Supporting information

EXPLORING THE SUBSISTENCE OF SOLVATION CONSEQUENCES OF L-ASPARAGINE AND L-GLUTAMINE PREVAILING IN AQUEOUS IONIC LIQUID SOLUTIONS BY PHYSICOCHEMICAL AND COMPUTATIONAL INVESTIGATIONS

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Tel: +91-353-2776381, Fax: +91 353 2699001

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### Tables

**Table S1.** Experimental density ($\rho$), viscosity ($\eta$) and molar refraction ($R_M$) of different molality (0.001, 0.003, 0.005) mol·kg$^{-1}$ of aqueous (BTBAC) ionic liquid solutions at temperatures $T$ = (293.15 - 313.15) K at atmospheric pressure 0.1MPa $^{a,b}$

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<th>Molality of BTBAC(IL) /mol·kg$^{-1}$</th>
<th>$T$(K)</th>
<th>$10^3 \cdot \rho$/(kg·m$^{-3}$)</th>
<th>$\eta$/(mPa·s)</th>
<th>$R_M$/(m$^3$·mol$^{-1}$)</th>
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$^a$ Standard uncertainties $u$ are $u(\rho) = 0.00037$ g·cm$^{-3}$, $u(T) = 0.01K$, $u(P) = 0.01$MPa, $u(\eta) = 0.022$ mPa·S., $u(nD) = 0.0005$. $^b$ Standard uncertainty in molality considering the purity of mass of the studied samples is expected to be about 0.0003 mol·kg$^{-1}$. $^c$ Molality for the above system has been stated per kg of (IL + water) as a solvent mixture, (0.68 denotes as the level of confidence of the measurements). Symbol ‘[IL]’ denotes as molality of ionic liquid. Wave length of light source for refractive index measurement was, $\lambda = 589.3$ nm.
Table S2. Experimental values of refractive index ($n_D$) and specific conductance ($\kappa$) of different molality (0.001, 0.003, 0.005) mol·kg$^{-1}$ of aqueous IL (BTBAC) solutions at temperatures $T=(293.15 - 313.15)$ K at atmospheric pressure 0.1MPa $^{a,b}$

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<tr>
<th>Molality of BTBAC(IL)/ (mol·kg$^{-1}$)</th>
<th>$T$/K</th>
<th>$n_D$</th>
<th>$\kappa$/(mS/cm)</th>
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$^a$ Standard uncertainties $u$ are $u(\rho) = 0.00037$ g.cm$^{-3}$, $u(T) = 0.01K$, $u(P)=0.01$MPa, $u(\kappa)=0.021$(mScm$^{-1}$), $u(n_D) = 0.0005$ and $u(T) = 0.01K$, $^b$ Standard uncertainty in molality considering the purity of mass of the studied samples is expected to be about 0.0003 mol·kg$^{-1}$. $^c$ Molality for the above system has been stated per kg of (IL + water) as a solvent mixture, (0.68 denotes as the level of confidence of the measurements). Wavelength of light source for refractive index measurement was, $\lambda=589.3$nm. Symbol ‘[IL]’ denotes as ionic liquid.
Table S3. Density ($\rho$) of L-Asn in aqueous (BTBAC) ionic liquid solutions at temperatures $T= (293.15 - 313.15)$ K at atmospheric pressure 0.1MPa $^{a,b}$

<table>
<thead>
<tr>
<th>Molality of L-Asn in Aq. BTBAC(IL) / (mol·kg$^{-1}$)</th>
<th>$T=293.15$K $10^{-3}\rho$ (kg·m$^{-3}$)</th>
<th>$T=298.15$K $10^{-3}\rho$ (kg·m$^{-3}$)</th>
<th>$T=303.15$K $10^{-3}\rho$ (kg·m$^{-3}$)</th>
<th>$T=308.15$K $10^{-3}\rho$ (kg·m$^{-3}$)</th>
<th>$T=313.15$K $10^{-3}\rho$ (kg·m$^{-3}$)</th>
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$^a$ Standard uncertainties $u$ are $u(\rho) = 0.00037$ g.cm$^{-3}$, $u(T) = 0.01$K, $u(P) = 0.01$MPa

$^b$ Standard uncertainty in molality considering the purity of mass of the studied samples is expected to be about 0.0003 mol· kg$^{-1}$. 

$^c$ Molality for the above system has been stated per kg of (IL + water) as a solvent mixture, (0.68 denotes as the level of confidence of the measurements). Symbol ‘[IL]’ denotes as ionic liquid.
Table S4. Density ($\rho$) of L-Gln in aqueous (BTBAC) ionic liquid solutions at temperatures $T= (293.15 - 313.15)$ K at atmospheric pressure 0.1MPa $^{a,b}$

<table>
<thead>
<tr>
<th>Molality of L-Gln in Aq. BTBAC(IL)/ (mol·kg$^{-1}$)</th>
<th>$T=293.15K$</th>
<th>$T=298.15K$</th>
<th>$T=303.15K$</th>
<th>$T=308.15K$</th>
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<td>$10^{-3}\rho$ (kg·m$^{-3}$)</td>
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$^a$ Standard uncertainties $u$ are $u(\rho) = 0.00037$ g·cm$^{-3}$, $u(T) = 0.01K$, $u(P)=0.01$MPa, $^b$ Standard uncertainty in molality considering the purity of mass of the studied samples is expected to be about 0.0003 mol· kg$^{-1}$. $^c$ Molality for the above system has been stated per kg of (IL + water) as
a solvent mixture, (0.68 denotes as the level of confidence of the measurements). Symbol ‘[IL]’ denotes as ionic liquid.

Table S5. Density ($\rho$) of L-Asn and L-Gln in aqueous solutions at temperatures $T= (293.15 - 313.15)$ K at atmospheric pressure 0.1MPa$^a, b$

<table>
<thead>
<tr>
<th>Molality of Amino acid(AA) in Aq. Soln./(mol·kg$^{-1}$)</th>
<th>$T=293.15K$ 10$^{-3}$ $\rho$ (kg·m$^{-3}$)</th>
<th>$T=298.15K$ 10$^{-3}$ $\rho$ (kg·m$^{-3}$)</th>
<th>$T=303.15K$ 10$^{-3}$ $\rho$ (kg·m$^{-3}$)</th>
<th>$T=308.15K$ 10$^{-3}$ $\rho$ (kg·m$^{-3}$)</th>
<th>$T=313.15K$ 10$^{-3}$ $\rho$ (kg·m$^{-3}$)</th>
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<td>0.99837</td>
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<td>1.00028</td>
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<tr>
<td>L-Gln+ Aq. Solution</td>
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<td></td>
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<tr>
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</tr>
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</tr>
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<td>0.99710</td>
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</tbody>
</table>

$^a$ Standard uncertainties $u$ are $u(\rho) = 0.00037$ g·cm$^{-3}$, $u (T) = 0.01K$, $u(P)=0.01$MPa, $^b$ Standard uncertainty in molality considering the purity of mass of the studied samples is expected to be about 0.0003 mol· kg$^{-1}$. (0.68 denotes as the level of confidence of the measurements), Symbol [AA], denotes as amino acid.
Table S6. Viscosity ($\eta$) and Molar refraction ($R_M$) of L-Asn in aqueous (BTBAC) ionic liquid solutions at temperatures $T =$ (293.15 - 313.15) K at atmospheric pressure 0.1MPa $^c$.

<table>
<thead>
<tr>
<th>Molality of L-Asn in Aq. BTBAC(IL) / (mol·kg$^{-1}$)</th>
<th>$T$=293.15K $\eta$ (Pa·s) $R_M$</th>
<th>$T$=298.15K $\eta$(mPa·s) $R_M$</th>
<th>$T$=303.15K $\eta$(mPa·s) $R_M$</th>
<th>$T$=308.15K $\eta$(mPa·s) $R_M$</th>
<th>$T$=313.15K $\eta$(mPa·s) $R_M$</th>
</tr>
</thead>
<tbody>
<tr>
<td>L-Asn+ 0.001mol· kg$^{-1}$ aq. BTBAC Soln.</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.010</td>
<td>0.959</td>
<td>27.17</td>
<td>0.919</td>
<td>27.18</td>
<td>0.882</td>
</tr>
<tr>
<td>0.025</td>
<td>0.965</td>
<td>27.16</td>
<td>0.925</td>
<td>27.17</td>
<td>0.888</td>
</tr>
<tr>
<td>0.040</td>
<td>0.970</td>
<td>27.15</td>
<td>0.931</td>
<td>27.17</td>
<td>0.894</td>
</tr>
<tr>
<td>0.055</td>
<td>0.975</td>
<td>27.14</td>
<td>0.936</td>
<td>27.16</td>
<td>0.899</td>
</tr>
<tr>
<td>0.070</td>
<td>0.980</td>
<td>27.13</td>
<td>0.941</td>
<td>27.15</td>
<td>0.905</td>
</tr>
<tr>
<td>0.085</td>
<td>0.984</td>
<td>27.12</td>
<td>0.946</td>
<td>27.15</td>
<td>0.910</td>
</tr>
<tr>
<td>L-Asn+ 0.003mol· kg$^{-1}$ aq. BTBAC Soln.</td>
<td></td>
<td></td>
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<td></td>
<td></td>
</tr>
<tr>
<td>0.010</td>
<td>0.967</td>
<td>27.18</td>
<td>0.926</td>
<td>27.20</td>
<td>0.885</td>
</tr>
<tr>
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<td>0.974</td>
<td>27.17</td>
<td>0.932</td>
<td>27.19</td>
<td>0.892</td>
</tr>
<tr>
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<td>0.938</td>
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</tr>
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<td>0.943</td>
<td>27.17</td>
<td>0.904</td>
</tr>
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<td>27.14</td>
<td>0.948</td>
<td>27.16</td>
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</tr>
<tr>
<td>0.085</td>
<td>0.995</td>
<td>27.13</td>
<td>0.954</td>
<td>27.16</td>
<td>0.915</td>
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<tr>
<td>L-Asn+ 0.005mol· kg$^{-1}$ aq. BTBAC Soln.</td>
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<td></td>
<td></td>
</tr>
<tr>
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<td>0.935</td>
<td>27.21</td>
<td>0.898</td>
</tr>
<tr>
<td>0.025</td>
<td>0.985</td>
<td>27.18</td>
<td>0.941</td>
<td>27.20</td>
<td>0.904</td>
</tr>
<tr>
<td>0.040</td>
<td>0.992</td>
<td>27.17</td>
<td>0.947</td>
<td>27.19</td>
<td>0.910</td>
</tr>
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<td>27.17</td>
<td>0.952</td>
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</tr>
<tr>
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<td>1.008</td>
<td>27.15</td>
<td>0.964</td>
<td>27.17</td>
<td>0.929</td>
</tr>
</tbody>
</table>

$^c$ Standard uncertainties $u$ are $u (\eta)=0.022$ mPa·S., $u (T) = 0.01$K, $u (P)=0.01$MPa $^b$ Standard uncertainty in molality considering the purity of mass of the studied samples is expected to be about 0.0003 mol·kg$^{-1}$. $^c$ Molality for the above system has been stated per kg of (IL + water) as
a solvent mixture, (0.68 denotes as the level of confidence of the measurements). Symbol ‘[IL]’
denotes as ionic liquid.

Table S7. Viscosity ($\eta$) and Molar refraction ($R_M$) of L-Gln in aqueous (BTBAC) ionic liquid
solutions at temperatures $T= (293.15 -313.15) \text{ K}$ at atmospheric pressure 0.1MPa $^{c*,b}$

| Molality of L-Gln in Aq. BTBAC(IL)/ (mol·kg$^{-1}$) | $T=293.15K$ | $T=298.15K$ | $T=303.15K$ | $T=308.15K$ | $T=313.15K$
<table>
<thead>
<tr>
<th></th>
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<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$\eta$ (Pa·s)</td>
<td>$R_M$</td>
<td>$\eta$ (mPa·s)</td>
<td>$R_M$</td>
<td>$\eta$ (mPa·s)</td>
</tr>
<tr>
<td>L-Gln+ 0.001mol·kg$^{-1}$ aq. BTBAC Soln.</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
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<td>30.04</td>
<td>0.921</td>
<td>30.07</td>
<td>0.884</td>
</tr>
<tr>
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<td>0.930</td>
<td>30.05</td>
<td>0.893</td>
</tr>
<tr>
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<td>30.01</td>
<td>0.939</td>
<td>30.04</td>
<td>0.902</td>
</tr>
<tr>
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<td>30.00</td>
<td>0.948</td>
<td>30.03</td>
<td>0.912</td>
</tr>
<tr>
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<td>29.99</td>
<td>0.956</td>
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<td>0.921</td>
</tr>
<tr>
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<td>29.98</td>
<td>0.965</td>
<td>30.01</td>
<td>0.929</td>
</tr>
<tr>
<td>L-Gln+ 0.003mol·kg$^{-1}$ aq. BTBAC Soln.</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.010</td>
<td>0.969</td>
<td>30.05</td>
<td>0.929</td>
<td>30.07</td>
<td>0.888</td>
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<td>0.896</td>
</tr>
<tr>
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<td>30.02</td>
<td>0.947</td>
<td>30.05</td>
<td>0.906</td>
</tr>
<tr>
<td>0.055</td>
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<td>30.01</td>
<td>0.957</td>
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<td>0.917</td>
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<td>0.977</td>
<td>30.03</td>
<td>0.936</td>
</tr>
<tr>
<td>L-Gln+ 0.005mol·kg$^{-1}$ aq. BTBAC Soln.</td>
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<td>0.900</td>
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<td>0.909</td>
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<td>30.05</td>
<td>0.960</td>
<td>30.06</td>
<td>0.919</td>
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<tr>
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<td>0.929</td>
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<td>0.990</td>
<td>30.04</td>
<td>0.950</td>
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Standard uncertainties $u$ are $u(\eta)=0.022\ \text{mPa}\cdot\text{S}$, $(T)=0.01\text{K}$, $u(P)=0.01\text{MPa}$. Standard uncertainty in molality considering the purity of mass of the studied samples is expected to be about 0.0003 $\text{mol}\cdot\text{kg}^{-1}$. Molality for the above system has been stated per kg of (IL + water) as a solvent mixture, (0.68 denotes as the level of confidence of the measurements). Symbol ‘[IL]’ denotes as ionic liquid.

Table S8. Apparent molar volume, $(V_\phi)$ and $(\eta/\eta^0 - 1)/\sqrt{m}$ of L-Asn solution in (0.001, 0.003, 0.005) $\text{mol} \cdot \text{kg}^{-1}$ aqueous BTBAC solution at temperatures $T=\{293.15, \ldots, 313.15\}\text{K}$ temperatures and at atmospheric pressure 0.1MPa.$^a$.$^b$.

<table>
<thead>
<tr>
<th>Molality of L-Asn (AA) in Aq. BTBAC (IL)/(mol·kg⁻¹)</th>
<th>$T=293.15\text{K}$</th>
<th>$T=298.15\text{K}$</th>
<th>$T=303.15\text{K}$</th>
<th>$T=308.15\text{K}$</th>
<th>$T=313.15\text{K}$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$10^6\cdot V_\phi/\sqrt{m}$</td>
<td>$10^6\cdot V_\phi/(\eta/\eta^0 - 1)/\sqrt{m}$</td>
<td>$10^6\cdot V_\phi/(\eta/\eta^0 - 1)/\sqrt{m}$</td>
<td>$10^6\cdot V_\phi/(\eta/\eta^0 - 1)/\sqrt{m}$</td>
<td>$10^6\cdot V_\phi/(\eta/\eta^0 - 1)/\sqrt{m}$</td>
</tr>
<tr>
<td>L-Asn+ 0.001 mol·kg⁻¹ aq. BTBAC Soln.</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.010</td>
<td>77.58</td>
<td>0.063</td>
<td>80.35</td>
<td>0.066</td>
<td>82.47</td>
</tr>
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<td>0.083</td>
<td>81.31</td>
</tr>
<tr>
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<td>78.19</td>
<td>0.098</td>
<td>80.40</td>
</tr>
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<td>77.63</td>
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<td>79.64</td>
</tr>
<tr>
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<td>0.115</td>
<td>78.94</td>
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<td>0.111</td>
<td>76.34</td>
<td>0.123</td>
<td>78.34</td>
</tr>
<tr>
<td>L-Asn+ 0.003 mol·kg⁻¹ aq. BTBAC Soln.</td>
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<td>83.43</td>
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<td>0.122</td>
<td>78.34</td>
</tr>
<tr>
<td>L-Asn + 0.005 mol·kg⁻¹ aq. BTBAC Soln.</td>
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<td>84.94</td>
</tr>
<tr>
<td>Molality of L-Gln (AA) in Aq. BTBAC(IL)/ (mol·kg⁻¹)</td>
<td>( T = 293.15 ) K</td>
<td>( T = 298.15 ) K</td>
<td>( T = 303.15 ) K</td>
<td>( T = 308.15 ) K</td>
<td>( T = 313.15 ) K</td>
</tr>
<tr>
<td>--------------------------------------------------</td>
<td>-----------------</td>
<td>-----------------</td>
<td>-----------------</td>
<td>-----------------</td>
<td>-----------------</td>
</tr>
<tr>
<td></td>
<td>( 10^6 \cdot \phi ) / (( \eta / \eta^0 - 1 )) / ( m )</td>
<td>( 10^6 \cdot \phi ) / (( \eta / \eta^0 - 1 )) / ( m )</td>
<td>( 10^6 \cdot \phi ) / (( \eta / \eta^0 - 1 )) / ( m )</td>
<td>( 10^6 \cdot \phi ) / (( \eta / \eta^0 - 1 )) / ( m )</td>
<td>( 10^6 \cdot \phi ) / (( \eta / \eta^0 - 1 )) / ( m )</td>
</tr>
<tr>
<td>L-Gln+ 0.001mol·kg⁻¹ aq. BTBAC Soln.</td>
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</tr>
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<td>91.40</td>
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</tr>
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<td>86.73</td>
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<td>86.88</td>
</tr>
<tr>
<td>L-Gln+ 0.003mol·kg⁻¹ aq. BTBAC Soln.</td>
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<td></td>
<td></td>
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<td></td>
</tr>
<tr>
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<td>89.36</td>
<td>0.083</td>
<td>92.40</td>
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</tbody>
</table>

\(^c\) Standard uncertainties \( u \) are \( (V φ) = 5 \times 10^{-5} \text{ m}^3\cdot\text{mol}^{-1} \), \( (\eta) = 0.022 \text{ mPa} \cdot \text{S} \), \( (T) = 0.01 \text{K} \), \( u (P) = 0.01 \text{MPa} \), \(^b\) Standard uncertainty in molality considering the purity of mass of the studied samples is expected to be about 0.0003 mol·kg⁻¹. \(^c\) molality for the above system has been stated per kg of (IL + water) as a solvent mixture, (0.68 denotes as the level of confidence of the measurements). Symbol ‘[AA]’ denotes as Amino acid. Symbol ‘[IL]’ denotes as ionic liquid.

Table S9. Apparent molar volume, \( (V φ) \) and \( (\eta/\eta^0 - 1)/\sqrt{m} \) of L-Gln solution in (0.001, 0.003 ,0.005) mol·kg⁻¹ in aqueous (BTBAC) solution at different temperatures \( T = (293.15 - 313.15) \text{K} \) at atmospheric pressure 0.1MPa \(^c\), \(^b\).
<table>
<thead>
<tr>
<th>L-Gln + 0.005mol· kg⁻¹ aq. BTBAC Soln.</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.010</td>
</tr>
<tr>
<td>0.025</td>
</tr>
<tr>
<td>0.040</td>
</tr>
<tr>
<td>0.055</td>
</tr>
<tr>
<td>0.070</td>
</tr>
<tr>
<td>0.085</td>
</tr>
</tbody>
</table>

Standard uncertainties \( u \) are \( u(V\varphi) = 5 \times 10^{-5} \text{ m}^3\text{ mol}^{-1} \), \( u(\eta) = 0.022 \text{ mPa} \cdot \text{s} \), \( T = 0.01 \text{K} \), \( u(P) = 0.01 \text{MPa} \). Standard uncertainty in molality considering the purity of mass of the studied samples is expected to be about 0.0003 mol· kg⁻¹. Molality for the above system has been stated per kg of (IL + water) as a solvent mixture, (0.68 denotes as the level of confidence of the measurements). Symbol ‘[AA]’ denotes as Amino acid. Symbol ‘[IL]’ denotes as ionic liquid.

**Table S10.** Apparent molar volume, \( V\varphi \) of L-Asn/L-Gln in aqueous solution at different temperatures \( T = (293.15 - 313.15) \text{ K} \) at atmospheric pressure 0.1MPa c.

<table>
<thead>
<tr>
<th>Molality of Amino acid (AA) in Aq. Soln./(mol·kg⁻¹)</th>
<th>( T=293.15 \text{K} )</th>
<th>( T=298.15 \text{K} )</th>
<th>( T=303.15 \text{K} )</th>
<th>( T=308.15 \text{K} )</th>
<th>( T=313.15 \text{K} )</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>( 10^6 V\varphi )</td>
<td>( 10^6 V\varphi )</td>
<td>( 10^6 V\varphi )</td>
<td>( 10^6 V\varphi )</td>
<td>( 10^6 V\varphi )</td>
</tr>
<tr>
<td></td>
<td>/(m³·mol⁻¹)</td>
<td>/(m³·mol⁻¹)</td>
<td>/(m³·mol⁻¹)</td>
<td>/(m³·mol⁻¹)</td>
<td>/(m³·mol⁻¹)</td>
</tr>
<tr>
<td>L-Asn + Aq. Solution</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.010</td>
<td>77.09</td>
<td>80.04</td>
<td>82.02</td>
<td>83.05</td>
<td>85.07</td>
</tr>
<tr>
<td>0.025</td>
<td>76.45</td>
<td>78.89</td>
<td>80.54</td>
<td>81.80</td>
<td>83.49</td>
</tr>
<tr>
<td>0.040</td>
<td>75.94</td>
<td>78.21</td>
<td>80.00</td>
<td>80.79</td>
<td>82.61</td>
</tr>
<tr>
<td>0.055</td>
<td>75.37</td>
<td>77.78</td>
<td>79.46</td>
<td>80.24</td>
<td>81.96</td>
</tr>
<tr>
<td>0.070</td>
<td>75.00</td>
<td>77.48</td>
<td>78.65</td>
<td>79.56</td>
<td>81.35</td>
</tr>
<tr>
<td>0.085</td>
<td>74.56</td>
<td>76.92</td>
<td>78.24</td>
<td>78.99</td>
<td>80.81</td>
</tr>
<tr>
<td>L-Gln + Aq. Solution</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.010</td>
<td>87.54</td>
<td>90.57</td>
<td>91.62</td>
<td>92.68</td>
<td>93.76</td>
</tr>
<tr>
<td>0.025</td>
<td>86.86</td>
<td>89.71</td>
<td>90.56</td>
<td>91.43</td>
<td>92.31</td>
</tr>
</tbody>
</table>

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Table S11. Data of limiting molar expansibilities \((E^0_\phi)\) for (L-Asn+ Aq. BTBAC) system in aqueous soln. of BTBAC at temperatures \(T = (293.15 - 313.15)\) K and at atmospheric pressure \(0.1\text{MPa}^{a,b}\)

<table>
<thead>
<tr>
<th>Molality of BTBAC(IL) /((\text{mol}\cdot\text{kg}^{-1}))</th>
<th>(T=293.15\text{K})</th>
<th>(T=298.15\text{K})</th>
<th>(T=303.15\text{K})</th>
<th>(T=308.15\text{K})</th>
<th>(T=313.15\text{K})</th>
</tr>
</thead>
<tbody>
<tr>
<td>(10^6\cdot E^0_\phi/\text{(m}^3\cdot\text{mol}^{-1}\cdot\text{K}^{-1}))</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.001</td>
<td>0.6232(0.6050)d</td>
<td>0.5282</td>
<td>0.4332</td>
<td>0.3382</td>
<td>0.2432</td>
</tr>
<tr>
<td>0.003</td>
<td>0.6513</td>
<td>0.5443</td>
<td>0.4373</td>
<td>0.3303</td>
<td>0.2233</td>
</tr>
<tr>
<td>0.005</td>
<td>0.7346</td>
<td>0.5936</td>
<td>0.4526</td>
<td>0.3116</td>
<td>0.1706</td>
</tr>
</tbody>
</table>

\(^a\) Standard uncertainties \(u\) are \(u(V_\phi) = 5 \times 10^{-5} \text{m}^3\cdot\text{mol}^{-1}\), \((T) = 0.01\text{K}, u(P)= 0.01\text{MPa}, \). Symbol ‘[AA]’ denotes as amino acid. (0.68 denotes as the level of confidence of the measurements).

\(^b\) Molality for the above system has been stated per kg of (IL + water) as a solvent mixture, (0.68 denotes as the level of confidence of the measurements). \(^d\) This Value was taken from ref.26.

Table S12. Data of limiting molar expansibilities \((E^0_\phi)\) for (L-Gln+ Aq. BTBAC) system in aqueous solutions of IL (BTBAC) at temperatures \(T= (293.15 - 313.15)\) K at atmospheric pressure \(0.1\text{MPa}^{a,b}\)

<table>
<thead>
<tr>
<th>Molality of BTBAC(IL) /((\text{mol}\cdot\text{kg}^{-1}))</th>
<th>(T=293.15\text{K})</th>
<th>(T=298.15\text{K})</th>
<th>(T=303.15\text{K})</th>
<th>(T=308.15\text{K})</th>
<th>(T=313.15\text{K})</th>
</tr>
</thead>
<tbody>
<tr>
<td>(10^6\cdot E^0_\phi/\text{(m}^3\cdot\text{mol}^{-1}\cdot\text{K}^{-1}))</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>((\delta E^0_\phi/\delta T)_P \cdot 10^6/\text{(m}^3\cdot\text{mol}^{-1}\cdot\text{K}^{-2}))</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

\(^a\) Standard uncertainties \(u\) are \(u(T) = 0.01\text{K}, u(P)= 0.01\text{MPa}, \). Standard uncertainty in molality considering the purity of mass of the studied samples is expected to be about 0.0003 mol· kg\(^{-1}\).
Table S13. Limiting apparent molar volumes ($V_\varphi^0$), experimental slopes ($S_V^*$), of L-Asn/L-Gln in aqueous solutions at various working temperatures and atmospheric pressure at 0.1 MPa.

<table>
<thead>
<tr>
<th>Temperature/K</th>
<th>$10^6 \cdot V_\varphi^0 / (m^3 \cdot mol^{-1})$</th>
<th>$10^6 \cdot S_V^* / (m^3 \cdot mol^{-3/2} \cdot kg^{1/2})$</th>
<th>$10^6 \cdot V_\varphi^0 / (m^3 \cdot mol^{-1})$</th>
<th>$10^6 \cdot S_V^* / (m^3 \cdot mol^{-3/2} \cdot kg^{1/2})$</th>
</tr>
</thead>
<tbody>
<tr>
<td>293.15</td>
<td>78.52</td>
<td>-13.35</td>
<td>89.07</td>
<td>-15.00</td>
</tr>
<tr>
<td>298.15</td>
<td>81.58</td>
<td>-16.31</td>
<td>92.93</td>
<td>-21.66</td>
</tr>
<tr>
<td>303.15</td>
<td>83.84</td>
<td>-19.26</td>
<td>94.20</td>
<td>-24.39</td>
</tr>
<tr>
<td>308.15</td>
<td>85.15</td>
<td>-21.13</td>
<td>95.69</td>
<td>-28.18</td>
</tr>
<tr>
<td>313.15</td>
<td>87.11</td>
<td>-21.88</td>
<td>96.86</td>
<td>-29.47</td>
</tr>
</tbody>
</table>

$^a$ Standard uncertainties $u$ are $u (T) = 0.01K$, $u (P)= 0.01MPa$. $^b$ Standard uncertainty in molality considering the purity of mass of the studied samples is expected to be about 0.0003 mol· kg$^{-1}$. $^c$ Molality for the above system has been stated per kg of (IL + water) as a solvent mixture,(0.68 denotes as the level of confidence of the measurements). $^e$ This value was taken from ref (72). Symbol ‘[IL]’ denotes as ionic liquid.

Table S14. The values of viscosity $B$-coefficients and $dB/dT$ of L-Asn solution in different concentrations of IL at temperatures $T= (293.15 - 313.15)$ K at atmospheric pressure 0.1 MPa.

<table>
<thead>
<tr>
<th>Temperature /K</th>
<th>L-Asn in 0.001 mol· kg$^{-1}$ aq. BTBAC Soln.</th>
<th>L-Asn in 0.003 mol· kg$^{-1}$ aq. BTBAC Soln.</th>
<th>L-Asn in 0.005 mol· kg$^{-1}$ aq. BTBAC Soln.</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$B$</td>
<td>$B$</td>
<td>$B$</td>
</tr>
<tr>
<td>293.15</td>
<td>0.253</td>
<td>0.296</td>
<td>0.336</td>
</tr>
<tr>
<td>298.15</td>
<td>0.301</td>
<td>0.346</td>
<td>0.364</td>
</tr>
<tr>
<td>303.15</td>
<td>0.335</td>
<td>0.400</td>
<td>0.421</td>
</tr>
<tr>
<td></td>
<td>$dB/dT$</td>
<td>$dB/dT$</td>
<td>$dB/dT$</td>
</tr>
<tr>
<td>293.15</td>
<td>0.009</td>
<td>0.009</td>
<td>0.009</td>
</tr>
<tr>
<td>298.15</td>
<td>0.012</td>
<td>0.012</td>
<td>0.012</td>
</tr>
<tr>
<td>303.15</td>
<td>0.012</td>
<td>0.012</td>
<td>0.012</td>
</tr>
</tbody>
</table>

S13
Table S15. The values of viscosity $B$-coefficients and $dB/dT$ of L-Gln solution in different concentrations of IL at temperatures $T= (293.15 - 313.15)$ K at atmospheric pressure 0.1 MPa.$^a$

<table>
<thead>
<tr>
<th>Temperature /K</th>
<th>L-Gln in 0.001 mol·kg$^{-1}$ aq. BTBAC Soln.</th>
<th>L-Gln in 0.003 mol·kg$^{-1}$ aq. BTBAC Soln.</th>
<th>L-Gln in 0.005 mol·kg$^{-1}$ aq. BTBAC Soln.</th>
<th>$dB/dT$</th>
</tr>
</thead>
<tbody>
<tr>
<td>293.15</td>
<td>0.481</td>
<td>0.549</td>
<td>0.628</td>
<td>0.014</td>
</tr>
<tr>
<td>298.15</td>
<td>0.555</td>
<td>0.631</td>
<td>0.684</td>
<td>0.013</td>
</tr>
<tr>
<td>303.15</td>
<td>0.614</td>
<td>0.679</td>
<td>0.712</td>
<td>0.012</td>
</tr>
<tr>
<td>308.15</td>
<td>0.689</td>
<td>0.735</td>
<td>0.782</td>
<td></td>
</tr>
<tr>
<td>313.15</td>
<td>0.768</td>
<td>0.839</td>
<td>0.900</td>
<td></td>
</tr>
</tbody>
</table>

$^a$ Standard uncertainties $u$ are $u(T) = 0.01K$, $u(P)= 0.01MPa$, $u(\eta)= 0.022 mPa\cdot S$. $^b$ Standard uncertainty in molality considering the purity of mass of the studied samples is expected to be about 0.0003 mol· kg$^{-1}$. $^c$ Molality for the above system has been stated per kg of (IL + water) as a solvent mixture, (0.68 denotes as the level of confidence of the measurements).

Table S16. Refractive index ($n_D$) and specific electrical conductivity ($\kappa$) of L-Asn in aqueous IL (BTBAC) solution at different temperatures $T= (293.15 - 313.15)$K at atmospheric pressure 0.1MPa $^{a,b}$

<table>
<thead>
<tr>
<th>Molality of L-Asn (AA) in Aq. BTBAC(IL)/(mol·kg$^{-1}$)</th>
<th>$T=293.15K$</th>
<th>$T=298.15K$</th>
<th>$T=303.15K$</th>
<th>$T=308.15K$</th>
<th>$T=313.15K$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$n_D$ $\kappa$ (mS/cm)</td>
<td>$n_D$ $\kappa$ (mS/cm)</td>
<td>$n_D$ $\kappa$ (mS/cm)</td>
<td>$n_D$ $\kappa$ (mS/cm)</td>
<td>$n_D$ $\kappa$ (mS/cm)</td>
<td>$n_D$ $\kappa$ (mS/cm)</td>
</tr>
<tr>
<td>L-Asn + 0.001 mol·kg$^{-1}$ aq. BTBAC Soln.</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Temperature (°C)</td>
<td>Refractive Index ($n_D$)</td>
<td>Specific Electrical Conductivity ($\kappa$)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>------------------</td>
<td>--------------------------</td>
<td>------------------------------------------</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.010</td>
<td>1.3325 0.457 1.3322 0.482 1.3321 0.503 1.3319 0.520 1.3317 0.553</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.025</td>
<td>1.3326 0.517 1.3324 0.574 1.3322 0.590 1.3321 0.615 1.3318 0.657</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.040</td>
<td>1.3328 0.570 1.3326 0.653 1.3324 0.683 1.3323 0.709 1.3320 0.773</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.055</td>
<td>1.3330 0.635 1.3328 0.749 1.3326 0.776 1.3325 0.796 1.3322 0.859</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.070</td>
<td>1.3332 0.698 1.3330 0.826 1.3328 0.859 1.3327 0.888 1.3324 0.951</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.085</td>
<td>1.3334 0.860 1.3333 0.920 1.3331 0.943 1.3330 0.983 1.3326 1.098</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**L-Asn + 0.003 mol· kg$^{-1}$ aq. BTBAC Soln.**

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>Refractive Index ($n_D$)</th>
<th>Specific Electrical Conductivity ($\kappa$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.010</td>
<td>1.3326 0.516 1.3324 0.545 1.3323 0.572 1.3321 0.607 1.3319 0.639</td>
<td></td>
</tr>
<tr>
<td>0.025</td>
<td>1.3328 0.603 1.3326 0.634 1.3324 0.663 1.3322 0.714 1.3320 0.753</td>
<td></td>
</tr>
<tr>
<td>0.040</td>
<td>1.3330 0.678 1.3328 0.720 1.3326 0.765 1.3324 0.809 1.3322 0.884</td>
<td></td>
</tr>
<tr>
<td>0.055</td>
<td>1.3332 0.716 1.3330 0.812 1.3328 0.854 1.3326 0.913 1.3324 0.954</td>
<td></td>
</tr>
<tr>
<td>0.070</td>
<td>1.3334 0.783 1.3332 0.903 1.3330 0.935 1.3329 0.999 1.3326 1.128</td>
<td></td>
</tr>
<tr>
<td>0.085</td>
<td>1.3336 0.934 1.3335 0.997 1.3333 1.052 1.3331 1.080 1.3328 1.153</td>
<td></td>
</tr>
</tbody>
</table>

**L-Asn + 0.005 mol· kg$^{-1}$ aq. BTBAC Soln.**

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>Refractive Index ($n_D$)</th>
<th>Specific Electrical Conductivity ($\kappa$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.010</td>
<td>1.3328 0.589 1.3326 0.660 1.3325 0.748 1.3322 0.813 1.3321 0.899</td>
<td></td>
</tr>
<tr>
<td>0.025</td>
<td>1.3330 0.728 1.3327 0.771 1.3326 0.832 1.3323 0.889 1.3322 0.937</td>
<td></td>
</tr>
<tr>
<td>0.040</td>
<td>1.3332 0.805 1.3329 0.870 1.3328 0.917 1.3325 0.967 1.3323 1.045</td>
<td></td>
</tr>
<tr>
<td>0.055</td>
<td>1.3334 0.886 1.3331 0.965 1.3330 1.020 1.3327 1.040 1.3325 1.109</td>
<td></td>
</tr>
<tr>
<td>0.070</td>
<td>1.3336 1.021 1.3333 1.053 1.3332 1.080 1.3329 1.123 1.3327 1.268</td>
<td></td>
</tr>
<tr>
<td>0.085</td>
<td>1.3339 1.070 1.3336 1.114 1.3335 1.163 1.3332 1.210 1.3329 1.380</td>
<td></td>
</tr>
</tbody>
</table>

$^a$ standard uncertainties $u$ are $u(T) = 0.01K$, $u(P) = 0.01MPa$, $u(k) = 0.021(mScm^{-1})$, $u(n_D) = 0.0005$. $^b$ Standard uncertainty in molality considering the purity of mass of the studied samples is expected to be about 0.0003 mol· kg$^{-1}$. $^c$ Molality for the above system has been stated per kg of (IL + water) as a solvent mixture, (0.68 denotes as the level of confidence of the measurements). Wave length of light source for refractive index measurement was, $\lambda = 589.3nm$. Symbol ‘[IL]’ denotes as ionic liquid.

**Table S17.** Refractive index ($n_D$) and specific electrical conductivity ($\kappa$) of L-Gln in aqueous IL (BTBAC) solution at different temperatures $T= (293.15 - 313.15) K$ at atmospheric pressure 0.01MPa $^a,b$
Molality of L-Gln (AA) in Aq. BTBAC(IL)/ (mol·kg⁻¹)

<table>
<thead>
<tr>
<th>T=293.15K</th>
<th>T=298.15K</th>
<th>T=303.15K</th>
<th>T=308.15K</th>
<th>T=313.15K</th>
</tr>
</thead>
<tbody>
<tr>
<td>nD κ (mS/cm)</td>
<td>nD κ (mS/cm)</td>
<td>nD κ (mS/cm)</td>
<td>nD κ (mS/cm)</td>
<td>nD κ (mS/cm)</td>
</tr>
</tbody>
</table>

L-Gln + 0.001 mol· kg⁻¹ aq. BTBAC Soln.

| 0.010 | 1.3324 | 0.331 | 1.3322 | 0.352 | 1.3320 | 0.382 | 1.3318 | 0.410 | 1.3315 | 0.452 |
| 0.025 | 1.3325 | 0.408 | 1.3323 | 0.453 | 1.3321 | 0.486 | 1.3319 | 0.523 | 1.3317 | 0.553 |
| 0.040 | 1.3327 | 0.479 | 1.3325 | 0.557 | 1.3323 | 0.582 | 1.3321 | 0.614 | 1.3319 | 0.662 |
| 0.055 | 1.3329 | 0.551 | 1.3327 | 0.640 | 1.3325 | 0.692 | 1.3323 | 0.710 | 1.3321 | 0.769 |
| 0.070 | 1.3331 | 0.646 | 1.3330 | 0.756 | 1.3327 | 0.790 | 1.3325 | 0.819 | 1.3324 | 0.865 |
| 0.085 | 1.3333 | 0.733 | 1.3332 | 0.847 | 1.3330 | 0.896 | 1.3328 | 0.903 | 1.3327 | 0.994 |

L-Gln + 0.003 mol· kg⁻¹ aq. BTBAC Soln.

| 0.010 | 1.3325 | 0.419 | 1.3323 | 0.441 | 1.3321 | 0.463 | 1.3319 | 0.496 | 1.3316 | 0.536 |
| 0.025 | 1.3326 | 0.492 | 1.3325 | 0.543 | 1.3322 | 0.570 | 1.3320 | 0.597 | 1.3318 | 0.642 |
| 0.040 | 1.3328 | 0.619 | 1.3327 | 0.683 | 1.3324 | 0.702 | 1.3322 | 0.724 | 1.3320 | 0.764 |
| 0.055 | 1.3330 | 0.713 | 1.3329 | 0.784 | 1.3326 | 0.819 | 1.3324 | 0.821 | 1.3322 | 0.806 |
| 0.070 | 1.3332 | 0.809 | 1.3331 | 0.902 | 1.3328 | 0.923 | 1.3326 | 0.943 | 1.3325 | 1.035 |
| 0.085 | 1.3334 | 0.868 | 1.3334 | 0.975 | 1.3330 | 1.030 | 1.3329 | 1.050 | 1.3327 | 1.155 |

L-Gln + 0.005 mol· kg⁻¹ aq. BTBAC Soln.

| 0.010 | 1.3327 | 0.513 | 1.3325 | 0.542 | 1.3324 | 0.582 | 1.3322 | 0.612 | 1.3318 | 0.654 |
| 0.025 | 1.3329 | 0.592 | 1.3326 | 0.641 | 1.3325 | 0.670 | 1.3323 | 0.690 | 1.3319 | 0.728 |
| 0.040 | 1.3331 | 0.692 | 1.3328 | 0.768 | 1.3327 | 0.774 | 1.3325 | 0.796 | 1.3321 | 0.867 |
| 0.055 | 1.3333 | 0.768 | 1.3330 | 0.871 | 1.3329 | 0.876 | 1.3327 | 0.906 | 1.3323 | 1.003 |
| 0.070 | 1.3335 | 0.911 | 1.3332 | 0.980 | 1.3331 | 0.989 | 1.3329 | 1.010 | 1.3326 | 1.128 |
| 0.085 | 1.3338 | 0.990 | 1.3335 | 1.060 | 1.3333 | 1.080 | 1.3332 | 1.090 | 1.3328 | 1.186 |

\(^a\) Standard uncertainties \(u\) are \(u(T) = 0.01\), \(u(P) = 0.01\)MPa, \(u(k) = 0.021\) (mScm⁻¹), \(u(n_D) = 0.0005\). \(^b\) Standard uncertainty in molality considering the purity of mass of the studied samples is expected to be about 0.0003 mol· kg⁻¹. \(^c\) Molality for the above system has been stated per kg of (IL + water) as a solvent mixture, \((0.68\) denotes as the level of confidence of the measurements). Wave length of light source for refractive index measurement was, \(\lambda = 589.3\)nm. Symbol '[IL]' denotes as ionic liquid.
**Table S18.** UV-Vis Spectroscopic data for the Benesi-Hildebrand double reciprocal plot of (BTBAC+L-Asn) system at 298.15K.

<table>
<thead>
<tr>
<th>Tem./K</th>
<th>IL/μM</th>
<th>[AA] μM</th>
<th>A₀</th>
<th>A</th>
<th>ΔA</th>
<th>[AA]/M⁻¹</th>
<th>1/ΔA</th>
<th>Intercept</th>
<th>slope</th>
<th>Ka/M⁻¹×10⁻³</th>
<th>ΔG/kJ mol⁻¹</th>
</tr>
</thead>
<tbody>
<tr>
<td>300</td>
<td>20</td>
<td>0.44027</td>
<td>0.45956</td>
<td>0.01929</td>
<td>0.0500</td>
<td>51.8403</td>
<td>5.9241</td>
<td>919.52</td>
<td>6.44</td>
<td>-16.03</td>
<td></td>
</tr>
<tr>
<td>300</td>
<td>40</td>
<td>0.44207</td>
<td>0.47520</td>
<td>0.03493</td>
<td>0.0250</td>
<td>28.6286</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>298.15</td>
<td>300</td>
<td>60</td>
<td>0.44207</td>
<td>0.48683</td>
<td>0.04656</td>
<td>0.0166</td>
<td>21.4776</td>
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<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>300</td>
<td>80</td>
<td>0.44207</td>
<td>0.49470</td>
<td>0.05443</td>
<td>0.0125</td>
<td>18.3621</td>
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</tr>
<tr>
<td>300</td>
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<td>0.06488</td>
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<tr>
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<td>120</td>
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<td>0.08267</td>
<td>0.0088</td>
<td>12.0962</td>
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<td></td>
<td></td>
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</tbody>
</table>

The standard uncertainty of u(T) = 0.01K

**Table S19.** UV-Vis Spectroscopic data for the Benesi-Hildebrand double reciprocal plot of (BTBAC+L-Gln) system at 298.15K.

<table>
<thead>
<tr>
<th>Tem./K</th>
<th>IL/μM</th>
<th>[AA] μM</th>
<th>A₀</th>
<th>A</th>
<th>ΔA</th>
<th>[AA]/M⁻¹</th>
<th>1/ΔA</th>
<th>Intercept</th>
<th>slope</th>
<th>Ka/M⁻¹×10⁻³</th>
<th>ΔG/kJ mol⁻¹</th>
</tr>
</thead>
<tbody>
<tr>
<td>300</td>
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<td>0.44027</td>
<td>0.48763</td>
<td>0.03881</td>
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<td>16.09</td>
<td>-18.30</td>
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<tr>
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<td>40</td>
<td>0.44207</td>
<td>0.50090</td>
<td>0.06063</td>
<td>0.0250</td>
<td>16.4927</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>298.15</td>
<td>300</td>
<td>60</td>
<td>0.44207</td>
<td>0.51862</td>
<td>0.07835</td>
<td>0.0166</td>
<td>12.7632</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>300</td>
<td>80</td>
<td>0.44207</td>
<td>0.52547</td>
<td>0.08520</td>
<td>0.0125</td>
<td>11.7370</td>
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<tr>
<td>300</td>
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<td>0.0100</td>
<td>10.1424</td>
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</tr>
<tr>
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<td>120</td>
<td>0.44207</td>
<td>0.55208</td>
<td>0.11184</td>
<td>0.0088</td>
<td>8.9410</td>
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</tr>
</tbody>
</table>

The standard uncertainty of u(T) = 0.01K
Figure S1. Benesi double reciprocal plot of (BTBAC+L-Asn) system
Figure S2. Benesi double reciprocal plot of (BTBAC+L-Gln) system

\[ y = 392.59x + 6.3179 \]
\[ R^2 = 0.9963 \]