pentene	5.00	465	9.65	0.4	1.50
1-Hexene	5.20	525	11.65	0.3	1.50
1-Heptene	5.44	575	13.51	0.3	1.50
Benzene	4.80	410	10.6	0	8.69
Toluene	5.00	720	12.3	0.37	8.69
Acetone	4.62	250	6.42	2.88	0

Table 3. Data sources for experimental solubilities and for ionic-liquid densities

	Solubility	Density
Gases in NaCl	32	33
Gases in RbCl	32	33
Gases in [BMIM] [PF ₆]	5 and 7 *	21
Gases in [BMIM] [BF ₄]	6 and 7 *	22
Solutes in [MMIM][CH ₃ SO ₄]	17	17
Solutes in [MMIM][CH ₃ OC ₂ H ₄ SO ₄]	17	17
Solutes in [MMIM][(CH ₃) ₂ PO ₄]	17	17
Solutes in [MMIM][(CF ₃ SO ₂) ₂ N]	16	16
Solutes in [EMIM][(CF ₃ SO ₂) ₂ N]	16 and 14	16
Solutes in [EMIM] [C ₂ H ₅ SO ₄]	16	16
Solutes in [BMIM][(CF ₃ SO ₂) ₂ N]	16	16
Solutes in [PY][C ₂ H ₅ OC ₂ H ₄ SO ₄]	17	17
Solutes in [EPY][(CF ₃ SO ₂) ₂ N]	17	17
Solutes in [BMPY][BF ₄]	9	20

* For gases with low solubilities, Ref. 7 gives Henry's constants that are more accurate than those in Ref. 5 and Ref. 6.

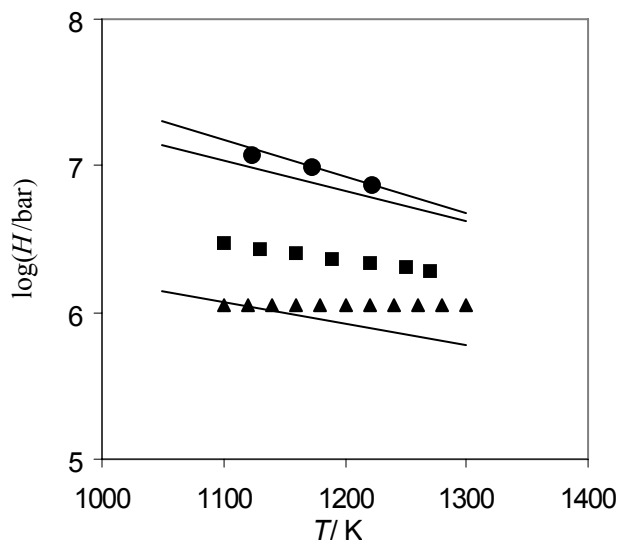


Fig. 1(a) Henry's constants for some gases at very high temperatures in molten NaCl.

Experimental: ● Ar; ■ CO₂; ▲ HCl. Lines: Perturbed-hard-sphere theory.

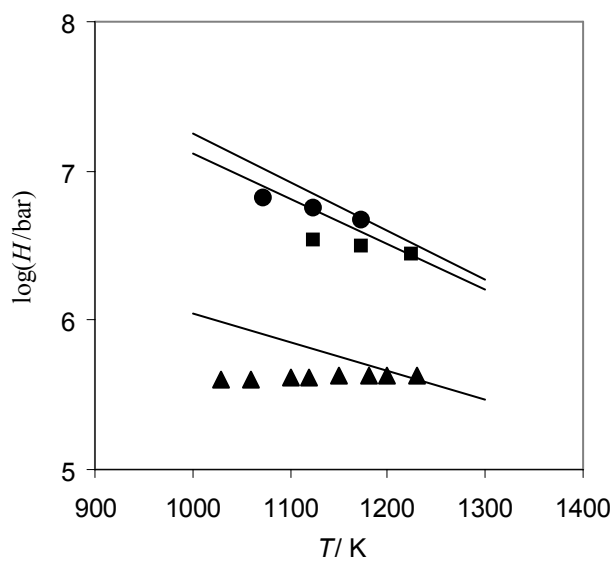


Fig. 1(b) Henry's constants for some gases at very high temperatures in molten RbCl.

Experimental: ● Ar; ■ CO₂; ▲ HCl. Lines: Perturbed-hard-sphere theory.

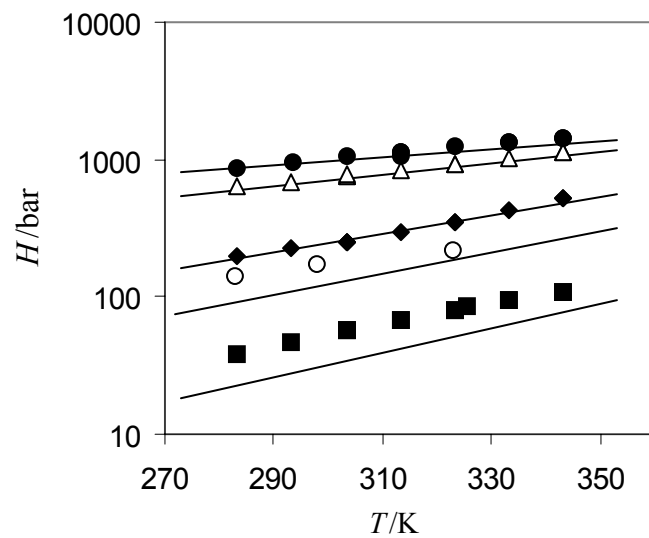


Fig. 2 Henry's constants for some gases in [BMIM] [PF₆]

Experimental: ● Argon; △ Methane; ◆ Ethane; ○ Ethylene; ■ Carbon dioxide. Lines: Perturbed-hard-sphere theory.

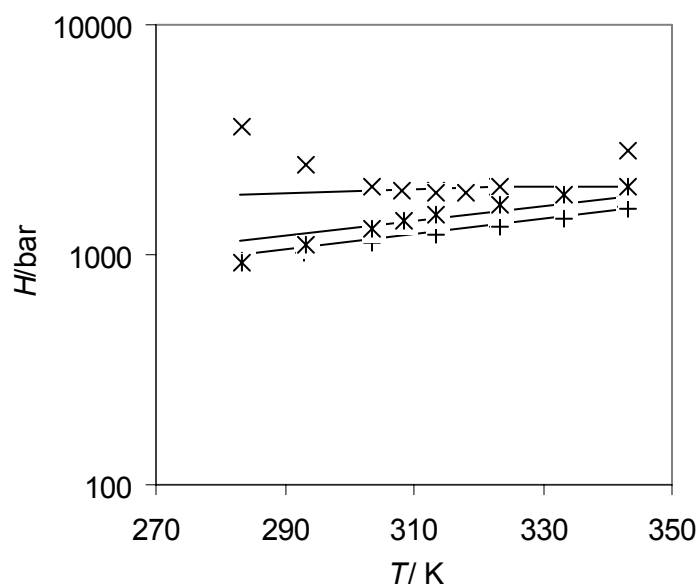


Fig. 3(a) Henry's constants for some gases in [BMIM] [PF₆]

Experimental: × Hydrogen; * Nitrogen; + Oxygen. Lines: Perturbed-hard-sphere theory.

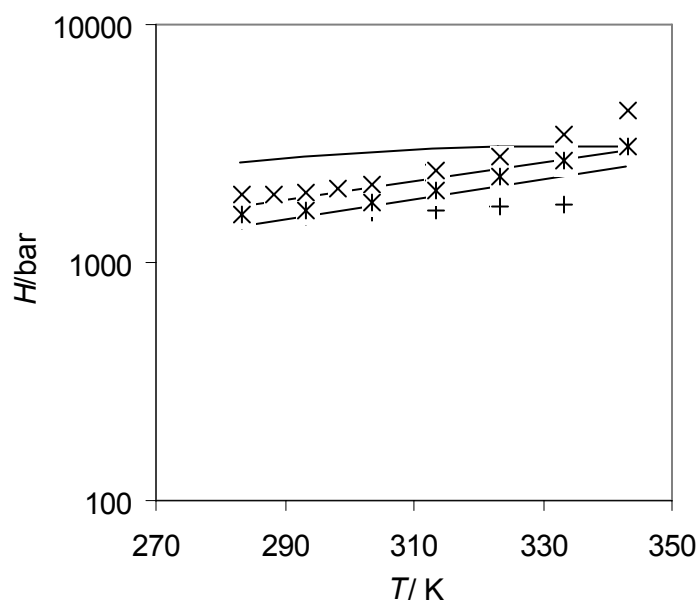


Fig. 3(b) Henry's constants for some gases in [BMIM] [BF₄]

Experimental: × Hydrogen; * Nitrogen; + Oxygen. Lines: Perturbed-hard-sphere theory.

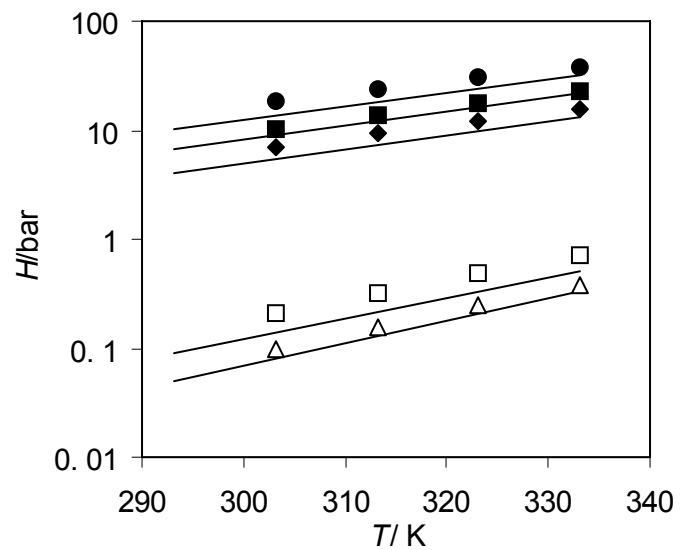


Fig.4 Henry's constants for some solutes in [MMIM] [(CF₃SO₂)₂N].

Experimental: ● n-Pentane; ■ 1-Pentene; ◆ Cyclopentane; □ Benzene; △ Toluene.

Lines: Perturbed-hard-sphere theory.

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Appendix. Calculated and Observed Henry's Constants for Solutes in Ionic Liquids

Table A1. Henry's constants for solutes in [MMIM][(CF₃SO₂)₂N] at 30 and 60 °C, bar

	30 °C		60 °C	
	calc	expt	calc	expt
n-Pentane	14.6	18.2	33.3	37.8
n-Hexane	7.79	9.77	19.7	23.1
n-Heptane	4.80	5.13	13.4	13.8
Cyclopentane	5.82	6.93	14.1	15.6
Cyclohexane	2.94	3.64	7.92	9.12
1-Pentene	9.36	10.2	21.9	22.6
1-Hexene	4.95	5.13	12.9	13.0
1-Heptene	2.91	2.64	8.41	7.50
Benzene	0.151	0.211	0.537	0.701
Toluene	0.0843	0.0977	0.331	0.380

Table A2. Henry's constants for solutes in [EMIM][(CF₃SO₂)₂N] at 20 and 50 °C, bar

	20 °C		50 °C	
	calc	expt	calc	expt
n-Pentane	7.60	10.2	18.6	23.2
n-Hexane	3.85	4.81	10.6	12.7
n-Heptane	2.25	2.26	6.88	6.90
Cyclopentane	3.16	3.65	8.19	9.13
Cyclohexane	1.52	1.74	4.44	4.80
1-Pentene	4.95	5.75	12.5	14.0
1-Hexene	2.51	2.60	7.06	7.37
1-Heptene	1.39	1.22	4.39	3.98
Benzene	0.0742	0.117	0.291	0.431
Toluene	0.0431	0.0526	0.185	0.220
Acetone	0.0580	0.0974	0.224	0.332

Table A3. Henry's constants for solutes in [BMIM][(CF₃SO₂)₂N] at 20 and 50 °C, bar

	20 °C		50 °C	
	calc	expt	calc	expt
n-Pentane	4.97	5.65	12.0	13.1
n-Hexane	2.53	2.41	6.82	6.65
n-Heptane	1.46	1.04	4.36	3.39
Cyclopentane	2.27	2.12	5.77	5.45
Cyclohexane	1.11	0.941	3.15	2.75
1-Pentene	3.37	3.50	8.34	8.91
1-Hexene	1.72	1.49	4.75	4.35
1-Heptene	0.950	0.652	2.92	2.18
Benzene	0.0565	0.0868	0.216	0.321
Toluene	0.0379	0.0353	0.156	0.156

Table A4. Henry's constants for solutes in[EMIM] [C₂H₅SO₄] at 30 and 60 °C, bar

	30 °C		60 °C	
	calc	expt	calc	expt
n-Hexane	25.9	17.6	70.9	52.9
n-Heptane	16.8	14.8	51.6	39.9
Cyclopentane	16.1	9.10	41.6	31.2
Cyclohexane	8.28	9.09	24.1	21.2
1-Hexene	15.3	14.4	42.9	32.9
1-Heptene	9.43	8.74	29.8	22.2
Benzene	0.447	0.430	1.66	1.45
Toluene	0.200	0.260	0.846	1.00

Table A5. Henry's constants for solutes in [MMIM] [CH₃SO₄] at 30 and 60 °C, bar

	30 °C		60 °C	
	calc	expt	calc	expt
n-Pentane	55.3	36.4	152	60.5
n-Hexane	27.7	27.7	88.1	53.7
n-Heptane	16.8	23.3	61.2	49.2
Cyclopentane	15.6	28.6	46.1	41.9
Cyclohexane	7.22	22.5	24.6	44.9
1-Pentene	29.6	36.2	88.4	62.8
1-Hexene	15.1	29.3	49.4	55.4
1-Heptene	8.62	22.2	32.3	47.4
Benzene	0.491	1.15	2.05	3.03
Toluene	0.119	0.836	0.611	2.30

Table A6. Henry's constants for solutes in[MMIM] [CH₃OC₂H₄SO₄] at 50 and 60 °C, bar

	50 °C		60 °C	
	calc	expt	calc	expt
n-Pentane	103	103	134	123
n-Hexane	62.8	89.0	85.1	119
n-Heptane	45.3	70.2	63.4	100
Cyclopentane	36.2	44.1	48.2	57.0
Cyclohexane	20.6	37.7	28.5	50.7
1-Pentene	62.5	56.3	82.4	70.4
1-Hexene	37.4	46.0	51.0	58.1
1-Heptene	25.6	36.2	36.3	46.5
Benzene	1.21	1.53	1.82	2.13
Toluene	0.629	1.21	0.978	1.72
Acetone	1.03	1.72	1.53	2.42

Table A7. Henry's constants for solutes in [MMIM] [(CH₃)₂PO₄] at 30 and 60 °C, bar

	30 °C		60 °C	
	calc	expt	calc	expt
Cyclohexane	7.69	7.78	23.4	22.3
1-Heptene	8.68	8.98	28.9	28.1
Benzene	0.474	0.559	1.81	1.87
Toluene	0.178	0.353	0.791	1.34

Table A8. Henry's constants for solutes in [PY] [(C₂H₅OC₂H₄SO₄) at 30 and 60 °C, bar

	30 °C		60 °C	
	calc	expt	calc	expt
n-Hexane	12.0	11.1	34.3	28.1
n-Heptane	7.21	8.59	23.2	23.3
Cyclopentane	8.31	8.04	22.3	18.2
Cyclohexane	4.00	5.86	12.1	14.9
1-Pentene	14.4	7.67	37.4	13.7
1-Hexene	7.28	5.88	21.3	11.3
Benzene	0.252	0.600	0.968	1.92
Toluene	0.0978	0.338	0.432	1.02

Table A9. Henry's constants for solutes in [EPY] [(CF₃SO₂)₂N] at 30 and 60 °C, bar

	30 °C		60 °C	
	calc	expt	calc	expt
n-Pentane	13.8	17.1	31.3	37.2
n-Hexane	7.48	8.33	18.9	20.4
n-Heptane	4.66	4.14	13.0	11.4
Cyclopentane	5.76	5.78	13.8	13.1
Cyclohexane	2.97	2.98	7.93	7.50
1-Pentene	9.00	8.79	21.0	19.2
1-Hexene	4.86	4.30	12.5	11.0
1-Heptene	2.89	2.25	8.29	6.63
Benzene	0.151	0.199	0.533	0.716
Toluene	0.0956	0.0904	0.365	0.377
Acetone	0.114	0.170	0.398	0.530

Table A10. Henry's constants for solutes in [BMPY] [BF₄] at 40 and 60 °C, bar

	40 °C		60 °C	
	calc	expt	calc	expt
n-Hexane	19.1	22.0	36.0	40.1
n-Heptane	12.4	10.5	25.1	21.0
Cyclohexane	7.07	7.04	13.8	12.6
Benzene	0.463	0.395	1.05	0.843
Toluene	0.240	0.206	0.590	0.488
Acetone	0.386	0.496	0.868	1.01