

Electronic Supplementary Information

Efficient Separation of Surfactant and Organic Solvent by CO₂

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1. Experimental

Materials: TX-45 and TX-100 were provided by Sigma. TX-114 and Tween 80 were purchased from Shanghai ShineGene Molecular Bio-Technologies, Inc. AOT was purchased from Aldrich. Ethyl acetate, chloroform, benzene, toluene and 2,5-dimethylfuran were all analytical grade and purchased from Beijing Chemical Works. CO₂ (>99.95% purity) was provided by Beijing Analytical Instrument Factory.

Phase behaviour investigation: The apparatus and experimental procedures for studying the phase behaviour were similar to those reported previously.^[1] It consisted mainly of a high-pressure view cell, a constant temperature water bath, a high-pressure syringe pump, a pressure gauge, a magnetic stirrer, and a gas cylinder. The volume of the view cell could be changed in the range of 20 to 45 mL by changing the position of piston of the cell. In a typical experiment, the air in the view cell was replaced by CO₂. 1.0 mL of surfactant/organic solvent solution was injected into the cell, and the cell was placed in the constant temperature water bath (35 °C). After the thermal equilibrium had been reached, a suitable amount of CO₂ was charged into the view cell. The magnetic stirrer in the cell was started to accelerate the mixing of CO₂ and liquid. The pressure was unchanged with time as equilibrium was reached. The phase behaviour was observed at different pressures, the cloud point pressure and merging pressure were recorded.

Determination of volume expansion and CO₂ solubility: The apparatus to measure the volume expansion and CO₂ solubility at cloud point pressure was similar to those above. In the experiments, 10.0 mL of surfactant/organic solvent solution was injected into the view cell, and the cell was placed in the constant temperature water bath (35 °C). After the thermal equilibrium had been reached, a suitable amount of CO₂ was charged into the cell. The volume of the solution at equilibrium condition was known from the level of the liquid surface, and the volume expansion coefficient (ΔV) could be calculated on the basis of the volumes of the liquid before

and after dissolution of CO₂. For the CO₂ solubility determination, the liquid at cloud point pressure was sampled into the sample bomb. During the sampling, the volume of the view cell was adjusted to keep the pressure unchanged. The solubility was calculated from the masses of the liquid and the CO₂ in the sample bomb. The mass of the liquid was known from the masses of the sample bomb before and after sampling; the mass of the CO₂ was known from the masses of the sample bomb before and after releasing the gas in the sample.^[2]

UV-Vis spectra: The UV-Vis spectra were determined by a TU-1201 Model spectrophotometer (Beijing General Instrument Company).

2. Results

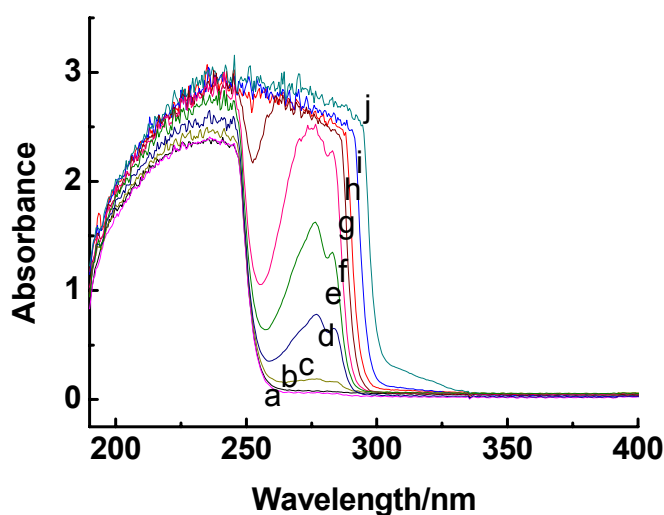


Fig. S1 UV-Vis spectra of TX100/ethyl acetate solutions of different concentrations at 35 °C. The surfactant concentrations are 0 (a), 0.00005 mol% (b), 0.0005 mol% (c), 0.005 mol% (d), 0.02 mol% (e), 0.04 mol% (f), 0.13 mol% (g), 0.2 mol% (h), 1.0 mol% (i), 5.0 mol% (j).

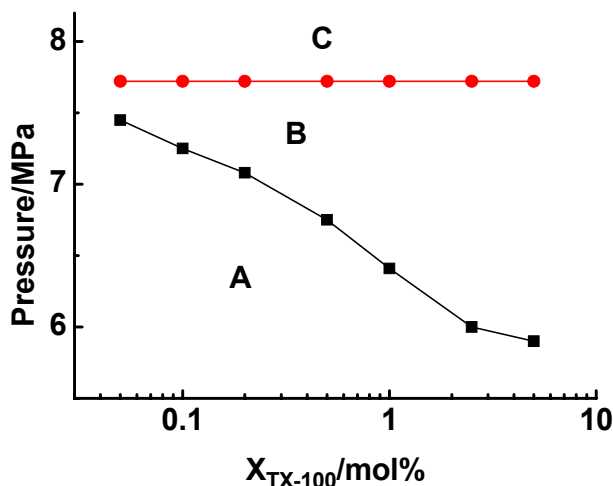
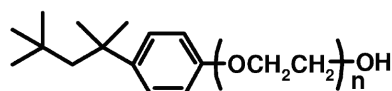
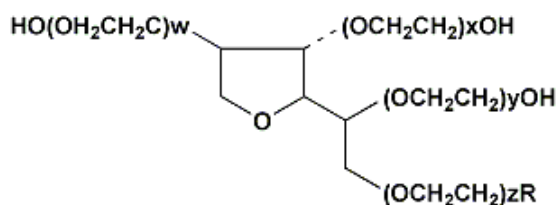


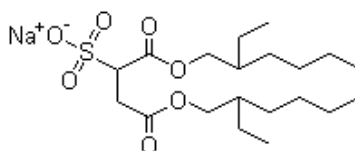
Fig. S2 Dependence of cloud point pressure (■) and merging pressure (●) of TX-100/ethyl acetate solution on the initial surfactant concentration (X_{TX-100}) at 35 °C. The phase regions of A, B and C correspond to Fig. 1a and 1b, 1c and 1d, 1e, respectively.



TX-45: $n=5$; TX-114: $n=7.5$; TX-100: $n=10$



Tween 80: $w+x+y+z=20$, $R=-\text{OCO}(\text{C}_{17}\text{H}_{33})$



AOT

Fig. S3 Molecular structures of the surfactants used in this work.

References

- [1] J. L. Zhang, B. X. Han, C. X. Zhang, W. Li and X. Y. Feng, *Angew. Chem. Int. Ed.* 2008, **47**, 3012.
- [2] J. L. Zhang, B. X. Han, Y. J. Zhao, J. S. Li, M Q. Hou and G. Y. Yang, *Chem. Commun.* 2011, **47**, 1033.