

## **Supporting Information**

Supplemental information to the manuscript:

### **Aggregation Behavior of Nitrophenoxy-tailed Quaternary Ammonium Surfactants**

Xu Huang, Yuchun Han, Yingxiong Wang, and Yilin Wang<sup>\*</sup>

*Key Laboratory of Colloid and Interface Science, Institute of Chemistry, Chinese Academy of Sciences, Beijing 100080, People's Republic of China*

The supporting information provides additional experimental results. These results are complementary and do not present any novel finding or facts exceeding the principal information of the paper. Nevertheless, the results obtained for an extended experimental range may be of interest for some readers. Moreover, they can be taken as further justification of the discussion and conclusions.

**Table S1. The observed  $^1\text{H}$  Chemical Shifts Assignments (in ppm) of N10TAB at different concentrations**

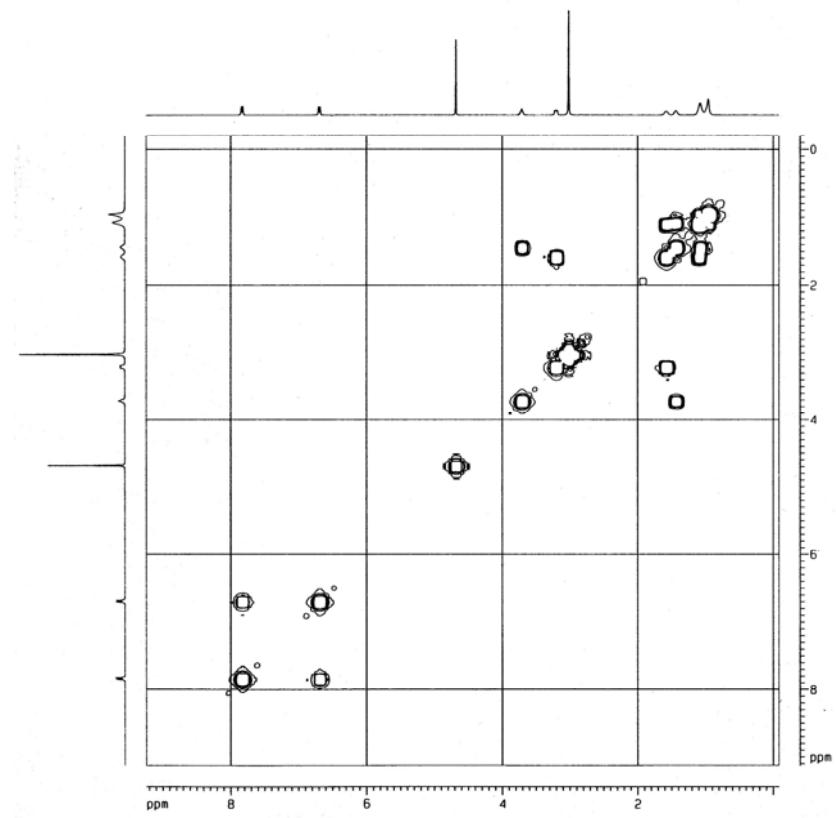
concentration (mM)	proton				
	H <sub>a</sub>	H <sub>b</sub>	H <sub>c</sub>	H <sub>g</sub>	H <sub>h</sub>
1.0	8.119	6.972	4.067	3.146 <sup>a</sup>	2.945
	8.095	6.949	4.051 4.034		
1.5	8.120	6.972	4.067	3.148 <sup>a</sup>	2.947
	8.096	6.949	4.051 4.035		
2.0	8.120	6.972	4.067	3.148 <sup>a</sup>	2.948
	8.096	6.949	4.051 4.034		
3.0	8.119	6.972	4.067	3.149 <sup>a</sup>	2.948
	8.095	6.949	4.051 4.035		
4.0	8.115	6.969	4.063	3.148 <sup>a</sup>	2.948
	8.093	6.946	4.047 4.031		
5.0	8.112	6.965	4.060	3.148 <sup>a</sup>	2.948
	8.089	6.942	4.044 4.028		
6.0	8.104	6.957	4.050	3.149 <sup>a</sup>	2.950
	8.081	6.934	4.034 4.018		
8.0	8.066	6.919	4.002	3.155 <sup>a</sup>	2.959
	8.044	9.897	3.987 3.971		
10.0	8.015	6.868	3.938	3.170 <sup>a</sup>	2.977
	7.933	6.845	3.922 3.906		
15.0	7.932	6.786	3.819 <sup>b</sup>	3.174 <sup>b</sup>	2.988
	7.910	6.764			
20	7.904	6.758	3.784 <sup>b</sup>	3.183 <sup>b</sup>	2.998
	7.882	6.736			
30.0	7.868	6.724	3.740 <sup>b</sup>	3.191 <sup>b</sup>	3.007
	7.846	6.702			
50.0	7.844	6.702	3.710 <sup>b</sup>	3.206 <sup>b</sup>	3.018
	7.822	6.679			

<sup>a</sup> middle value of the quintuple peak.    <sup>b</sup> broad peak.

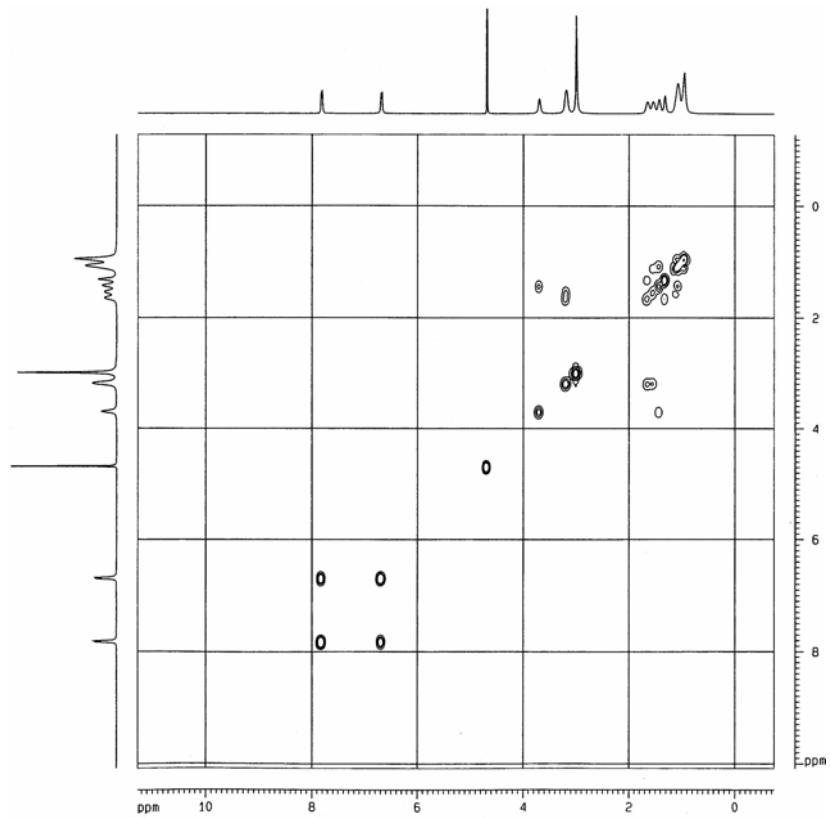
**Table S2. The observed  $^1\text{H}$  Chemical Shifts Assignments (in ppm) of N10-6-10N at different concentrations**

concentration (mM)	proton				
	$\text{H}_a$	$\text{H}_b$	$\text{H}_c$	$\text{H}_g (\text{H}_g')$	$\text{H}_h$
0.35	8.119	6.972	3.998		
	8.095	6.949	3.982 3.966	3.096 <sup>a</sup>	2.883
0.40	8.120	6.972	3.992		
	8.096	6.949	3.975 3.959	3.096 <sup>a</sup>	2.884
0.50	8.120	6.972	3.978		
	8.096	6.949	3.962 3.946	3.096 <sup>a</sup>	2.886
0.60	8.119	6.972	3.964		
	8.095	6.949	3.948 3.933	3.097 <sup>a</sup>	2.892
0.80	8.115	6.969	3.911		
	8.093	6.946	3.899 3.885	3.098 <sup>a</sup>	2.894
1.0	8.112	6.965			
	8.089	6.942	3.869 <sup>b</sup>	3.100 <sup>a</sup>	2.898
1.5	8.104	6.957			
	8.081	6.934	3.792 <sup>b</sup>	3.104 <sup>b</sup>	2.916
2.0	8.066	6.919			
	8.044	9.897	3.764 <sup>b</sup>	3.107 <sup>b</sup>	2.923
3.0	8.015	6.868			
	7.933	6.845	3.734 <sup>b</sup>	3.114 <sup>b</sup>	2.933
5.0	7.932	6.786			
	7.910	6.764	3.697 <sup>b</sup>	3.141 <sup>b</sup>	2.956
8.0	7.904	6.758			
	7.882	6.736	3.689 <sup>b</sup>	3.148 <sup>b</sup>	2.963
12.0	7.868	6.724			
	7.846	6.702	3.684 <sup>b</sup>	3.156 <sup>b</sup>	2.969
20.0	7.844	6.702			
	7.822	6.679	3.674 <sup>b</sup>	3.168 <sup>b</sup>	2.979

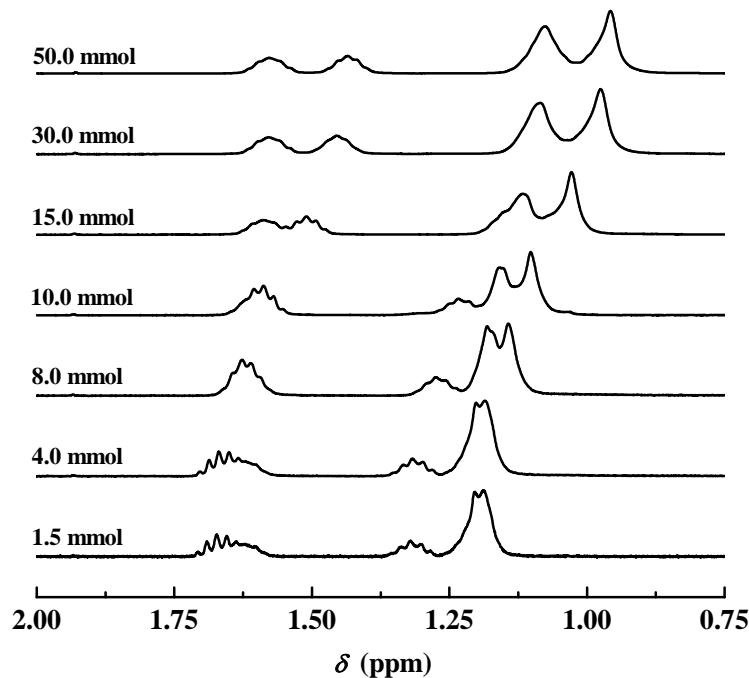
<sup>a</sup> middle value of the quintuple peak.    <sup>b</sup> broad peak.



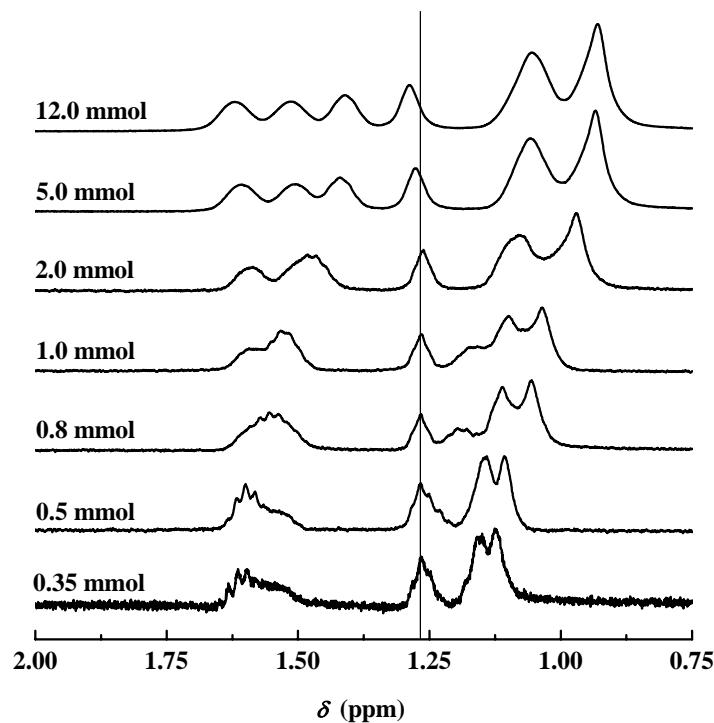
**Figure S1.** COSY spectrum of 50.0 mM N10TAB in  $\text{D}_2\text{O}$ .



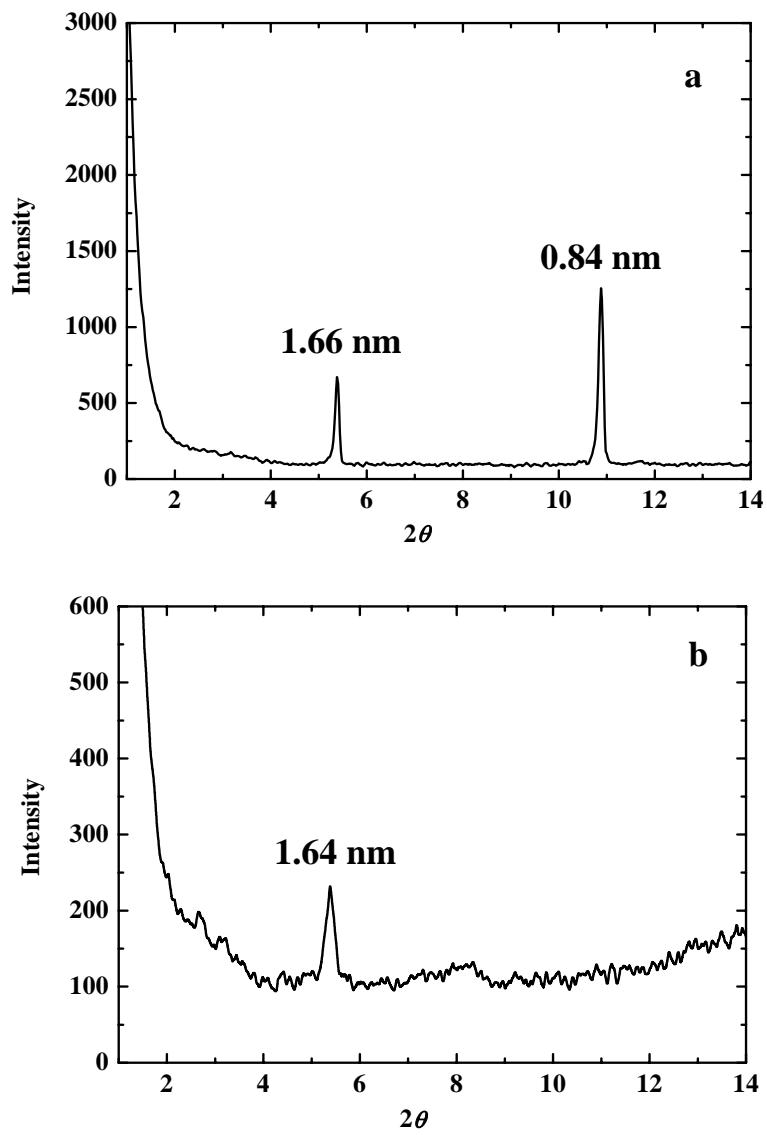
**Figure S2.** COSY spectrum of 20.0 mM N10-6-10N in  $\text{D}_2\text{O}$ .



**Figure S3.** Expansion of the chemical shifts between 2.00 and 0.75 ppm in  $^1\text{H}$ -NMR of N10TAB in  $\text{D}_2\text{O}$  at different concentrations.



**Figure S4.** Expansion of the chemical shifts between 2.00 and 0.75 ppm in  $^1\text{H}$ -NMR of N10-6-10N in  $\text{D}_2\text{O}$  at different concentrations. The vertical line denotes the downfield shifts of  $\text{H}_c$  with the increase of concentration.



**Figure S5.** XRD data of (a) N10TAB and (b) N10-6-10N.