Supporting Information

Counterion-Mediated Assembly of Fluorocarbon–Hydrocarbon Surfactant Mixtures at the Air-Liquid Interface: A Molecular Dynamics Study

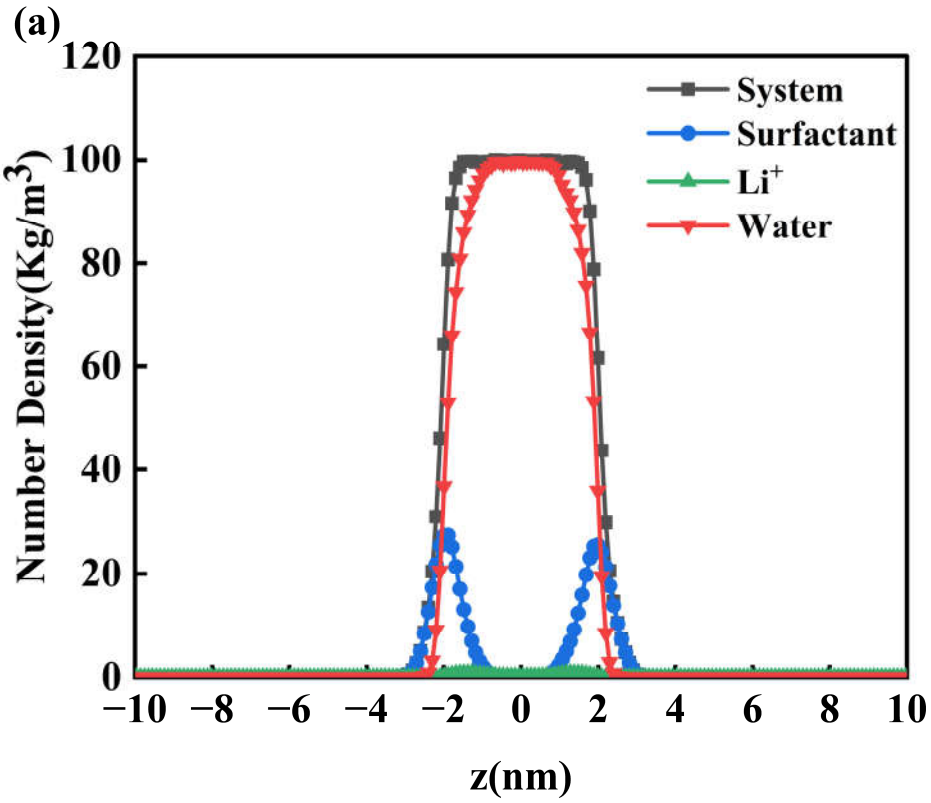
Xiaolong Quan,† Tong Tong,† Tao Li, Dawei Han, Baolong Cui, Jing Xiong, Zekai Cui, Hao Guo, Jinqing Jiao,* Yuechang Wei,*

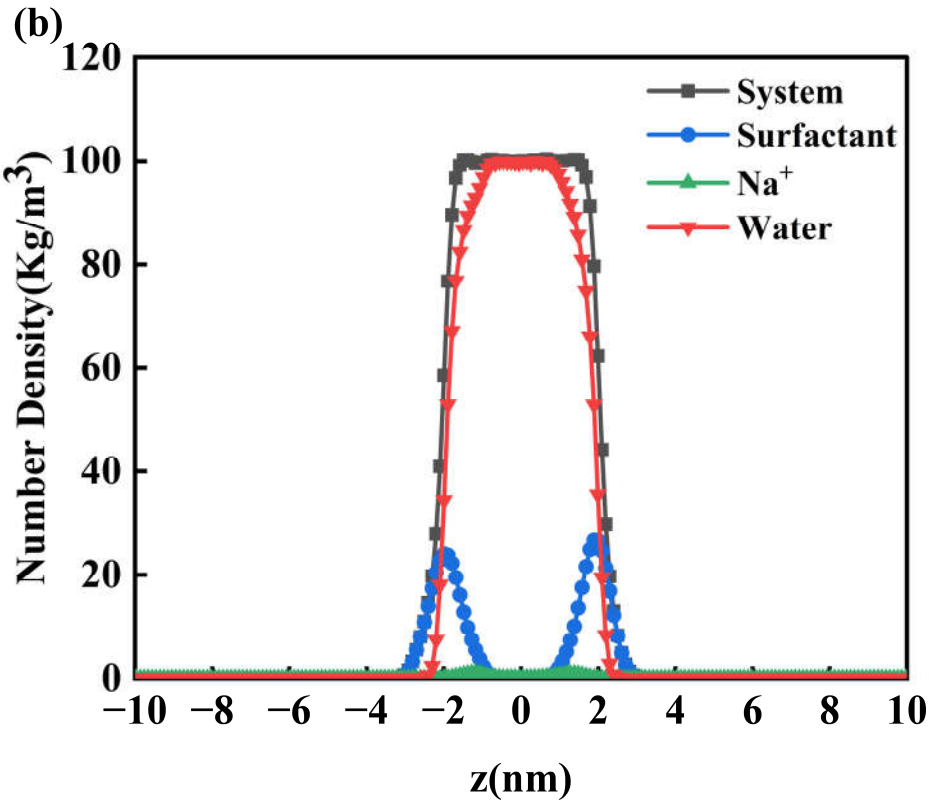
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1D-Density


(a)
120
100
80
60
40
20
0
Number Density(Kg/m3)
−10 −8 −6 −4 −2 0 2 4 6 8 10
z(nm)
System
Surfactant
Li+
Water


(b)
120
100
80
60
40
20
0
Number Density(Kg/m3)
−10 −8 −6 −4 −2 0 2 4 6 8 10
z(nm)
System
Surfactant
Na+
Water

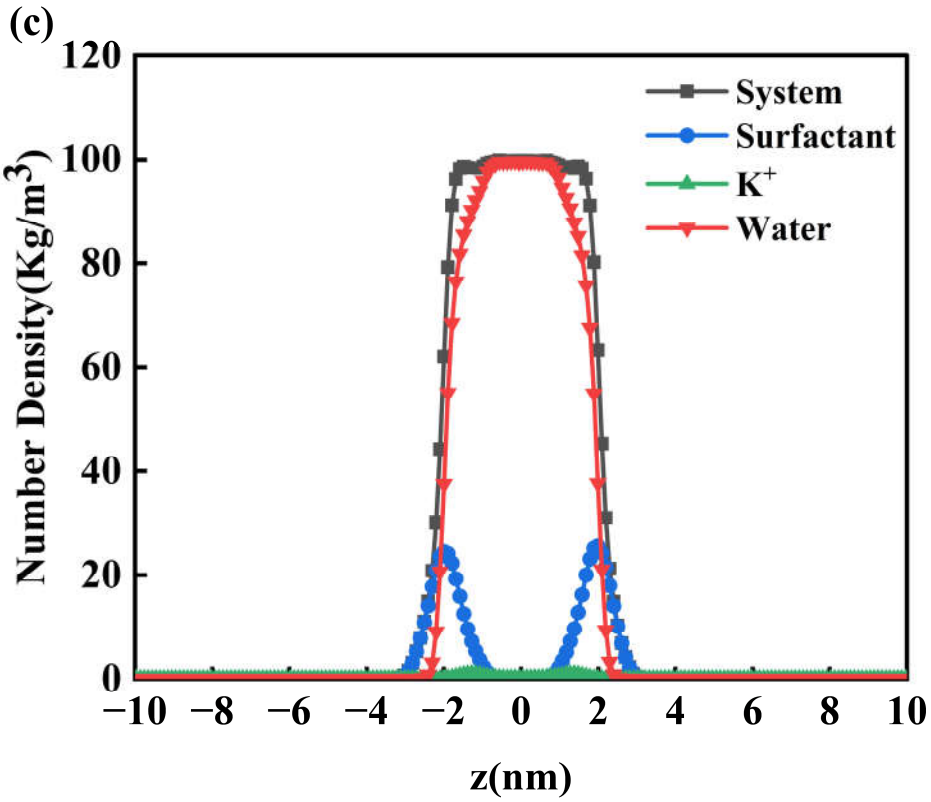


Figure S1. Z-axis Number Density Profiles of PFH_XA/SDS Mixed Surfactant Systems and Counterion Distributions: (a-c) PFH_XA/SDS Ratios of Li^+, Na^+, K^+.

model of the system

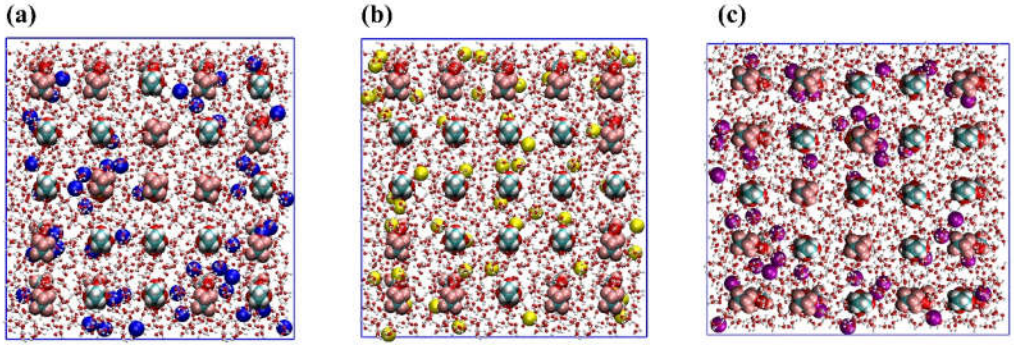


Figure S2. The top views initial model of the system: (a-c) PFH_XA/SDS Ratios of Li^+, Na^+, K^+.

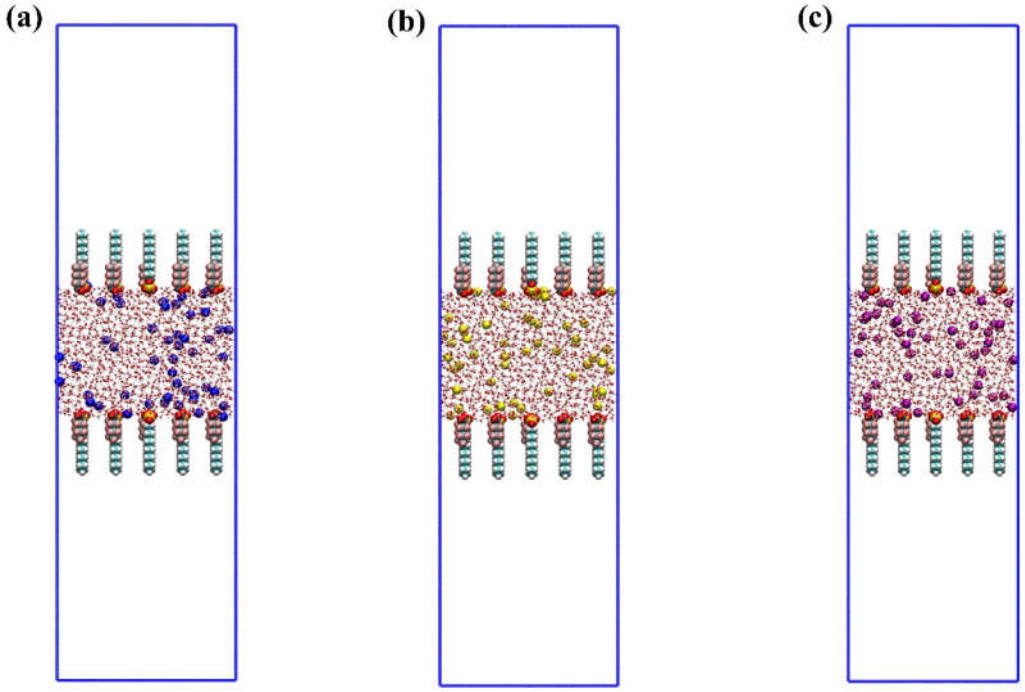


Figure S3. The front views initial model of the system: (a-c) PFH_XA/SDS Ratios of Li^+, Na^+, K^+.

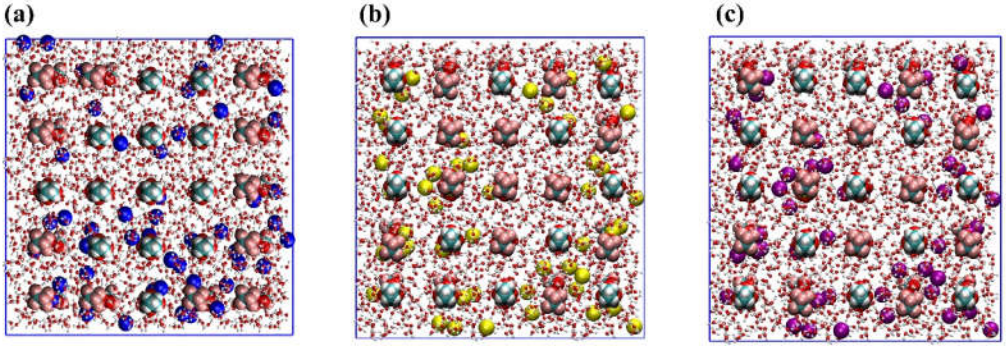


Figure S4. The top view initial model of the recreate system: (a-c) PFH_XA/SDS Ratios of Li^+, Na^+, K^+.

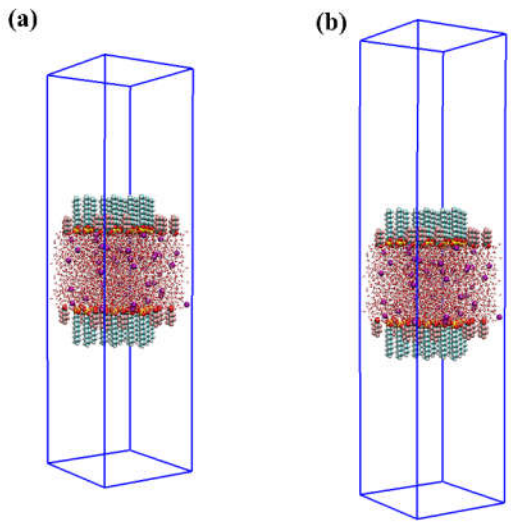


Figure S5. Initial System Model (Z-Axis Dimension of 20 nm) (a) and Enlarged System Model (Z-Axis Dimension of 25 nm) (b): PFH_XA/SDS Ratios of K^+.

RESP Maximum and minimum Distribution of Surfactant

Table S1 RESP Maximum Distribution of Surfactant PFH_XA Ions

maximum	kcal/mol	X(Å)	Y(Å)	Z(Å)
1	-90.441526	-3.457569	-1.666483	1.070191
2	-86.286182	-1.793424	-0.654316	3.157295
3	-72.065471	-1.147691	-0.974294	-1.656539
4	-57.150847	0.027469	0.524927	1.908423
5	-42.249386	1.377731	0.134922	-1.888691
6	-47.102882	2.358627	-2.07857	-0.782204
7	-41.131792	2.959724	2.088707	0.243272
8	-34.21389	3.305456	0.069359	1.768411
9	-35.182362	3.381485	1.343936	-1.341053
10	-27.706962	4.653997	-1.050172	-0.434795
11	-47.495968	5.437433	1.275275	0.357716

Table S2 RESP Minimum Distribution of Surfactant PFBS Ions

minimum	kcal/mol	X(Å)	Y(Å)	Z(Å)
1	-0.21163757	-5.758951	-132.80469	-5.355592
2	-0.2058297	-5.600911	-129.160196	-3.795364
3	-0.20509696	-5.580972	-128.700396	-2.732543
4	-0.08373824	-2.278633	-52.546585	3.805272

Table S3 RESP Maximum Distribution of Surfactant SDS Ions

maximum	kcal/mol	X(Å)	Y(Å)	Z(Å)
1	-0.02070436	-0.563394	-12.992193	-12.259596
2	-0.02294668	-0.624411	-14.399269	-10.564338
3	-0.02295046	-0.624514	-14.401644	-10.554064
4	-0.02685515	-0.730766	-16.851878	-9.20907
5	-0.02683965	-0.730344	-16.842151	-9.195839
6	-0.0295373	-0.803751	-18.534954	-8.120172
7	-0.02952745	-0.803483	-18.528768	-8.058189
8	-0.03268385	-0.889373	-20.509446	-6.725506
9	-0.03268674	-0.889452	-20.511259	-6.669089
10	-0.03630915	-0.988022	-22.784358	-5.613716
11	-0.03630029	-0.987781	-22.778796	-5.607688
12	-0.04070267	-1.107576	-25.541331	-4.303494
13	-0.04069849	-1.107462	-25.538708	-4.31776
14	-0.04568924	-1.243267	-28.670456	-3.124821
15	-0.04568969	-1.24328	-28.670734	-3.121588
16	-0.0519848	-1.414578	-32.620981	-1.879797
17	-0.05198176	-1.414496	-32.619077	-1.819737
18	-0.05928611	-1.613257	-37.202627	-0.768238
19	-0.05929369	-1.613463	-37.207387	-0.742234
20	-0.1821441	-4.956393	-114.297246	5.607892
21	-0.178387	-4.854157	-111.939628	6.662039
22	-0.18783521	-5.111256	-117.868471	8.098931
23	-0.18780016	-5.110302	-117.846476	8.043336
24	-0.15534	-4.22704	-97.4779	8.545812

Table S4 RESP Minimum Distribution of Surfactant SDS Ions

minimum	kcal/mol	X(Å)	Y(Å)	Z(Å)
1	-0.03445	-0.93735	-21.6158	-11.6191
2	-0.03451	-0.93919	-21.6582	-10.796
3	-0.03451	-0.9392	-21.6584	-10.7831
4	-0.20505	-5.5796	-128.669	5.929655
5	-0.20501	-5.5786	-128.646	5.894115
6	-0.19838	-5.39824	-124.486	7.06313
7	-0.1984	-5.39881	-124.5	7.028385
8	-0.19936	-5.42493	-125.102	7.467786
9	-0.19935	-5.42445	-125.091	7.472617
10	-0.20296	-5.5227	-127.357	8.386073
11	-0.20296916	-5.523072	-127.36518	8.460124

Detailed parameters of topology files

SDS.itp

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h1    1    1.007941    0.000000    A    2.471353E-01    6.568880E-02
os    8    15.999405    0.000000    A    3.000012E-01    7.112800E-01
s6    16    32.064787    0.000000    A    3.563595E-01    1.046000E+00
o    8    15.999405    0.000000    A    2.959922E-01    8.786400E-01

[ moleculetype ]
; name    nrexcl
SDS    3

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     2    c3    1    MOL    C2    2    0.11738414    12.010736
     3    hc    1    MOL    H3    3    0.06022224    1.007941
     4    hc    1    MOL    H4    4    0.06022224    1.007941
     5    hc    1    MOL    H5    5    0.06022224    1.007941
     6    c3    1    MOL    C6    6    -0.00987108    12.010736
     7    hc    1    MOL    H7    7    -0.01427893    1.007941
     8    hc    1    MOL    H8    8    -0.01427893    1.007941
     9    c3    1    MOL    C9    9    -0.03697414    12.010736
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12	hc	1	MOL	H12	12	-0.00056846
1.007941						
13	hc	1	MOL	H13	13	-0.00056846
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16	hc	1	MOL	H16	16	-0.01475950
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17	hc	1	MOL	H17	17	-0.01475950
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21	c3	1	MOL	C21	21	0.00843912
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22	hc	1	MOL	H22	22	0.00110041
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1.007941						
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28	hc	1	MOL	H28	28	-0.02786062
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29	hc	1	MOL	H29	29	-0.02786062
1.007941						
30	c3	1	MOL	C30	30	-0.09655935
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31	hc	1	MOL	H31	31	-0.00324552
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1.007941
     36        h1          1        MOL       H36          36     -0.02070795
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1.007941
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     39        s6          1        MOL       S39          39      1.11657032
32.064787
     40        o           1        MOL       O40          40     -0.59228433
15.999405
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DRIH method
     2         7          1          0.110016       3.072732E+05       ; C2-H7,
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     6         9          1          0.153943       2.617181E+05       ; C6-C9,
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C2-C1-H5, DRIH method
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C1-C2-H8, DRIH method
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C6-C2-H7, DRIH method
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C6-C2-H8, DRIH method
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H25-C21-C26, DRIH method
21 26 27 1 113.529 3.524159E+02 ;
C21-C26-C27, DRIH method
21 26 28 1 109.274 1.326522E+02 ;
C21-C26-H28, DRIH method
21 26 29 1 109.274 1.326572E+02 ;
C21-C26-H29, DRIH method
27 26 28 1 109.174 1.327108E+02 ;
C27-C26-H28, DRIH method
27 26 29 1 109.175 1.327111E+02 ;
C27-C26-H29, DRIH method
28 26 29 1 106.151 4.991992E+01 ;
H28-C26-H29, DRIH method
26 27 30 1 113.282 3.486095E+02 ;
C26-C27-C30, DRIH method

26 27 31 1 109.185 1.328595E+02 ;
C26-C27-H31, DRIH method
26 27 32 1 109.185 1.328620E+02 ;
C26-C27-H32, DRIH method
30 27 31 1 109.385 1.310722E+02 ;
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31 27 32 1 106.170 4.998243E+01 ;
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27 30 33 1 112.653 3.446953E+02 ;
C27-C30-C33, DRIH method
27 30 34 1 110.050 1.261131E+02 ;
C27-C30-H34, DRIH method
27 30 35 1 110.050 1.261134E+02 ;
C27-C30-H35, DRIH method
33 30 34 1 108.609 1.303667E+02 ;
C33-C30-H34, DRIH method
33 30 35 1 108.609 1.303686E+02 ;
C33-C30-H35, DRIH method
34 30 35 1 106.675 5.061107E+01 ;
H34-C30-H35, DRIH method
30 33 36 1 110.675 1.881884E+02 ;
C30-C33-H36, DRIH method
30 33 37 1 110.675 1.881844E+02 ;
C30-C33-H37, DRIH method
30 33 38 1 106.385 4.000860E+02 ;
C30-C33-O38, DRIH method
36 33 37 1 107.127 7.936205E+01 ;
H36-C33-H37, DRIH method
36 33 38 1 111.014 1.541018E+02 ;
H36-C33-O38, DRIH method
37 33 38 1 111.015 1.541019E+02 ;
H37-C33-O38, DRIH method
33 38 39 1 113.132 6.683723E+02 ;
C33-O38-S39, DRIH method
38 39 40 1 102.727 4.396403E+02 ;
O38-S39-O40, DRIH method
38 39 41 1 102.725 4.396708E+02 ;
O38-S39-O41, DRIH method
38 39 42 1 103.377 6.270696E+02 ;
O38-S39-O42, DRIH method
40 39 41 1 115.550 2.832937E+02 ;
O40-S39-O41, DRIH method

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    40          39          42          1          114.928          2.823754E+02          ;
O40-S39-O42, DRIH method
    41          39          42          1          114.929          2.823735E+02          ;
O41-S39-O42, DRIH method

[ angles ] ; bond-bond cross term
; atom_i   atom_j   atom_k   functype     r0_ij (nm)    r0_jk (nm)      k
(kJ/mol/nm^2)
      2          1          3          3          0.153727          0.109658
4.077426E+03          ; C2-C1-H3
      2          1          4          3          0.153727          0.109749
4.891827E+03          ; C2-C1-H4
      2          1          5          3          0.153727          0.109749
4.891841E+03          ; C2-C1-H5
      3          1          4          3          0.109658          0.109749
2.097844E+03          ; H3-C1-H4
      3          1          5          3          0.109658          0.109749
2.097817E+03          ; H3-C1-H5
      4          1          5          3          0.109749          0.109749
2.095536E+03          ; H4-C1-H5
      1          2          6          3          0.153727          0.153985
7.876479E+03          ; C1-C2-C6
      1          2          7          3          0.153727          0.110016
4.901173E+03          ; C1-C2-H7
      1          2          8          3          0.153727          0.110016
4.901093E+03          ; C1-C2-H8
      6          2          7          3          0.153985          0.110016
5.159592E+03          ; C6-C2-H7
      6          2          8          3          0.153985          0.110016
5.159629E+03          ; C6-C2-H8
      7          2          8          3          0.110016          0.110016
2.864910E+03          ; H7-C2-H8
      2          6          9          3          0.153985          0.153943
7.916531E+03          ; C2-C6-C9
      2          6         10          3          0.153985          0.110115
4.931684E+03          ; C2-C6-H10
      2          6         11          3          0.153985          0.110115
4.931614E+03          ; C2-C6-H11
      9          6         10          3          0.153943          0.110115
5.002771E+03          ; C9-C6-H10
      9          6         11          3          0.153943          0.110115
5.002311E+03          ; C9-C6-H11
     10          6         11          3          0.110115          0.110115
2.736213E+03          ; H10-C6-H11
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     6          9         12          3          0.153943       0.110108
4.975547E+03       ; C6-C9-H12
     6          9         13          3          0.153943       0.110108
4.975191E+03       ; C6-C9-H13
     6          9         14          3          0.153943       0.153961
7.928884E+03       ; C6-C9-C14
    12          9         13          3          0.110108       0.110108
2.738034E+03       ; H12-C9-H13
    12          9         14          3          0.110108       0.153961
5.017865E+03       ; H12-C9-C14
    13          9         14          3          0.110108       0.153961
5.018057E+03       ; H13-C9-C14
     9         14         15          3          0.153961       0.153959
7.940129E+03       ; C9-C14-C15
     9         14         16          3          0.153961       0.110106
4.947045E+03       ; C9-C14-H16
     9         14         17          3          0.153961       0.110106
4.946876E+03       ; C9-C14-H17
    15         14         16          3          0.153959       0.110106
5.046004E+03       ; C15-C14-H16
    15         14         17          3          0.153959       0.110106
5.045958E+03       ; C15-C14-H17
    16         14         17          3          0.110106       0.110106
2.741991E+03       ; H16-C14-H17
    14         15         18          3          0.153959       0.153961
7.923220E+03       ; C14-C15-C18
    14         15         19          3          0.153959       0.110109
4.957010E+03       ; C14-C15-H19
    14         15         20          3          0.153959       0.110109
4.957252E+03       ; C14-C15-H20
    18         15         19          3          0.153961       0.110109
5.036033E+03       ; C18-C15-H19
    18         15         20          3          0.153961       0.110109
5.035755E+03       ; C18-C15-H20
    19         15         20          3          0.110109       0.110109
2.744184E+03       ; H19-C15-H20
    15         18         21          3          0.153961       0.153965
7.940297E+03       ; C15-C18-C21
    15         18         22          3          0.153961       0.110112
4.934161E+03       ; C15-C18-H22
    15         18         23          3          0.153961       0.110113
4.934136E+03       ; C15-C18-H23
    21         18         22          3          0.153965       0.110112
5.070815E+03       ; C21-C18-H22
```

21 18 23 3 0.153965 0.110113
5.070372E+03 ; C21-C18-H23
22 18 23 3 0.110112 0.110113
2.750272E+03 ; H22-C18-H23
18 21 24 3 0.153965 0.110115
4.935030E+03 ; C18-C21-H24
18 21 25 3 0.153965 0.110115
4.934880E+03 ; C18-C21-H25
18 21 26 3 0.153965 0.153964
7.915298E+03 ; C18-C21-C26
24 21 25 3 0.110115 0.110115
2.752919E+03 ; H24-C21-H25
24 21 26 3 0.110115 0.153964
5.055986E+03 ; H24-C21-C26
25 21 26 3 0.110115 0.153964
5.055869E+03 ; H25-C21-C26
21 26 27 3 0.153964 0.153960
8.008297E+03 ; C21-C26-C27
21 26 28 3 0.153964 0.110104
4.901017E+03 ; C21-C26-H28
21 26 29 3 0.153964 0.110105
4.900995E+03 ; C21-C26-H29
27 26 28 3 0.153960 0.110104
5.069469E+03 ; C27-C26-H28
27 26 29 3 0.153960 0.110105
5.069369E+03 ; C27-C26-H29
28 26 29 3 0.110104 0.110105
2.749555E+03 ; H28-C26-H29
26 27 30 3 0.153960 0.153982
7.832277E+03 ; C26-C27-C30
26 27 31 3 0.153960 0.110105
4.909099E+03 ; C26-C27-H31
26 27 32 3 0.153960 0.110104
4.909512E+03 ; C26-C27-H32
30 27 31 3 0.153982 0.110105
5.310456E+03 ; C30-C27-H31
30 27 32 3 0.153982 0.110104
5.309839E+03 ; C30-C27-H32
31 27 32 3 0.110105 0.110104
2.831492E+03 ; H31-C27-H32
27 30 33 3 0.153982 0.153078
8.233886E+03 ; C27-C30-C33
27 30 34 3 0.153982 0.109839
4.371672E+03 ; C27-C30-H34

```
    27          30          35          3          0.153982       0.109839
4.371580E+03        ; C27-C30-H35
    33          30          34          3          0.153078       0.109839
4.480751E+03        ; C33-C30-H34
    33          30          35          3          0.153078       0.109839
4.480926E+03        ; C33-C30-H35
    34          30          35          3          0.109839       0.109839
2.513451E+03        ; H34-C30-H35
    30          33          36          3          0.153078       0.109820
4.186274E+03        ; C30-C33-H36
    30          33          37          3          0.153078       0.109820
4.186152E+03        ; C30-C33-H37
    30          33          38          3          0.153078       0.145086
1.649022E+04        ; C30-C33-O38
    36          33          37          3          0.109820       0.109820
3.682514E+03        ; H36-C33-H37
    36          33          38          3          0.109820       0.145086
1.319827E+04        ; H36-C33-O38
    37          33          38          3          0.109820       0.145086
1.319722E+04        ; H37-C33-O38
    33          38          39          3          0.145086       0.189082
1.760604E+04        ; C33-O38-S39
    38          39          40          3          0.189082       0.163394
3.953157E+03        ; O38-S39-O40
    38          39          41          3          0.189082       0.163394
3.952643E+03        ; O38-S39-O41
    38          39          42          3          0.189082       0.164306
7.585390E+03        ; O38-S39-O42
    40          39          41          3          0.163394       0.163394
8.644500E+03        ; O40-S39-O41
    40          39          42          3          0.163394       0.164306
8.003586E+03        ; O40-S39-O42
    41          39          42          3          0.163394       0.164306
8.002934E+03        ; O41-S39-O42

[ dihedrals ] ; propers
; atom_i    atom_j    atom_k    atom_l    functype      d0 (Deg.)      k
(kJ/mol/rad^2)        ; Case of functype=2
; atom_i    atom_j    atom_k    atom_l    functype    phase (Deg.)    kd (kJ/mol)
pn          ; Case of functype=9
      1           2           6           9           2          -179.999
3.730266E+01          ; C1-C2-C6-C9, DRIH method
      1           2           6          10           2           -57.821
3.879407E+01          ; C1-C2-C6-H10, DRIH method
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     1        2        6       11        2          57.822
3.879532E+01       ; C1-C2-C6-H11, DRIH method
     2        6        9       12        2         -57.854
3.864634E+01       ; C2-C6-C9-H12, DRIH method
     2        6        9       13        2          57.856
3.864554E+01       ; C2-C6-C9-H13, DRIH method
     2        6        9       14        2        -179.998
3.741211E+01       ; C2-C6-C9-C14, DRIH method
     3        1        2        6        2        -179.991
3.869429E+01       ; H3-C1-C2-C6, DRIH method
     3        1        2        7        2         -58.003
4.051704E+01       ; H3-C1-C2-H7, DRIH method
     3        1        2        8        2          58.021
4.051645E+01       ; H3-C1-C2-H8, DRIH method
     4        1        2        6        2         -59.788
3.840104E+01       ; H4-C1-C2-C6, DRIH method
     4        1        2        7        2          62.199
4.227779E+01       ; H4-C1-C2-H7, DRIH method
     4        1        2        8        2         178.224
3.997019E+01       ; H4-C1-C2-H8, DRIH method
     5        1        2        6        2          59.806
3.840082E+01       ; H5-C1-C2-C6, DRIH method
     5        1        2        7        2        -178.206
3.997138E+01       ; H5-C1-C2-H7, DRIH method
     5        1        2        8        2         -62.182
4.227683E+01       ; H5-C1-C2-H8, DRIH method
     6        9       14       15        2         179.993
3.813157E+01       ; C6-C9-C14-C15, DRIH method
     6        9       14       16        2          57.854
3.889943E+01       ; C6-C9-C14-H16, DRIH method
     6        9       14       17        2         -57.866
3.889802E+01       ; C6-C9-C14-H17, DRIH method
     7        2        6        9        2          57.801
3.911590E+01       ; H7-C2-C6-C9, DRIH method
     7        2        6       10        2         179.980
3.995633E+01       ; H7-C2-C6-H10, DRIH method
     7        2        6       11        2         -64.377
4.260776E+01       ; H7-C2-C6-H11, DRIH method
     8        2        6        9        2         -57.799
3.911507E+01       ; H8-C2-C6-C9, DRIH method
     8        2        6       10        2          64.379
4.260725E+01       ; H8-C2-C6-H10, DRIH method
     8        2        6       11        2        -179.978
3.995612E+01       ; H8-C2-C6-H11, DRIH method
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     9         14         15         18          2        -179.997
3.825049E+01       ; C9-C14-C15-C18, DRIH method
     9         14         15         19          2         -57.847
3.892171E+01       ; C9-C14-C15-H19, DRIH method
     9         14         15         20          2          57.852
3.892045E+01       ; C9-C14-C15-H20, DRIH method
    10          6          9         12          2        -179.981
3.991071E+01       ; H10-C6-C9-H12, DRIH method
    10          6          9         13          2         -64.271
4.249935E+01       ; H10-C6-C9-H13, DRIH method
    10          6          9         14          2          57.875
3.892287E+01       ; H10-C6-C9-C14, DRIH method
    11          6          9         12          2          64.272
4.250002E+01       ; H11-C6-C9-H12, DRIH method
    11          6          9         13          2         179.982
3.991013E+01       ; H11-C6-C9-H13, DRIH method
    11          6          9         14          2         -57.872
3.892347E+01       ; H11-C6-C9-C14, DRIH method
    12          9         14         15          2          57.842
3.913670E+01       ; H12-C9-C14-C15, DRIH method
    12          9         14         16          2         -64.298
4.251771E+01       ; H12-C9-C14-H16, DRIH method
    12          9         14         17          2         179.983
3.993128E+01       ; H12-C9-C14-H17, DRIH method
    13          9         14         15          2         -57.854
3.913657E+01       ; H13-C9-C14-C15, DRIH method
    13          9         14         16          2        -179.993
3.993101E+01       ; H13-C9-C14-H16, DRIH method
    13          9         14         17          2          64.287
4.251635E+01       ; H13-C9-C14-H17, DRIH method
    14         15         18         21          2         179.997
3.848951E+01       ; C14-C15-C18-C21, DRIH method
    14         15         18         22          2         -57.858
3.903057E+01       ; C14-C15-C18-H22, DRIH method
    14         15         18         23          2          57.852
3.903178E+01       ; C14-C15-C18-H23, DRIH method
    15         18         21         24          2         -57.843
3.894059E+01       ; C15-C18-C21-H24, DRIH method
    15         18         21         25          2          57.840
3.893989E+01       ; C15-C18-C21-H25, DRIH method
    15         18         21         26          2         179.999
3.814582E+01       ; C15-C18-C21-C26, DRIH method
    16         14         15         18          2         -57.845
3.902115E+01       ; H16-C14-C15-C18, DRIH method
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    16         14         15         19          2          64.306
4.251219E+01        ; H16-C14-C15-H19, DRIH method
    16         14         15         20          2        -179.996
3.994149E+01        ; H16-C14-C15-H20, DRIH method
    17         14         15         18          2          57.849
3.902065E+01        ; H17-C14-C15-C18, DRIH method
    17         14         15         19          2         180.000
3.994237E+01        ; H17-C14-C15-H19, DRIH method
    17         14         15         20          2         -64.302
4.251115E+01        ; H17-C14-C15-H20, DRIH method
    18         21         26         27          2         179.991
3.820156E+01        ; C18-C21-C26-C27, DRIH method
    18         21         26         28          2          57.868
3.901677E+01        ; C18-C21-C26-H28, DRIH method
    18         21         26         29          2         -57.883
3.901602E+01        ; C18-C21-C26-H29, DRIH method
    19         15         18         21          2          57.836
3.909329E+01        ; H19-C15-C18-C21, DRIH method
    19         15         18         22          2         179.982
3.990718E+01        ; H19-C15-C18-H22, DRIH method
    19         15         18         23          2         -64.309
4.249812E+01        ; H19-C15-C18-H23, DRIH method
    20         15         18         21          2         -57.842
3.909277E+01        ; H20-C15-C18-C21, DRIH method
    20         15         18         22          2          64.304
4.249701E+01        ; H20-C15-C18-H22, DRIH method
    20         15         18         23          2        -179.987
3.990698E+01        ; H20-C15-C18-H23, DRIH method
    21         26         27         30          2        -179.999
3.736855E+01        ; C21-C26-C27-C30, DRIH method
    21         26         27         31          2         -57.838
3.881718E+01        ; C21-C26-C27-H31, DRIH method
    21         26         27         32          2          57.838
3.881615E+01        ; C21-C26-C27-H32, DRIH method
    22         18         21         24          2         179.993
3.988879E+01        ; H22-C18-C21-H24, DRIH method
    22         18         21         25          2         -64.323
4.246887E+01        ; H22-C18-C21-H25, DRIH method
    22         18         21         26          2          57.835
3.885352E+01        ; H22-C18-C21-C26, DRIH method
    23         18         21         24          2          64.319
4.246923E+01        ; H23-C18-C21-H24, DRIH method
    23         18         21         25          2        -179.997
3.988840E+01        ; H23-C18-C21-H25, DRIH method
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    23          18          21          26           2          -57.838
3.885386E+01        ; H23-C18-C21-C26, DRIH method
    24          21          26          27           2           57.820
3.892693E+01        ; H24-C21-C26-C27, DRIH method
    24          21          26          28           2          -64.304
4.245160E+01        ; H24-C21-C26-H28, DRIH method
    24          21          26          29           2          179.945
3.983998E+01        ; H24-C21-C26-H29, DRIH method
    25          21          26          27           2          -57.835
3.892611E+01        ; H25-C21-C26-C27, DRIH method
    25          21          26          28           2         -179.959
3.984009E+01        ; H25-C21-C26-H28, DRIH method
    25          21          26          29           2           64.290
4.245002E+01        ; H25-C21-C26-H29, DRIH method
    26          27          30          33           2          179.996
3.753037E+01        ; C26-C27-C30-C33, DRIH method
    26          27          30          34           2          -58.644
3.896384E+01        ; C26-C27-C30-H34, DRIH method
    26          27          30          35           2           58.637
3.896531E+01        ; C26-C27-C30-H35, DRIH method
    27          30          33          36           2          -59.306
4.123483E+01        ; C27-C30-C33-H36, DRIH method
    27          30          33          37           2           59.303
4.123355E+01        ; C27-C30-C33-H37, DRIH method
    27          30          33          38           2          179.999
4.461772E+01        ; C27-C30-C33-O38, DRIH method
    28          26          27          30           2          -57.820
3.861222E+01        ; H28-C26-C27-C30, DRIH method
    28          26          27          31           2           64.341
4.243918E+01        ; H28-C26-C27-H31, DRIH method
    28          26          27          32           2         -179.983
3.986041E+01        ; H28-C26-C27-H32, DRIH method
    29          26          27          30           2           57.821
3.861180E+01        ; H29-C26-C27-C30, DRIH method
    29          26          27          31           2          179.982
3.986066E+01        ; H29-C26-C27-H31, DRIH method
    29          26          27          32           2          -64.342
4.243852E+01        ; H29-C26-C27-H32, DRIH method
    30          33          38          39           2         -179.988
4.899157E+01        ; C30-C33-O38-S39, DRIH method
    31          27          30          33           2           57.946
3.899089E+01        ; H31-C27-C30-C33, DRIH method
    31          27          30          34           2          179.306
3.998878E+01        ; H31-C27-C30-H34, DRIH method
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    31        27        30        35         2          -63.413
4.262268E+01        ; H31-C27-C30-H35, DRIH method
    32        27        30        33         2          -57.953
3.899005E+01        ; H32-C27-C30-C33, DRIH method
    32        27        30        34         2           63.406
4.262141E+01        ; H32-C27-C30-H34, DRIH method
    32        27        30        35         2         -179.312
3.998920E+01        ; H32-C27-C30-H35, DRIH method
    33        38        39        40         2          119.840
8.970097E+01        ; C33-O38-S39-O40, DRIH method
    33        38        39        41         2         -119.876
8.970976E+01        ; C33-O38-S39-O41, DRIH method
    33        38        39        42         2           -0.018
8.792772E+01        ; C33-O38-S39-O42, DRIH method
    34        30        33        36         2          178.518
4.202139E+01        ; H34-C30-C33-H36, DRIH method
    34        30        33        37         2          -62.873
4.584188E+01        ; H34-C30-C33-H37, DRIH method
    34        30        33        38         2           57.823
4.538001E+01        ; H34-C30-C33-O38, DRIH method
    35        30        33        36         2           62.869
4.584207E+01        ; H35-C30-C33-H36, DRIH method
    35        30        33        37         2         -178.521
4.202158E+01        ; H35-C30-C33-H37, DRIH method
    35        30        33        38         2          -57.826
4.537951E+01        ; H35-C30-C33-O38, DRIH method
    36        33        38        39         2           59.535
6.439067E+01        ; H36-C33-O38-S39, DRIH method
    37        33        38        39         2          -59.511
6.438522E+01        ; H37-C33-O38-S39, DRIH method
```

PFH$_X$A.itp

```
[ atomtypes ]
; name    at.num    mass    charge    ptype    sigma (nm)    epsilon (kJ/mol)
c3    6    12.010736    0.000000    A    3.399670E-01    4.577296E-01
f    9    18.998403    0.000000    A    3.118146E-01    2.552240E-01
c    6    12.010736    0.000000    A    3.399670E-01    3.598240E-01
o    8    15.999405    0.000000    A    2.959922E-01    8.786400E-01

[ moleculetype ]
; name    nrexcl
PFHXA    3

[ atoms ]
;   Index    type    residue    resname    atom    cgnr    charge    mass
     1    c3    1    MOL    C1    1    0.65938193    12.010736
     2    c3    1    MOL    C2    2    0.20868072    12.010736
     3    c3    1    MOL    C3    3    0.41499987    12.010736
     4    c3    1    MOL    C4    4    0.28942482    12.010736
     5    c3    1    MOL    C5    5    0.33657049    12.010736
     6    f    1    MOL    F6    6    -0.21045228    18.998403
     7    f    1    MOL    F7    7    -0.21000762    18.998403
     8    f    1    MOL    F8    8    -0.20966861    18.998403
     9    f    1    MOL    F9    9    -0.15570669    18.998403
    10    f    1    MOL    F10    10    -0.16848622    18.998403
    11    f    1    MOL    F11    11    -0.20921247    18.998403
    12    f    1    MOL    F12    12    -0.19698297    18.998403
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     13      f       1       MOL     F13     13      -0.18354705
18.998403
     14      f       1       MOL     F14     14      -0.20477902
18.998403
     15      f       1       MOL     F15     15      -0.25375507
18.998403
     16      f       1       MOL     F16     16      -0.24683263
18.998403
     17      c       1       MOL     C17     17       0.74448359
12.010736
     18      o       1       MOL     O18     18      -0.70875001
15.999405
     19      o       1       MOL     O19     19      -0.69536079
15.999405

[ bonds ]
; atom_i    atom_j    functype        r0 (nm)        k (kJ/mol/nm^2)
     1       2       1       0.154385        2.587223E+05        ; C1-C2,
DRIH method
     1       6       1       0.138412        3.449576E+05        ; C1-F6,
DRIH method
     1       7       1       0.137705        3.580219E+05        ; C1-F7,
DRIH method
     1       8       1       0.137982        3.548800E+05        ; C1-F8,
DRIH method
     2       3       1       0.155018        2.519975E+05        ; C2-C3,
DRIH method
     2       9       1       0.139465        3.440676E+05        ; C2-F9,
DRIH method
     2       10      1       0.139306        3.461769E+05        ; C2-F10,
DRIH method
     3       4       1       0.155363        2.431614E+05        ; C3-C4,
DRIH method
     3       11      1       0.139934        3.356723E+05        ; C3-F11,
DRIH method
     3       12      1       0.139629        3.391629E+05        ; C3-F12,
DRIH method
     4       5       1       0.154021        2.491763E+05        ; C4-C5,
DRIH method
     4       13      1       0.139858        3.346371E+05        ; C4-F13,
DRIH method
     4       14      1       0.140090        3.300306E+05        ; C4-F14,
DRIH method
     5       15      1       0.141647        2.976212E+05        ; C5-F15,
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DRIH method
5 16 1 0.141721 3.021871E+05 ; C5-F16,
DRIH method
5 17 1 0.158354 1.617261E+05 ; C5-C17,
DRIH method
17 18 1 0.127046 5.910028E+05 ; C17-
O18, DRIH method
17 19 1 0.126214 6.124872E+05 ; C17-
O19, DRIH method

[angles]
; atom_i atom_j atom_k functype a0 (Deg.) k (kJ/mol/rad^2)
2 1 6 1 109.530 4.842664E+02 ;
C2-C1-F6, DRIH method
2 1 7 1 111.777 4.653960E+02 ;
C2-C1-F7, DRIH method
2 1 8 1 111.292 4.644317E+02 ;
C2-C1-F8, DRIH method
6 1 7 1 107.552 3.017802E+02 ;
F6-C1-F7, DRIH method
6 1 8 1 107.825 2.926047E+02 ;
F6-C1-F8, DRIH method
7 1 8 1 108.714 2.995705E+02 ;
F7-C1-F8, DRIH method
1 2 3 1 115.307 5.296114E+02 ;
C1-C2-C3, DRIH method
1 2 9 1 106.166 2.245655E+02 ;
C1-C2-F9, DRIH method
1 2 10 1 106.468 2.237951E+02 ;
C1-C2-F10, DRIH method
3 2 9 1 110.377 2.017650E+02 ;
C3-C2-F9, DRIH method
3 2 10 1 109.536 2.094423E+02 ;
C3-C2-F10, DRIH method
9 2 10 1 108.733 8.272421E+01 ;
F9-C2-F10, DRIH method
2 3 4 1 115.440 5.287963E+02 ;
C2-C3-C4, DRIH method
2 3 11 1 106.506 2.367255E+02 ;
C2-C3-F11, DRIH method
2 3 12 1 106.093 2.342774E+02 ;
C2-C3-F12, DRIH method
4 3 11 1 109.971 2.120558E+02 ;
C4-C3-F11, DRIH method

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     4          3          12          1          110.332        2.038879E+02     ;
C4-C3-F12, DRIH method
    11          3          12          1          108.180        8.336373E+01     ;
F11-C3-F12, DRIH method
     3          4           5          1          116.331        5.181101E+02     ;
C3-C4-C5, DRIH method
     3          4          13          1          105.593        2.419758E+02     ;
C3-C4-F13, DRIH method
     3          4          14          1          105.489        2.308227E+02     ;
C3-C4-F14, DRIH method
     5          4          13          1          110.989        2.095912E+02     ;
C5-C4-F13, DRIH method
     5          4          14          1          109.425        1.969828E+02     ;
C5-C4-F14, DRIH method
    13          4          14          1          108.643        7.963867E+01     ;
F13-C4-F14, DRIH method
     4          5          15          1          105.456        2.681969E+02     ;
C4-C5-F15, DRIH method
     4          5          16          1          106.319        2.329393E+02     ;
C4-C5-F16, DRIH method
     4          5          17          1          115.033        3.828535E+02     ;
C4-C5-C17, DRIH method
    15          5          16          1          105.997        9.303725E+01     ;
F15-C5-F16, DRIH method
    15          5          17          1          113.083        2.031242E+02     ;
F15-C5-C17, DRIH method
    16          5          17          1          110.322        1.567112E+02     ;
F16-C5-C17, DRIH method
     5         17          18          1          111.647        4.004102E+02     ;
C5-C17-O18, DRIH method
     5         17          19          1          115.106        3.981908E+02     ;
C5-C17-O19, DRIH method
    18         17          19          1          133.224        4.887620E+02     ;
O18-C17-O19, DRIH method

[ angles ] ; bond-bond cross term
; atom_i   atom_j   atom_k   functype     r0_ij (nm)    r0_jk (nm)      k
(kJ/mol/nm^2)
     2          1           6          3          0.154385       0.138412
1.382165E+04         ; C2-C1-F6
     2          1           7          3          0.154385       0.137705
1.160314E+04         ; C2-C1-F7
     2          1           8          3          0.154385       0.137982
1.216627E+04         ; C2-C1-F8
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     6         1         7         3         0.138412  0.137705
3.882471E+04      ; F6-C1-F7
     6         1         8         3         0.138412  0.137982
3.798914E+04      ; F6-C1-F8
     7         1         8         3         0.137705  0.137982
3.738043E+04      ; F7-C1-F8
     1         2         3         3         0.154385  0.155018
1.821919E+04      ; C1-C2-C3
     1         2         9         3         0.154385  0.139465
1.832715E+04      ; C1-C2-F9
     1         2        10         3         0.154385  0.139306
1.764728E+04      ; C1-C2-F10
     3         2         9         3         0.155018  0.139465
1.266076E+04      ; C3-C2-F9
     3         2        10         3         0.155018  0.139306
1.349503E+04      ; C3-C2-F10
     9         2        10         3         0.139465  0.139306
3.533633E+04      ; F9-C2-F10
     2         3         4         3         0.155018  0.155363
1.802954E+04      ; C2-C3-C4
     2         3        11         3         0.155018  0.139934
1.801985E+04      ; C2-C3-F11
     2         3        12         3         0.155018  0.139629
1.957235E+04      ; C2-C3-F12
     4         3        11         3         0.155363  0.139934
1.149352E+04      ; C4-C3-F11
     4         3        12         3         0.155363  0.139629
1.179583E+04      ; C4-C3-F12
    11         3        12         3         0.139934  0.139629
3.524968E+04      ; F11-C3-F12
     3         4         5         3         0.155363  0.154021
1.864799E+04      ; C3-C4-C5
     3         4        13         3         0.155363  0.139858
2.036897E+04      ; C3-C4-F13
     3         4        14         3         0.155363  0.140090
2.079703E+04      ; C3-C4-F14
     5         4        13         3         0.154021  0.139858
9.905021E+03      ; C5-C4-F13
     5         4        14         3         0.154021  0.140090
1.493040E+04      ; C5-C4-F14
    13         4        14         3         0.139858  0.140090
3.419778E+04      ; F13-C4-F14
     4         5        15         3         0.154021  0.141647
1.759900E+04      ; C4-C5-F15
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     4          5          16          3          0.154021       0.141721
1.798846E+04        ; C4-C5-F16
     4          5          17          3          0.154021       0.158354
1.279757E+04        ; C4-C5-C17
    15          5          16          3          0.141647       0.141721
3.357959E+04        ; F15-C5-F16
    15          5          17          3          0.141647       0.158354
5.468785E+03        ; F15-C5-C17
    16          5          17          3          0.141721       0.158354
7.253260E+03        ; F16-C5-C17
     5         17          18          3          0.158354       0.127046
4.705772E+04        ; C5-C17-O18
     5         17          19          3          0.158354       0.126214
4.249290E+04        ; C5-C17-O19
    18         17          19          3          0.127046       0.126214
5.569632E+04        ; O18-C17-O19

[ dihedrals ] ; propers
; atom_i    atom_j    atom_k    atom_l    functype      d0 (Deg.)      k
(kJ/mol/rad^2)        ; Case of functype=2
; atom_i    atom_j    atom_k    atom_l    functype    phase (Deg.)    kd (kJ/mol)
pn          ; Case of functype=9
     1          2          3          4          2         -162.176
5.412045E+01          ; C1-C2-C3-C4, DRIH method
     1          2          3         11          2          -39.802
6.642954E+01          ; C1-C2-C3-F11, DRIH method
     1          2          3         12          2           75.297
6.652788E+01          ; C1-C2-C3-F12, DRIH method
     2          3          4          5          2         -162.661
5.490107E+01          ; C2-C3-C4-C5, DRIH method
     2          3          4         13          2          -39.085
6.746976E+01          ; C2-C3-C4-F13, DRIH method
     2          3          4         14          2           75.859
6.871547E+01          ; C2-C3-C4-F14, DRIH method
     3          2          1          6          2         -168.763
7.596564E+01          ; C3-C2-C1-F6, DRIH method
     3          2          1          7          2           72.141
7.535797E+01          ; C3-C2-C1-F7, DRIH method
     3          2          1          8          2          -49.630
7.021865E+01          ; C3-C2-C1-F8, DRIH method
     3          4          5         15          2          -37.650
6.475966E+01          ; C3-C4-C5-F15, DRIH method
     3          4          5         16          2           74.614
6.441029E+01          ; C3-C4-C5-F16, DRIH method
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     3     4     5    17     2   -162.966
5.165929E+01     ; C3-C4-C5-C17, DRIH method
     4     3     2     9     2    -41.900
6.830518E+01     ; C4-C3-C2-F9, DRIH method
     4     3     2    10     2     77.791
7.055201E+01     ; C4-C3-C2-F10, DRIH method
     4     5    17    18     2    -49.068
7.404582E+01     ; C4-C5-C17-O18, DRIH method
     4     5    17    19     2    132.437
6.922454E+01     ; C4-C5-C17-O19, DRIH method
     5     4     3    11     2     76.833
7.099483E+01     ; C5-C4-C3-F11, DRIH method
     5     4     3    12     2    -42.421
6.776174E+01     ; C5-C4-C3-F12, DRIH method
     6     1     2     9     2     68.683
8.061965E+01     ; F6-C1-C2-F9, DRIH method
     6     1     2    10     2    -47.062
8.487263E+01     ; F6-C1-C2-F10, DRIH method
     7     1     2     9     2    -50.413
8.050997E+01     ; F7-C1-C2-F9, DRIH method
     7     1     2    10     2   -166.158
8.807710E+01     ; F7-C1-C2-F10, DRIH method
     8     1     2     9     2   -172.183
8.335207E+01     ; F8-C1-C2-F9, DRIH method
     8     1     2    10     2     72.071
8.140336E+01     ; F8-C1-C2-F10, DRIH method
     9     2     3    11     2     80.474
7.705697E+01     ; F9-C2-C3-F11, DRIH method
     9     2     3    12     2   -164.427
8.275251E+01     ; F9-C2-C3-F12, DRIH method
    10     2     3    11     2   -159.835
8.365192E+01     ; F10-C2-C3-F11, DRIH method
    10     2     3    12     2    -44.736
7.377701E+01     ; F10-C2-C3-F12, DRIH method
    11     3     4    13     2   -159.591
8.419614E+01     ; F11-C3-C4-F13, DRIH method
    11     3     4    14     2    -44.647
7.416646E+01     ; F11-C3-C4-F14, DRIH method
    12     3     4    13     2     81.155
7.721035E+01     ; F12-C3-C4-F13, DRIH method
    12     3     4    14     2   -163.901
8.362993E+01     ; F12-C3-C4-F14, DRIH method
    13     4     5    15     2   -158.388
7.974847E+01     ; F13-C4-C5-F15, DRIH method
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    13          4          5          16          2          -46.124
6.958147E+01        ; F13-C4-C5-F16, DRIH method
    13          4          5          17          2           76.296
6.689778E+01        ; F13-C4-C5-C17, DRIH method
    14          4          5          15          2           81.722
7.659092E+01        ; F14-C4-C5-F15, DRIH method
    14          4          5          16          2         -166.014
8.150943E+01        ; F14-C4-C5-F16, DRIH method
    14          4          5          17          2          -43.594
6.496221E+01        ; F14-C4-C5-C17, DRIH method
    15          5         17          18          2         -170.317
9.120235E+01        ; F15-C5-C17-O18, DRIH method
    15          5         17          19          2           11.188
9.118248E+01        ; F15-C5-C17-O19, DRIH method
    16          5         17          18          2           71.174
9.497806E+01        ; F16-C5-C17-O18, DRIH method
    16          5         17          19          2         -107.321
8.154691E+01        ; F16-C5-C17-O19, DRIH method
```