

Supporting Information

The effect of hydroxyl on the phase behavior of quaternary ammonium gemini surfactant

Xuepeng Wu, Caili Dai,* Sisi Fang, Hao Li, Yining Wu, Xin Sun, Mingwei Zhao†

*School of Petroleum Engineering, State Key Laboratory of Heavy Oil Processing,
China University of Petroleum (East China), Qingdao, Shandong, 266580, China*

* **Caili Dai:** Fax: +86-532-86981161; Tel: +86-532-86981183;
Email: daicl@upc.edu.cn

† **Mingwei Zhao:** Fax: +86-532-86981161; Tel: +86-532-86981183;
Email: zhaomingwei@upc.edu.cn

Experiment section

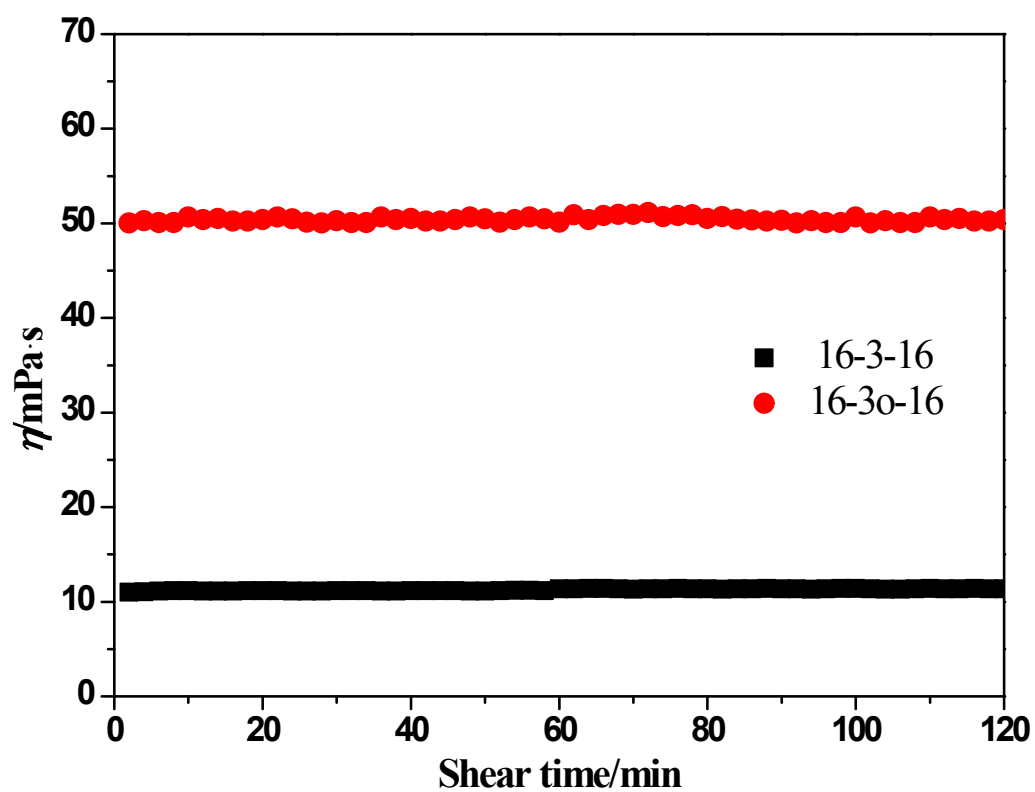


Fig. S1 The shear viscosity of 16-3-16 and 16-3OH-16 as a function of shear time at 170 s^{-1} and $70 \text{ }^\circ\text{C}$.

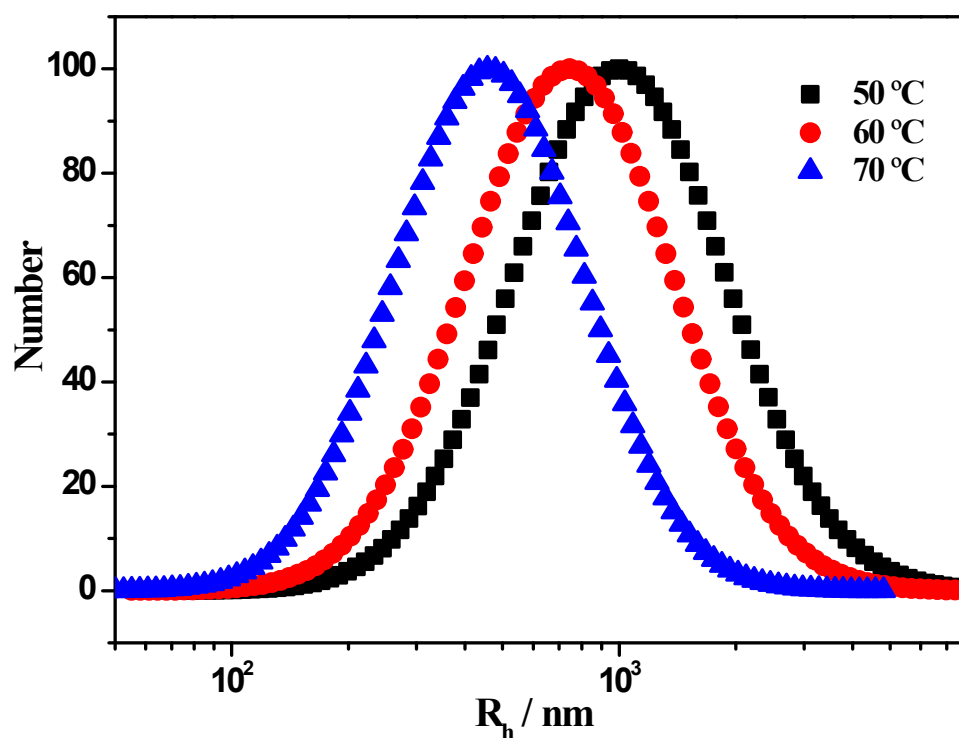


Fig. S2 Apparent hydrodynamic diameter distribution of 50 mM 16-3OH-16 at different temperatures.

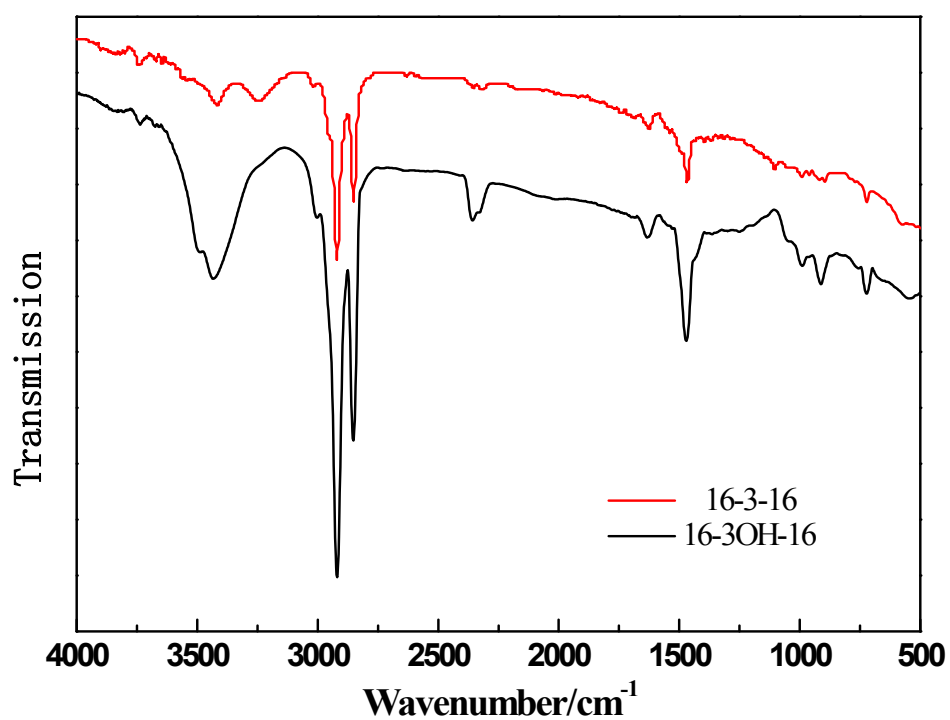


Fig. S3 FTIR spectra for samples of 16-3-16 and 16-3OH-16 in dry solid state (KBr disks method).

Simulation section

Table S1 Interaction energy & contributors

Systems	Energy, kcal/mol		
	Interaction energy	vdW	Electrostatic
16-3-16	-424.953	-15.419	-408.652
16-3OH-16	-438.036	-13.673	-423.513

Natural bond orbitals calculations were performed using NBO program as implemented in the Gaussian09 package at the B3LYP method and 6-31G basis set in order to study second-order interactions.

Table S2 Selected natural atomic charges and natural electron configuration for the
16-3-16

Atom	Net charge	Electron configuration
N1-117	-0.14826	[core]2S(0.63)2p(2.01)
N2-64	-0.14905	[core]2S(0.63)2p(2.01)
C1-65	-0.13498	[core]2S(0.52)2p(1.61)3p(0.01)
C2-53	-0.25633	[core]2S(0.52)2p(1.73)
C3-50	-0.13474	[core]2S(0.52)2p(1.61)3p(0.01)

Table S3 Selected natural atomic charges and natural electron configuration for the
16-3OH-16

Atom	Net charge	Electron configuration
N1-116	-0.14867	[core]2S(0.63)2p(2.01)
N2-63	-0.14951	[core]2S(0.63)2p(2.02)
C1-64	-0.14944	[core]2S(0.52)2p(1.62)3p(0.01)
C2-53	0.01876	[core]2S(0.48)2p(1.50)3p(0.01)
C3-50	-0.14848	[core]2S(0.52)2p(1.63)3p(0.01)
O1-125	-0.37505	[core]2S(0.85)2p(2.52)

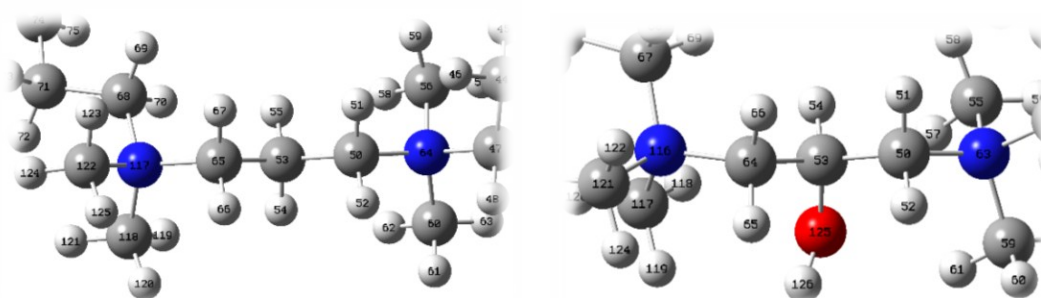


Fig. 4S Atom label in the simulation structural of 16-3-16 (left) and 16-3OH-16
(right).

Table S4 Second order perturbation theory analysis of Fock matrix in NBO basis
corresponding to the intramolecular bonds of the 16-3OH-16.

Donor	Acceptor	E_h (kcal/mol)	E (a.u.)	F (a.u.)
LP O125	BD* C53-C64	2.03	0.63	0.045
	BD*C59-H61	1.06	0.79	0.037
	BD*C50 - C53	3.72	0.63	0.061

E_h means energy of hyperconjugative interactions (stabilization energy in KJ/mol)

E (a.u.) means energy difference between donor and acceptor i and j NBO orbitals

F (a.u.) is the Fock matrix elements between i and j NBO orbitals.

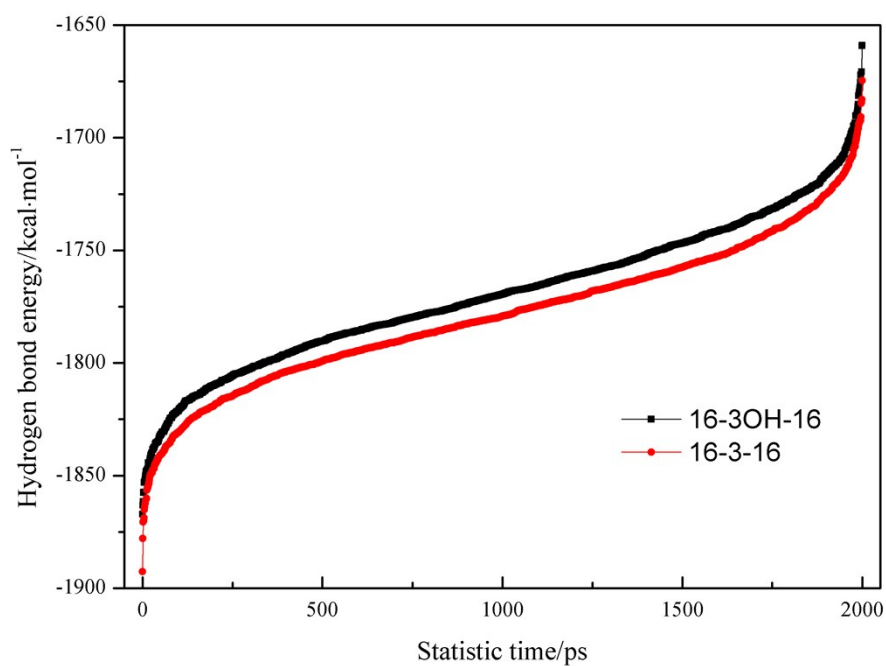


Fig. 5S The average hydrogen bond energy of two system over the entire stimulate
time.

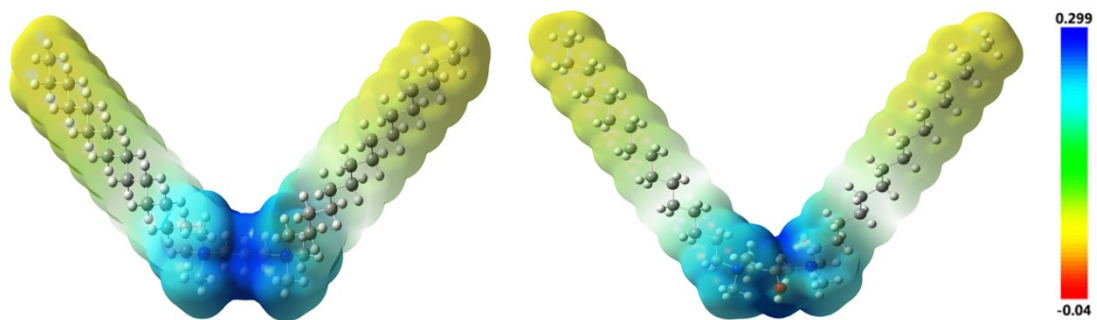


Fig. 6S Electrostatic potentials, in hartrees, at the 0.001 e/bohr^3 isodensity surfaces of 16-3-16 and 16-3OH-16 counterions in water medium.

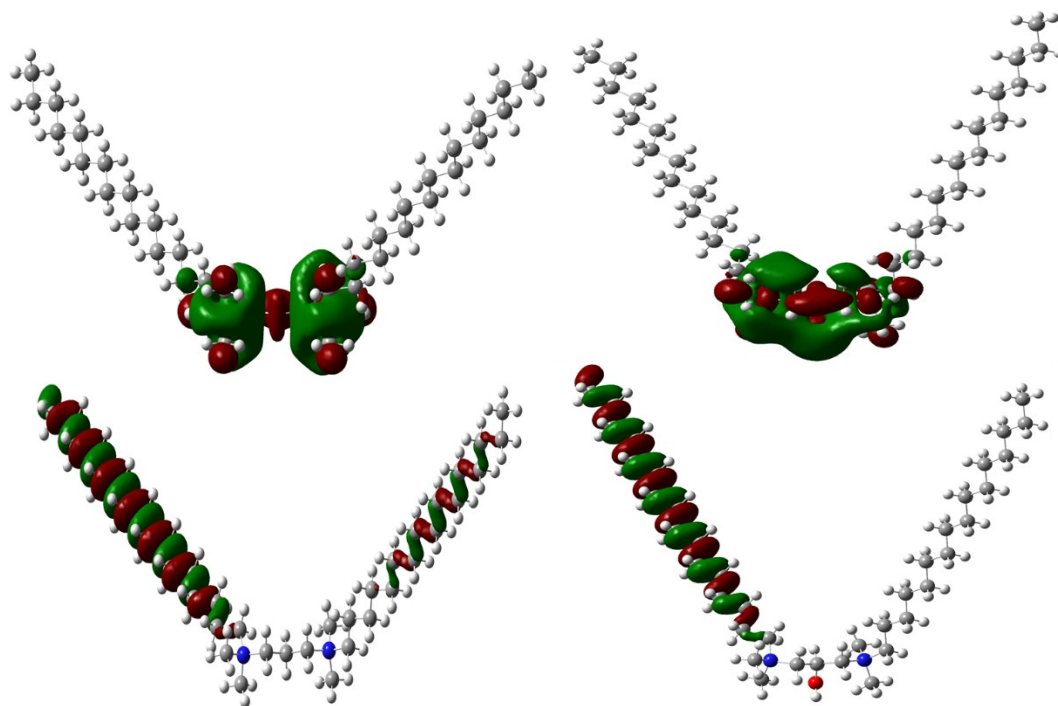


Fig. 7S The optimized configurations of 16-3-16 and 16-3OH-16 HOMO-LUMO for the respective compounds in water medium.