Supplementary Material

Aggregation Behavior of Cetyldimethylethylammonium Bromide under the Influence of Bovine Serum Albumin in Aqueous/ Electrolyte Solutions at Various Temperatures and Compositions: Conductivity and Molecular Dynamics Study

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SM Table 1

Thermodynamic parameters of transfer for the micellization of BSA mediated CDMEAB solution (with/without salt of different ionic strength)\textsuperscript{a}

| System | Medium | $I_{\text{Salt}}$/mmol.kg\textsuperscript{-1} | $T$/K | $\Delta G^0_{1,\text{m, tr}}$ | $\Delta G^0_{2,\text{m, tr}}$ | $\Delta G^0_{3,\text{m, tr}}$ | $\Delta H^0_{1,\text{m, tr}}$ | $\Delta H^0_{2,\text{m, tr}}$ | $\Delta H^0_{3,\text{m, tr}}$ | $\Delta C^0_{1,\text{m, tr}}$ | $\Delta C^0_{2,\text{m, tr}}$ | $\Delta C^0_{3,\text{m, tr}}$ |
|--------|--------|----------------------------------|------|---------------------|---------------------|---------------------|---------------------|---------------------|---------------------|---------------------|---------------------|---------------------|
|        |        |                                  |      | kJ mol\textsuperscript{-1} | kJ mol\textsuperscript{-1} | kJ mol\textsuperscript{-1} | kJ mol\textsuperscript{-1} | kJ mol\textsuperscript{-1} | kJ mol\textsuperscript{-1} | kJ K\textsuperscript{-1} mol\textsuperscript{-1} | kJ K\textsuperscript{-1} mol\textsuperscript{-1} | kJ K\textsuperscript{-1} mol\textsuperscript{-1} |
| BSA+CDMEAB | H\textsubscript{2}O | 0.00 | 298.15 | 0.92 | -2.11 | 0.55 | 25.02 | -13.04 | -8.59 | -1.60 | -0.16 | -0.38 |
|          |       |      | 303.15 | 3.48 | 3.46 | 2.20 | 17.48 | -14.02 | -10.13 | -1.87 | -0.13 | -0.43 |
|          |       |      | 308.15 | 2.10 | 1.02 | 2.69 | 5.70 | -13.94 | -12.53 | -2.13 | -0.08 | -0.49 |
|          |       |      | 313.15 | 3.54 | 2.40 | 2.07 | -5.16 | -14.49 | -15.35 | -2.40 | -0.04 | -0.53 |
|          |       |      | 318.15 | 1.95 | 4.17 | 0.73 | -16.05 | -15.20 | -18.20 | -2.66 | 0.00 | -0.58 |
|          |       |      | 323.15 | 5.30 | 1.81 | 0.66 | -31.65 | -14.38 | -20.82 | -2.90 | 0.04 | -0.63 |
| BSA+CDMEAB | H\textsubscript{2}O+NaCl | 1.50 | 298.15 | 3.06 | 5.43 | 4.94 | -36.42 | -85.60 | -16.27 | 1.41 | 3.07 | 0.40 |
|          |       |      | 303.15 | 1.20 | 2.98 | 1.65 | -29.74 | -72.31 | -15.41 | 1.52 | 3.60 | 0.55 |
|          |       |      | 308.15 | 1.55 | 0.92 | 2.69 | -21.73 | -51.49 | -11.20 | 1.66 | 4.16 | 0.70 |
|          |       |      | 313.15 | 3.20 | 1.00 | 2.11 | -11.92 | -27.09 | -6.80 | 1.80 | 4.71 | 0.88 |
|          |       |      | 318.15 | 2.00 | 0.84 | 1.72 | -3.46 | -2.98 | -2.43 | 1.94 | 5.27 | 1.03 |
|          |       |      | 323.15 | 1.05 | 1.07 | 1.74 | 6.69 | 23.30 | 2.78 | 2.07 | 5.81 | 1.19 |
| BSA+CDMEAB | H\textsubscript{2}O+Na\textsubscript{2}SO\textsubscript{4} | 1.50 | 298.15 | 5.35 | 5.13 | 4.70 | -51.25 | -4.92 | -1.52 | 2.06 | 0.08 | 0.02 |
|          |       |      | 303.15 | 5.80 | 6.28 | 3.19 | -41.27 | -4.34 | -1.60 | 2.18 | 0.10 | 0.05 |
|          |       |      | 308.15 | 4.42 | 4.63 | 2.77 | -30.34 | -3.44 | -1.14 | 2.29 | 0.13 | 0.07 |
|          |       |      | 313.15 | 4.49 | 6.23 | 4.01 | -17.08 | -3.28 | -0.42 | 2.42 | 0.16 | 0.14 |
|          |       |      | 318.15 | 4.85 | 6.30 | 4.02 | -5.84 | -2.51 | 0.06 | 2.54 | 0.19 | 0.15 |
|          |       |      | 323.15 | 4.65 | 5.75 | 3.77 | 7.39 | -1.07 | 0.88 | 2.66 | 0.21 | 0.18 |

\textsuperscript{a}Relative standard uncertainties ($u_r$) limits are $u_r(\Delta G^0_{\text{m, tr}})$, $u_r(\Delta H^0_{\text{m, tr}})$, and $u_r(\Delta C^0_{\text{p, m, tr}})$ are 0.03, 0.04, and 0.04 respectively.
SM Fig. 1. Plot of $\ln (Xc^*_1)$ versus $T$ for (BSA+CDMEAB) system containing 0.03 mmol.kg$^{-1}$ BSA in aqueous solution.
SM Fig. 2. Representative plots of contribution of enthalpy, $\Delta H_{1,m}^0$ (■) and entropy, $-T \Delta S_{1,m}^0$ (●) to $\Delta G_{1,m}^0$ for (CDMEAB+BSA) mixed system containing 0.03 mmol.kg$^{-1}$ BSA in (a) water, (b) aqueous solution of NaCl (ionic strength, $I = 1.50$ mmol.kg$^{-1}$) and (c) aqueous solution of Na$_2$SO$_4$ (ionic strength, $I = 1.50$ mmol.kg$^{-1}$)
SM Fig. 3. Plot of enthalpy-entropy compensation event for (BSA+CDMEAB) systems having 0.03 mmol.kg\(^{-1}\) BSA solution in an aqueous medium for \(c_1^*\)
SM Fig. 4. Interaction of sodium ion (in purple) with four negatively charged amino acid residues of BSA (obtained from a simulation snapshot at 20 ns)
SM Fig. 5. Simulation snapshots of BSA+CDMEAB in (A) H₂O and (B) H₂O+NaCl