Supplementary Information

Phase and Rheological Behavior of a Gemini Cationic Surfactant Aqueous System

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1. ^{1}H NMR spectral data, elemental analysis dates and IR spectrogram of 12-3(OH)-12(2Cl)

^{1}HNMR: δH (400MHz,$CDCl_3$), 0.88(t,6H,$2CH_3CH_2$), 1.20~1.45(m,36H,$2CH_3(CH_2)_9$), 1.80(m,4H,$2CH_3(CH_2)_9CH_2$), 2.16(1H,OH), 3.39~3.42(s,12H,$4NCH_3$), 3.52(t,4H,$2CH_3(CH_2)_{10}CH_2$), 3.67(d,4H,$2CHCH_2$), 5.19(m,1H,$CHCH_2$)

Elemental analysis: measured value (theoretical value) (%): C 66.31(67.03), H 12.10(12.25), N 4.85(5.05), Cl,12.08(12.25).

IR spectrogram:

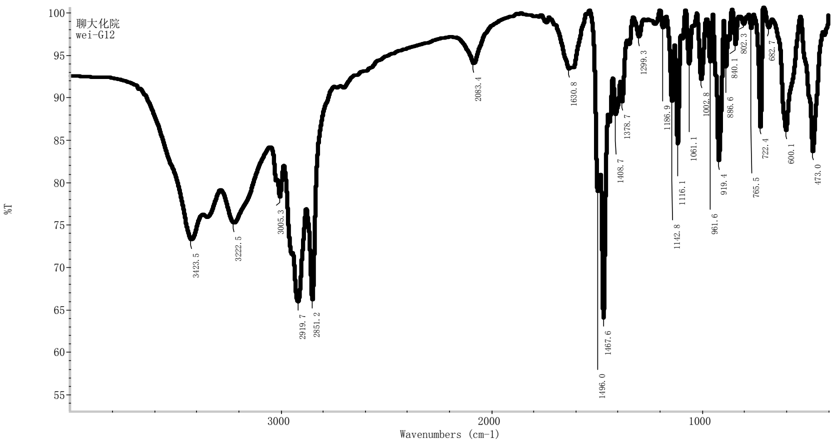

Fig.1

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在 3222.5cm^{-1}(-OH), 2919.7 cm^{-1}(-CH_3)，2851 cm^{-1}(-CH2), 1467.6 cm^{-1}(C - N^+ - C), 3423 cm^{-1}(H_2O).

2. Photograph of 12-3(OH)-12(2Cl) 42 wt% taken at 25°C with crossed polarizer

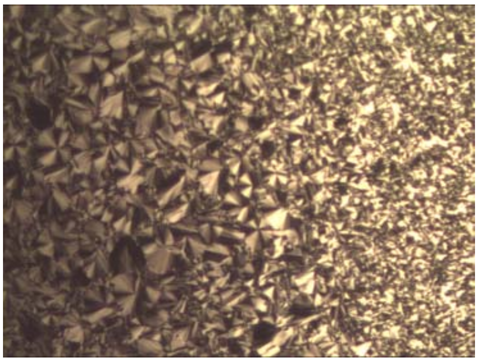
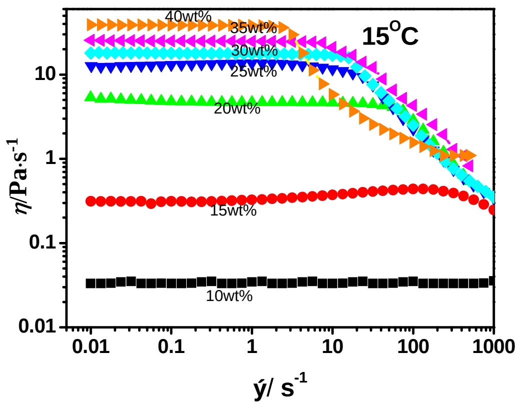


Fig.2

3. Curves of apparent viscosity (η) versus shear rate (ý) for aqueous solutions of 12-3(OH)-12(2Cl) at different concentrations and temperatures.

■, 10wt%; ●,15wt%; ▲, 20wt%; ▼,25wt%; ◆,30wt%; ◀;35wt%; ▶,40wt%



Electronic Supplementary Material (ESI) for Soft Matter

4.

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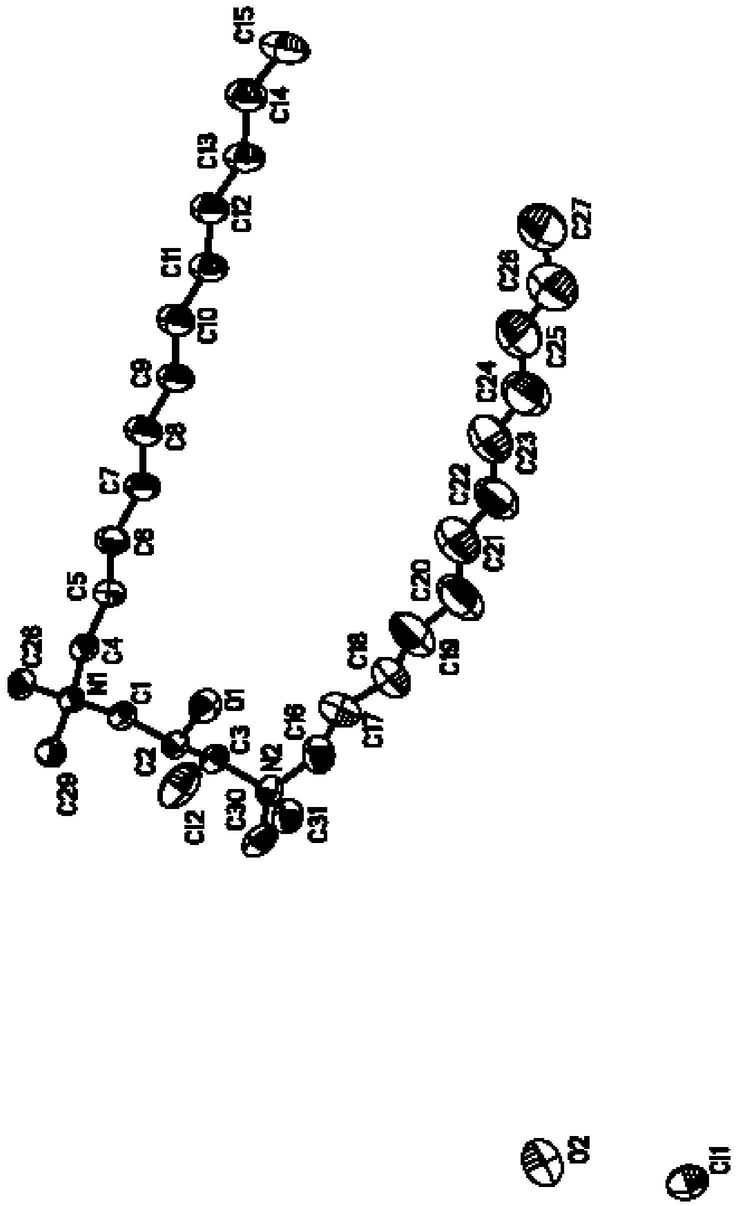
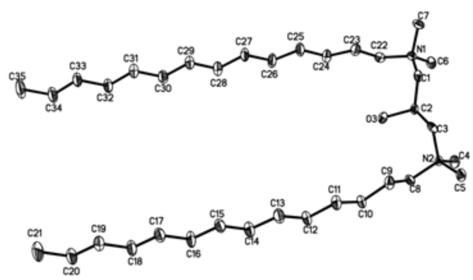


(B) The molecular structures of the R_{14-16}-3(OH)- R_{14-16} (2Br)



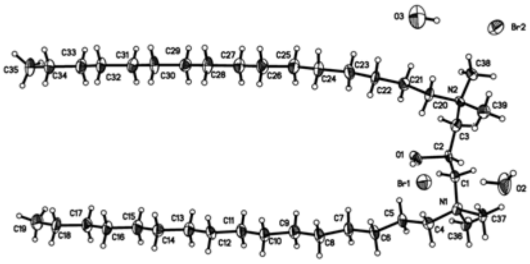


Fig.5

Explain: We have not made the crystal of 12-3(OH)- 12(2Br) So far, taking into account the similarity of molecular structures of R_{14-16}-3(OH)- R_{14-16} (2Br) and R_{12-16}-3(OH)- R_{12-16} (2Cl), using the structures of 14-3(OH)- 14 (2Br) and 14-3(OH)- 14 (2Cl) as a compare.

(C) Hydrogen bonds between the pendant hydroxyl group and halide ions and crystallization water molecules: (A) 12-3(OH)-12(2Cl), (B) 14-3(OH)-14(2Br)

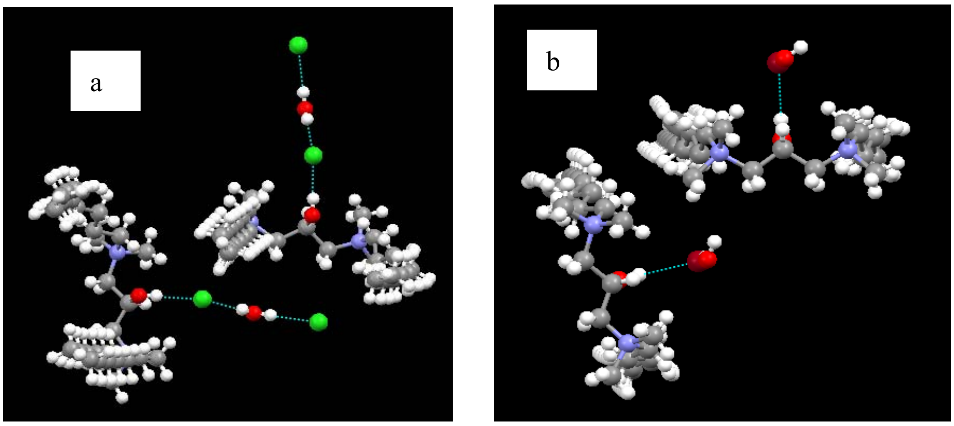


Fig. 6

5. Zero-shear apparent viscosity of 12-3(OH)-12(2Cl) as a function of concentration at different temperatures. (a) 15 °C; (b) 20 °C ; (C) 25 °C

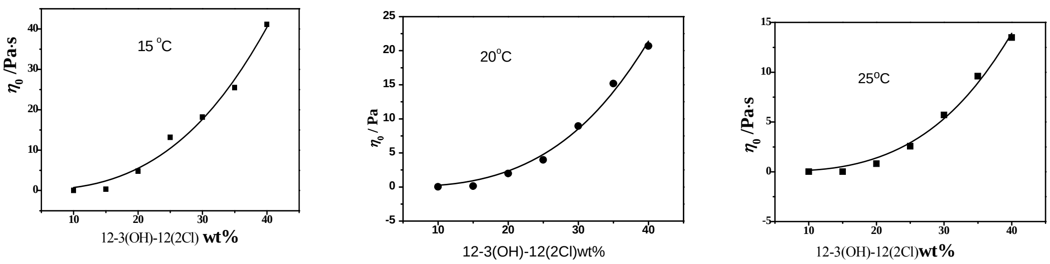


Fig.7

6. The Storage modulus (closed symbol) and loss modulus (open symbol) as a function of angular frequency for solutions with different 12-3(OH)-12(2Cl)wt% which are indicated in the figures (a) at 20 °C and the corresponding Cole–Cole plots (b).

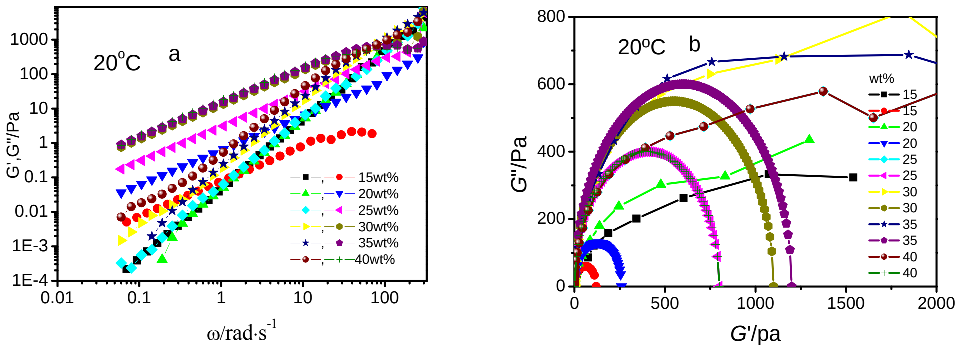


Fig.8

The Storage modulus (closed symbol) and loss modulus (open symbol) as a function of angular frequency for solutions with different 12-3(OH)-12(2Cl)wt% which are indicated in the figures (a) at 25 °C and the corresponding Cole–Cole plots (b).

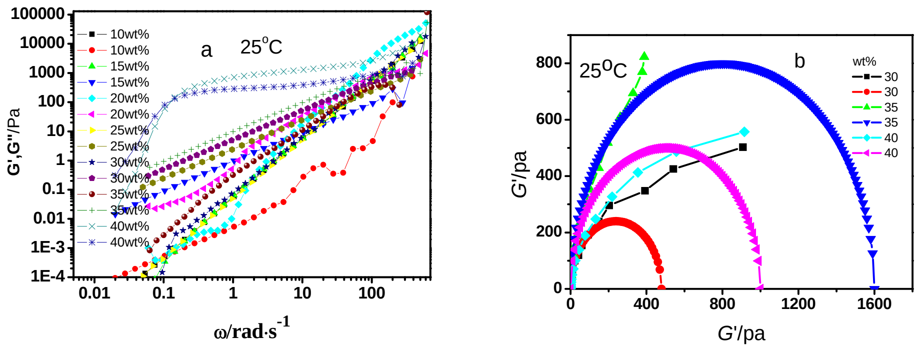


Fig. 9

7. Shear-rate dependence ($\dot{\gamma}$) of steady-shear viscosity (η, closed symbol) and frequency dependence(ω) of absolute value of complex viscosity ($|\eta^*|$, open symbol) for 12-3(OH)-12(2Cl) solution with different wt% which are indicated in the figures.

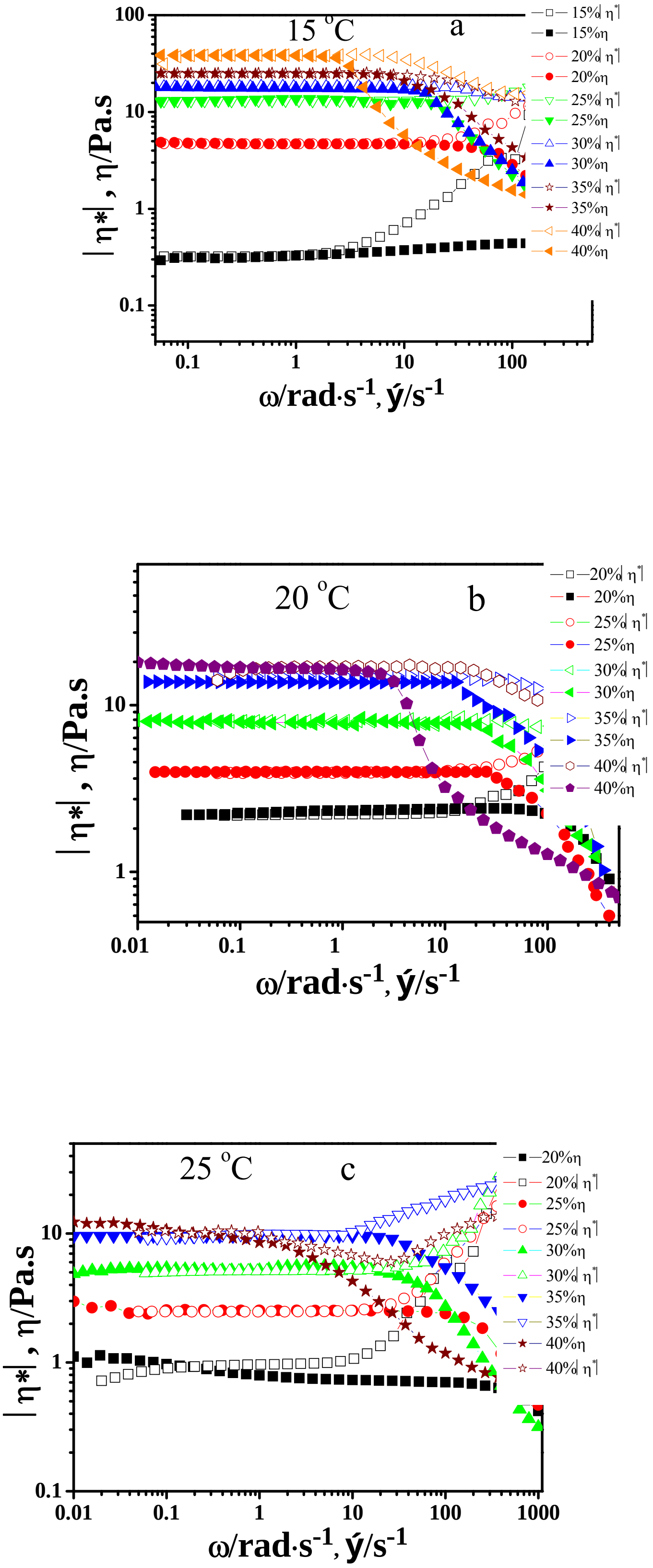

15 °C
a
|η*|, η/Pa.s
ω/rad·s-1, ý/s-1
15%|η*|
15%η
20%|η*|
20%η
25%|η*|
25%η
30%|η*|
30%η
35%|η*|
35%η
40%|η*|
40%η
20 °C
b
25 °C
c

Fig. 10

8. Schematic diagrams of the hydrogen bonds between micelles and the network structure

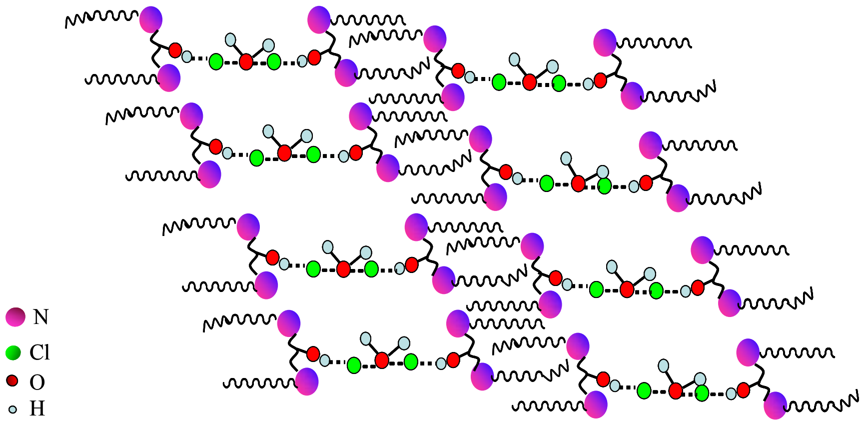


Fig. 11

9. Plot of shear stress (σ) vs. shear rate (ý) for different contents of 12-3(OH)-12(2Cl)(wt%) solutions at 15 °C(a), 20 °C (b) and 25 °C(c), respectively

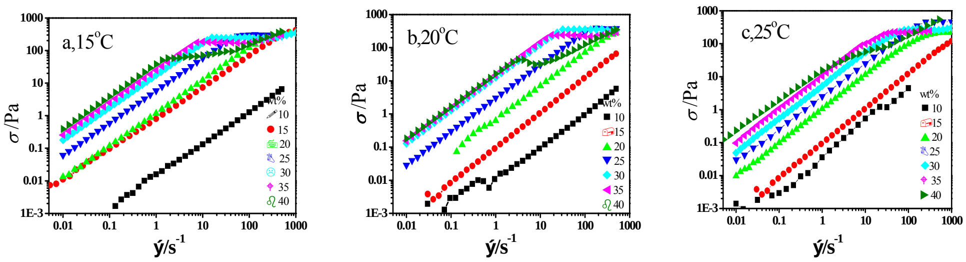


Fig.12

10. Photograph of the sample containing 30wt% 12-3(OH)-12(2Cl) at the end of the experiment

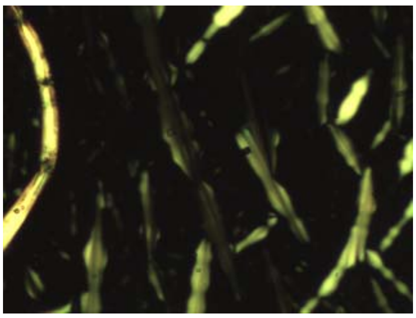


Fig. 13

11. Tables

Table 1 Crystallographic parameters of $R_{12\text{-}16}$-3(OH)- $R_{12\text{-}16}$- (2Cl) and $R_{14\text{-}16}$--3(OH)- $R_{14\text{-}16}$- (2Br)

Formula	$C_{31}H_{70}Cl_2N_2O_2$	$C_{35}H_{78}Cl_2N_2O_2$	$C_{39}H_{86}Cl_2N_2O_2$	Formula	$C_{35}H_{78}Br_2N_2O_3$	$C_{39}H_{88}Br_2N_2O_3$
Formula wt	573.79	629.89	686.00	Formula wt	736.80	792.93
Cryst syst	Monoclinic	Monoclinic	Monoclinic	Cryst syst	Orthorhombic	Orthorhombic
Space group	$P2_1/c$	$P2_1/c$	$P2_1/c$	Space group	Pbca	Pbca
a. Å	22.999(3)	25.402(3)	27.977(3)	*a*. Å	8.8000(9)	8.7630(7)
b. Å	9.6368(12)	9.5648(8)	9.5824(9)	*b*. Å	16.8741(18)	16.8491(15)
c. Å	17.2702(16)	17.1691(15)	17.1634(15)	*c*. Å	56.210(4)	61.244(4) A
α. °	90.00	90.00	90.00	α. °	90.00	90.00
β. °	100.665(2)	101.553(2)	102.438(2)	β. °	90.00	90.00
γ. °	90.00	90.00	90.00	γ. °	90.00	90.00
V. Å^3	3761.5(7)	4087.0(6)	4493.3(7)	V. Å^3	8346.8(13)	9042.6(12)
Z	4	4	4	Z	8	8
$D_{calc.}$ (g cm^{-3})	1.013	1.024	1.014	$D_{calc.}$ (g cm^{-3})	1.166	1.165
F(000)	1280	1408	1536	F(000)	3152	3440
M(Mo $K\alpha$) (mm^{-1})	0.198	0.187	0.175	M(Mo $K\alpha$) (mm^{-1})	1.973	1.826
Theta range	1.80-25.02	1.64-25.02	1.49-25.02	Theta range	2.43 -25.02	2.42 - 25.02
Reflections measured	18430	20837	21982	Reflections measured	39506	42522
Unique reflections	6635	7151	7853	Unique reflections	7353	7976
R(int)	0.0592	0.1463	0.1112	R(int)	0.1324	0.1451
GOF	1.000	0.999	0.999	GOF	1.169	1.078
Final R_1 [I>2σ(I)]	0.0591	0.0758	0.0838	Final R_1 [I>2σ(I)]	0.1202	0.1405
Final wR_2 [I>2σ(I)]	0.1326	0.1002	0.1673	Final wR_2 [I>2σ(I)]	0.2151	0.2799

Table 2 Flow activation energy of 12-3(OH)-12(2Cl) at different concentrations

12-3(OH)-12(2Cl)wt%	15	20	25	30	35	40
E_a/kJ·mol^{-1}	100.05	58.55	54.26	38.24	32.01	36.74

Table 3 ω^c date of 12-3(OH)-12(2Cl) at different temperatures

12-3(OH)-12(2Cl) wt%	15	20	25	30	35	40
15°C	1.767	14.017	17.55	16.05	7.811	2.476
20 °C	1.232	16.328	24.89	21.02	12.69	2.484
25 °C		0.269	18.263	24.166	9.841	1.928