Activity coefficients at infinite dilution of aroma compounds in water: effect of temperature and salt concentration.

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ABSTRACT

Activity coefficients at infinite dilution in water have been determined for some aroma compounds detected in brown crab liquid effluent produced during boiling (1-octen-3-ol, 1-penten-3-ol, 3-methylbutanal, hexanal, benzaldehyde, 2,3-pentadione and ethyl acetate) by using the headspace gas chromatography technique (HSGC). Experimental data have been obtained over the temperature range of 40ºC to 50ºC. In this work, activity coefficients at infinite dilution for different type of systems have been considered: one component solute + water and multicomponent solute + water. No significant differences were observed between activity coefficients obtained in these two types of systems. Additionally the effect of salt concentration at 40ºC has been studied by varying salt concentration from 0 to 1.71

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mol/kg. Experimental data were fitted as a function of salt concentration by using the Setschenow equation obtaining the salting out coefficient.

1. INTRODUCTION

Knowledge of the thermodynamic behavior of dilute aqueous solutions is necessary for a correct design of processes to separate dilute compounds such as aroma recovery from food streams. In previous work (1), it has been reported that the pervaporation technique is a promising alternative to recover the volatile fraction from brown crab processing effluent. Pervaporation is a membrane process that has been considered in the last years as an alternative to conventional methods to recover aroma compounds, since the addition of chemical solvents is avoided (2). Based on the solution/diffusion model the flux of component i through the membrane is proportional to the difference in partial vapor pressure at both sides of the membrane $\left(x_i \gamma_i p_i^s - y_i p_p\right)$. In pervaporation of dilute aqueous solutions, activity coefficients at infinite dilution in water (γ_i^∞) are used as feed-side activity coefficients due to the very low concentrations of aroma compounds in the feed. Activity coefficients at infinite dilution provide an insight into the chemical and physical interactions between water (solvent) and aroma compounds (solute molecules) in the absence of solute-solute interactions.

The affinity of a solvent towards a volatile compound can be expressed using Henry's law:

$$H = \lim_{x_i \to 0} \frac{p_i}{x_i}$$

[1]

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where p_i is the partial pressure of the volatile component and x_i its mole fraction at infinite dilution. The activity coefficient at infinite dilution of the volatile compound in the solvent is determined by taking into account the vapor pressure of the volatile compound at the same temperature, p_i^s (3):

$$\gamma_i^\infty = \frac{H}{p_i^s} \qquad\qquad [2]$$

Both, Henry constant and γ_i^∞, allow the evaluation of affinity of the aroma compound and the solvent (water) (4).

Different techniques have been developed to determine γ_i^∞ in water. Sherman et al. (5) emphasize that each method is most suitable in a certain range of relative volatility at infinite dilution, $\alpha_{i,w}^\infty$, defined as:

$$\alpha_{i,w}^\infty = \frac{p_i^s}{p_w^s} \gamma_i^\infty \qquad\qquad [3]$$

In this study the headspace gas chromatography has been used to determine γ_i^∞. The headspace gas chromatography is useful not only for analytical purposes (6), but also provides a valuable tool to obtain thermodynamically reliable data (7). Static headspace methods are based on measurements of gas-liquid thermodynamic equilibrium . This technique has a range of applicability from low relative volatility systems (around 0.5) to systems of relative volatilities up to 1000 (5).

In this work, the activity coefficients at infinite dilution of seven volatile compounds found in the brown crab processing effluent (1-octen-3-ol, 1-penten-3-ol, 3-methylbutanal, hexanal, benzaldehyde, 2,3-pentadione and ethyl acetate) have been determined by using

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the headspace gas chromatography technique (HS-GC). These coefficients were determined at three different temperatures over the range 40ºC to 50ºC. In food systems the volatility of aroma compounds is dependent on the presence of nonvolatile components such as sugars, salts, lipids and other macromolecular compounds (8). In the particular case of aroma recovery from brown crab effluent, the effect of the presence of salts must be considered. Therefore, the effect of sodium chloride on activity coefficients at infinite dilution has been analyzed by varying the salt concentration in the range 0 to 1.7 mol/kg at 40ºC, since it is well known that the presence of salts and other electrolytes may increase or decrease the value of γ_i^∞ (9).

2. EXPERIMENTAL SECTION

2.1. Materials

The volatile compounds, whose activity coefficients at infinite dilution have been determined in theis work, belong to different chemical classes: alcohols such as 1-octen-3-ol (Sigma Aldrich, 98 %), 1-penten-3-ol (Sigma Aldrich, 99 %); aldehydes such as 3-methylbutanal (Sigma Aldrich, 97 %), hexanal (Sigma Aldrich, 98 %), benzaldehyde (Sigma Aldrich, >=99 %); ketones such as 2,3-pentadione (Sigma Aldrich, 98 %) and esters as ethyl acetate (Sigma Aldrich, HPLC grade). The volatile compounds were used as received. Milli-Q-Millipore ultra pure water was used in this work. Water was degassed by ultrasound (Selecta, Ultrasons-H). Sodium chloride was supplied by Sigma ($\geq$ 99.5 % purity).

2.2. Systems

Activity coefficients at infinite dilution, γ_i^∞, have been determined for systems of various types. First, γ_i^∞ has been obtained for binary systems consisting of a volatile compound and water at three different temperatures, 40ºC, 45ºC and 50ºC. The headspace oven could not be regulated below 40ºC and this value was the lowest temperature studied in this work. Subsequently, γ_i^∞ has been obtained for a system formed by all the aroma compounds previously considered and water at 40ºC. Finally the effect of salt on γ_i^∞ has been determined for a multicomponent solute and water system at 40 ºC in the range 0 to 1.7 mol/kg of salt concentration.

2.3. Apparatus and procedure

Activity coefficients at infinite dilution were determined by headspace gas chromatography (HS-GC). The HS-GC consists of a gas chromatograph (Hewlett Packard GC 6890) and a headspace sampler (Hewlett Packard 7694E).

To determine γ_i^∞, glass vials (ca. 20 cm^3) were filled gravimetrically with different mixtures of the corresponding system varying the mole fraction of the volatile compound in the liquid phase. To obtain one activity coefficient at infinite dilution, seven measurements were performed to determine the vapor solute partial pressure as a function of the solute concentration. The interval of infinite dilution region cannot be evaluated a priori. For highly associated compounds, this region is smaller than 10^{-4} mole fraction and can be as small as 10^{-6} or 10^{-7} (10). In our case, mole fraction of the aroma compounds was kept below $2 \cdot 10^{-4}$ in all cases. In this concentration range results are obtained under Henry's law conditions (see section 3.1). Solutions were prepared from a concentrated solution (approximately 1000 ppm) in water or in a salty water mixture. This mixture was stored at

4ºC to avoid losses of volatile compounds and diluted for the different solutions concentrations. The vials were filled about half way (ca. 10 cm^3) and immediately sealed properly with a pressure-tight rubber septum and a special aluminum lid to ensure that the headspace gases do not escape. Equilibrium between gas and liquid phases is reached in the headspace oven. After reaching equilibrium, an aliquot of the vapor phase is withdrawn and transported and analyzed in the GC. The GC column was a 007 FFAP 25 m × 0.25 mm bonded phase fused silica capillary column. The injector and flame ionization detector were at 200 ºC and 250ºC respectively. The oven was operated at programmed temperature, from 40ºC to 220ºC. At least three replicates of each experiment were made.

Equilibrium time was determined for each of the investigated systems. For that, different glass vials were prepared with the same concentration and kept in the headspace oven for different increasing time intervals. When the peak areas obtained in the GC were constant, phase equilibrium was assumed to be reached.

Calibration was performed according to Whitehead and Sandler (11) by using pure components at different temperatures to determine the relationship between solute vapor pressure and peak area. This way, for mixtures, the solute partial pressure in equilibrium with the dilute solution can be obtained from the saturation pressure calibration curves. For all the components and range of conditions considered in this work, the pure component peak area was linearly proportional to vapor pressure with a linear correlation coefficient above 0.99.

Vapor pressure correlations of the pure compounds were obtained or predicted considering experimental data found in the literature by using Aspen Plus (2008) (12) except for 2,3-

pentadione, which Antoine constants were obtained from the literature (13). The equation for the extended Antoine vapor pressure model is:

$$\ln\left(p_i^s/kPa\right) = C_{1,i} + \frac{C_{2,i}}{(T/K) + C_{3,i}} + C_{4,i}(T/K) + C_{5,i}\ln(T/K) + C_{6,i}(T/K)^{C_{7,i}} \qquad [4]$$

Coefficients for the extended Antoine equation are listed in Table 1. The uncertainty in the pure solute vapor pressure has not been considered in γ_i^∞ calculation since the way the vapor pressure data have been obtained is unknown. Similar procedure has been followed in the literature (14, 15)

3. RESULTS AND DISCUSSION

When determining γ_i^∞ by headspace, it must be taken into account that the liquid phase composition in equilibrium with the vapor phase does not correspond with the liquid composition calculated from the amounts weighed, since a certain amount has been vaporized during equilibration. This correction has been calculated as indicated by Brendel and Sandler (9). Due to the large difference in the molar volume of a liquid and a gas, the correction in the liquid phase was not very important. For the systems studied in this work the relative deviation between the initial and the real liquid phase composition was always lower than 2 %. This correction, though small, was included in all the results. Additionally, as it was pointed out by Whitehead and Sandler (11) the greatest source of experimental error in the activity coefficient at infinite dilution calculation comes from the solute peak area determination.

3.1 Binary systems: solute + solvent

The values of γ_i^∞ for the aroma compounds selected in this work have been determined at three different temperatures, 40ºC, 45ºC and 50ºC. The partial pressures of the volatile compounds in the vapor phase in the vials were calculated from the calibration with pure components and the detector response. This solute partial pressure has been found to be a linear function of the aroma mole fraction in the liquid phase. As an example, Figure 1 shows this behavior for benzaldehyde at the three different temperatures studied in this work. In this graph, the uncertainties for the mole fraction and the partial pressure have been also represented. Henry's law constant can be calculated from the slope of the variation of partial pressure with mole fraction according to Equation 1 (3). This slope is independent of mole fraction, which indicates that results were obtained under Henry´s law conditions in the interval of infinite dilution. Activity coefficients were directly deduced from H values by using Equation 2. The H and γ_i^∞ values for each volatile compound at the three temperatures are listed in Table 2 together with the uncertainties for the activity coefficients calculated. The uncertainties for γ_i^∞ are expressed through the relative standard deviations calculated from the uncertainties of the experimental variables (24). Relative standard deviations range from 4% to a maximum of 17%. For most experimental points relative standard deviation is less than 10 %, with a mean value of 9%. The maximum value of 17% corresponds to 1-octen-3-ol. Brendel and Sandler (9) pointed out that the error of the HS-GC technique can be as high as 25%, especially for compounds with low solubility and high values of activity coefficient at infinite dilution, as is the case of 1-octen-3-ol.

The temperature dependence of γ_i^∞ can be expressed by an Arrhenius type relationship (26):

$$\ln \gamma_i^\infty = a + \frac{b}{(T/K)} \qquad [5]$$

In general γ_i^∞ slightly increase with increasing temperature. Figure 2 shows the logarithms of γ_i^∞ as a function of the reciprocal temperature and the corresponding Arrhenius fit.

Table 2 also reports some activity coefficients found in the literature for the compounds studied in this work. For some of the compounds, differences can be appreciated among the different values reported in the literature. In this regard Barrera Zapata et al. (25) emphasize that accurate data for γ_i^∞ are not abundant and even for common systems like ethanol in water at room temperature, the experimental values reported for γ_i^∞ can vary by a factor of two. Figure 3 shows the logarithms of the activity coefficients at infinite dilution obtained in this work for ethyl acetate as a function of the reciprocal temperature, together with the data found in the literature. From linear regression analysis of all the data, an activity coefficient of 67.8 can be estimated for ethyl acetate at 298.15 K. For the rest of the compounds limited published data do not allow precise comparison with the results of the present work. For hexanal, benzaldehyde and 1-octen-3ol a value of γ_i^∞ of 694, 501 and 1753 respectively at 298.15 K can be extrapolated from the experimental data reported in this work.

3.2 Multicomponent solute + solvent system

Activity coefficients at infinite dilution for each volatile compound previously considered in this work were also determined in a mixture formed by all the volatile compounds (multicomponent solute) and the solvent (water). Table 3 shows the γ_i^∞ values obtained for each compound in this multicomponent mixture at 40ºC and the values obtained at the same temperature in a single component solute mixture. This Table also presents the uncertainty of γ_i^∞ through the percentage of the relative standard deviation. As an example, Figure 4

shows the solute partial pressure in the vapor phase as a function of the mole fraction of the liquid phase in the single component solute mixture and in the multicomponent solute mixture for ethylacetate. The values obtained for multicomponent solute-water mixtures at 40ºC are similar to those obtained for single solute component-water mixtures concluding that no interactions take place among the volatile compounds in the range studied in this work. So, in this case, a mixture with (n-1) components at a composition close to zero and the solvent at a composition close to 1 is similar to the situation of having (n-1) binary mixtures formed by the solvent and the (n-1) components, always infinitely diluted (10). Similar results were obtained for Bao and Han (27) in the study of the infinite dilution activity coefficients for various types of systems.

3.2 Effect of salt on activity coefficients at infinite dilution

The effect of salt concentration on γ_i^∞ has been evaluated by varying the sodium chloride concentration from 0 to 1.71 mol/kg (0% to 10 wt%) at 40ºC. Henry's constants have been calculated through the slope of solute partial pressure in the vapor phase as a function of mole fraction of the solute in the liquid phase. Activity coefficients were then deduced from equation (2). The experimental values are listed in Table 4. As a general trend, the values of γ_i^∞ increase with increasing salt concentration; this effect is referred as "salting out" since an increase of the activity coefficient value involves lower solubility values.

Brendel and Sandler (9) proposed the following equation to correlate γ_i^∞ in salty solutions based on the Setschenow empirical equation to correlate solubilities of substances in salty solutions:

$$\ln\left(\frac{\gamma_i^\infty}{\gamma_{i,o}^\infty}\right) = k_i c_s \qquad\qquad [8]$$

where γ_i^∞ is the activity coefficient at infinite dilution in salty solutions, $\gamma_{i,o}^\infty$ the activity coefficient at infinite dilution in pure water, c_s the salt concentration and the proportionality factor, k_i, is the salting-out coefficient. Brendel and Sandler (9) report a dependence of k on temperature but this effect has not been studied in this work. The values of the salting out coefficients at 40ºC are provided in Table 4. The correlation factor was higher than 0.98 for the all the compounds considered in this work. According to equation 3, the relative volatility would also increase with salt concentration due to the salting out effect.

4. Conclusions

The Henry's law constant and the activity coefficient at infinite dilution of seven volatile compounds found in brown crab boiling effluent have been determined by using the headspace gas chromatograpy technique. Experimental data have been obtained at three different temperatures 40ºC, 45ºC and 50ºC. The temperature dependence of activity coefficients at infinite dilution can be expressed by an Arrhenius type expression.

Comparing the γ_i^∞ obtained in a single component solute aqueous solution with those obtained in a multicomponent solute aqueous solution, it can be concluded that no, or little, interactions take place among the volatile compounds in the concentration range studied in this work. However, one should keep in mind that the number of volatile compounds identified in the brown crab boiling effluent was more than 150 compounds, including aldehydes, ketones, alcohols, esters, aromatic compounds and sulphur and nitrogen-containing compounds (1).

Finally, the effect of salt concentration has been studied by varying the sodium chloride concentration from 0 to 1.71 mol/kg. As a general rule, activity coefficients at infinite

dilution for all the volatile compounds considered I nthis work increase as the salt concentration increases, showing a salting out effect.

Nomenclature

c_s = salt concentration

H = Henry constant

k = salting out coeffficient

p = pressure

R = gas constant

T = temperature

γ = activity coefficient

α = relative volatility

Upperscripts:

s: saturation

∞: Infinite dilution

Subscripts:

i = component

w = water

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Table 1. Coefficients for the extended Antoine Equation, Eq. [4].

Compound	C_1	C_2	C_3	C_4	C_5	C_6	C_7	Reference
Water	66.74	-7258.2	0	0	-7.30	$4.17 \cdot 10^{-6}$	2	Aspen Plus
Ethylacetate	59.92	-6227.6	0	0	-6.41	$1.79 \cdot 10^{-17}$	6	Aspen Plus
3-Methylbutanal	54.11	-6192.1	0	0	-5.52	$1.17 \cdot 10^{-17}$	6	Aspen Plus
2,3-Pentadione	13.77	-2756.6	-82.1	0	0	0	0	[13]
1-Penten-3-ol	87.19	-8981.7	0	0	-9.98	$1.72 \cdot 10^{-17}$	6	Aspen Plus*
Hexanal	74.60	-7776.8	0	0	-8.45	$1.51 \cdot 10^{-17}$	6	Aspen Plus
Benzaldehyde	109.37	-9331.2	0	0	-14.64	$1.19 \cdot 10^{-2}$	1	Aspen Plus
1-Octen-3-ol	91.50	-10339.1	0	0	-10.47	$9.46 \cdot 10^{-18}$	6	Aspen Plus*

(*) predicted

Table 2. Experimental values of Henry's law constant (H_i), γ_i^∞ obtained with Eq. 2 andliterature values of γ_i^∞.

Compound	T (K)	H_i, kPa	γ_i^∞	RSD (γ_i^∞ %)	γ_i^∞ (literature)
Ethylacetate	313.15	1761 ± 102	69	6	$68.3^{25°C,[16]}$ $68.2^{25°C,[17]}$
	318.15	2267 ± 125	72	4	$63.9^{15°C,[18]}$ $65.3^{25°C,[18]}$
	323.15	2860 ± 165	74	4	$84.5^{40°C,[18]}$ $66.8^{50°C,[18]}$
3-Methylbutanal	313.15	2190 ± 193	160	9	$161^{-,[19]}$
	318.15	2870 ± 240	166	9	$46.4^{98-99°C,[14]}$
	323.15	3982 ± 320	185	8	
2,3-Pentadione	313.15	1087 ± 94	173	9	
	318.15	1582 ± 138	195	9	
	323.15	2133 ± 146	207	7	
1-Penten-3-ol	313.15	153 ± 13	47	9	
	318.15	211 ± 23	48	10	
	323.15	315 ± 54	54	11	
Hexanal	313.15	2097 ± 283	625	14	$813^{25°C,[5]}$ $121.1^{98-99°C,[14]}$
	318.15	2754 ± 321	634	14	$1213^{25°C,[16]}$
	323.15	3291 ± 431	591	13	$1012-1000^{20-25°C,[20]}$
Benzaldehyde	313.15	241 ± 19	545	8	$559^{20-22°C,[21]}$ $1001^{25°C,[16]}$
	318.15	333 ± 26	559	8	$1485.5^{25°C,[22]}$ $251^{100°C,[15]}$
	323.15	454 ± 28	574	6	
1-Octen-3-ol	313.15	413 ± 70	2179	17	$3568^{25°C,[17]}$ $3386^{25°C,[23]}$
	318.15	623 ± 73	2310	12	
	323.15	943 ± 84	2487	9	

Table 3. Activity coefficients at infinite dilution obtained in a single component solute aqueous solution and in a multicomponent solute aqueous solution at 40ºC.

Compound	γ_i^∞ Single component solute mixture	RSD (%)	γ_i^∞ Multicomponent solute mixture	RSD (%)
Ethylacetate	69	6	71	8
3-Methylbutanal	160	9	179	9
2,3-Pentadione	172	9	160	9
1-Penten-3-ol	47	9	49	8
Hexanal	625	14	601	14
Benzaldehyde	545	8	570	9
1-Octen-3-ol	2179	17	2164	10

Table 4. Activity coefficients at infinite dilution at 40ºC at different salt concentrations And salting out coefficients, k_i, at 40ºC.

| Compound	c_s (mol/kg)	γ_i^∞	RSD (%)	r^2	k_i
Ethylacetate	0.00	71	8		
	0.34	86	8	0.995	0.58 ± 0.05
	0.86	121	6		
	1.71	186	6		
3-Methylbutanal	0.00	179	9		
	0.34	200	12	0.996	0.39 ± 0.03
	0.86	244	9		
	1.71	350	9		
2,3-Pentadione	0.00	160	6		
	0.34	196	18	0.984	0.43 ± 0.07
	0.86	236	17		
	1.71	324	18		
1-Penten-3-ol	0.00	49	8		
	0.34	56	14	0.990	0.37 ± 0.03
	0.86	66	14		
	1.71	--			
Hexanal	0.00	601	14		
	0.34	768	10	0.996	0.62 ± 0.07
	0.86	1029	10		
	1.71	1644	10		
Benzaldehyde	0.00	570	9		
	0.34	646	4	0.992	0.34 ± 0.04
	0.86	788	5		
	1.71	1003	6		
1-Octen-3-ol	0.00	2164	10		
	0.34	2493	11	0.995	0.56 ± 0.05
	0.86	3537	11		
	1.71	5679	9		

List of Figure Caption

Figure 1. Partial pressure of benzaldehyde as a function of mole fraction in the liquid phase at three different temperatures (♦ 40ºC, ■ 45ºC, ▲ 50ºC). Standard deviation for each data has been drawn.
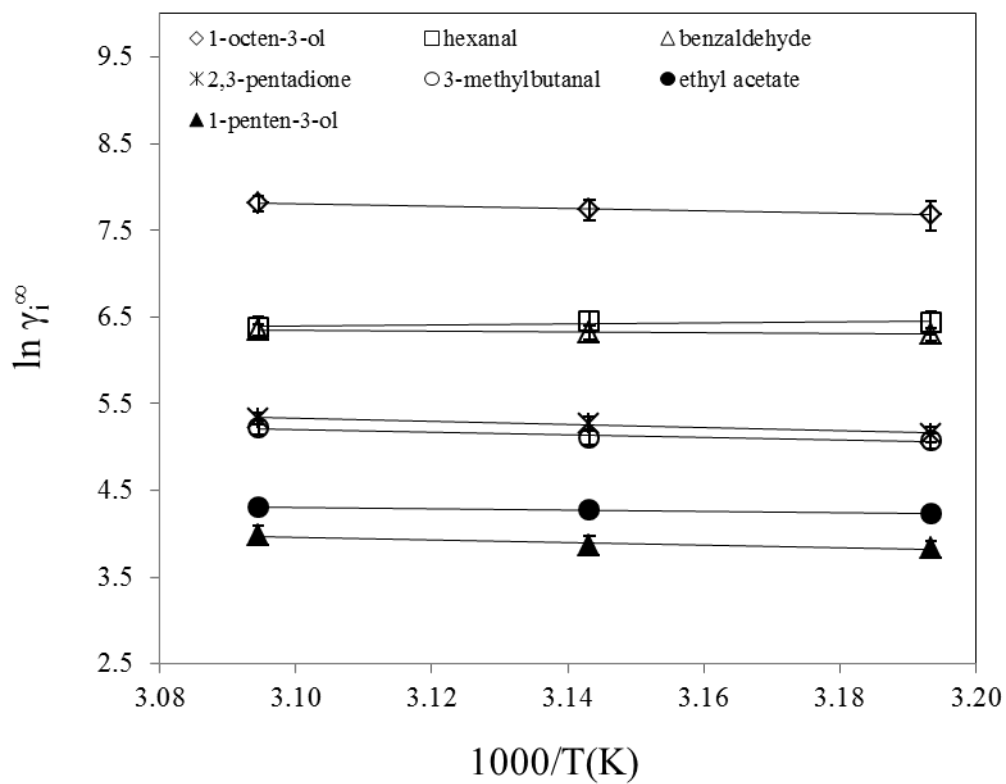
Figure 2. Arrehnius plot of the activity coefficients at infinite dilution for the volatile compounds studied in this work. Standard deviation for each data has been drawn.

Figure 3. Values of the activity coefficients at infinite dilution for ethyl acetate as a function of temperature (○ data obtained in this work, ● literature values from Table 2).

Figure 4. Partial pressure of ethylacetate as a function of mole fraction in the liquid phase at 40ºC (♦ Multicomponent solute mixture, ◊ single component solute mixture). Standard deviation for each data has been drawn.
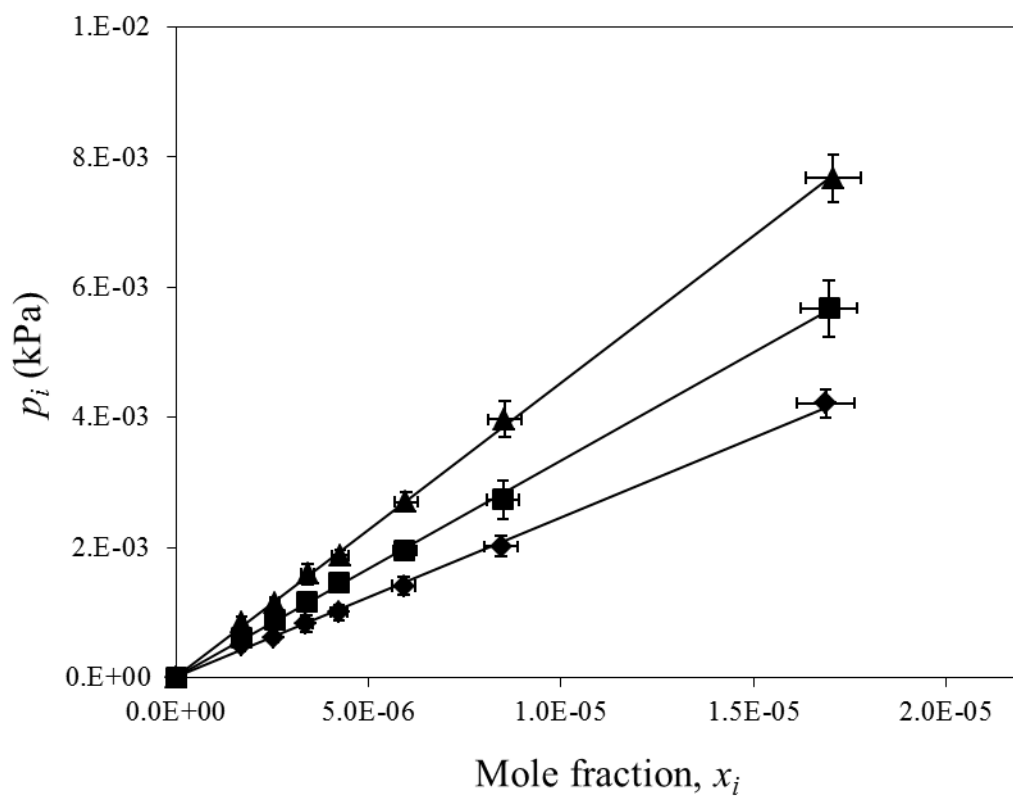
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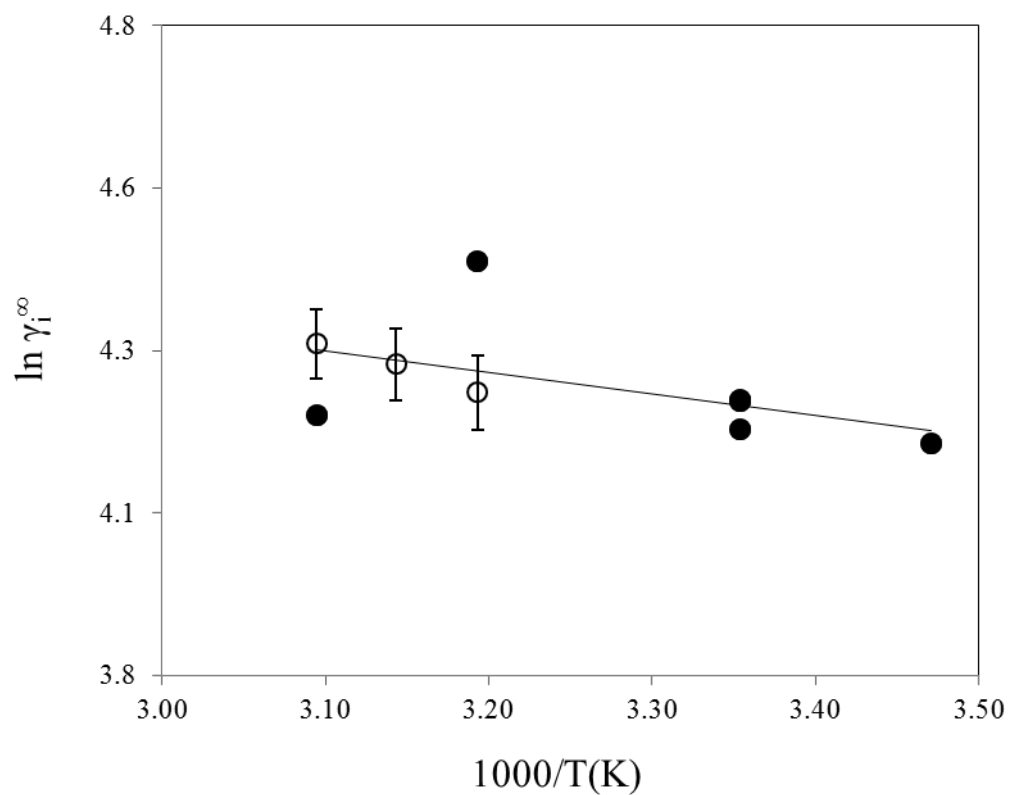
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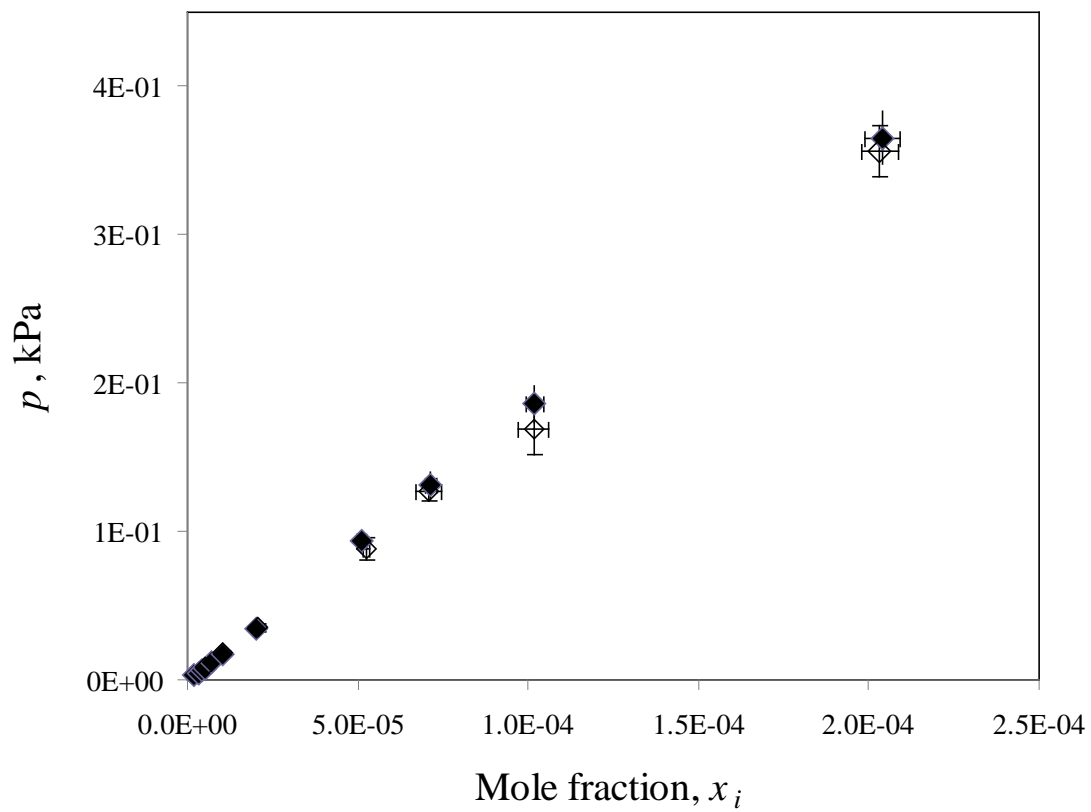
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