1 **Molecular Dynamics of Synergistic Behavior at the Air-Water**

2 **Interface: Mixed Cationic-anionic Fluorocarbon-Hydrocarbon**

3 **Surfactants**

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model of the system

**Figure. S1** The top view initial model of the system (a) PFB-MC/1-OA = 1:0 (b) PFB-MC/1-OA = 2:1 (c) PFB-MC/1-OA = 1:1 (d) PFB-MC/1-OA = 1:2 (e) PFB-MC/1-OA = 0:1
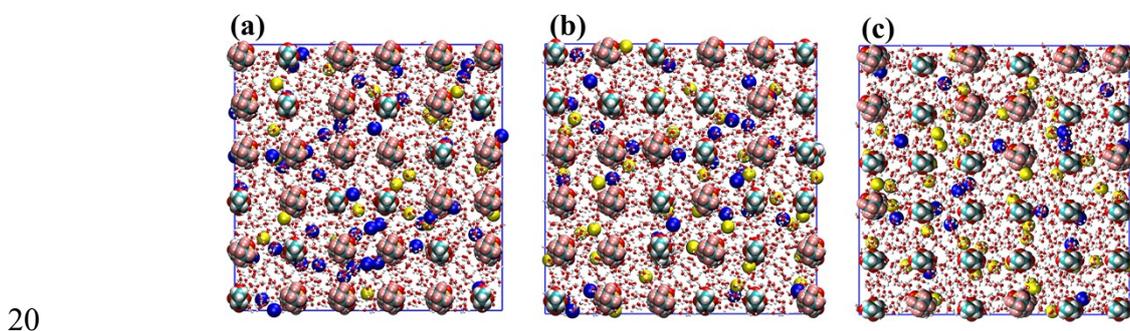
Figure. S2 The top view initial model of the recreate system (a) PFB-MC/1-OA = 2:1 (b) PFB-MC/1-OA = 1:1 (c) PFB-MC/1-OA = 1:2
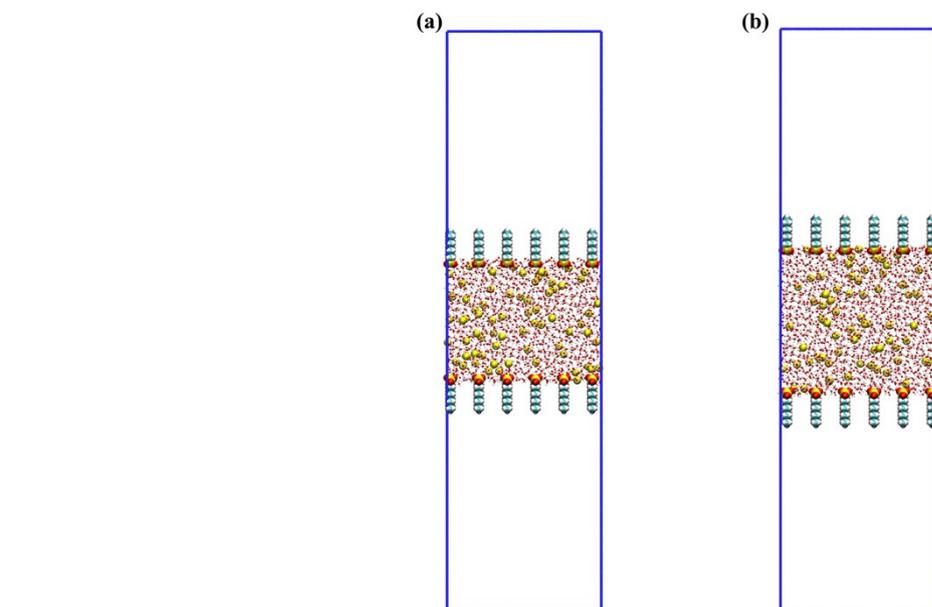

Figure S3. The initial models of the system with water layer thicknesses of 4 nm (a) and 5 nm (b) for PFB-MC/1-OA ratios of 0:1.

26 1D-Density

27

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(c)

29

(d)

30
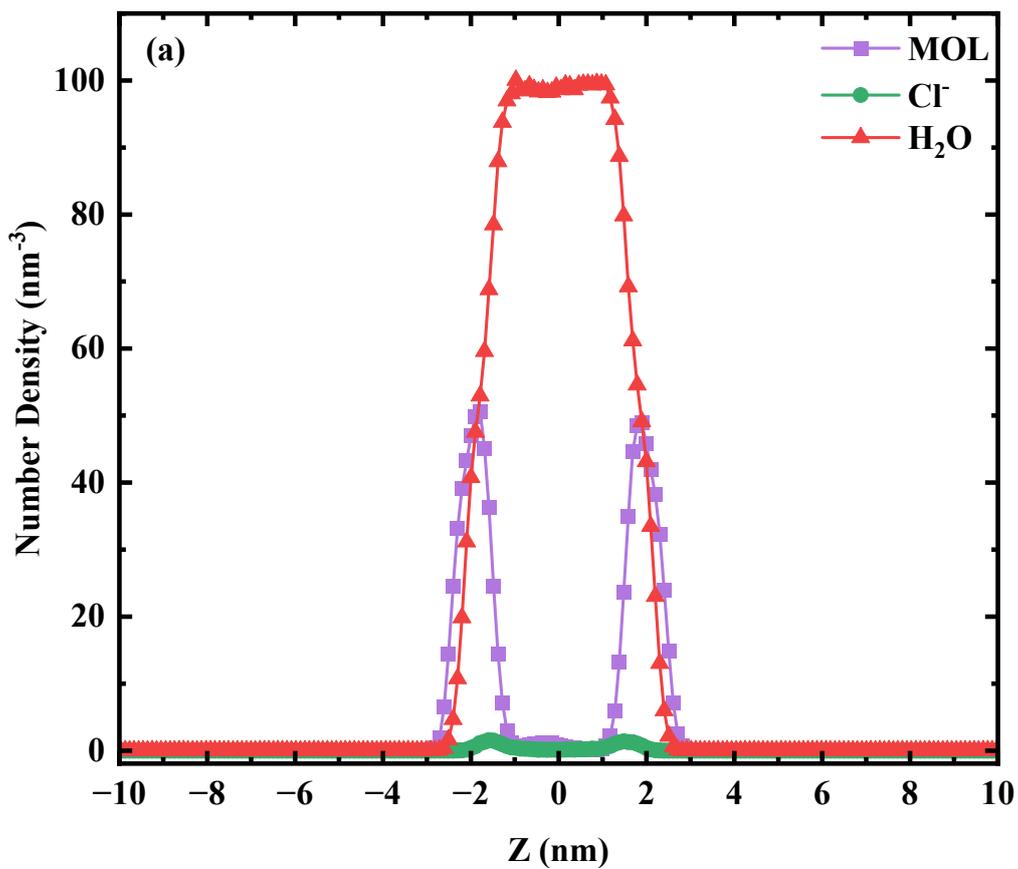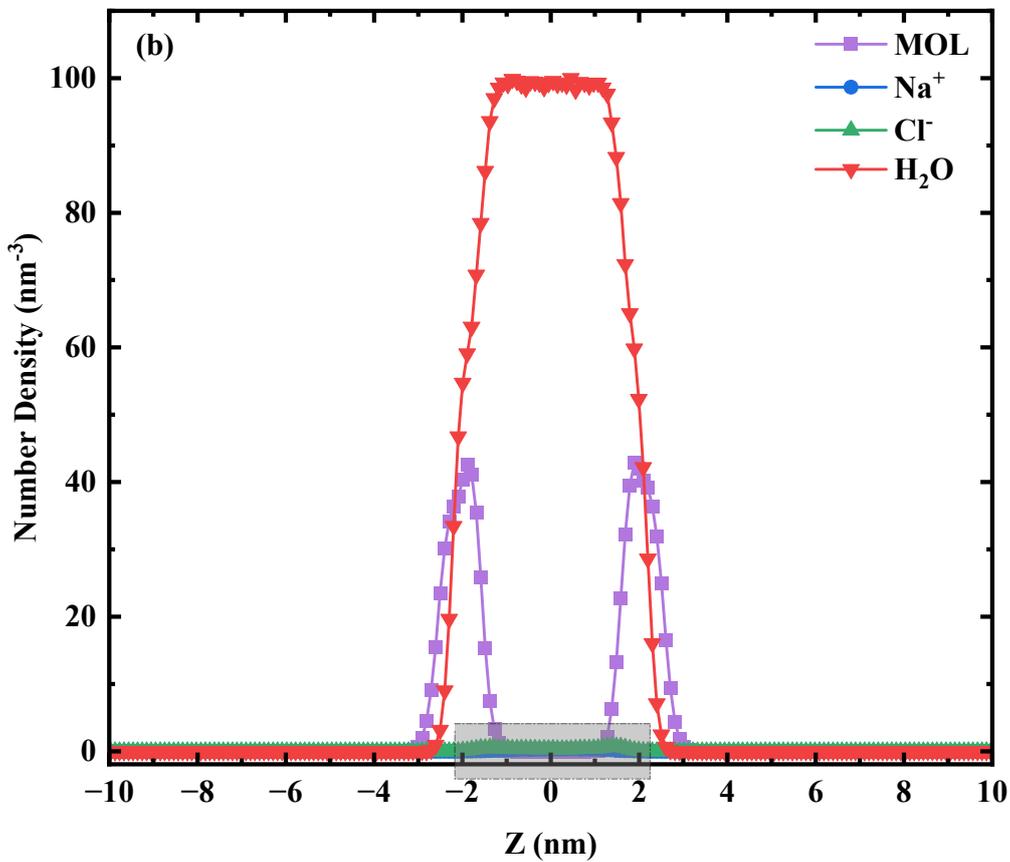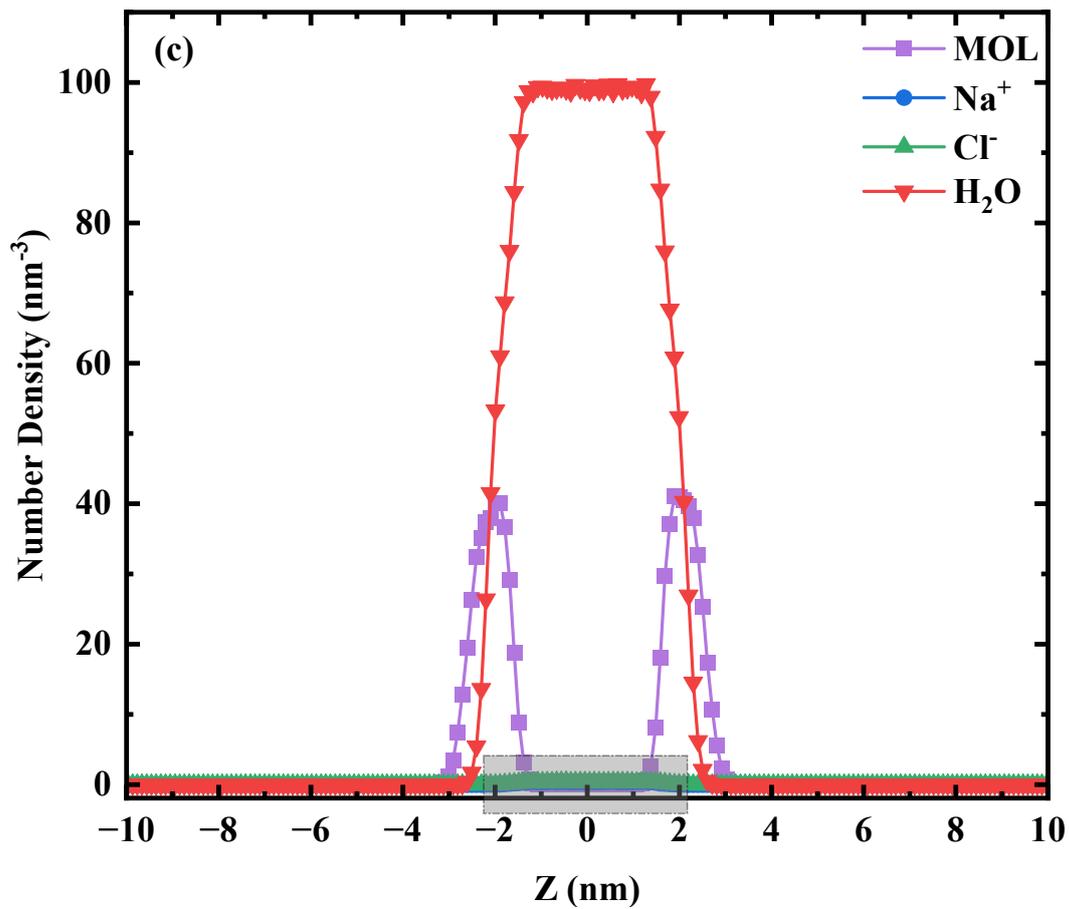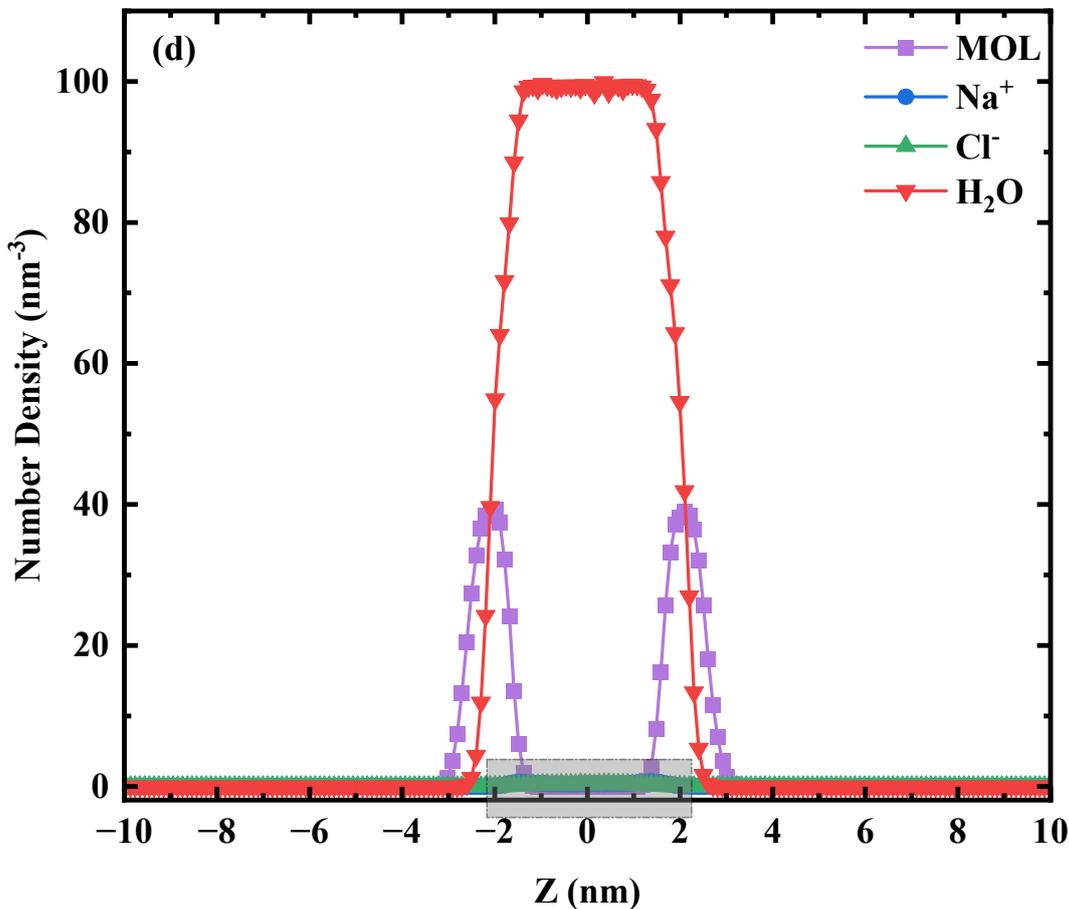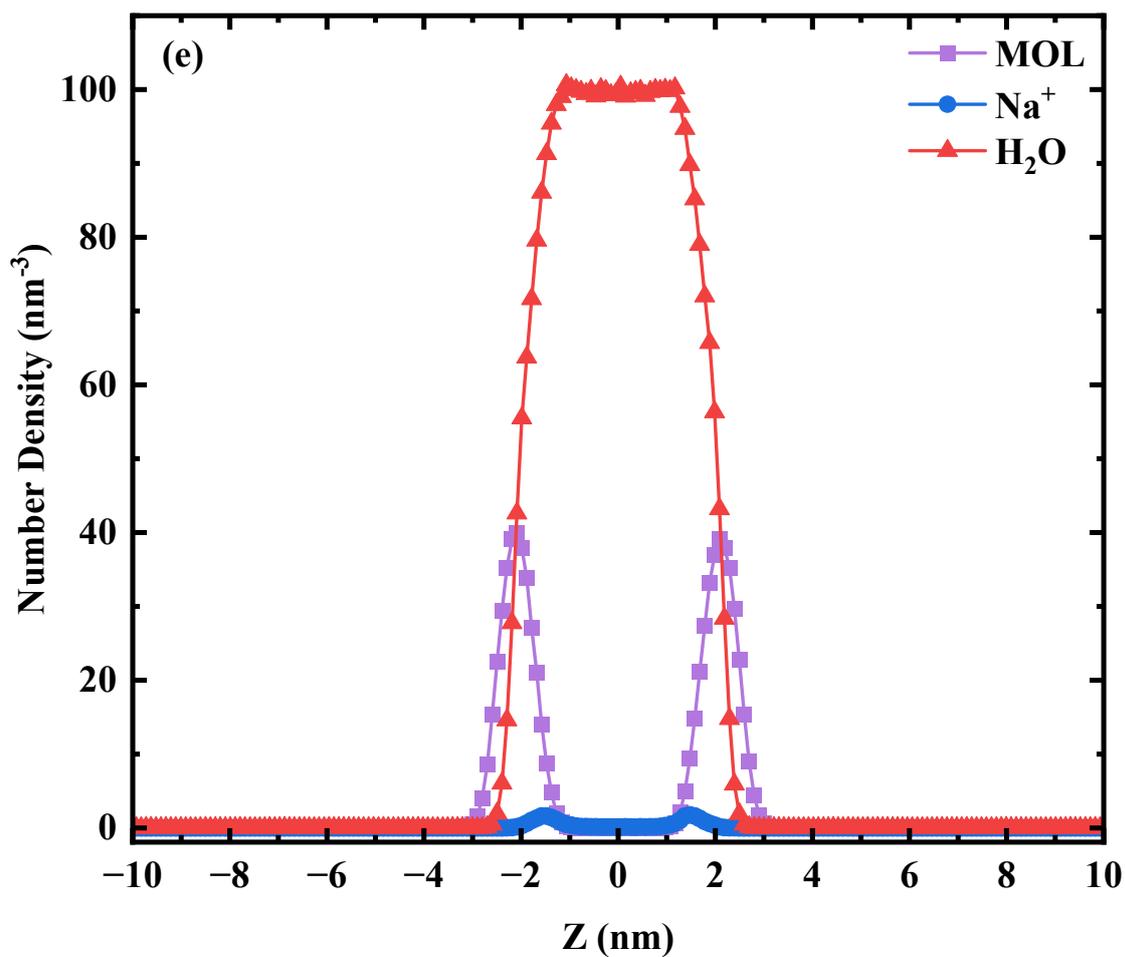
Figure S4. Z-axis distribution of number densities (a) PFB-MC/1-OA = 1:0 (b) PFB-MC/1-OA = 2:1 (c) PFB-MC/1-OA = 1:1 (d) PFB-MC/1-OA = 1:2 (e) PFB-MC/1-OA = 0:1.

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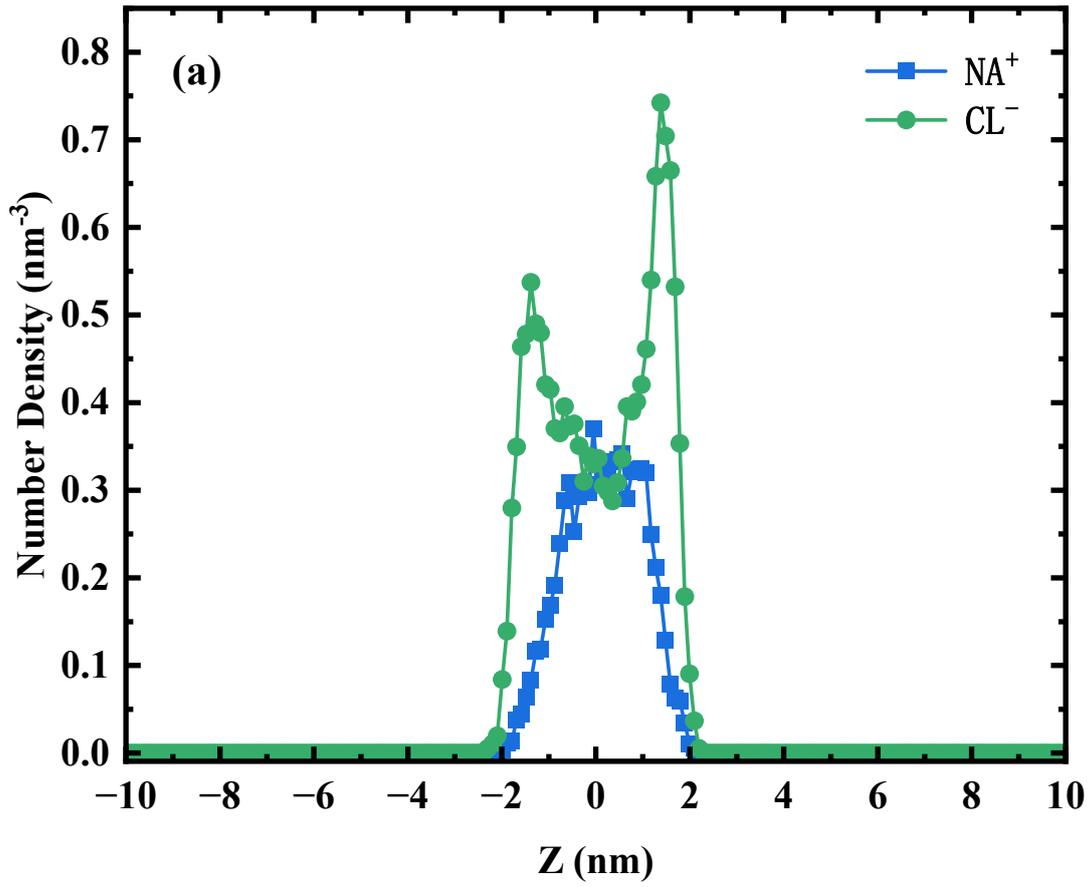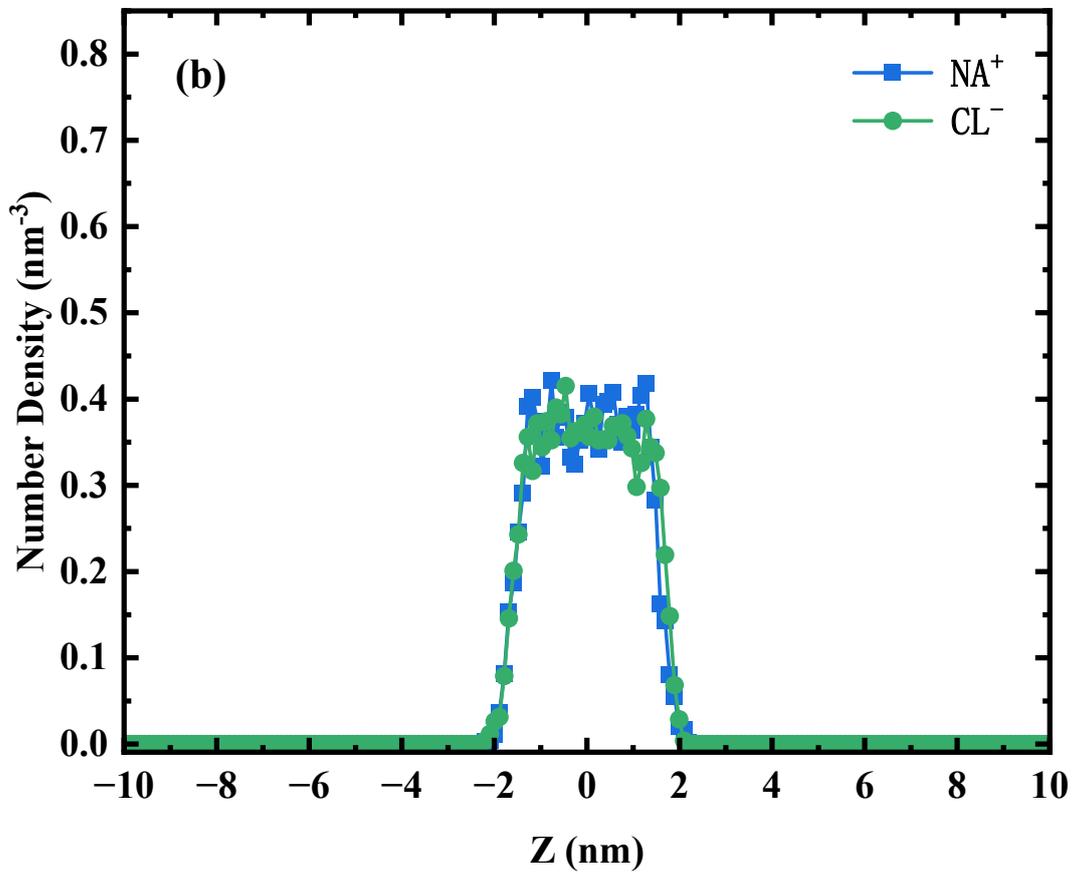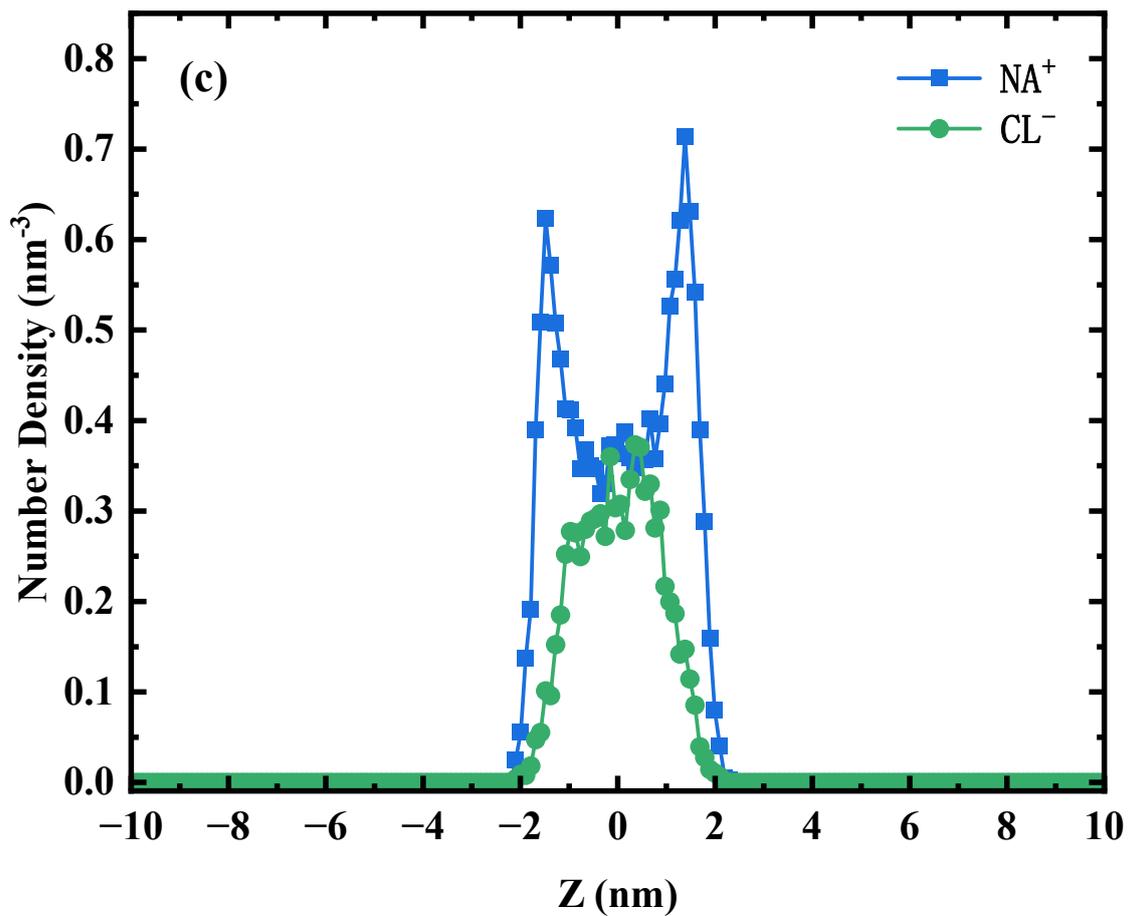
Figure S5 Z-axis distribution of number densities in mixed system (a) PFB-MC/1-OA = 2:1

(b) PFB-MC/1-OA = 1:1 (c) PFB-MC/1-OA = 1:2.

41 Detailed parameters of topology files

42 PFB-MC.itp

43 [moleculetype]

44 ; name   nrexcl

45 PFB-MC   3

46

47 [atoms]

48 ; Index   type   residue   resname   atom   cgnr   charge   mass

Index	type	residue	resname	atom	cgnr	charge	mass
49 1	c3	1	MOL	C1	1	0.38630423	50 12.010736
51 2	c3	1	MOL	C2	2	0.14363258	52 12.010736
53 3	c3	1	MOL	C3	3	0.22102457	54 12.010736
55 4	c3	1	MOL	C4	4	0.03733211	56 12.010736
57 5	f	1	MOL	F5	5	-0.09365470	58 18.998403
59 6	f	1	MOL	F6	6	-0.10629787	60 18.998403
61 7	f	1	MOL	F7	7	-0.11494802	

62	18.998403						
63	8	f	1	MOL	F8	8	-0.07239060
64	18.998403						
65	9	f	1	MOL	F9	9	-0.07893600
66	18.998403						
67	10	f	1	MOL	F10	10	-0.09993404
68	18.998403						
69	11	f	1	MOL	F11	11	-0.13825585
70	18.998403						
71	12	f	1	MOL	F12	12	-0.03612519
72	18.998403						
73	13	f	1	MOL	F13	13	-0.06555029
74	18.998403						
75	14	s6	1	MOL	S14	14	0.87168130
76	32.064787						
77	15	o	1	MOL	O15	15	-0.43763937
78	15.999405						
79	16	o	1	MOL	O16	16	-0.38098913
80	15.999405						
81	17	n3	1	MOL	N17	17	-0.65996229
82	14.006703						
83	18	hn	1	MOL	H18	18	0.39307088

84	1.007941						
85	19	c3	1	MOL	C19	19	0.31636510
86	12.010736						
87	20	c3	1	MOL	C20	20	-0.09011922
88	12.010736						
89	21	h1	1	MOL	H21	21	0.01770142
90	1.007941						
91	22	h1	1	MOL	H22	22	0.01770142
92	1.007941						
93	23	c3	1	MOL	C23	23	-0.24981353
94	12.010736						
95	24	hc	1	MOL	H24	24	0.08737701
96	1.007941						
97	25	hc	1	MOL	H25	25	0.08737701
98	1.007941						
99	26	hx	1	MOL	H26	26	0.16215708
100	1.007941						
101	27	hx	1	MOL	H27	27	0.16215708
102	1.007941						
103	28	hn	1	MOL	H28	28	0.35002768
104	1.007941						
105	29	n4	1	MOL	N29	29	0.00880602

106 14.006703

| 107 | 30 | c3 | 1 | MOL | C30 | 30 | -0.45119007 |

108 12.010736

| 109 | 31 | hx | 1 | MOL | H31 | 31 | 0.21045303 |

110 1.007941

| 111 | 32 | hx | 1 | MOL | H32 | 32 | 0.21045303 |

112 1.007941

| 113 | 33 | hx | 1 | MOL | H33 | 33 | 0.21045303 |

114 1.007941

| 115 | 34 | c3 | 1 | MOL | C34 | 34 | -0.34287118 |

116 12.010736

| 117 | 35 | hx | 1 | MOL | H35 | 35 | 0.17486760 |

118 1.007941

| 119 | 36 | hx | 1 | MOL | H36 | 36 | 0.17486760 |

120 1.007941

| 121 | 37 | hx | 1 | MOL | H37 | 37 | 0.17486760 |

122 1.007941

123

124   [bonds]

125   ; atom_i atom_j functype   r0 (nm)   k (kJ/mol/nm^2)

126   1   2   1   0.155389   2.467929E+05   ; C1-C2, DRIH

127 method

128	1	5	1	0.133166	4.071290E+05	; C1-F5, DRIH
129	method					
130	1	6	1	0.133987	3.938268E+05	; C1-F6, DRIH
131	method					
132	1	7	1	0.133815	3.952800E+05	; C1-F7, DRIH
133	method					
134	2	3	1	0.155443	2.442864E+05	; C2-C3, DRIH
135	method					
136	2	8	1	0.134595	3.972445E+05	; C2-F8, DRIH
137	method					
138	2	9	1	0.135464	3.812073E+05	; C2-F9, DRIH
139	method					
140	3	4	1	0.155337	2.428070E+05	; C3-C4, DRIH
141	method					
142	3	10	1	0.135336	3.810860E+05	; C3-F10, DRIH
143	method					
144	3	11	1	0.136231	3.630831E+05	; C3-F11, DRIH
145	method					
146	4	12	1	0.133683	4.023830E+05	; C4-F12, DRIH
147	method					
148	4	13	1	0.135282	3.649358E+05	; C4-F13, DRIH
149	method					

150	4	14	1	0.190782	1.432446E+05 ; C4-S14, DRIH
151	method				
152	14	15	1	0.146875	5.495640E+05 ; S14-O15, DRIH
153	method				
154	14	16	1	0.144959	6.155814E+05 ; S14-O16, DRIH
155	method				
156	14	17	1	0.165882	2.688670E+05 ; S14-N17, DRIH
157	method				
158	17	18	1	0.101441	4.318770E+05 ; N17-H18, DRIH
159	method				
160	17	19	1	0.146927	3.129959E+05 ; N17-C19, DRIH
161	method				
162	19	20	1	0.154383	2.555698E+05 ; C19-C20, DRIH
163	method				
164	19	21	1	0.109416	3.167316E+05 ; C19-H21, DRIH
165	method				
166	19	22	1	0.109285	3.210857E+05 ; C19-H22, DRIH
167	method				
168	20	23	1	0.153373	2.677554E+05 ; C20-C23, DRIH
169	method				
170	20	24	1	0.109421	3.183093E+05 ; C20-H24, DRIH
171	method				

172	20	25	1	0.109387	3.191526E+05	; C20-H25, DRIH
173	method					
174	23	26	1	0.109154	3.241077E+05	; C23-H26, DRIH
175	method					
176	23	27	1	0.109399	3.205481E+05	; C23-H27, DRIH
177	method					
178	23	29	1	0.152797	2.289728E+05	; C23-N29, DRIH
179	method					
180	28	29	1	0.102559	3.944276E+05	; H28-N29, DRIH
181	method					
182	29	30	1	0.150539	2.590139E+05	; N29-C30, DRIH
183	method					
184	29	34	1	0.150895	2.534838E+05	; N29-C34, DRIH
185	method					
186	30	31	1	0.108993	3.309597E+05	; C30-H31, DRIH
187	method					
188	30	32	1	0.109001	3.307655E+05	; C30-H32, DRIH
189	method					
190	30	33	1	0.109053	3.305552E+05	; C30-H33, DRIH
191	method					
192	34	35	1	0.109069	3.294482E+05	; C34-H35, DRIH
193	method					

194	34	36	1	0.108933	3.329083E+05	; C34-H36, DRIH
195	method					
196	34	37	1	0.109037	3.298079E+05	; C34-H37, DRIH
197	method					

198

199 [angles]

200 ; atom_i atom_j atom_k functype a0 (Deg.) k (kJ/mol/rad^2)

201	2	1	5	1	109.032	4.913679E+02	; C2-
202	C1-F5, DRIH method						
203	2	1	6	1	109.812	5.131750E+02	; C2-
204	C1-F6, DRIH method						
205	2	1	7	1	110.069	5.123328E+02	; C2-
206	C1-F7, DRIH method						
207	5	1	6	1	109.455	3.132873E+02	; F5-
208	C1-F6, DRIH method						
209	5	1	7	1	109.293	3.175054E+02	; F5-
210	C1-F7, DRIH method						
211	6	1	7	1	109.164	3.151555E+02	; F6-
212	C1-F7, DRIH method						
213	1	2	3	1	114.404	5.059364E+02	; C1-
214	C2-C3, DRIH method						
215	1	2	8	1	108.510	2.029429E+02	; C1-

216	C2-F8, DRIH method						
217	1	2	9	1	108.180	2.016184E+02	; C1-
218	C2-F9, DRIH method						
219	3	2	8	1	108.065	2.104123E+02	; C3-
220	C2-F8, DRIH method						
221	3	2	9	1	107.955	2.063720E+02	; C3-
222	C2-F9, DRIH method						
223	8	2	9	1	109.672	8.897392E+01	; F8-
224	C2-F9, DRIH method						
225	2	3	4	1	113.769	4.876774E+02	; C2-
226	C3-C4, DRIH method						
227	2	3	10	1	109.268	2.116850E+02	; C2-
228	C3-F10, DRIH method						
229	2	3	11	1	109.270	2.085036E+02	; C2-
230	C3-F11, DRIH method						
231	4	3	10	1	108.854	2.144307E+02	; C4-
232	C3-F10, DRIH method						
233	4	3	11	1	107.222	2.282253E+02	; C4-
234	C3-F11, DRIH method						
235	10	3	11	1	108.313	9.152912E+01	; F10-
236	C3-F11, DRIH method						
237	3	4	12	1	111.004	1.987646E+02	; C3-

238	C4-F12, DRIH method						
239	3	4	13	1	108.776	1.991823E+02	; C3-
240	C4-F13, DRIH method						
241	3	4	14	1	113.856	4.868951E+02	; C3-
242	C4-S14, DRIH method						
243	12	4	13	1	109.858	9.043871E+01	; F12-
244	C4-F13, DRIH method						
245	12	4	14	1	106.445	1.868969E+02	; F12-
246	C4-S14, DRIH method						
247	13	4	14	1	106.774	2.001801E+02	; F13-
248	C4-S14, DRIH method						
249	4	14	15	1	103.637	2.040387E+02	; C4-
250	S14-O15, DRIH method						
251	4	14	16	1	107.216	2.008309E+02	; C4-
252	S14-O16, DRIH method						
253	4	14	17	1	106.554	5.049964E+02	; C4-
254	S14-N17, DRIH method						
255	15	14	16	1	123.544	1.036722E+02	; O15-
256	S14-O16, DRIH method						
257	15	14	17	1	105.929	2.105154E+02	; O15-
258	S14-N17, DRIH method						
259	16	14	17	1	108.817	1.777651E+02	; O16-

260	S14-N17, DRIH method						
261	14	17	18	1	113.576	2.677294E+02	; S14-
262	N17-H18, DRIH method						
263	14	17	19	1	120.064	5.942509E+02	; S14-
264	N17-C19, DRIH method						
265	18	17	19	1	118.847	2.472895E+02	; H18-
266	N17-C19, DRIH method						
267	17	19	20	1	110.665	4.642280E+02	; N17-
268	C19-C20, DRIH method						
269	17	19	21	1	110.701	1.749403E+02	; N17-
270	C19-H21, DRIH method						
271	17	19	22	1	106.970	1.681431E+02	; N17-
272	C19-H22, DRIH method						
273	20	19	21	1	111.782	1.623811E+02	; C20-
274	C19-H21, DRIH method						
275	20	19	22	1	110.343	1.542175E+02	; C20-
276	C19-H22, DRIH method						
277	21	19	22	1	106.175	5.882052E+01	; H21-
278	C19-H22, DRIH method						
279	19	20	23	1	115.569	3.847051E+02	; C19-
280	C20-C23, DRIH method						
281	19	20	24	1	108.539	1.398159E+02	; C19-

282 C20-H24, DRIH method

283   19   20   25   1   108.824   1.452656E+02   ; C19-

284 C20-H25, DRIH method

285   23   20   24   1   109.821   1.427173E+02   ; C23-

286 C20-H24, DRIH method

287   23   20   25   1   107.842   1.505847E+02   ; C23-

288 C20-H25, DRIH method

289   24   20   25   1   105.801   4.711249E+01   ; H24-

290 C20-H25, DRIH method

291   20   23   26   1   110.487   1.444835E+02   ; C20-

292 C23-H26, DRIH method

293   20   23   27   1   113.349   1.316719E+02   ; C20-

294 C23-H27, DRIH method

295   20   23   29   1   113.524   6.278623E+02   ; C20-

296 C23-N29, DRIH method

297   26   23   27   1   107.869   5.309133E+01   ; H26-

298 C23-H27, DRIH method

299   26   23   29   1   105.009   1.849928E+02   ; H26-

300 C23-N29, DRIH method

301   27   23   29   1   106.090   1.878100E+02   ; H27-

302 C23-N29, DRIH method

303   23   29   28   1   106.244   5.795745E+01   ; C23-

304 N29-H28, DRIH method

| 305 | 23 | 29 | 30 | 1 | 111.009 | 2.028011E+02 | ; C23- |

306 N29-C30, DRIH method

| 307 | 23 | 29 | 34 | 1 | 114.204 | 2.088544E+02 | ; C23- |

308 N29-C34, DRIH method

| 309 | 28 | 29 | 30 | 1 | 107.442 | 5.621122E+01 | ; H28- |

310 N29-C30, DRIH method

| 311 | 28 | 29 | 34 | 1 | 106.447 | 5.973121E+01 | ; H28- |

312 N29-C34, DRIH method

| 313 | 30 | 29 | 34 | 1 | 111.047 | 2.026724E+02 | ; C30- |

314 N29-C34, DRIH method

| 315 | 29 | 30 | 31 | 1 | 108.886 | 3.374338E+02 | ; N29- |

316 C30-H31, DRIH method

| 317 | 29 | 30 | 32 | 1 | 109.222 | 3.378771E+02 | ; N29- |

318 C30-H32, DRIH method

| 319 | 29 | 30 | 33 | 1 | 108.501 | 3.374056E+02 | ; N29- |

320 C30-H33, DRIH method

| 321 | 31 | 30 | 32 | 1 | 110.098 | 1.414139E+02 | ; H31- |

322 C30-H32, DRIH method

| 323 | 31 | 30 | 33 | 1 | 109.952 | 1.386289E+02 | ; H31- |

324 C30-H33, DRIH method

| 325 | 32 | 30 | 33 | 1 | 110.147 | 1.399058E+02 | ; H32- |

326 C30-H33, DRIH method

327   29   34   35   1   108.227   3.360063E+02   ; N29-

328 C34-H35, DRIH method

329   29   34   36   1   109.460   3.583962E+02   ; N29-

330 C34-H36, DRIH method

331   29   34   37   1   108.155   3.490619E+02   ; N29-

332 C34-H37, DRIH method

333   35   34   36   1   111.651   1.439548E+02   ; H35-

334 C34-H36, DRIH method

335   35   34   37   1   109.802   1.362082E+02   ; H35-

336 C34-H37, DRIH method

337   36   34   37   1   109.472   1.436319E+02   ; H36-

338 C34-H37, DRIH method

339

340   [angles] ; bond-bond cross term

341   ; atom_i atom_j atom_k functype r0_ij (nm) r0_jk (nm)   k (kJ/mol/nm^2)

342   2   1   5   3   0.155389   0.133166   1.882445E+04

343   ; C2-C1-F5

344   2   1   6   3   0.155389   0.133987   1.857239E+04

345   ; C2-C1-F6

346   2   1   7   3   0.155389   0.133815   1.771504E+04

347   ; C2-C1-F7

348	5	1	6	3	0.133166	0.133987	4.755793E+04
349	; F5-C1-F6						
350	5	1	7	3	0.133166	0.133815	4.815618E+04
351	; F5-C1-F7						
352	6	1	7	3	0.133987	0.133815	4.721050E+04
353	; F6-C1-F7						
354	1	2	3	3	0.155389	0.155443	1.810541E+04
355	; C1-C2-C3						
356	1	2	8	3	0.155389	0.134595	1.632735E+04
357	; C1-C2-F8						
358	1	2	9	3	0.155389	0.135464	1.632810E+04
359	; C1-C2-F9						
360	3	2	8	3	0.155443	0.134595	2.059068E+04
361	; C3-C2-F8						
362	3	2	9	3	0.155443	0.135464	2.062466E+04
363	; C3-C2-F9						
364	8	2	9	3	0.134595	0.135464	4.534865E+04
365	; F8-C2-F9						
366	2	3	4	3	0.155443	0.155337	1.818061E+04
367	; C2-C3-C4						
368	2	3	10	3	0.155443	0.135336	1.643739E+04
369	; C2-C3-F10						

370	2	3	11	3	0.155443	0.136231	1.490990E+04
371	; C2-C3-F11						
372	4	3	10	3	0.155337	0.135336	2.028434E+04
373	; C4-C3-F10						
374	4	3	11	3	0.155337	0.136231	1.959414E+04
375	; C4-C3-F11						
376	10	3	11	3	0.135336	0.136231	4.619977E+04
377	; F10-C3-F11						
378	3	4	12	3	0.155337	0.133683	1.725833E+04
379	; C3-C4-F12						
380	3	4	13	3	0.155337	0.135282	1.654045E+04
381	; C3-C4-F13						
382	3	4	14	3	0.155337	0.190782	1.639006E+04
383	; C3-C4-S14						
384	12	4	13	3	0.133683	0.135282	4.384892E+04
385	; F12-C4-F13						
386	12	4	14	3	0.133683	0.190782	1.765931E+04
387	; F12-C4-S14						
388	13	4	14	3	0.135282	0.190782	1.595542E+04
389	; F13-C4-S14						
390	4	14	15	3	0.190782	0.146875	-2.989052E+03
391	; C4-S14-O15						

392	4	14	16	3	0.190782	0.144959	-3.804864E+03
393	; C4-S14-O16						
394	4	14	17	3	0.190782	0.165882	-1.353775E+02
395	; C4-S14-N17						
396	15	14	16	3	0.146875	0.144959	-5.772634E+03
397	; O15-S14-O16						
398	15	14	17	3	0.146875	0.165882	1.024076E+04
399	; O15-S14-N17						
400	16	14	17	3	0.144959	0.165882	6.187132E+03
401	; O16-S14-N17						
402	14	17	18	3	0.165882	0.101441	3.610517E+03
403	; S14-N17-H18						
404	14	17	19	3	0.165882	0.146927	2.434791E+04
405	; S14-N17-C19						
406	18	17	19	3	0.101441	0.146927	-1.888816E+03
407	; H18-N17-C19						
408	17	19	20	3	0.146927	0.154383	2.411113E+04
409	; N17-C19-C20						
410	17	19	21	3	0.146927	0.109416	9.551602E+03
411	; N17-C19-H21						
412	17	19	22	3	0.146927	0.109285	4.721538E+03
413	; N17-C19-H22						

414	20	19	21	3	0.154383	0.109416	4.297605E+03
415	; C20-C19-H21						
416	20	19	22	3	0.154383	0.109285	4.594315E+03
417	; C20-C19-H22						
418	21	19	22	3	0.109416	0.109285	2.694372E+03
419	; H21-C19-H22						
420	19	20	23	3	0.154383	0.153373	1.165562E+04
421	; C19-C20-C23						
422	19	20	24	3	0.154383	0.109421	1.797977E+03
423	; C19-C20-H24						
424	19	20	25	3	0.154383	0.109387	4.369948E+03
425	; C19-C20-H25						
426	23	20	24	3	0.153373	0.109421	3.703793E+03
427	; C23-C20-H24						
428	23	20	25	3	0.153373	0.109387	2.757998E+03
429	; C23-C20-H25						
430	24	20	25	3	0.109421	0.109387	2.259958E+03
431	; H24-C20-H25						
432	20	23	26	3	0.153373	0.109154	3.844459E+03
433	; C20-C23-H26						
434	20	23	27	3	0.153373	0.109399	5.048128E+03
435	; C20-C23-H27						

436	20	23	29	3	0.153373	0.152797	1.892973E+04
437	; C20-C23-N29						
438	26	23	27	3	0.109154	0.109399	2.115115E+03
439	; H26-C23-H27						
440	26	23	29	3	0.109154	0.152797	3.579857E+03
441	; H26-C23-N29						
442	27	23	29	3	0.109399	0.152797	4.508942E+03
443	; H27-C23-N29						
444	23	29	28	3	0.152797	0.102559	4.774977E+03
445	; C23-N29-H28						
446	23	29	30	3	0.152797	0.150539	1.135273E+04
447	; C23-N29-C30						
448	23	29	34	3	0.152797	0.150895	9.948979E+03
449	; C23-N29-C34						
450	28	29	30	3	0.102559	0.150539	3.668456E+03
451	; H28-N29-C30						
452	28	29	34	3	0.102559	0.150895	4.503013E+03
453	; H28-N29-C34						
454	30	29	34	3	0.150539	0.150895	1.062195E+04
455	; C30-N29-C34						
456	29	30	31	3	0.150539	0.108993	3.233846E+03
457	; N29-C30-H31						

458	29	30	32	3	0.150539	0.109001	3.292064E+03
459	; N29-C30-H32						
460	29	30	33	3	0.150539	0.109053	4.275582E+03
461	; N29-C30-H33						
462	31	30	32	3	0.108993	0.109001	1.534402E+03
463	; H31-C30-H32						
464	31	30	33	3	0.108993	0.109053	1.477296E+03
465	; H31-C30-H33						
466	32	30	33	3	0.109001	0.109053	1.433538E+03
467	; H32-C30-H33						
468	29	34	35	3	0.150895	0.109069	4.341486E+03
469	; N29-C34-H35						
470	29	34	36	3	0.150895	0.108933	3.350185E+03
471	; N29-C34-H36						
472	29	34	37	3	0.150895	0.109037	2.976845E+03
473	; N29-C34-H37						
474	35	34	36	3	0.109069	0.108933	9.045900E+02
475	; H35-C34-H36						
476	35	34	37	3	0.109069	0.109037	1.492227E+03
477	; H35-C34-H37						
478	36	34	37	3	0.108933	0.109037	1.490258E+03
479	; H36-C34-H37						

480

481 [dihedrals] ; propers

482 ; atom_i atom_j atom_k atom_l functype d0 (Deg.) k (kJ/mol/rad^2) ; Case
483 of functype=2

484 ; atom_i atom_j atom_k atom_l functype phase (Deg.) kd (kJ/mol) pn ; Case
485 of functype=9

486   1   2   3   4   2   165.216   5.501244E+01   ;
487 C1-C2-C3-C4, DRIH method

488   1   2   3   10   2   -72.913   6.797000E+01   ;
489 C1-C2-C3-F10, DRIH method

490   1   2   3   11   2   45.434   7.014663E+01   ;
491 C1-C2-C3-F11, DRIH method

492   2   3   4   12   2   42.082   6.549520E+01   ;
493 C2-C3-C4-F12, DRIH method

494   2   3   4   13   2   -78.905   7.028344E+01   ;
495 C2-C3-C4-F13, DRIH method

496   2   3   4   14   2   162.172   5.210252E+01   ;
497 C2-C3-C4-S14, DRIH method

498   3   2   1   5   2   169.998   7.542723E+01   ;
499 C3-C2-C1-F5, DRIH method

500   3   2   1   6   2   50.080   7.325384E+01   ;
501 C3-C2-C1-F6, DRIH method

502	3	2	1	7	2	-70.126	7.660367E+01	;

503 C3-C2-C1-F7, DRIH method

504	3	4	14	15	2	151.120	8.472903E+01	;

505 C3-C4-S14-O15, DRIH method

506	3	4	14	16	2	-76.778	6.859521E+01	;

507 C3-C4-S14-O16, DRIH method

508	3	4	14	17	2	39.605	7.444749E+01	;

509 C3-C4-S14-N17, DRIH method

510	4	3	2	8	2	-73.809	7.117386E+01	;

511 C4-C3-C2-F8, DRIH method

512	4	3	2	9	2	44.741	6.991651E+01	;

513 C4-C3-C2-F9, DRIH method

514	4	14	17	18	2	-74.814	5.023196E+01	;

515 C4-S14-N17-H18, DRIH method

516	4	14	17	19	2	74.597	5.905141E+01	;

517 C4-S14-N17-C19, DRIH method

518	5	1	2	8	2	49.269	8.645564E+01	;

519 F5-C1-C2-F8, DRIH method

520	5	1	2	9	2	-69.651	8.365828E+01	;

521 F5-C1-C2-F9, DRIH method

522	6	1	2	8	2	-70.649	8.558021E+01	;

523 F6-C1-C2-F8, DRIH method

| 524 | 6 | 1 | 2 | 9 | 2 | 170.431 | 8.527121E+01 | ; |

525 F6-C1-C2-F9, DRIH method

| 526 | 7 | 1 | 2 | 8 | 2 | 169.145 | 8.740507E+01 | ; |

527 F7-C1-C2-F8, DRIH method

| 528 | 7 | 1 | 2 | 9 | 2 | 50.225 | 8.629376E+01 | ; |

529 F7-C1-C2-F9, DRIH method

| 530 | 8 | 2 | 3 | 10 | 2 | 48.062 | 7.752231E+01 | ; |

531 F8-C2-C3-F10, DRIH method

| 532 | 8 | 2 | 3 | 11 | 2 | 166.410 | 8.469321E+01 | ; |

533 F8-C2-C3-F11, DRIH method

| 534 | 9 | 2 | 3 | 10 | 2 | 166.611 | 8.206349E+01 | ; |

535 F9-C2-C3-F10, DRIH method

| 536 | 9 | 2 | 3 | 11 | 2 | -75.041 | 8.144385E+01 | ; |

537 F9-C2-C3-F11, DRIH method

| 538 | 10 | 3 | 4 | 12 | 2 | -80.018 | 7.694374E+01 | ; |

539 F10-C3-C4-F12, DRIH method

| 540 | 10 | 3 | 4 | 13 | 2 | 158.995 | 8.507576E+01 | ; |

541 F10-C3-C4-F13, DRIH method

| 542 | 10 | 3 | 4 | 14 | 2 | 40.072 | 6.663090E+01 | ; |

543 F10-C3-C4-S14, DRIH method

| 544 | 11 | 3 | 4 | 12 | 2 | 163.017 | 8.148157E+01 | ; |

545 F11-C3-C4-F12, DRIH method

546	11	3	4	13	2	42.029	7.945049E+01	;

547 F11-C3-C4-F13, DRIH method

548	11	3	4	14	2	-76.894	7.121577E+01	;

549 F11-C3-C4-S14, DRIH method

550	12	4	14	15	2	-86.253	8.590705E+01	;

551 F12-C4-S14-O15, DRIH method

552	12	4	14	16	2	45.848	7.659234E+01	;

553 F12-C4-S14-O16, DRIH method

554	12	4	14	17	2	162.232	7.821634E+01	;

555 F12-C4-S14-N17, DRIH method

556	13	4	14	15	2	31.062	9.087507E+01	;

557 F13-C4-S14-O15, DRIH method

558	13	4	14	16	2	163.164	8.119484E+01	;

559 F13-C4-S14-O16, DRIH method

560	13	4	14	17	2	-80.453	8.233422E+01	;

561 F13-C4-S14-N17, DRIH method

562	14	17	19	20	2	85.664	5.110855E+01	;

563 S14-N17-C19-C20, DRIH method

564	14	17	19	21	2	-38.843	4.057052E+01	;

565 S14-N17-C19-H21, DRIH method

566	14	17	19	22	2	-154.100	4.484969E+01	;

567 S14-N17-C19-H22, DRIH method

568	15	14	17	18	2	175.271	9.258084E+01	;

569 O15-S14-N17-H18, DRIH method

570	15	14	17	19	2	-35.318	9.112091E+01	;

571 O15-S14-N17-C19, DRIH method

572	16	14	17	18	2	40.495	7.185781E+01	;

573 O16-S14-N17-H18, DRIH method

574	16	14	17	19	2	-170.095	8.194380E+01	;

575 O16-S14-N17-C19, DRIH method

576	17	19	20	23	2	-159.808	8.252392E+01	;

577 N17-C19-C20-C23, DRIH method

578	17	19	20	24	2	-35.965	5.353843E+01	;

579 N17-C19-C20-H24, DRIH method

580	17	19	20	25	2	78.729	5.583712E+01	;

581 N17-C19-C20-H25, DRIH method

582	18	17	19	20	2	-126.509	4.407865E+01	;

583 H18-N17-C19-C20, DRIH method

584	18	17	19	21	2	108.984	4.107677E+01	;

585 H18-N17-C19-H21, DRIH method

586	18	17	19	22	2	-6.274	3.585317E+01	;

587 H18-N17-C19-H22, DRIH method

588	19	20	23	26	2	-146.786	5.076100E+01	;

589 C19-C20-C23-H26, DRIH method

| 590 | 19 | 20 | 23 | 27 | 2 | -25.583 | 3.889020E+01 | ; |

591 C19-C20-C23-H27, DRIH method

| 592 | 19 | 20 | 23 | 29 | 2 | 95.558 | 5.695042E+01 | ; |

593 C19-C20-C23-N29, DRIH method

| 594 | 20 | 23 | 29 | 28 | 2 | 48.130 | 3.147030E+01 | ; |

595 C20-C23-N29-H28, DRIH method

| 596 | 20 | 23 | 29 | 30 | 2 | 164.639 | 4.330028E+01 | ; |

597 C20-C23-N29-C30, DRIH method

| 598 | 20 | 23 | 29 | 34 | 2 | -68.890 | 5.391992E+01 | ; |

599 C20-C23-N29-C34, DRIH method

| 600 | 21 | 19 | 20 | 23 | 2 | -35.919 | 4.585445E+01 | ; |

601 H21-C19-C20-C23, DRIH method

| 602 | 21 | 19 | 20 | 24 | 2 | 87.924 | 4.592077E+01 | ; |

603 H21-C19-C20-H24, DRIH method

| 604 | 21 | 19 | 20 | 25 | 2 | -157.382 | 4.144294E+01 | ; |

605 H21-C19-C20-H25, DRIH method

| 606 | 22 | 19 | 20 | 23 | 2 | 81.993 | 5.072570E+01 | ; |

607 H22-C19-C20-C23, DRIH method

| 608 | 22 | 19 | 20 | 24 | 2 | -154.164 | 4.262320E+01 | ; |

609 H22-C19-C20-H24, DRIH method

| 610 | 22 | 19 | 20 | 25 | 2 | -39.470 | 4.341952E+01 | ; |

611 H22-C19-C20-H25, DRIH method

| 612 | 23 | 29 | 30 | 31 | 2 | -176.717 | 4.482127E+01 | ; |

613 C23-N29-C30-H31, DRIH method

| 614 | 23 | 29 | 30 | 32 | 2 | -56.458 | 4.417359E+01 | ; |

615 C23-N29-C30-H32, DRIH method

| 616 | 23 | 29 | 30 | 33 | 2 | 63.628 | 4.379841E+01 | ; |

617 C23-N29-C30-H33, DRIH method

| 618 | 23 | 29 | 34 | 35 | 2 | -58.102 | 4.202271E+01 | ; |

619 C23-N29-C34-H35, DRIH method

| 620 | 23 | 29 | 34 | 36 | 2 | 63.791 | 4.880560E+01 | ; |

621 C23-N29-C34-H36, DRIH method

| 622 | 23 | 29 | 34 | 37 | 2 | -177.005 | 4.369909E+01 | ; |

623 C23-N29-C34-H37, DRIH method

| 624 | 24 | 20 | 23 | 26 | 2 | 90.044 | 4.196900E+01 | ; |

625 H24-C20-C23-H26, DRIH method

| 626 | 24 | 20 | 23 | 27 | 2 | -148.753 | 4.801704E+01 | ; |

627 H24-C20-C23-H27, DRIH method

| 628 | 24 | 20 | 23 | 29 | 2 | -27.612 | 4.214966E+01 | ; |

629 H24-C20-C23-N29, DRIH method

| 630 | 25 | 20 | 23 | 26 | 2 | -24.796 | 4.430040E+01 | ; |

631 H25-C20-C23-H26, DRIH method

| 632 | 25 | 20 | 23 | 27 | 2 | 96.407 | 4.492455E+01 | ; |

633 H25-C20-C23-H27, DRIH method

| 634 | 25 | 20 | 23 | 29 | 2 | -142.452 | 4.917695E+01 | ; |

635 H25-C20-C23-N29, DRIH method

| 636 | 26 | 23 | 29 | 28 | 2 | -72.662 | 3.381445E+01 | ; |

637 H26-C23-N29-H28, DRIH method

| 638 | 26 | 23 | 29 | 30 | 2 | 43.848 | 4.399603E+01 | ; |

639 H26-C23-N29-C30, DRIH method

| 640 | 26 | 23 | 29 | 34 | 2 | 170.318 | 5.035773E+01 | ; |

641 H26-C23-N29-C34, DRIH method

| 642 | 27 | 23 | 29 | 28 | 2 | 173.261 | 3.459394E+01 | ; |

643 H27-C23-N29-H28, DRIH method

| 644 | 27 | 23 | 29 | 30 | 2 | -70.230 | 4.271399E+01 | ; |

645 H27-C23-N29-C30, DRIH method

| 646 | 27 | 23 | 29 | 34 | 2 | 56.241 | 4.150892E+01 | ; |

647 H27-C23-N29-C34, DRIH method

| 648 | 28 | 29 | 30 | 31 | 2 | -60.946 | 3.338447E+01 | ; |

649 H28-N29-C30-H31, DRIH method

| 650 | 28 | 29 | 30 | 32 | 2 | 59.312 | 3.335490E+01 | ; |

651 H28-N29-C30-H32, DRIH method

| 652 | 28 | 29 | 30 | 33 | 2 | 179.399 | 3.344992E+01 | ; |

653 H28-N29-C30-H33, DRIH method

| 654 | 28 | 29 | 34 | 35 | 2 | -175.004 | 3.391175E+01 | ; |

655 H28-N29-C34-H35, DRIH method

| 656 | 28 | 29 | 34 | 36 | 2 | -53.112 | 3.419062E+01 | ; |

657 H28-N29-C34-H36, DRIH method

| 658 | 28 | 29 | 34 | 37 | 2 | 66.092 | 3.278750E+01 | ; |

659 H28-N29-C34-H37, DRIH method

| 660 | 30 | 29 | 34 | 35 | 2 | 68.350 | 4.224944E+01 | ; |

661 C30-N29-C34-H35, DRIH method

| 662 | 30 | 29 | 34 | 36 | 2 | -169.758 | 4.502496E+01 | ; |

663 C30-N29-C34-H36, DRIH method

| 664 | 30 | 29 | 34 | 37 | 2 | -50.554 | 4.145878E+01 | ; |

665 C30-N29-C34-H37, DRIH method

| 666 | 31 | 30 | 29 | 34 | 2 | 55.087 | 4.396626E+01 | ; |

667 H31-C30-N29-C34, DRIH method

| 668 | 32 | 30 | 29 | 34 | 2 | 175.346 | 4.509663E+01 | ; |

669 H32-C30-N29-C34, DRIH method

| 670 | 33 | 30 | 29 | 34 | 2 | -64.568 | 4.399271E+01 | ; |

671 H33-C30-N29-C34, DRIH method

672

673 **1-OA.itp**

674 [moleculetype]

675 ; name   nrexcl

676 1-OA   3

677

678 [atoms]

679 ; Index   type   residue   resname   atom   cgnr   charge   mass

680   1   c3   1   MOL   C1   1   -0.25374112

681 12.010736

682   2   c3   1   MOL   C2   2   0.11213405

683 12.010736

684   3   h1   1   MOL   H3   3   0.06842264

685 1.007941

686   4   h1   1   MOL   H4   4   0.06842264

687 1.007941

688   5   c3   1   MOL   C5   5   0.02372227

689 12.010736

690   6   hc   1   MOL   H6   6   -0.00720387

691 1.007941

692   7   hc   1   MOL   H7   7   -0.00720387

693 1.007941

694	8	c3	1	MOL	C8	8	0.04250598
695	12.010736						
696	9	hc	1	MOL	H9	9	-0.02275900
697	1.007941						
698	10	hc	1	MOL	H10	10	-0.02275900
699	1.007941						
700	11	hc	1	MOL	H11	11	-0.02154117
701	1.007941						
702	12	hc	1	MOL	H12	12	-0.02154117
703	1.007941						
704	13	c3	1	MOL	C13	13	-0.00658163
705	12.010736						
706	14	c3	1	MOL	C14	14	-0.00714000
707	12.010736						
708	15	hc	1	MOL	H15	15	-0.01297870
709	1.007941						
710	16	hc	1	MOL	H16	16	-0.01297870
711	1.007941						
712	17	c3	1	MOL	C17	17	0.12778662
713	12.010736						
714	18	hc	1	MOL	H18	18	0.00074076
715	1.007941						

716	19	hc	1	MOL	H19	19	0.00074076
717	1.007941						
718	20	c3	1	MOL	C20	20	-0.24854561
719	12.010736						
720	21	hc	1	MOL	H21	21	-0.02234380
721	1.007941						
722	22	hc	1	MOL	H22	22	-0.02234380
723	1.007941						
724	23	hc	1	MOL	H23	23	0.05305333
725	1.007941						
726	24	hc	1	MOL	H24	24	0.05305333
727	1.007941						
728	25	hc	1	MOL	H25	25	0.05305333
729	1.007941						
730	26	s6	1	MOL	S26	26	0.88463518
731	32.064787						
732	27	o	1	MOL	O27	27	-0.60431712
733	15.999405						
734	28	o	1	MOL	O28	28	-0.59713493
735	15.999405						
736	29	o	1	MOL	O29	29	-0.59715738
737	15.999405						

738

[bonds]

; atom_i atom_j functype   r0 (nm)   k (kJ/mol/nm^2)

741	1	2	1	0.152563	2.663415E+05	; C1-C2, DRIH

742 method

743	1	3	1	0.109562	3.141027E+05	; C1-H3, DRIH

744 method

745	1	4	1	0.109562	3.141012E+05	; C1-H4, DRIH

746 method

747	1	26	1	0.183645	1.681734E+05	; C1-S26, DRIH

748 method

749	2	5	1	0.153412	2.567887E+05	; C2-C5, DRIH

750 method

751	2	6	1	0.109679	3.123618E+05	; C2-H6, DRIH

752 method

753	2	7	1	0.109679	3.123621E+05	; C2-H7, DRIH

754 method

755	5	8	1	0.153427	2.578053E+05	; C5-C8, DRIH

756 method

757	5	9	1	0.110045	3.026487E+05	; C5-H9, DRIH

758 method

759	5	10	1	0.110045	3.026476E+05	; C5-H10, DRIH

760	method					
761	8	11	1	0.109946	3.053144E+05	; C8-H11, DRIH
762	method					
763	8	12	1	0.109946	3.053133E+05	; C8-H12, DRIH
764	method					
765	8	13	1	0.153380	2.585967E+05	; C8-C13, DRIH
766	method					
767	13	14	1	0.153364	2.591292E+05	; C13-C14, DRIH
768	method					
769	13	15	1	0.109994	3.040938E+05	; C13-H15, DRIH
770	method					
771	13	16	1	0.109994	3.040940E+05	; C13-H16, DRIH
772	method					
773	14	17	1	0.153371	2.594715E+05	; C14-C17, DRIH
774	method					
775	14	18	1	0.109973	3.047853E+05	; C14-H18, DRIH
776	method					
777	14	19	1	0.109973	3.047859E+05	; C14-H19, DRIH
778	method					
779	17	20	1	0.153195	2.640275E+05	; C17-C20, DRIH
780	method					
781	17	21	1	0.109882	3.064708E+05	; C17-H21, DRIH

782 method

783   17   22   1   0.109881   3.064727E+05   ; C17-H22, DRIH
784 method

785   20   23   1   0.109572   3.150316E+05   ; C20-H23, DRIH
786 method

787   20   24   1   0.109626   3.145204E+05   ; C20-H24, DRIH
788 method

789   20   25   1   0.109626   3.145190E+05   ; C20-H25, DRIH
790 method

791   26   27   1   0.148967   4.943792E+05   ; S26-O27, DRIH
792 method

793   26   28   1   0.149223   4.858050E+05   ; S26-O28, DRIH
794 method

795   26   29   1   0.149222   4.858186E+05   ; S26-O29, DRIH
796 method

797

798   [angles]

799   ; atom_i atom_j atom_k functype   a0 (Deg.)   k (kJ/mol/rad^2)

800   2   1   3   1   111.382   1.109620E+02   ; C2-
801 C1-H3, DRIH method

802   2   1   4   1   111.381   1.109576E+02   ; C2-
803 C1-H4, DRIH method

| 804 | 2 | 1 | 26 | 1 | 112.467 | 3.395122E+02 | ; C2- |

805 C1-S26, DRIH method

| 806 | 3 | 1 | 4 | 1 | 108.118 | 4.665041E+01 | ; H3- |

807 C1-H4, DRIH method

| 808 | 3 | 1 | 26 | 1 | 106.605 | 1.163372E+02 | ; H3- |

809 C1-S26, DRIH method

| 810 | 4 | 1 | 26 | 1 | 106.604 | 1.163318E+02 | ; H4- |

811 C1-S26, DRIH method

| 812 | 1 | 2 | 5 | 1 | 113.765 | 3.312877E+02 | ; C1- |

813 C2-C5, DRIH method

| 814 | 1 | 2 | 6 | 1 | 108.132 | 1.293415E+02 | ; C1- |

815 C2-H6, DRIH method

| 816 | 1 | 2 | 7 | 1 | 108.130 | 1.293380E+02 | ; C1- |

817 C2-H7, DRIH method

| 818 | 5 | 2 | 6 | 1 | 110.060 | 1.225712E+02 | ; C5- |

819 C2-H6, DRIH method

| 820 | 5 | 2 | 7 | 1 | 110.059 | 1.225671E+02 | ; C5- |

821 C2-H7, DRIH method

| 822 | 6 | 2 | 7 | 1 | 106.407 | 4.794074E+01 | ; H6- |

823 C2-H7, DRIH method

| 824 | 2 | 5 | 8 | 1 | 113.418 | 3.340161E+02 | ; C2- |

825 C5-C8, DRIH method

826	2	5	9	1	109.566	1.254069E+02	; C2-
827	C5-H9, DRIH method						
828	2	5	10	1	109.566	1.254090E+02	; C2-
829	C5-H10, DRIH method						
830	8	5	9	1	109.090	1.278591E+02	; C8-
831	C5-H9, DRIH method						
832	8	5	10	1	109.090	1.278600E+02	; C8-
833	C5-H10, DRIH method						
834	9	5	10	1	105.829	4.777833E+01	; H9-
835	C5-H10, DRIH method						
836	5	8	11	1	109.141	1.274413E+02	; C5-
837	C8-H11, DRIH method						
838	5	8	12	1	109.141	1.274388E+02	; C5-
839	C8-H12, DRIH method						
840	5	8	13	1	113.914	3.385019E+02	; C5-
841	C8-C13, DRIH method						
842	11	8	12	1	105.816	4.761773E+01	; H11-
843	C8-H12, DRIH method						
844	11	8	13	1	109.257	1.283781E+02	; H11-
845	C8-C13, DRIH method						
846	12	8	13	1	109.256	1.283781E+02	; H12-
847	C8-C13, DRIH method						

848	8	13	14	1	113.802	3.392823E+02	; C8-
849	C13-C14, DRIH method						
850	8	13	15	1	109.275	1.276770E+02	; C8-
851	C13-H15, DRIH method						
852	8	13	16	1	109.275	1.276711E+02	; C8-
853	C13-H16, DRIH method						
854	14	13	15	1	109.176	1.282535E+02	; C14-
855	C13-H15, DRIH method						
856	14	13	16	1	109.176	1.282552E+02	; C14-
857	C13-H16, DRIH method						
858	15	13	16	1	105.831	4.767793E+01	; H15-
859	C13-H16, DRIH method						
860	13	14	17	1	113.823	3.394577E+02	; C13-
861	C14-C17, DRIH method						
862	13	14	18	1	109.291	1.275907E+02	; C13-
863	C14-H18, DRIH method						
864	13	14	19	1	109.290	1.275847E+02	; C13-
865	C14-H19, DRIH method						
866	17	14	18	1	109.154	1.286192E+02	; C17-
867	C14-H18, DRIH method						
868	17	14	19	1	109.154	1.286182E+02	; C17-
869	C14-H19, DRIH method						

| 870 | 18 | 14 | 19 | 1 | 105.820 | 4.770128E+01 | ; H18- |

871 C14-H19, DRIH method

| 872 | 14 | 17 | 20 | 1 | 113.408 | 3.429247E+02 | ; C14- |

873 C17-C20, DRIH method

| 874 | 14 | 17 | 21 | 1 | 109.204 | 1.279241E+02 | ; C14- |

875 C17-H21, DRIH method

| 876 | 14 | 17 | 22 | 1 | 109.204 | 1.279260E+02 | ; C14- |

877 C17-H22, DRIH method

| 878 | 20 | 17 | 21 | 1 | 109.430 | 1.275658E+02 | ; C20- |

879 C17-H21, DRIH method

| 880 | 20 | 17 | 22 | 1 | 109.430 | 1.275648E+02 | ; C20- |

881 C17-H22, DRIH method

| 882 | 21 | 17 | 22 | 1 | 105.890 | 4.801252E+01 | ; H21- |

883 C17-H22, DRIH method

| 884 | 17 | 20 | 23 | 1 | 111.707 | 2.637665E+02 | ; C17- |

885 C20-H23, DRIH method

| 886 | 17 | 20 | 24 | 1 | 111.134 | 2.699589E+02 | ; C17- |

887 C20-H24, DRIH method

| 888 | 17 | 20 | 25 | 1 | 111.134 | 2.699478E+02 | ; C17- |

889 C20-H25, DRIH method

| 890 | 23 | 20 | 24 | 1 | 107.660 | 1.369120E+02 | ; H23- |

891 C20-H24, DRIH method

892	23	20	25	1	107.660	1.369107E+02	; H23-

893 C20-H25, DRIH method

894	24	20	25	1	107.344	1.364444E+02	; H24-

895 C20-H25, DRIH method

896	1	26	27	1	103.715	6.546967E+02	; C1-

897 S26-O27, DRIH method

898	1	26	28	1	104.049	6.816576E+02	; C1-

899 S26-O28, DRIH method

900	1	26	29	1	104.050	6.816158E+02	; C1-

901 S26-O29, DRIH method

902	27	26	28	1	114.467	3.035863E+02	; O27-

903 S26-O28, DRIH method

904	27	26	29	1	114.467	3.035918E+02	; O27-

905 S26-O29, DRIH method

906	28	26	29	1	114.242	3.059318E+02	; O28-

907 S26-O29, DRIH method

908

909 [angles] ; bond-bond cross term

910 ; atom_i   atom_j   atom_k   functype   r0_ij (nm)   r0_jk (nm)   k (kJ/mol/nm^2)

911	2	1	3	3	0.152563	0.109562	4.851409E+03

912   ; C2-C1-H3

913	2	1	4	3	0.152563	0.109562	4.851491E+03

914	; C2-C1-H4						
915	2	1	26	3	0.152563	0.183645	9.986385E+03
916	; C2-C1-S26						
917	3	1	4	3	0.109562	0.109562	1.999650E+03
918	; H3-C1-H4						
919	3	1	26	3	0.109562	0.183645	9.320733E+02
920	; H3-C1-S26						
921	4	1	26	3	0.109562	0.183645	9.319382E+02
922	; H4-C1-S26						
923	1	2	5	3	0.152563	0.153412	8.765801E+03
924	; C1-C2-C5						
925	1	2	6	3	0.152563	0.109679	5.863601E+03
926	; C1-C2-H6						
927	1	2	7	3	0.152563	0.109679	5.864288E+03
928	; C1-C2-H7						
929	5	2	6	3	0.153412	0.109679	4.847278E+03
930	; C5-C2-H6						
931	5	2	7	3	0.153412	0.109679	4.847513E+03
932	; C5-C2-H7						
933	6	2	7	3	0.109679	0.109679	2.541394E+03
934	; H6-C2-H7						
935	2	5	8	3	0.153412	0.153427	8.713447E+03

936	; C2-C5-C8						
937	2	5	9	3	0.153412	0.110045	5.950534E+03
938	; C2-C5-H9						
939	2	5	10	3	0.153412	0.110045	5.950933E+03
940	; C2-C5-H10						
941	8	5	9	3	0.153427	0.110045	5.315236E+03
942	; C8-C5-H9						
943	8	5	10	3	0.153427	0.110045	5.315521E+03
944	; C8-C5-H10						
945	9	5	10	3	0.110045	0.110045	3.218401E+03
946	; H9-C5-H10						
947	5	8	11	3	0.153427	0.109946	5.492264E+03
948	; C5-C8-H11						
949	5	8	12	3	0.153427	0.109946	5.492059E+03
950	; C5-C8-H12						
951	5	8	13	3	0.153427	0.153380	8.522585E+03
952	; C5-C8-C13						
953	11	8	12	3	0.109946	0.109946	3.036735E+03
954	; H11-C8-H12						
955	11	8	13	3	0.109946	0.153380	5.259223E+03
956	; H11-C8-C13						
957	12	8	13	3	0.109946	0.153380	5.259897E+03

958	; H12-C8-C13						
959	8	13	14	3	0.153380	0.153364	8.560891E+03
960	; C8-C13-C14						
961	8	13	15	3	0.153380	0.109994	5.628965E+03
962	; C8-C13-H15						
963	8	13	16	3	0.153380	0.109994	5.629309E+03
964	; C8-C13-H16						
965	14	13	15	3	0.153364	0.109994	5.336049E+03
966	; C14-C13-H15						
967	14	13	16	3	0.153364	0.109994	5.335599E+03
968	; C14-C13-H16						
969	15	13	16	3	0.109994	0.109994	3.096432E+03
970	; H15-C13-H16						
971	13	14	17	3	0.153364	0.153371	8.488262E+03
972	; C13-C14-C17						
973	13	14	18	3	0.153364	0.109973	5.478890E+03
974	; C13-C14-H18						
975	13	14	19	3	0.153364	0.109973	5.478517E+03
976	; C13-C14-H19						
977	17	14	18	3	0.153371	0.109973	5.363622E+03
978	; C17-C14-H18						
979	17	14	19	3	0.153371	0.109973	5.363893E+03

980	; C17-C14-H19						
981	18	14	19	3	0.109973	0.109973	3.049275E+03
982	; H18-C14-H19						
983	14	17	20	3	0.153371	0.153195	8.388200E+03
984	; C14-C17-C20						
985	14	17	21	3	0.153371	0.109882	5.745327E+03
986	; C14-C17-H21						
987	14	17	22	3	0.153371	0.109881	5.744770E+03
988	; C14-C17-H22						
989	20	17	21	3	0.153195	0.109882	5.298304E+03
990	; C20-C17-H21						
991	20	17	22	3	0.153195	0.109881	5.298487E+03
992	; C20-C17-H22						
993	21	17	22	3	0.109882	0.109881	3.188155E+03
994	; H21-C17-H22						
995	17	20	23	3	0.153195	0.109572	4.779416E+03
996	; C17-C20-H23						
997	17	20	24	3	0.153195	0.109626	5.575009E+03
998	; C17-C20-H24						
999	17	20	25	3	0.153195	0.109626	5.575191E+03
1000	; C17-C20-H25						
1001	23	20	24	3	0.109572	0.109626	2.490924E+03

1002   ; H23-C20-H24

1003   23   20   25   3   0.109572   0.109626   2.490950E+03

1004   ; H23-C20-H25

1005   24   20   25   3   0.109626   0.109626   2.501880E+03

1006   ; H24-C20-H25

1007   1   26   27   3   0.183645   0.148967   8.293024E+03

1008   ; C1-S26-O27

1009   1   26   28   3   0.183645   0.149223   9.374970E+03

1010   ; C1-S26-O28

1011   1   26   29   3   0.183645   0.149222   9.374324E+03

1012   ; C1-S26-O29

1013   27   26   28   3   0.148967   0.149223   7.346307E+03

1014   ; O27-S26-O28

1015   27   26   29   3   0.148967   0.149222   7.346687E+03

1016   ; O27-S26-O29

1017   28   26   29   3   0.149223   0.149222   8.129384E+03

1018   ; O28-S26-O29

1019

1020   [dihedrals] ; propers

1021   ; atom_i atom_j atom_k atom_l functype   d0 (Deg.)   k (kJ/mol/rad^2)   ; Case

1022 of functype=2

1023   ; atom_i atom_j atom_k atom_l functype phase (Deg.) kd (kJ/mol) pn   ; Case

1024	of functype=9							
1025	1	2	5	8	2	179.999	3.672017E+01	;
1026	C1-C2-C5-C8, DRIH method							
1027	1	2	5	9	2	-57.848	3.728205E+01	;
1028	C1-C2-C5-H9, DRIH method							
1029	1	2	5	10	2	57.845	3.728168E+01	;
1030	C1-C2-C5-H10, DRIH method							
1031	2	1	26	27	2	179.998	6.924459E+01	;
1032	C2-C1-S26-O27, DRIH method							
1033	2	1	26	28	2	-59.967	6.745119E+01	;
1034	C2-C1-S26-O28, DRIH method							
1035	2	1	26	29	2	59.962	6.744855E+01	;
1036	C2-C1-S26-O29, DRIH method							
1037	2	5	8	11	2	-57.594	3.654782E+01	;
1038	C2-C5-C8-H11, DRIH method							
1039	2	5	8	12	2	57.611	3.654732E+01	;
1040	C2-C5-C8-H12, DRIH method							
1041	2	5	8	13	2	-179.992	3.563625E+01	;
1042	C2-C5-C8-C13, DRIH method							
1043	3	1	2	5	2	-60.400	3.451001E+01	;
1044	H3-C1-C2-C5, DRIH method							
1045	3	1	2	6	2	62.185	3.899513E+01	;

1046 H3-C1-C2-H6, DRIH method

1047	3	1	2	7	2	177.017	3.597336E+01	;

1048 H3-C1-C2-H7, DRIH method

1049	3	1	26	27	2	57.653	6.767273E+01	;

1050 H3-C1-S26-O27, DRIH method

1051	3	1	26	28	2	177.689	6.694277E+01	;

1052 H3-C1-S26-O28, DRIH method

1053	3	1	26	29	2	-62.383	7.089335E+01	;

1054 H3-C1-S26-O29, DRIH method

1055	4	1	2	5	2	60.393	3.451041E+01	;

1056 H4-C1-C2-C5, DRIH method

1057	4	1	2	6	2	-177.023	3.597248E+01	;

1058 H4-C1-C2-H6, DRIH method

1059	4	1	2	7	2	-62.190	3.899662E+01	;

1060 H4-C1-C2-H7, DRIH method

1061	4	1	26	27	2	-57.660	6.767288E+01	;

1062 H4-C1-S26-O27, DRIH method

1063	4	1	26	28	2	62.376	7.089472E+01	;

1064 H4-C1-S26-O28, DRIH method

1065	4	1	26	29	2	-177.695	6.694288E+01	;

1066 H4-C1-S26-O29, DRIH method

1067	5	2	1	26	2	179.995	3.314755E+01	;

1068	C5-C2-C1-S26, DRIH method							
1069	5	8	13	14	2	-179.997	3.612331E+01	;
1070	C5-C8-C13-C14, DRIH method							
1071	5	8	13	15	2	57.687	3.670647E+01	;
1072	C5-C8-C13-H15, DRIH method							
1073	5	8	13	16	2	-57.682	3.670731E+01	;
1074	C5-C8-C13-H16, DRIH method							
1075	6	2	1	26	2	-57.420	3.456126E+01	;
1076	H6-C2-C1-S26, DRIH method							
1077	6	2	5	8	2	58.480	3.684414E+01	;
1078	H6-C2-C5-C8, DRIH method							
1079	6	2	5	9	2	-179.367	3.766193E+01	;
1080	H6-C2-C5-H9, DRIH method							
1081	6	2	5	10	2	-63.674	4.034372E+01	;
1082	H6-C2-C5-H10, DRIH method							
1083	7	2	1	26	2	57.412	3.456347E+01	;
1084	H7-C2-C1-S26, DRIH method							
1085	7	2	5	8	2	-58.485	3.684387E+01	;
1086	H7-C2-C5-C8, DRIH method							
1087	7	2	5	9	2	63.668	4.034402E+01	;
1088	H7-C2-C5-H9, DRIH method							
1089	7	2	5	10	2	179.361	3.766201E+01	;

1090	H7-C2-C5-H10, DRIH method							
1091	8	13	14	17	2	-179.984	3.534660E+01	;
1092	C8-C13-C14-C17, DRIH method							
1093	8	13	14	18	2	-57.671	3.674790E+01	;
1094	C8-C13-C14-H18, DRIH method							
1095	8	13	14	19	2	57.703	3.674748E+01	;
1096	C8-C13-C14-H19, DRIH method							
1097	9	5	8	11	2	179.989	3.744211E+01	;
1098	H9-C5-C8-H11, DRIH method							
1099	9	5	8	12	2	-64.806	4.011089E+01	;
1100	H9-C5-C8-H12, DRIH method							
1101	9	5	8	13	2	57.591	3.663112E+01	;
1102	H9-C5-C8-C13, DRIH method							
1103	10	5	8	11	2	64.824	4.011165E+01	;
1104	H10-C5-C8-H11, DRIH method							
1105	10	5	8	12	2	-179.971	3.744216E+01	;
1106	H10-C5-C8-H12, DRIH method							
1107	10	5	8	13	2	-57.574	3.663149E+01	;
1108	H10-C5-C8-C13, DRIH method							
1109	11	8	13	14	2	57.669	3.673859E+01	;
1110	H11-C8-C13-C14, DRIH method							
1111	11	8	13	15	2	-64.647	4.013621E+01	;

1112 H11-C8-C13-H15, DRIH method

| 1113 | 11 | 8 | 13 | 16 | 2 | 179.984 | 3.760226E+01 | ; |

1114 H11-C8-C13-H16, DRIH method

| 1115 | 12 | 8 | 13 | 14 | 2 | -57.663 | 3.673762E+01 | ; |

1116 H12-C8-C13-C14, DRIH method

| 1117 | 12 | 8 | 13 | 15 | 2 | -179.979 | 3.760154E+01 | ; |

1118 H12-C8-C13-H15, DRIH method

| 1119 | 12 | 8 | 13 | 16 | 2 | 64.652 | 4.013684E+01 | ; |

1120 H12-C8-C13-H16, DRIH method

| 1121 | 13 | 14 | 17 | 20 | 2 | -179.997 | 3.601719E+01 | ; |

1122 C13-C14-C17-C20, DRIH method

| 1123 | 13 | 14 | 17 | 21 | 2 | -57.678 | 3.673575E+01 | ; |

1124 C13-C14-C17-H21, DRIH method

| 1125 | 13 | 14 | 17 | 22 | 2 | 57.684 | 3.673428E+01 | ; |

1126 C13-C14-C17-H22, DRIH method

| 1127 | 14 | 17 | 20 | 23 | 2 | -179.996 | 3.685649E+01 | ; |

1128 C14-C17-C20-H23, DRIH method

| 1129 | 14 | 17 | 20 | 24 | 2 | -59.735 | 3.639392E+01 | ; |

1130 C14-C17-C20-H24, DRIH method

| 1131 | 14 | 17 | 20 | 25 | 2 | 59.742 | 3.639223E+01 | ; |

1132 C14-C17-C20-H25, DRIH method

| 1133 | 15 | 13 | 14 | 17 | 2 | -57.614 | 3.654973E+01 | ; |

1134 H15-C13-C14-C17, DRIH method

1135	15	13	14	18	2	64.700	4.020571E+01	;

1136 H15-C13-C14-H18, DRIH method

1137	15	13	14	19	2	-179.926	3.763499E+01	;

1138 H15-C13-C14-H19, DRIH method

1139	16	13	14	17	2	57.647	3.654887E+01	;

1140 H16-C13-C14-C17, DRIH method

1141	16	13	14	18	2	179.960	3.763483E+01	;

1142 H16-C13-C14-H18, DRIH method

1143	16	13	14	19	2	-64.666	4.020407E+01	;

1144 H16-C13-C14-H19, DRIH method

1145	18	14	17	20	2	57.615	3.687264E+01	;

1146 H18-C14-C17-C20, DRIH method

1147	18	14	17	21	2	179.934	3.763414E+01	;

1148 H18-C14-C17-H21, DRIH method

1149	18	14	17	22	2	-64.704	4.028496E+01	;

1150 H18-C14-C17-H22, DRIH method

1151	19	14	17	20	2	-57.609	3.687216E+01	;

1152 H19-C14-C17-C20, DRIH method

1153	19	14	17	21	2	64.710	4.028563E+01	;

1154 H19-C14-C17-H21, DRIH method

1155	19	14	17	22	2	-179.928	3.763273E+01	;

1156 H19-C14-C17-H22, DRIH method

| 1157 | 21 | 17 | 20 | 23 | 2 | 57.810 | 3.808950E+01 | ; |

1158 H21-C17-C20-H23, DRIH method

| 1159 | 21 | 17 | 20 | 24 | 2 | 178.071 | 3.764281E+01 | ; |

1160 H21-C17-C20-H24, DRIH method

| 1161 | 21 | 17 | 20 | 25 | 2 | -62.451 | 3.989287E+01 | ; |

1162 H21-C17-C20-H25, DRIH method

| 1163 | 22 | 17 | 20 | 23 | 2 | -57.803 | 3.808981E+01 | ; |

1164 H22-C17-C20-H23, DRIH method

| 1165 | 22 | 17 | 20 | 24 | 2 | 62.458 | 3.989391E+01 | ; |

1166 H22-C17-C20-H24, DRIH method

| 1167 | 22 | 17 | 20 | 25 | 2 | -178.064 | 3.764286E+01 | ; |

1168 H22-C17-C20-H25, DRIH method

1169

1170 **SPC/E.itp**

1171 [moleculetype]

1172 ; molnamenrexcl

1173 SOL   2

1174

1175 [atoms]

1176 ; nr   type   resnr residue   atom   cgnr   charge   mass

1177   1   OWSPCE   1   SOL   OW   1   -0.8476

1178   2   HWSPCE   1   SOL   HW1   1   0.4238

1179   3   HWSPCE   1   SOL   HW2   1   0.4238

1180

1181 #ifndef FLEXIBLE

1182 [settles]

1183 ; OW funct   doh dhh

1184 1 1   0.1 0.16330

1185

1186 [exclusions]

1187 1 2   3

1188 2 1   3

1189 3 1   2

```
1190    #else

1191    [ bonds ]

1192    ; i j   funct   length   force.c.

1193    1 2   1   0.1 345000  0.1      345000

1194    1 3   1   0.1 345000  0.1      345000

1195

1196    [ angles ]

1197    ; i j   k   funct   angle   force.c.

1198    2 1   3   1   109.47  383 109.47  383

1199    #endif
```