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# Micellar Transitions in Catanionic Ionic liquid - Ibuprofen Aqueous Mixtures; Effects of Composition and Dilution

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**Figure S1** UV-visible spectre of aqueous $C_{12}$mimCl + Ibu mixtures at various mole fractions of $C_{12}$mimCl ($x_{IL}$).

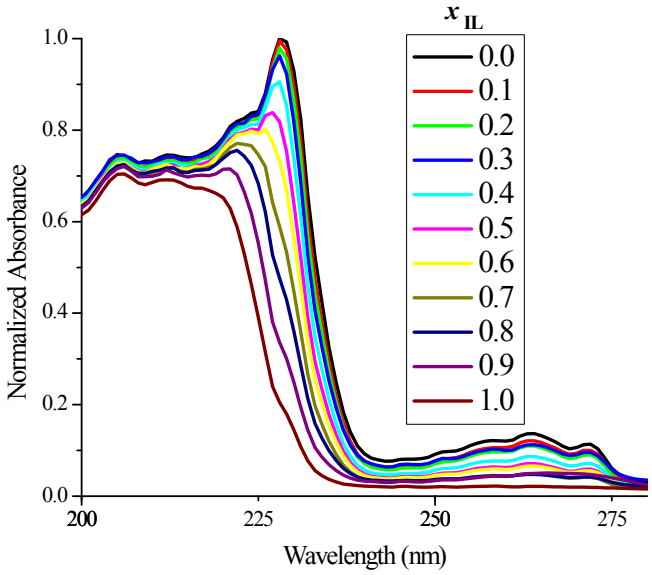


**Figure S2** Normalised fluorescence emission spectrum of Ibu in the presence of increasing amounts of $C_{12}$mimCl.

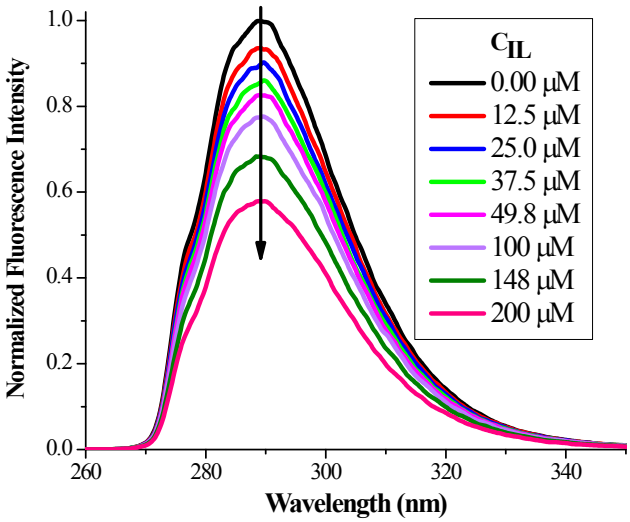

**Figure S3** (a) Stern-Volmer plots of fluorescence quenching of Ibu by $C_n$mimCl and (b) Binding constant determination for the $C_n mim^+Ibu^-$ complexes using changes in the fluorescence emission spectra of Ibu.

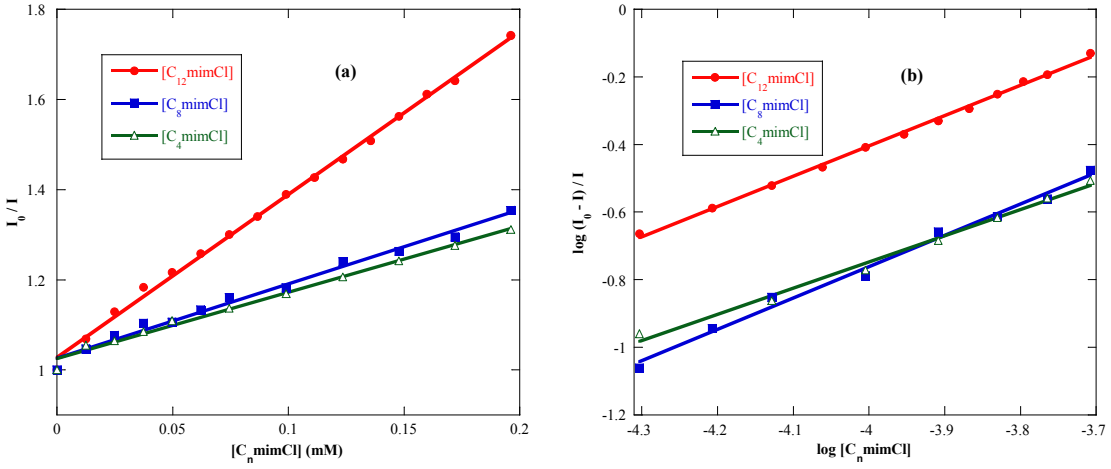


**Figure S4** Plots showing variation in the turbidity ($\tau$) with total mixture concentration for anionic dominated mole fractions ($x_{IL}$= 0.1 and 0.2) of $C_{12}$mimCl + Ibu aqueous mixtures.

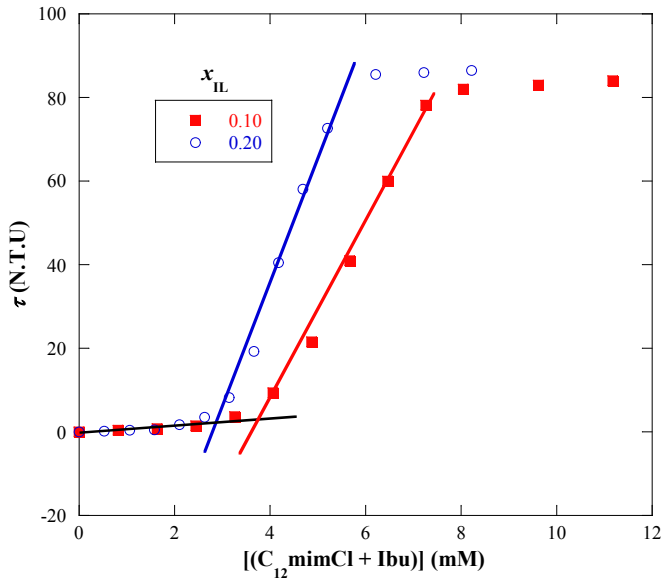

**Figure S5** Aggregate size distributions for $C_{12}$mimCl and Ibu at varied concentrations. The amplitudes for 900 mM Ibu, 10 mM $C_{12}$mimCl and 10mM Ibu have been shifted upwards by +20, +40 and +60 units respectively.

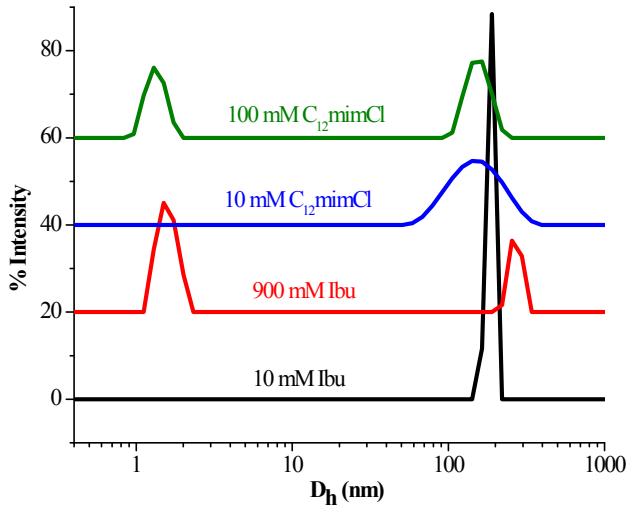


**Figure S6** $^1$H NMR spectra for pure $C_{12}$mimCl.

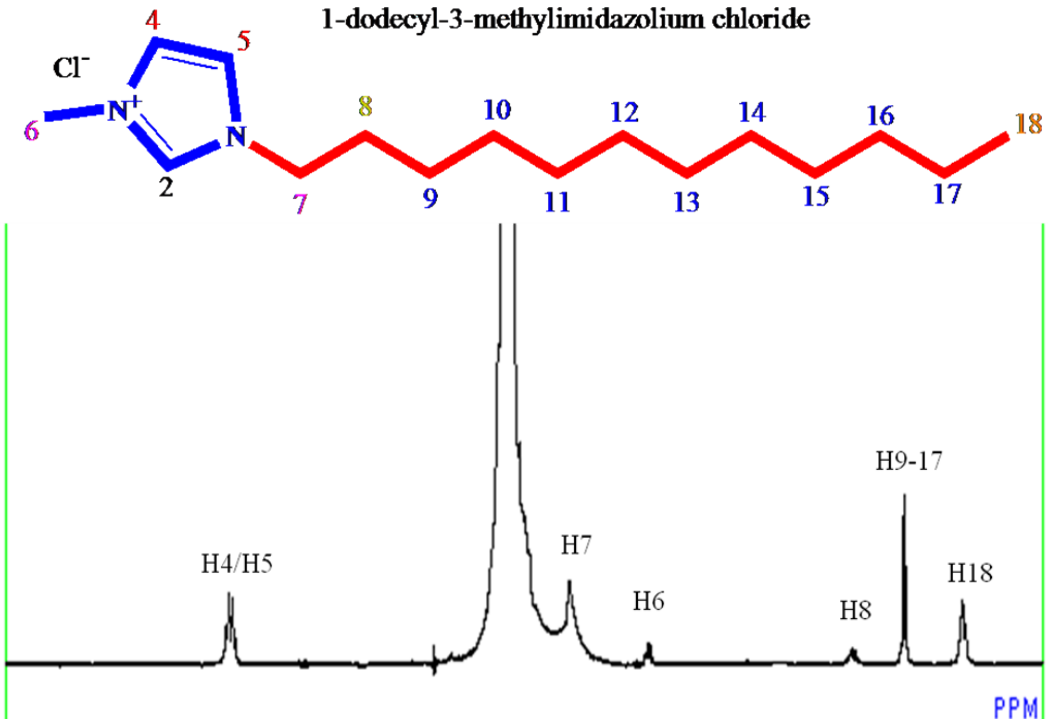

**Figure S7** $^{1}$H NMR spectra for pure Ibuprofen.

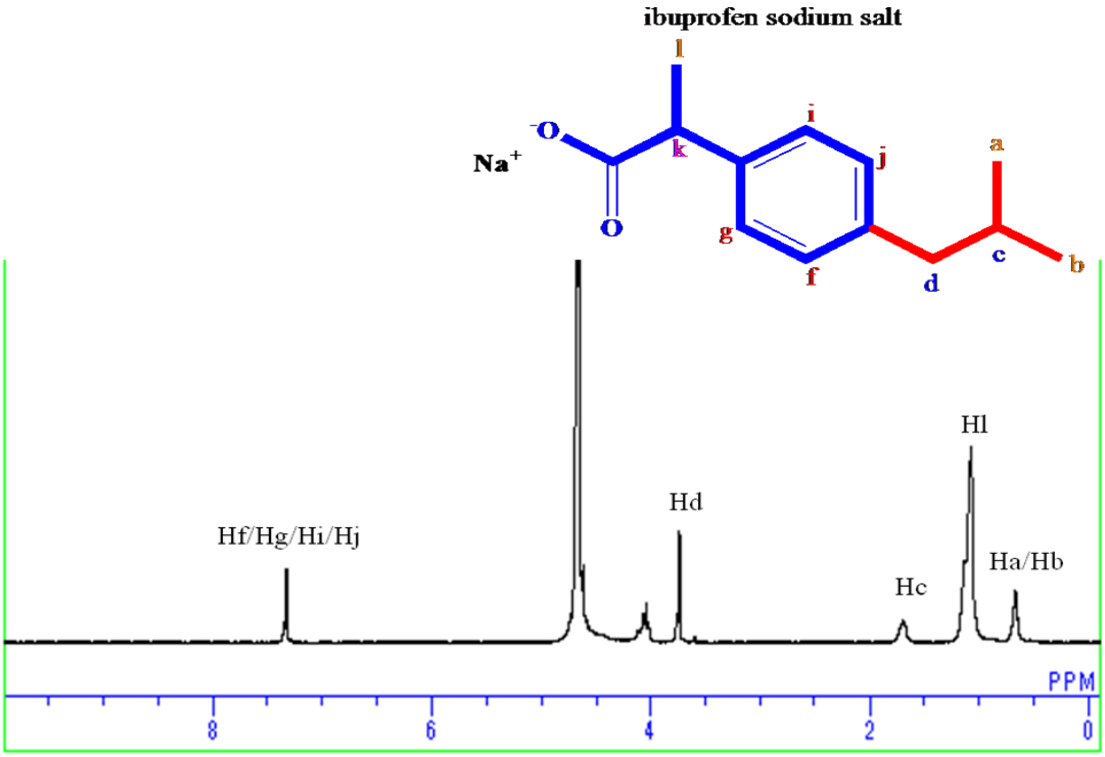


**Table S1** Effect of Dilution on the hydrodynamic diameters ($D_h$) of $C_{12}$mimCl + Ibu aqueous mixtures for anionic dominated mole fractions ($x_{IL}$ = 0.20) and cationic dominated mole fractions ($x_{IL}$ = 0.79) at total mixture concentrations of 10mM, 50mM, 100mM and 250mM.

| $x_{IL}$ | $D_h$ (nm) | | | |
|---|---|---|---|---|
| | 10 mM | 50 mM | 100 mM | 250 mM |
| 0.20 | 3458 ± 439.1 | 89.60 ± 27.10<br>21.89 ± 5.59 | 31.41 ± 7.69<br>11.88 ± 3.45 | 7.08 ± 1.66 |
| 0.79 | 4.64 ± 0.84<br>149.7 ± 24.6 | 2.76 ± 0.42<br>165.6 ± 25.1 | 2.60 ± 0.30<br>250.6 ± 66.5 | 1.95 ± 0.25<br>169.4 ± 17.9 |

**Table S2** Chemical shifts and observations for aromatic protons from $^1$H NMR measurements of $C_{12}$mimCl + Ibu mixtures at varying mole fractions ($x_{IL}$)

| $x_{IL}$ | $^1$H NMR chemical shift range in δ (ppm) for aromatic protons | | Observations |
|---|---|---|---|
| | H4 / H5 | Hf, Hg, Hi, Hj | |
| 0.00 | - | 7.318 (s)<br>7.333 (d) | (a) The aromatic protons of both the $C_{12}$mimCl and Ibu in all the catanionic mixtures appear upfield as compared to their pure counterparts.<br><br>(b) On moving from cationic rich to anionic dominated mole fractions, a downfield shifting of all the signals is observed. |
| 0.10 | 6.737 (s)<br>6.932(s) | 6.974 (d)<br>7.146 (d) | |
| 0.20 | 6.833 (s)<br>7.015 (s) | 6.966 (d)<br>7.152 (d) | |
| 0.30 | 6.812 (s)<br>6.986 (s) | 6.860 (d)<br>7.065 (d) | |
| 0.60 | 6.988 (s) | 6.828 (d)<br>7.044 (d) | |
| 0.70 | 6.747 (d)<br>7.028 (d) | 7.098 (s)<br>7.183 (s) | |
| 0.80 | 6.779 (d)<br>7.060 (d) | 7.220 (s)<br>7.271 (s) | |
| Pure IL | 7.088 (d)<br>7.066 (d) | - | |

**Table S3** Chemical shifts and observations for aliphatic protons from $^1$H NMR measurements of $C_{12}$mimCl + Ibu mixtures at varying mole fractions ($x_{IL}$)

| $x_{IL}$ | $^1$H NMR chemical shift range in δ (ppm) for aliphatic protons | | | | Observations |
|---|---|---|---|---|---|
| | H8 / Hc | Hl | H9-17 | Ha / Hb / H18 | |
| 0.00 | 1.694 (s) | 1.073 (s) | - | 0.672 (t) | (a) The aliphatic protons of both the $C_{12}$mimCl and Ibu in all the catanionic mixtures appear upfield as compared to their pure counterparts.<br><br>(b) On moving from cationic rich to anionic dominated mole fractions, a downfield shifting of all the signals is observed. |
| 0.10 | 1.586-1.743 (m) | 1.115 (s) | 1.255 (d) | 0.699 (d) | |
| 0.20 | 1.589-1.722 (m) | 1.104 (s) | 1.251 (d) | 0.697 (d) | |
| 0.30 | 1.492-1.625 (m) | 1.011 (s) | 1.155 (d) | 0.600 (d) | |
| 0.60 | 1.476-1.587 (m) | 0.991 (s) | 1.133 (d) | 0.574 (d) | |
| 0.70 | 1.515 (s) | 1.095 (s) | 1.117 (d) | 0.550 (t) | |
| 90.80 | 1.616 (s) | 1.145 (s) | 1.170 (d) | 0.608 (t) | |
| Pure IL | 1.635-1.703 (m) | - | 1.209 (d) | 0.697 (t) | |