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Sphere-to-rod transitions of nonionic surfactant micelles in aqueous solution modeled by molecular dynamics simulations

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C12E5_CG.itp

```
[moleculetype]
; name exclusions
EO5      1
```

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[atoms]
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3      SNa      1      EO5      O1      3      0.000
4      SNa      1      EO5      O1      4      0.000
5      SNa      1      EO5      O1      5      0.000
6      SNa      1      EO5      O1      6      0.000
7      C1       1      EO5      C1      7      0.000
8      C1       1      EO5      C2      8      0.000
9      C1       1      EO5      C3      9      0.000
```

```
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6      7      1      0.370 1250
7      8      1      0.470 1250
8      9      1      0.470 1250
```

```
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;backbonebackbonebackbone angles
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3      4      5      1      130.00      50
4      5      6      1      130.00      50
5      6      7      2      120.00      25
6      7      8      2      180.00      25
7      8      9      2      180.00      25
```

```
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1      2      3      4      1      180.00      1.96      1
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1      2      3      4      1      0           0.33      3
1      2      3      4      1      0           0.12      4
2      3      4      5      1      180.00      1.96      1
2      3      4      5      1      0           0.18      2
2      3      4      5      1      0           0.33      3
2      3      4      5      1      0           0.12      4
3      4      5      6      1      180.00      1.96      1
3      4      5      6      1      0           0.18      2
3      4      5      6      1      0           0.33      3
3      4      5      6      1      0           0.12      4
```

C12E5_AA.itp

```
[ moleculetype ]
; Name          nrexcl
Other           3
```

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chargeB   massB
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  2      CT    1    CE5    C2     2     -0.18      12.01  ; qtot -0.36
  3      CT    1    CE5    C3     3     -0.18      12.01  ; qtot -0.54
  4      CT    1    CE5    C4     4     -0.18      12.01  ; qtot -0.72
  5      CT    1    CE5    C5     5     -0.18      12.01  ; qtot -0.9
  6      CT    1    CE5    C6     6     -0.18      12.01  ; qtot -1.08
  7      CT    1    CE5    C7     7     -0.18      12.01  ; qtot -1.26
  8      CT    1    CE5    C8     8     -0.18      12.01  ; qtot -1.44
  9      CT    1    CE5    C9     9      0.27      12.01  ; qtot -1.17
 10     OS    1    CE5    O1    10     -0.41       16  ; qtot -1.58
 11     CT    1    CE5    CA    10     0.079     12.01  ; qtot -1.501
 12     CT    1    CE5    CB    10     0.107     12.01  ; qtot -1.394
 13     OS    1    CE5    O2    11     -0.41       16  ; qtot -1.804
 14     CT    1    CE5    CC    11     0.079     12.01  ; qtot -1.725
 15     CT    1    CE5    CD    11     0.107     12.01  ; qtot -1.618
 16     OS    1    CE5    O3    12     -0.41       16  ; qtot -2.028
 17     CT    1    CE5    CE    12     0.079     12.01  ; qtot -1.949
 18     CT    1    CE5    CF    12     0.107     12.01  ; qtot -1.842
 19     OS    1    CE5    O4    13    -0.609       16  ; qtot -2.451
 20     CT    1    CE5    CG    14     -0.18      12.01  ; qtot -2.631
 21     CT    1    CE5    CH    15     -0.18      12.01  ; qtot -2.811
 22     CT    1    CE5    CI    16     -0.27      12.01  ; qtot -3.081
 23     HC    1    CE5    H1    17      0.09      1.008  ; qtot -2.991
 24     HC    1    CE5    H2    17      0.09      1.008  ; qtot -2.901
 25     HC    1    CE5    H3    18      0.09      1.008  ; qtot -2.811
 26     HC    1    CE5    H4    18      0.09      1.008  ; qtot -2.721
 27     HC    1    CE5    H5    19      0.09      1.008  ; qtot -2.631
 28     HC    1    CE5    H6    19      0.09      1.008  ; qtot -2.541
 29     HC    1    CE5    H7    20      0.09      1.008  ; qtot -2.451
 30     HC    1    CE5    H8    20      0.09      1.008  ; qtot -2.361
 31     HC    1    CE5    H9    21      0.09      1.008  ; qtot -2.271
 32     HC    1    CE5    HA    21      0.09      1.008  ; qtot -2.181
 33     HC    1    CE5    HB    22      0.09      1.008  ; qtot -2.091
 34     HC    1    CE5    HC    22      0.09      1.008  ; qtot -2.001
 35     HC    1    CE5    HD    23      0.09      1.008  ; qtot -1.911
 36     HC    1    CE5    HE    23      0.09      1.008  ; qtot -1.821
 37     HC    1    CE5    HF    24      0.09      1.008  ; qtot -1.731
 38     HC    1    CE5    HG    24      0.09      1.008  ; qtot -1.641
 39     H1    1    CE5    HH    25    -0.015      1.008  ; qtot -1.656
 40     H1    1    CE5    HI    25    -0.015      1.008  ; qtot -1.671
 41     H1    1    CE5    HJ    26      0.06      1.008  ; qtot -1.611
 42     H1    1    CE5    HK    26      0.06      1.008  ; qtot -1.551
 43     H1    1    CE5    HL    26     0.052      1.008  ; qtot -1.499
 44     H1    1    CE5    HM    26     0.052      1.008  ; qtot -1.447
 45     H1    1    CE5    HN    27      0.06      1.008  ; qtot -1.387
 46     H1    1    CE5    HO    27      0.06      1.008  ; qtot -1.327
 47     H1    1    CE5    HP    27     0.052      1.008  ; qtot -1.275
 48     H1    1    CE5    HQ    27     0.052      1.008  ; qtot -1.223
 49     H1    1    CE5    HR    28      0.06      1.008  ; qtot -1.163
 50     H1    1    CE5    HS    28      0.06      1.008  ; qtot -1.103
 51     H1    1    CE5    HT    28     0.052      1.008  ; qtot -1.051
 52     H1    1    CE5    HU    28     0.052      1.008  ; qtot -0.999
 53     HO    1    CE5    HV    29     0.369      1.008  ; qtot -0.63
 54     HC    1    CE5    HW    30      0.09      1.008  ; qtot -0.54
 55     HC    1    CE5    HX    30      0.09      1.008  ; qtot -0.45
 56     HC    1    CE5    HY    31      0.09      1.008  ; qtot -0.36
 57     HC    1    CE5    HZ    31      0.09      1.008  ; qtot -0.27
 58     HC    1    CE5    H0    32      0.09      1.008  ; qtot -0.18
```

59	HC	1	CE5	H10	32	0.09	1.008	; qtot -0.09
60	HC	1	CE5	H11	32	0.09	1.008	; qtot 0
61	OS	1	CE5	O5	33	-0.41	16	; qtot -0.41
62	CT	1	CE5	CJ	33	0.079	12.01	; qtot -0.331
63	CT	1	CE5	CK	33	0.107	12.01	; qtot -0.224
64	OS	1	CE5	O6	34	-0.41	16	; qtot -0.634
65	CT	1	CE5	CL	34	0.079	12.01	; qtot -0.555
66	CT	1	CE5	CM	34	0.107	12.01	; qtot -0.448
67	H1	1	CE5	H12	35	0.06	1.008	; qtot -0.388
68	H1	1	CE5	H13	35	0.06	1.008	; qtot -0.328
69	H1	1	CE5	H14	35	0.052	1.008	; qtot -0.276
70	H1	1	CE5	H15	35	0.052	1.008	; qtot -0.224
71	H1	1	CE5	H16	36	0.06	1.008	; qtot -0.164
72	H1	1	CE5	H17	36	0.06	1.008	; qtot -0.104
73	H1	1	CE5	H18	36	0.052	1.008	; qtot -0.052
74	H1	1	CE5	H19	36	0.052	1.008	; qtot 0

[bonds]

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18	52	1
18	61	1
19	53	1

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65	71	1
65	72	1
66	73	1
66	74	1

[pairs]

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1	28	1	
1	56	1	
1	57	1	
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2	29	1	
2	30	1	
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9	35	1	

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68	70	1
71	73	1
71	74	1
72	73	1
72	74	1

[angles]

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19	66	74	1

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65	66	74	1
73	66	74	1

[dihedrals]

;	ai	aj	ak	al	funct
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11	12	13	14	9
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12	13	14	15	9
12	13	14	45	9
12	13	14	46	9
13	14	15	16	9
13	14	15	47	9
13	14	15	48	9
45	14	15	16	9
45	14	15	47	9
45	14	15	48	9
46	14	15	16	9
46	14	15	47	9
46	14	15	48	9
14	15	16	17	9
47	15	16	17	9
48	15	16	17	9
15	16	17	18	9
15	16	17	49	9
15	16	17	50	9
16	17	18	51	9
16	17	18	52	9
16	17	18	61	9
49	17	18	51	9
49	17	18	52	9
49	17	18	61	9
50	17	18	51	9
50	17	18	52	9
50	17	18	61	9
17	18	61	62	9
51	18	61	62	9
52	18	61	62	9
53	19	66	65	9

53	19	66	73	9
53	19	66	74	9
1	20	21	22	9
1	20	21	56	9
1	20	21	57	9
54	20	21	22	9
54	20	21	56	9
54	20	21	57	9
55	20	21	22	9
55	20	21	56	9
55	20	21	57	9
20	21	22	58	9
20	21	22	59	9
20	21	22	60	9
56	21	22	58	9
56	21	22	59	9
56	21	22	60	9
57	21	22	58	9
57	21	22	59	9
57	21	22	60	9
18	61	62	63	9
18	61	62	67	9
18	61	62	68	9
61	62	63	64	9
61	62	63	69	9
61	62	63	70	9
67	62	63	64	9
67	62	63	69	9
67	62	63	70	9
68	62	63	64	9
68	62	63	69	9
68	62	63	70	9
62	63	64	65	9
69	63	64	65	9
70	63	64	65	9
63	64	65	66	9
63	64	65	71	9
63	64	65	72	9
64	65	66	19	9
64	65	66	73	9
64	65	66	74	9
71	65	66	19	9
71	65	66	73	9
71	65	66	74	9
72	65	66	19	9
72	65	66	73	9
72	65	66	74	9

Figure S1. RDF of the distance between tail-tail COM in system 1

Figure S2. Evolution of cluster size distribution (A,B) and cluster number (C,D) for C_{12}E_5 in diluted system with 360 surfactants at $\chi=0.19$ (A,C) and concentrated system with 780 surfactants at $\chi=0.33$ (B,D)