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Published in:
Langmuir

DOI:
[10.1021/la203055t](https://doi.org/10.1021/la203055t)

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Document Version
Publisher's PDF, also known as Version of record

Publication date:
2011

[Link to publication in University of Groningen/UMCG research database](#)

Citation for published version (APA):

Velinova, M., Sengupta, D., Tadjer, A. V., & Marrink, S.-J. (2011). Sphere-to-Rod Transitions of Nonionic Surfactant Micelles in Aqueous Solution Modeled by Molecular Dynamics Simulations. *Langmuir*, 27(23), 14071-14077. <https://doi.org/10.1021/la203055t>

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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
```

```
[atoms]
1      SP2  1      EO5  OH   1      0.000
2      SNa  1      EO5  O1   2      0.000
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
```

```
[ bonds ]
; backbonebackbone bonds
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2      3      1      0.330 17000
3      4      1      0.330 17000
4      5      1      0.330 17000
5      6      1      0.330 17000
6      7      1      0.370 1250
7      8      1      0.470 1250
8      9      1      0.470 1250
```

```
[angles]
;backbonebackbonebackbone angles
1      2      3      1      130.00    50
2      3      4      1      130.00    50
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
```

```
[dihedrals]
1      2      3      4      1      180.00    1.96    1
1      2      3      4      1      0          0.18    2
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

[atoms]

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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	HO	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	61	1
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20	54	1
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65	72	1
66	73	1
66	74	1

[pairs]

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65	70	1
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68	69	1
68	70	1
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71	74	1
72	73	1
72	74	1

[angles]

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	2	1	24	1
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64	65	71	1
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71	65	72	1
19	66	65	1
19	66	73	1
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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12	13	14	15	9
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50	17	18	52	9
50	17	18	61	9
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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
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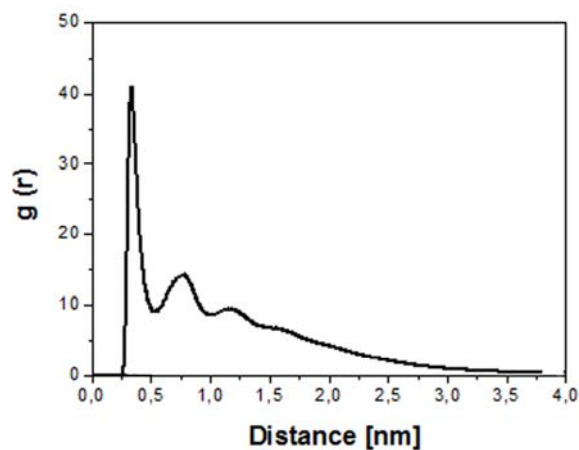


Figure S1. RDF of the distance between tail-tail COM in system 1

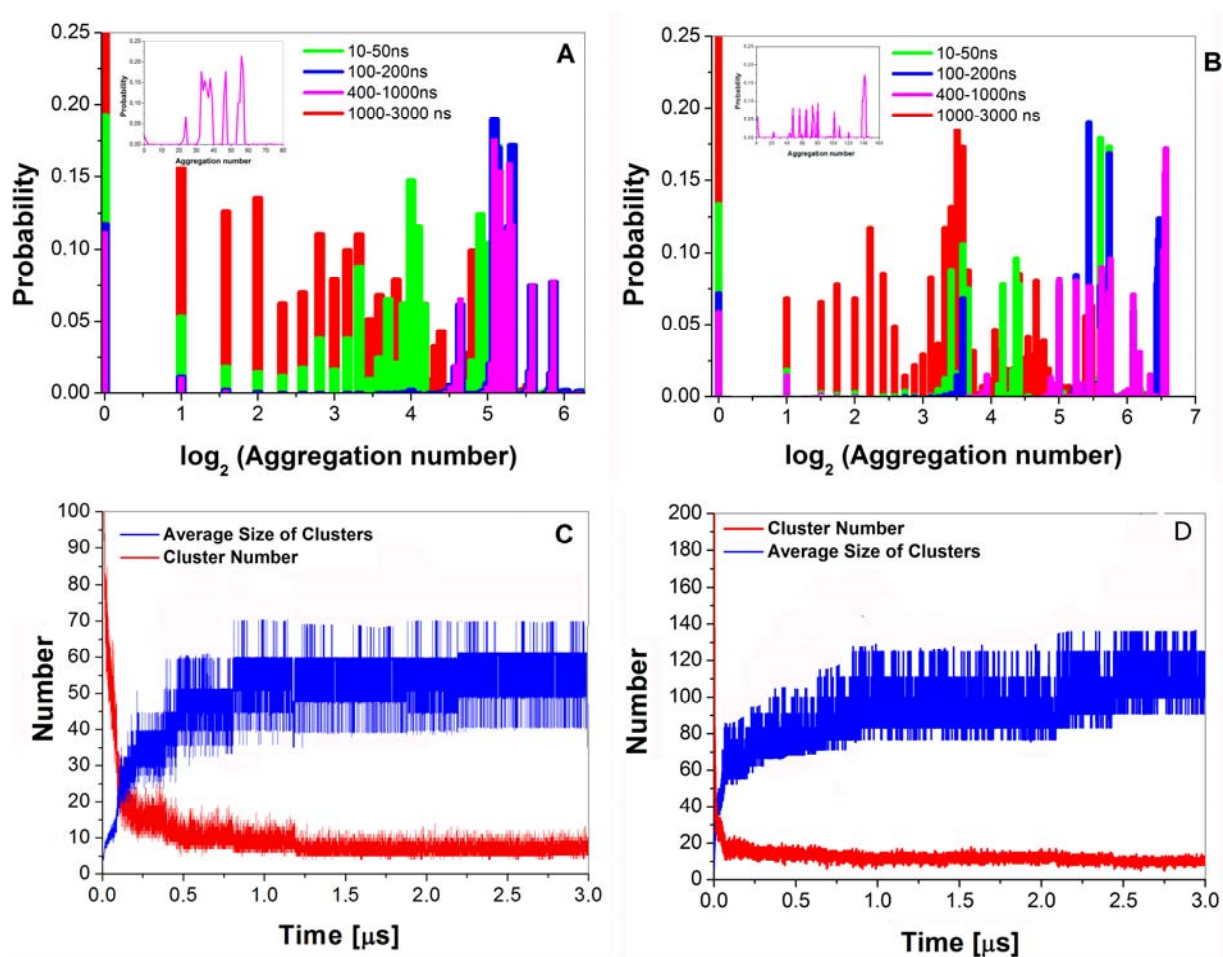


Figure S2. Evolution of cluster size distribution (A,B) and cluster number (C,D) for $C_{12}E_5$ in diluted system with 360 surfactants at $\chi=0.19$ (A,C) and concentrated system with 780 surfactants at $\chi=0.33$ (B,D)