**Supporting Information**

**Effect of changing alkyl chain in imidazolium based ionic liquid on the micellization behavior of anionic surfactant** **sodium hexadecyl sulfate in aqueous media**

**Harsh Kumar\*, Gagandeep Kaur**

Department of Chemistry, Dr B R Ambedkar National Institute of Technology, Jalandhar – 144011, Punjab, India

Email- [h.786.man@gmail.com](mailto:h.786.man@gmail.com), [manchandah@nitj.ac.in](mailto:manchandah@nitj.ac.in)

**Conductivity measurements**

**Table S1.** Specific conductivity*κ* (µS cm-1) of SHS in water and in (0.02, 0.05 and 0.10 wt. %) of [C3mim] [Br] at (298.15, 303.15 and 308.15 K).

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Concentration**  **(mM)** | ***κ* (µS cm-1)** | | | | | | | | | | | |
| **Water** | | | **0.02 wt.% [C3mim] [Br]** | | | **0.05 wt.% [C3mim] [Br]** | | | **0.10 wt.% [C3mim] [Br]** | | |
| **Temperature (K)** | | | **Temperature (K)** | | | **Temperature (K)** | | | **Temperature (K)** | | |
| **298.15** | **303.15** | **308.15** | **298.15** | **303.15** | **308.15** | **298.15** | **303.15** | **308.15** | **298.15** | **303.15** | **308.15** |
| 0.00746 | 5.64 | 7.88 | 9.15 | 213.8 | 219.5 | 225.7 | 355.9 | 365.8 | 374.3 | 542.1 | 594.0 | 645.2 |
| 0.01141 | 5.72 | 8.39 | 9.32 | 214.4 | 219.7 | 225.9 | 356.3 | 366.2 | 374.7 | 542.3 | 594.2 | 645.4 |
| 0.01632 | 5.87 | 8.51 | 9.77 | 214.8 | 220.3 | 226.4 | 356.7 | 366.5 | 375.0 | 542.5 | 594.4 | 645.6 |
| 0.02217 | 6.08 | 9.23 | 10.41 | 215.2 | 220.4 | 226.5 | 357.1 | 366.8 | 375.3 | 542.8 | 594.7 | 645.9 |
| 0.02893 | 6.58 | 9.38 | 10.77 | 215.4 | 220.5 | 226.7 | 357.3 | 367.4 | 375.9 | 543.2 | 594.8 | 646.0 |
| 0.03659 | 7.07 | 10.04 | 11.35 | 215.6 | 220.9 | 226.8 | 357.5 | 367.8 | 376.3 | 543.4 | 595.0 | 646.4 |
| 0.04510 | 7.34 | 10.58 | 11.89 | 216.5 | 221.6 | 227.7 | 358.4 | 367.7 | 376.2 | 543.7 | 595.3 | 646.7 |
| 0.05445 | 8.44 | 11.27 | 12.66 | 216.9 | 222.3 | 228.2 | 358.8 | 368.3 | 376.8 | 544.0 | 595.6 | 646.9 |
| 0.07279 | 8.75 | 11.95 | 13.33 | 217.6 | 222.5 | 228.6 | 359.5 | 368.8 | 377.8 | 544.3 | 595.9 | 647.9 |
| 0.09944 | 9.98 | 14.22 | 15.77 | 218.5 | 224.1 | 230.2 | 360.4 | 370.1 | 379.1 | 544.9 | 596.7 | 648.7 |
| 0.13346 | 12.63 | 16.19 | 17.89 | 219.5 | 225.5 | 231.4 | 361.4 | 371.7 | 380.7 | 545.6 | 597.8 | 649.8 |
| 0.17374 | 14.19 | 17.98 | 21.16 | 221.5 | 227.9 | 233.9 | 362.5 | 373.4 | 382.4 | 546.5 | 598.9 | 650.9 |
| 0.21904 | 16.97 | 21.17 | 24.42 | 222.9 | 230.4 | 236.3 | 363.7 | 375.4 | 384.4 | 547.6 | 600.5 | 652.5 |
| 0.26814 | 19.03 | 23.47 | 27.78 | 225.3 | 232.1 | 238.1 | 365.2 | 377.7 | 386.7 | 548.6 | 601.8 | 653.8 |
| 0.31983 | 20.91 | 25.82 | 29.77 | 226.8 | 235.2 | 241.3 | 366.7 | 380.4 | 389.1 | 549.7 | 603.4 | 655.2 |
| 0.37303 | 22.13 | 28.11 | 32.17 | 227.8 | 236.9 | 242.9 | 367.7 | 382.4 | 391.4 | 550.9 | 604.7 | 656.7 |
| 0.42678 | 23.85 | 29.91 | 34.92 | 229.5 | 238.4 | 244.5 | 368.9 | 383.7 | 392.9 | 551.5 | 605.9 | 657.9 |
| 0.49844 | 26.27 | 32.19 | 36.98 | 231.1 | 239.9 | 245.9 | 370.0 | 385.7 | 394.7 | 552.4 | 607.1 | 659.4 |
| 0.58032 | 29.35 | 34.95 | 40.92 | 233.2 | 242.7 | 248.6 | 371.6 | 387.8 | 396.9 | 553.5 | 608.7 | 660.9 |
| 0.66559 | 31.72 | 38.69 | 44.97 | 235.5 | 244.9 | 250.8 | 373.5 | 390.0 | 399.3 | 554.6 | 610.0 | 662.5 |
| 0.74912 | 34.53 | 41.83 | 49.06 | 237.4 | 248.0 | 254.1 | 375.3 | 392.1 | 401.9 | 555.8 | 611.6 | 664.2 |
| 0.83755 | 37.61 | 45.96 | 53.19 | 238.9 | 250.1 | 256.2 | 376.8 | 394.3 | 404.2 | 556.9 | 612.8 | 665.6 |

Standard uncertainties s are s (T) = ±0.1 K, s (*κ*) = ±0.0001 mS/cm.

**Table S2.** Specific conductivity*κ* (µS cm-1) of SHS in water and in (0.02, 0.05 and 0.10 wt. %) of [C4mim] [Br] at (298.15, 303.15 and 308.15 K).

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Concentration**  **(mM)** | ***κ* (µS cm-1)** | | | | | | | | |
| **0.02 wt.% [C4mim] [Br]** | | | **0.05 wt.% [C4mim] [Br]** | | | **0.10 wt.% [C4mim] [Br]** | | |
| **Temperature (K)** | | | **Temperature (K)** | | | **Temperature (K)** | | |
| **298.15** | **303.15** | **308.15** | **298.15** | **303.15** | **308.15** | **298.15** | **303.15** | **308.15** |
| 0.00746 | 208.7 | 211.9 | 215.4 | 299.5 | 317.2 | 336.2 | 485.2 | 535.0 | 579.3 |
| 0.01141 | 208.9 | 212.2 | 215.7 | 299.9 | 317.5 | 336.4 | 485.4 | 535.1 | 579.5 |
| 0.01632 | 209.2 | 212.4 | 216.6 | 300.1 | 317.9 | 336.9 | 485.7 | 535.3 | 579.7 |
| 0.02217 | 209.5 | 212.6 | 217.1 | 300.5 | 318.4 | 337.5 | 485.9 | 535.8 | 579.8 |
| 0.02893 | 210.1 | 212.8 | 218.0 | 300.7 | 318.6 | 337.7 | 486.0 | 536.1 | 580.1 |
| 0.03659 | 210.5 | 213.1 | 218.1 | 301.0 | 318.9 | 338.2 | 486.4 | 536.4 | 580.4 |
| 0.04510 | 210.8 | 213.4 | 219.0 | 301.1 | 319.3 | 339.0 | 486.6 | 536.9 | 580.7 |
| 0.05445 | 211.2 | 213.7 | 219.5 | 301.5 | 319.7 | 339.6 | 487.1 | 537.2 | 581.0 |
| 0.07279 | 211.9 | 214.8 | 220.1 | 302.3 | 320.4 | 340.4 | 487.5 | 537.9 | 581.4 |
| 0.09944 | 212.7 | 215.7 | 221.2 | 303.5 | 321.4 | 341.5 | 488.1 | 538.9 | 581.9 |
| 0.13346 | 213.7 | 217.2 | 222.9 | 304.6 | 323.2 | 343.0 | 489.0 | 540.3 | 582.9 |
| 0.17374 | 215.1 | 218.8 | 225.4 | 306.2 | 324.9 | 345.1 | 490.4 | 541.6 | 583.8 |
| 0.21904 | 216.7 | 220.9 | 227.5 | 307.5 | 326.9 | 347.3 | 491.7 | 543.5 | 584.8 |
| 0.26814 | 218.6 | 222.7 | 230.0 | 309.0 | 329.3 | 349.5 | 493.1 | 545.2 | 586.2 |
| 0.31983 | 219.9 | 224.4 | 232.8 | 310.5 | 331.9 | 351.9 | 494.5 | 547.2 | 587.4 |
| 0.37303 | 221.1 | 225.7 | 235.1 | 311.5 | 333.2 | 354.3 | 495.7 | 549.4 | 588.8 |
| 0.42678 | 222.2 | 227.2 | 237.2 | 312.7 | 334.7 | 355.8 | 496.6 | 550.8 | 589.9 |
| 0.49844 | 223.7 | 229.1 | 239.2 | 314.2 | 336.8 | 357.6 | 497.7 | 552.4 | 591.0 |
| 0.58032 | 225.7 | 231.1 | 242.2 | 315.9 | 338.8 | 360.1 | 499.1 | 554.5 | 592.2 |
| 0.66559 | 227.4 | 233.1 | 244.6 | 317.8 | 341.0 | 362.7 | 500.6 | 556.2 | 593.5 |
| 0.74912 | 229.3 | 235.3 | 247.5 | 319.5 | 343.5 | 365.3 | 502.1 | 558.3 | 594.8 |
| 0.83755 | 231.4 | 237.6 | 250.6 | 321.6 | 345.8 | 368.1 | 503.5 | 560.2 | 596.2 |

Standard uncertainties s are s (T) = ±0.1 0C, s (*κ*) = ±0.0001 mS/cm

**Fluorescence measurements**

**Table S3** Pyrene *II / IIII* values of SHS in water and in the presence of (0.02, 0.05 and 0.10 wt.%) of [C3mim][Br]

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  |  | **[C3mim][Br] / SHS** | | |
|  | **SHS / H2O** | **0.02wt. % of IL** | **0.05wt. % of IL** | **0.10wt. % of IL** |
| **Conc.(mM)** | ***II / IIII*** | ***II / IIII*** | ***II / IIII*** | ***II / IIII*** |
| 0.045102 | 1.32993 | 1.29238 | 1.22912 | 1.14059 |
| 0.054449 | 1.32826 | 1.29211 | 1.22900 | 1.14023 |
| 0.072788 | 1.32579 | 1.28954 | 1.22792 | 1.14044 |
| 0.09944 | 1.32209 | 1.28595 | 1.22986 | 1.13958 |
| 0.133465 | 1.31961 | 1.28099 | 1.22870 | 1.13869 |
| 0.17374 | 1.30054 | 1.27413 | 1.21966 | 1.13648 |
| 0.219044 | 1.20157 | 1.26039 | 1.20600 | 1.13486 |
| 0.268136 | 1.12469 | 1.21226 | 1.18160 | 1.12937 |
| 0.319827 | 1.11251 | 1.15617 | 1.15518 | 1.12117 |
| 0.373028 | 1.10807 | 1.11655 | 1.12543 | 1.10763 |
| 0.426783 | 1.10127 | 1.11195 | 1.09939 | 1.09174 |
| 0.498442 | 1.09177 | 1.10596 | 1.07341 | 1.07489 |
| 0.580319 | 1.09147 | 1.10230 | 1.07203 | 1.06761 |
| 0.665585 | - | 1.09650 | 1.07101 | 1.06648 |
| 0.749124 | - | 1.09398 | 1.06996 | 1.06541 |

**Table S4** Pyrene *II / IIII* values of SHS in the presence of (0.02, 0.05 and 0.10 wt.%) of [C4mim][Br]

|  |  |  |  |
| --- | --- | --- | --- |
|  | **[C4mim][Br]./ SHS** | | |
|  | **0.02wt. % of IL** | **0.05wt. % of IL** | **0.10wt. % of IL** |
| **Conc.(mM)** | ***II / IIII*** | ***II / IIII*** | ***II / IIII*** |
| 0.045102 | 1.09047 | 1.04518 | 1.04098 |
| 0.054449 | 1.08994 | 1.04491 | 1.04094 |
| 0.072788 | 1.08942 | 1.04469 | 1.04024 |
| 0.09944 | 1.08867 | 1.04420 | 1.03998 |
| 0.133465 | 1.08640 | 1.04326 | 1.03871 |
| 0.17374 | 1.08191 | 1.04197 | 1.03612 |
| 0.219044 | 1.07554 | 1.03849 | 1.03294 |
| 0.268136 | 1.06844 | 1.02934 | 1.02727 |
| 0.319827 | 1.05524 | 1.01971 | 1.01947 |
| 0.373028 | 1.04342 | 1.01003 | 1.00796 |
| 0.426783 | 1.04093 | 1.00310 | 0.99740 |
| 0.498442 | 1.03899 | 1.00197 | 0.98571 |
| 0.580319 | 1.03967 | 1.00120 | 0.98451 |
| 0.665585 | 1.03971 | 0.99975 | 0.98236 |
| 0.749124 | 1.03890 | 0.99969 | 0.98166 |

**UV-Visible spectroscopy**

**Table** **S5** Absorbance values of SHS in water and in the presence of (0.02, 0.05 and 0.10 wt.%) of [C3mim][Br] at 215 nm in aqueous media

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  |  | **Absorbance of SHS** | | | |
|  | **Conc.(mM) of SHS** | **Water** | **[C3mim][Br]** | | |
| **0.02wt. % of IL** | **0.05wt. % of IL** | **0.10wt. % of IL** |
|  | 0 | 0.023 | 1.530 | 3.028 | 3.293 |
| a | 0.054449 | 0.043 | 2.010 | 3.058 | 3.321 |
| b | 0.09944 | 0.088 | 2.196 | 3.085 | 3.351 |
| c | 0.17374 | 0.151 | 2.586 | 3.125 | 3.398 |
| d | 0.219044 | 0.195 | 2.961 | 3.148 | 3.423 |
| e | 0.268136 | 0.216 | 3.401 | 3.171 | 3.456 |
| f | 0.319827 | 0.238 | 3.539 | 3.213 | 3.477 |
| g | 0.373028 | 0.280 | 3.575 | 3.229 | 3.512 |
| h | 0.498442 | 0.346 | 3.664 | 3.270 | 3.531 |
| i | 0.580319 | 0.408 | 3.740 | 3.299 | 3.534 |
| j | 0.665585 | 0.451 | 3.754 | 3.333 | 3.546 |

**Table S6** Absorbance values of SHS in the presence of (0.02, 0.05 and 0.10 wt.%) of [C4mim][Br] at 215 nm in aqueous media

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | **Absorbance of SHS** | | | |
|  | **Conc.(mM)**  **of SHS** | **[C4mim][Br]** | | |
|  | **0.02wt. % of IL** | **0.05wt. % of IL** | **0.10wt. % of IL** |
|  | 0 | 2.998 | 2.955 | 3.127 |
| A | 0.09944 | 2.998 | 2.976 | 3.144 |
| B | 0.219044 | 2.999 | 3.000 | 3.171 |
| C | 0.268136 | 2.999 | 3.010 | 3.179 |
| D | 0.319827 | 3.003 | 3.022 | 3.192 |
| E | 0.426783 | 3.015 | 3.032 | 3.229 |
| F | 0.580319 | 3.033 | 3.050 | 3.290 |
| G | 0.665585 | 3.043 | 3.060 | 3.332 |

**Conductivity measurement** **of [C3mim][Br]/SHS**



**Figure S1** Plot of (a) standard free energy of micellization *ΔG0m* (b) standard enthalpy of micellization *ΔH0m* (c) standard entropy of micellization *ΔS0m* of SHS solutions in water and in the presence of (0.02, 0.05 and 0.10 wt.%) of [C3mim][Br] at different temperatures (298.15, 303.15 and 308.15 K) in the aqueous media.

**Conductivity measurement** **of [C4mim][Br]/SHS**



**Figure S2** Plot of (a) standard free energy of micellization *ΔG0m* (b) standard enthalpy of micellization *ΔH0m* (c) standard entropy of micellization *ΔS0m* of SHS solutions in water and in the presence of (0.02, 0.05 and 0.10 wt.%) of [C4mim][Br] at different temperatures (298.15, 303.15 and 308.15 K) in the aqueous media.

**FT-IR Spectroscopic Study**

**(A) 0.02wt. % of [C3mim][Br]**

**E:\research\C3,C4BR SHS\c3 c4 shs\figures tiff c3 c4\s3 a.tif**

**(B) 0.05wt. % of [C3mim][Br]**

E:\research\C3,C4BR SHS\c3 c4 shs\figures tiff c3 c4\s3 b.tif

**(C) 0.10wt. % of [C3mim][Br]**

**E:\research\C3,C4BR SHS\c3 c4 shs\figures tiff c3 c4\s3 c.tif**

**Figure S3** FT-IR spectra of SHS in (A) 0.02 wt. % (B) 0.05 wt. % (C) 0.10 wt. % of [C3mim][Br] in the absence of SHS and in the presence of SHS at concentration below CMC, at CMC and above CMC.

**(A) 0.02wt. % of [C4mim][Br]**

E:\research\C3,C4BR SHS\c3 c4 shs\figures tiff c3 c4\S4 A.tif

**(B) 0.05wt. % of [C4mim][Br]**

**E:\research\C3,C4BR SHS\c3 c4 shs\figures tiff c3 c4\S4 B.tif**

**(C) 0.10wt. % of [C4mim][Br]**

**E:\research\C3,C4BR SHS\c3 c4 shs\figures tiff c3 c4\S4 C.tif**

**Figure S4** FT-IR spectra of SHS in (A) 0.02 wt. % (B) 0.05 wt. % (C) 0.10 wt. % of [C4mim][Br] in the absence of SHS and in the presence of SHS at concentration below CMC, at CMC and above CMC.