Electronic Supplementary Information

Micellization, Surface Activities and Thermodynamics study of pyridinium-based

ionic liquids surfactants in aqueous solution

Dong Fu¹, Xiaoru Gao², Bo Huang¹, Jue Wang¹, Yao Sun¹, Weijun Zhang¹, Kan Kan^{1*}, Xiaochen Zhang^{1*}, Yang Xie¹, and Xin Sui¹

1. Heilongjiang Academy of Sciences Institute of Advanced Technology, Harbin 150020, China.

2. Harbin FRP research Institute, Harbin, Heilongjiang 150029, China.

E-mail: kankan.has@foxmail.com; xc_zhang.has@hotmail.com.

Characterizations of [C_nmpy][Br]

n-dodecyl-3-methylpyridinium bromide ([C12mpy][Br])

The title compound was buff crystals. Yield: 94%. ¹H NMR (CDCl₃, 400 MHz), δ: 9.490 (s, 1H), 9.304 (d, 1H), 8.266 (d, 1H), 8.034 (t, 1H), 4.929 (t, 2H), 2.633 (s, 3H), 2.035 (t, 2H), 1.487~1.103 (m, 18H), 0.842(t, 3H); ¹³C NMR (CDCl₃, 100 MHz), δ: 145.58, 144.67, 142.31, 139.61, 61.79, 31.88, 29.57, 29.31, 26.10, 22.66, 18.72, 14.11. FTIR (KBr), *v*/cm⁻¹: 2996, 2919, 2842, 1641, 1514, 1456, 1379, 1286, 723, 682.

n-tetradecyl-3-methylpyridinium bromide ([C14mpy][Br])

The title compound was withe crystals. Yield: 95%. ¹H NMR (CDCl₃, 400 MHz), δ: 9.433 (s, 1H), 9.288 (d, 1H), 8.262 (d, 1H), 8.003 (t, 1H), 4.959 (t, 2H), 2.648 (s, 3H), 2.024 (t, 2H), 1.478~1.132 (m, 22H), 0.866 (t, 3H); ¹³C NMR (CDCl₃, 100 MHz), δ: 145.53, 144.66, 142.28, 139.63, 127.70, 61.79, 31.92, 29.68, 29.64, 29.60, 29.53, 29.36, 26.11, 22.69, 18.76, 14.13. FTIR (KBr), *v*/cm⁻¹: 3006, 2919, 2847, 1631, 1502, 1467, 1369, 1236, 728, 682. n-hexadecyl-3-methylpyridinium bromide ([C₁₆mpy][Br])

The title compound was withe crystals. Yield: 95%. ¹H NMR (CDCl₃, 400 MHz), δ: 9.475 (s, 1H), 9.299 (d, 1H), 8.264 (d, 1H), 8.031 (t, 1H), 4.934 (t, 2H), 2.634 (s, 3H), 2.015 (t, 2H), 1.438~1.009 (m, 26H), 0.848 (t, 3H); ¹³C NMR (CDCl₃, 100 MHz), δ:145.56, 144.66, 142.31, 139.60, 127.77, 61.73, 32.04, 31.91, 29.68, 29.65, 29.61, 29.53, 29.37, 26.10, 22.68, 18.73, 14.12. FTIR (KBr), *v*/cm⁻¹: 3006, 2919, 2847, 1626, 1514, 1472, 1375, 1286, 718, 682.



Fig. S1. (¹H, ¹³C) NMR and FTIR spectrum of synthesized [C_nmpy][Br].



Fig. S2. The plots of absorption intensity vs. various concentrations of ILs solutions containing pyrene.



Fig. S3. Conductivity dependence of concentration for ILs in the presence of LiBr at different temperature.



Fig. S4. Conductivity dependence of concentration for ILs in the presence of NaBr at different temperature.



Fig. S5. Conductivity dependence of concentration for ILs in the presence of MgBr₂ at different temperature.



Fig. S6. Conductivity dependence of concentration for ILs in the presence of C₂H₅OH at different temperature.



Fig. S7. Conductivity dependence of concentration for ILs in the presence of C₃H₇OH at different temperature.



Fig. S8. Conductivity dependence of concentration for ILs in the presence of C₄H₉OH at different temperature.



Fig. S9. Conductivity dependence of concentration for ILs in the presence of $C_5H_{11}OH$ at different temperature.



Fig. S10. The dependence of the CMC on temperature for ILs

Table 15. Coefficients of polynomials $\log X_{CMC}=A+BT+CT^2$; the temperature $T^*(CMC)$, at the minimum criticalmicelle concentration, cmc* and T_0 at $\Delta H_m^{\vartheta}=0$.

	А	В	С	CMC*	T^*	T_0
[C ₁₂ mpy][Br]	7.57146	-0.0761	1.302×10 ⁻⁴	9.61	295.00	292.31
[C ₁₄ mpy][Br]	4.36697	-0.0606	1.048×10-4	2.35	288.72	287.90
[C ₁₆ mpy][Br]	1.54843	-0.0276	4.857×10-5	0.521	283.20	285.16

^a Units: *T*(K); B(K⁻¹); C(K⁻²); T^{*}, *T*₀(K); CMC^{*}(mmol·L⁻¹)