

## **Competitive double-switched Self-Assembled Cyclic Peptide Nanotubes: a dual internal and external control**

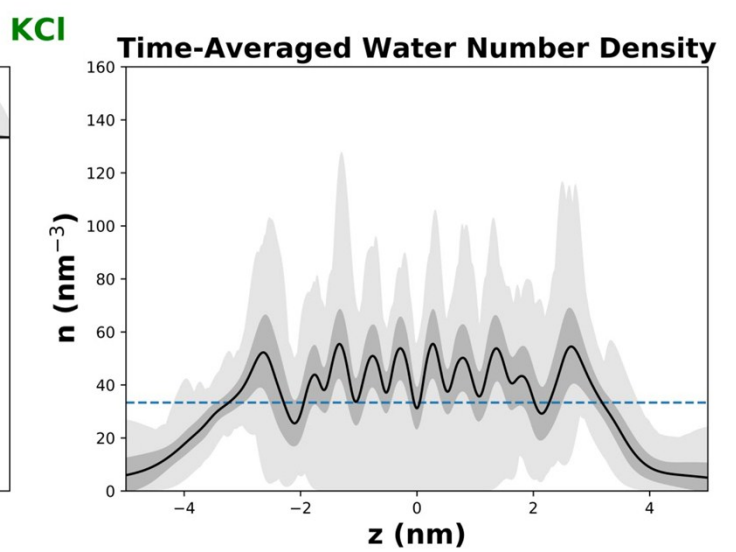
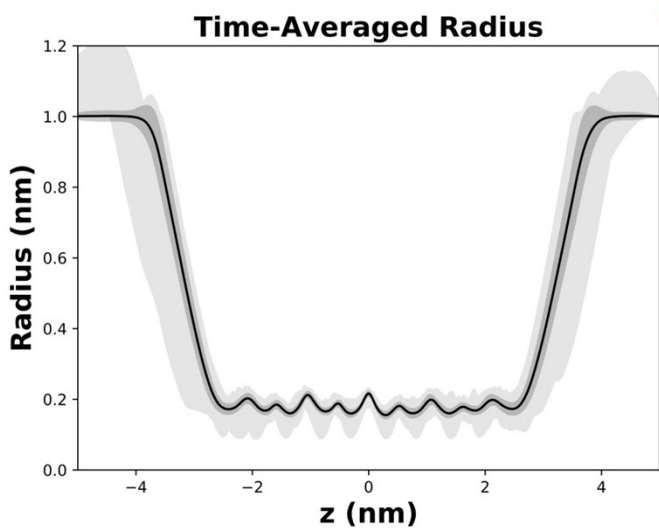
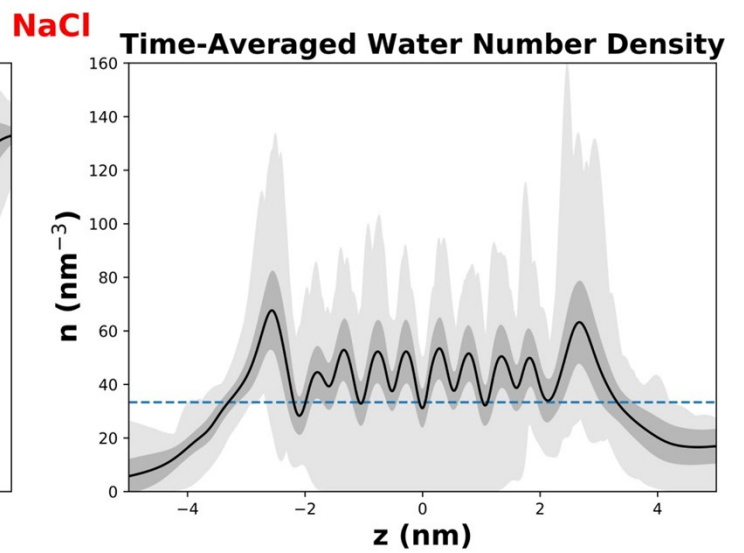
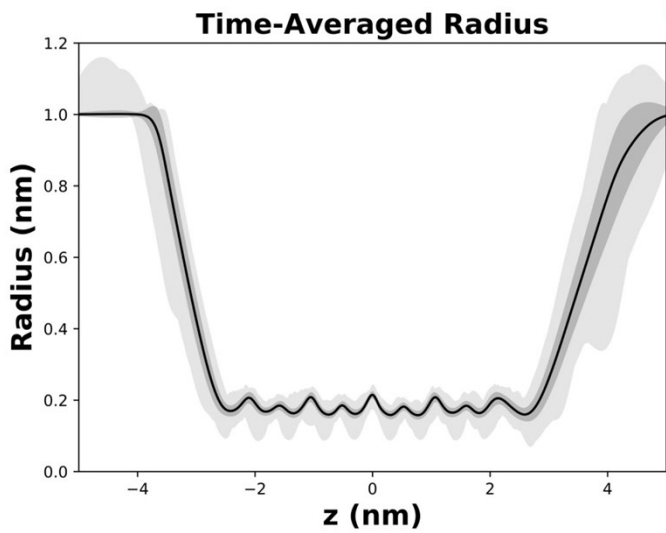
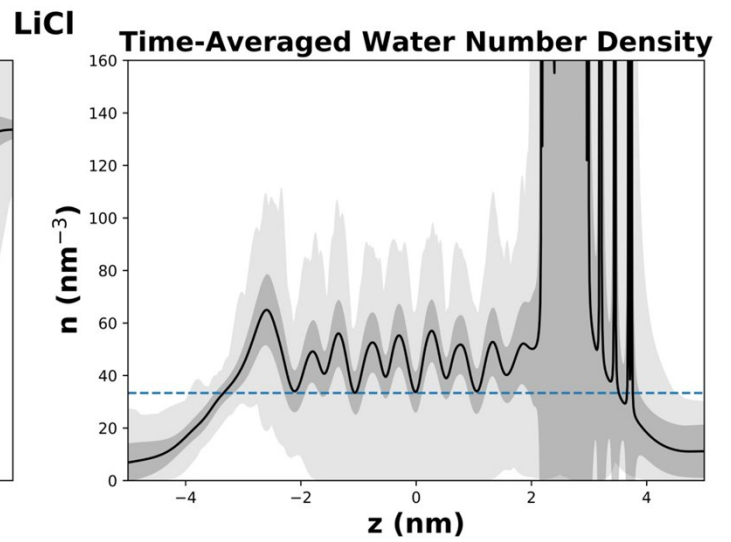
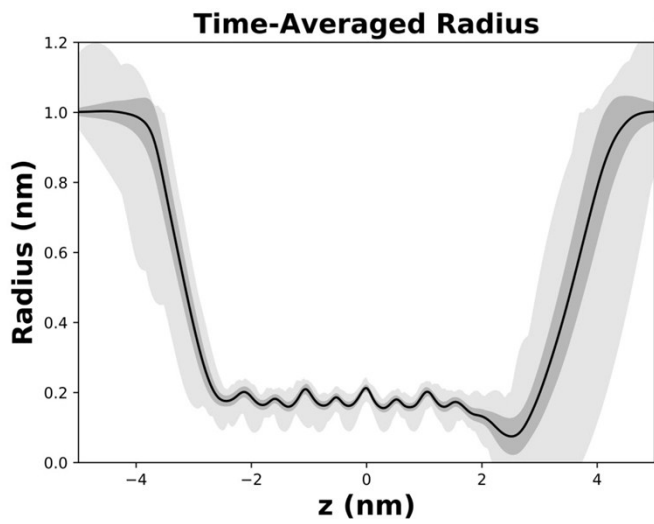
*Martín Calvelo, Juan R. Granja, Rebeca Garcia-Fandiño\**

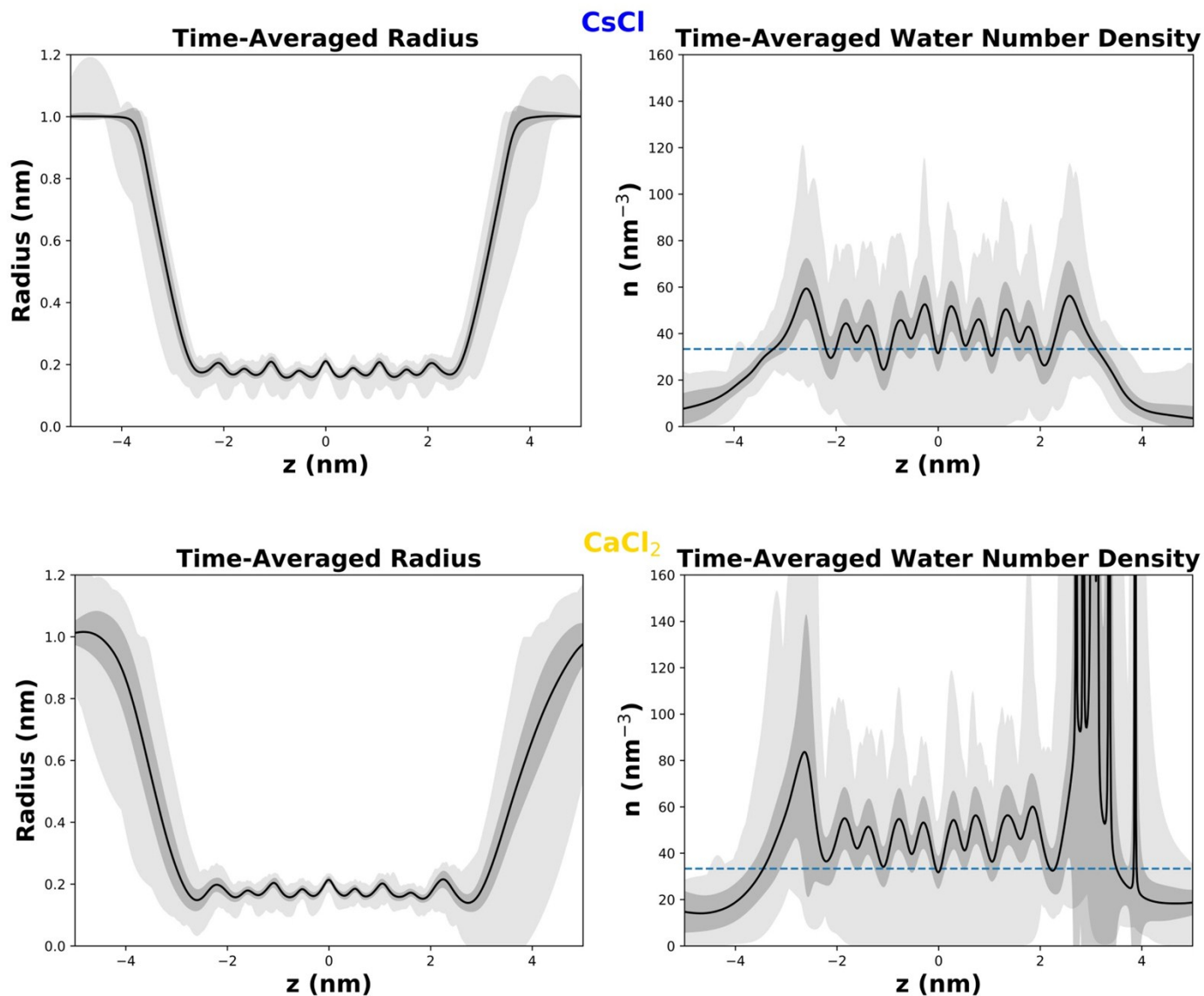
Centro Singular de Investigación en Química Biolóxica e Materiais Moleculares (CiQUS), Departamento de  
Química Orgánica, Universidade de Santiago de Compostela, 15782 Santiago de Compostela (Spain)

\*To whom correspondence should be addressed.

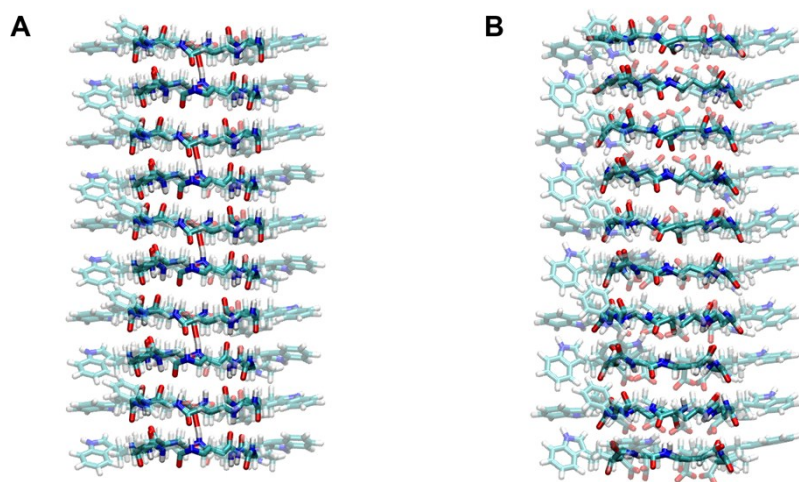
E-mail: [rebeca.garcia.fandino@usc.es](mailto:rebeca.garcia.fandino@usc.es)

## **Supporting Information**

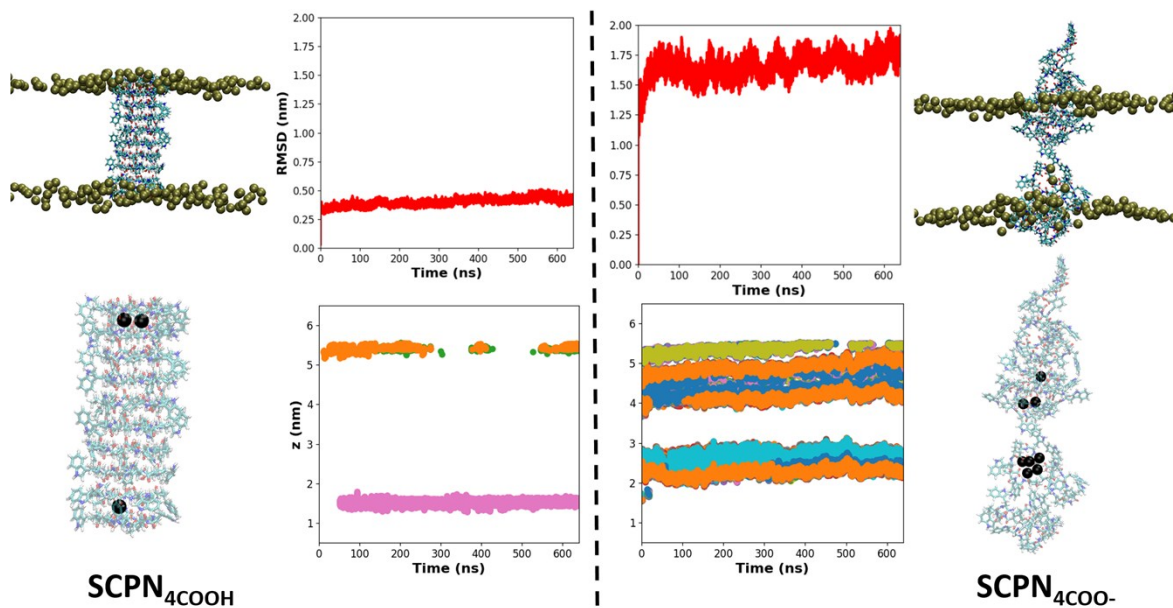




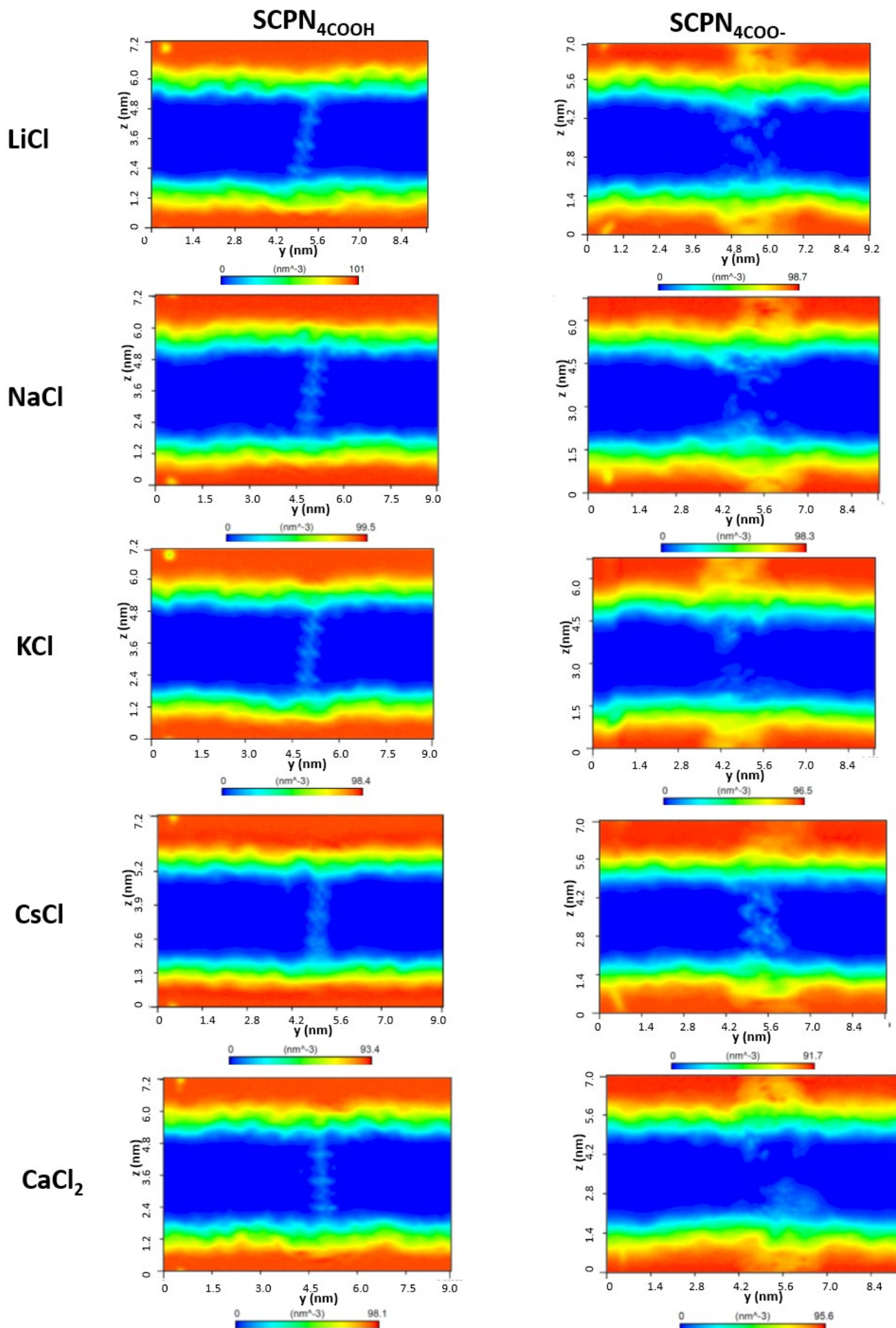
**Figure S1:** Minimum radius of SCPN<sub>4</sub>COOH (left) and 2D-density map for water inside the channels (right) for the simulations carried out in different salt concentrations, averaged from 200 ns.



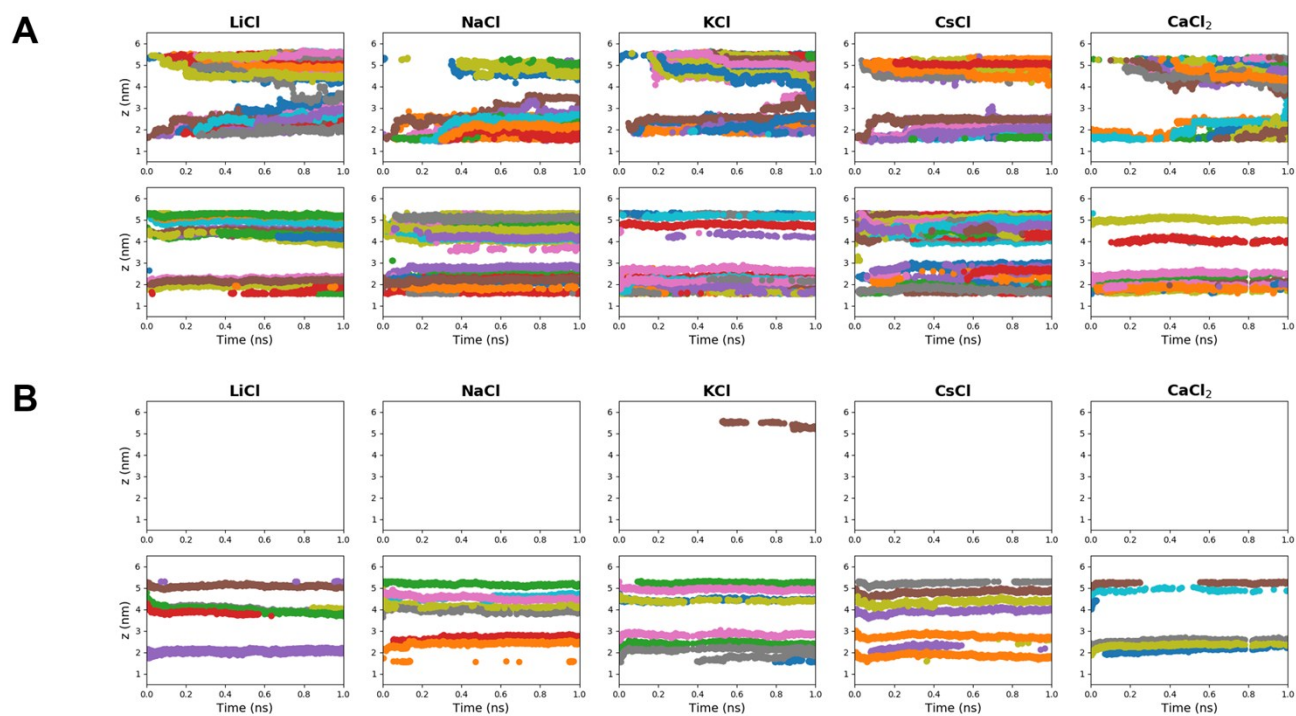
**Figure S2:** Snapshot of the initial structure of SCPN<sub>4</sub>COO<sup>-</sup> (A) and the same structure after minimization (B). It can be noticed that the H-bond network is already distorted just after the initial minimization (B).



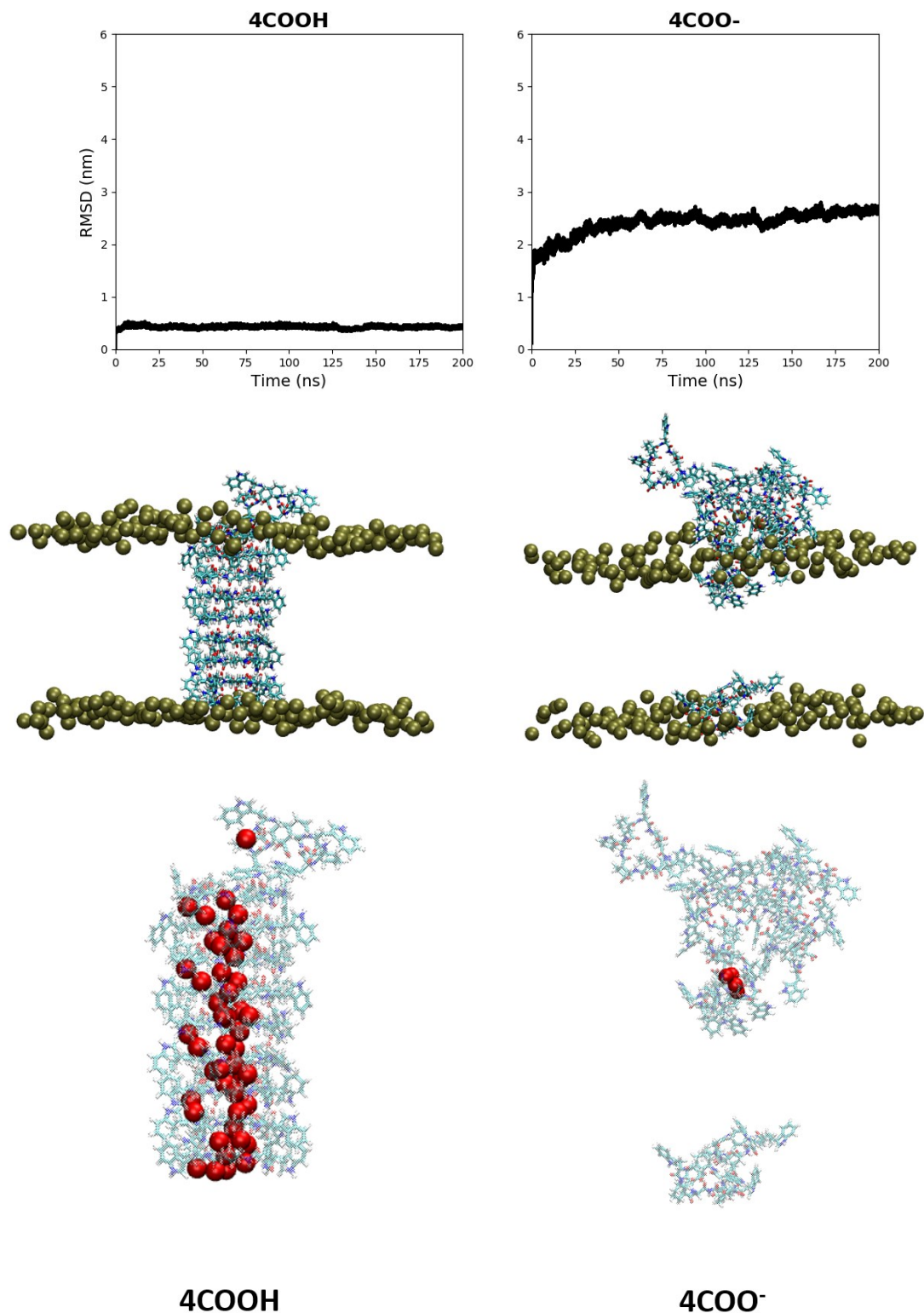
**Figure S3:** Snapshots ( $t = 640$  ns) of the two simulated  $\text{SCPN}_{4\text{COOH}}$  and  $\text{SCPN}_{4\text{COO}^-}$  in NaCl 0.5M. The graphics correspond to the RMSD for  $\text{SCPN}_{4\text{COOH}}$  and  $\text{SCPN}_{4\text{COO}^-}$  along 640 ns and considering all atoms of the SCPN (top) and to the Z-coordinate for each of the cations inside the SCPNs along the 640 ns trajectory. The nanotube z-region is comprehended between the region  $\approx 1-6$  nm. Each color corresponds to a different ion. Lipids, water and external ions have been removed for clarity. Brown spheres correspond to the phosphorous from the lipids and black circles are the corresponding ions.



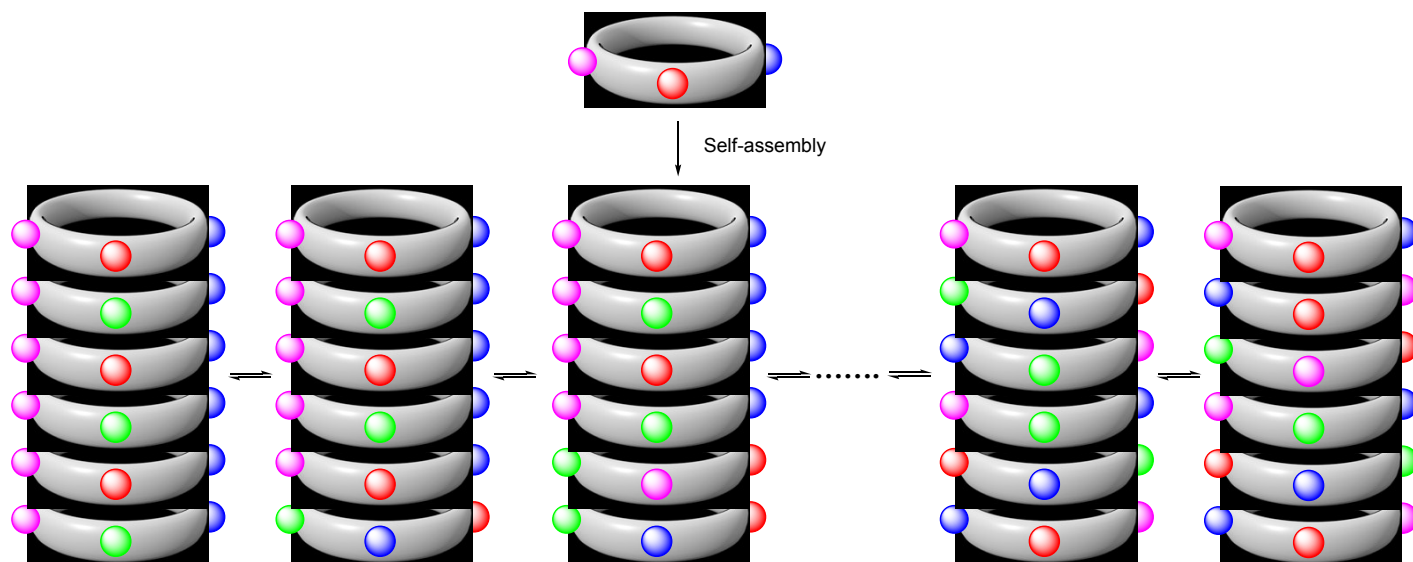
**Figure S4:** 2D-density map for water for the system  $\text{SCPN}_{4\text{COOH}}$  and  $\text{SCPN}_{4\text{COO}^-}$  simulated in different salt concentrations, averaged from 200 ns of MD simulation.



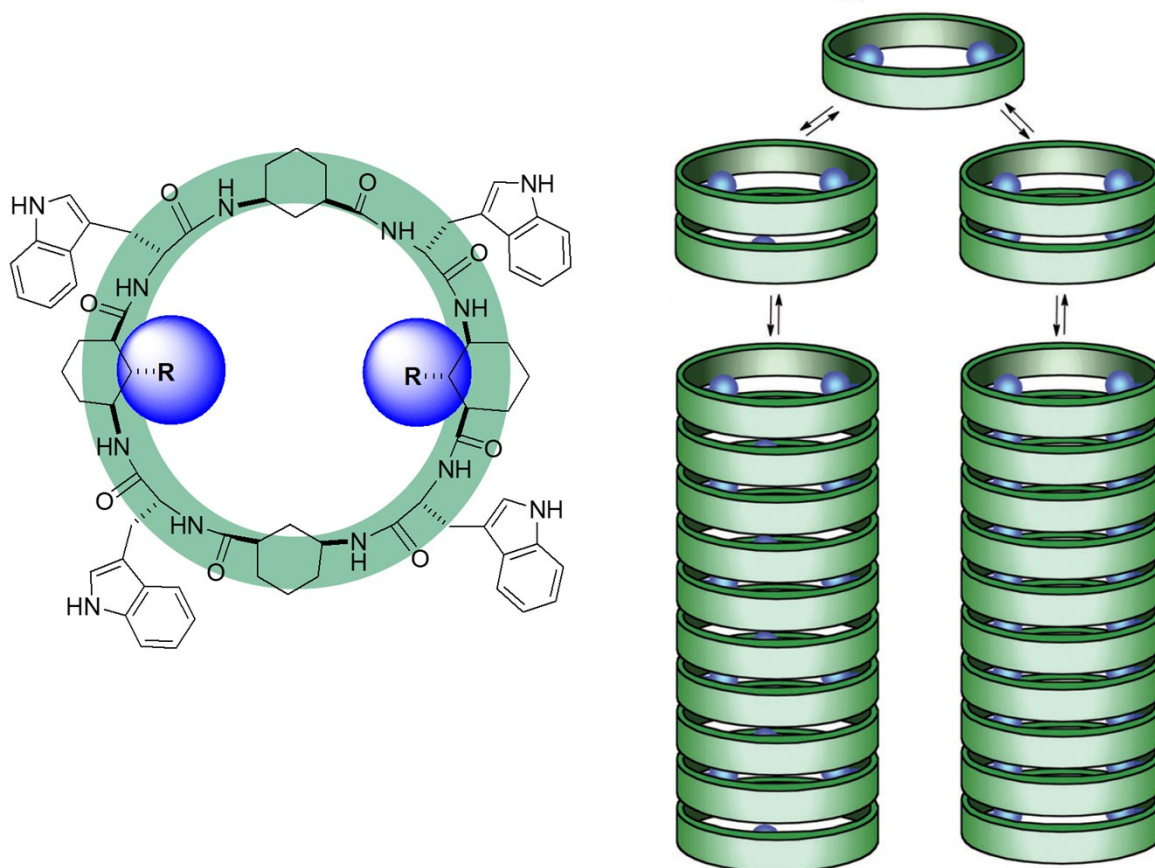
**Figure S5:** Detail of the filling of the channels with water molecules (A) and ions (B) for the protonated (top) and deprotonated (bottom) SCPNs,  $\text{SCP}_{\text{N}4\text{COOH}}$  and  $\text{SCP}_{\text{N}4\text{COO}^-}$ , respectively.



**Figure S6.** RMSD for the two derivatized nanotubes SCPN<sub>4</sub>COOH and SCPN<sub>4</sub>COO<sup>-</sup>, simulated without ions (except for the minima amount of Na<sup>+</sup> to maintain the system neutral in the case of SCPN<sub>4</sub>COO<sup>-</sup>), for 200 ns. Snapshots of the two simulated SCPN<sub>4</sub>COOH and SCPN<sub>4</sub>COO<sup>-</sup>, in these conditions after 200 ns of simulation. Lipids, water and external ions have been removed for clarity. Brown spheres correspond to the phosphorous from the lipids and red spheres correspond to the oxygen of water molecules.

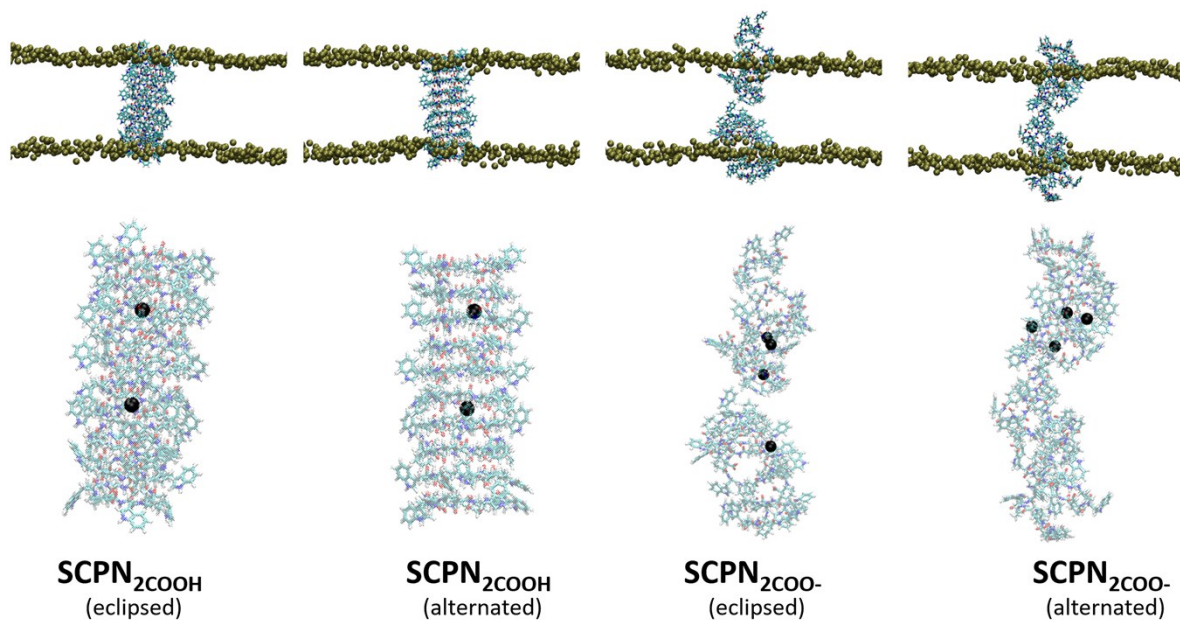


**Figure S7:** Illustration of the multiple possibilities of organization of the charged groups along the SCPN due to freedom of rotation among the CPs. For a clearer view, the charged groups are placed in the outer surface of the SCPNs.

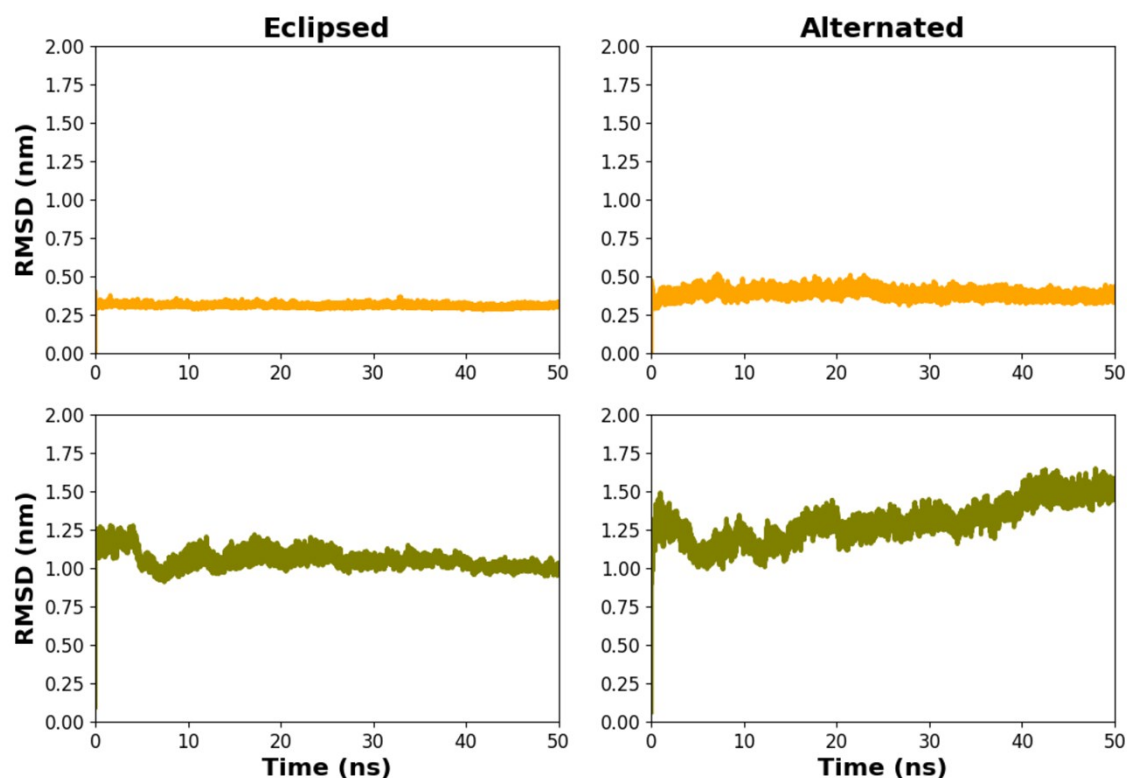


**Figure S8:** Functionalized CPs mimicking the intermediate protonated states with 2 COO<sup>-</sup> /COOH groups, SCPN<sub>2</sub>COOH and SCPN<sub>2</sub>COO<sup>-</sup>, leading to alternated or eclipsed conformation along the SCPN. R= COO<sup>-</sup> or COOH.

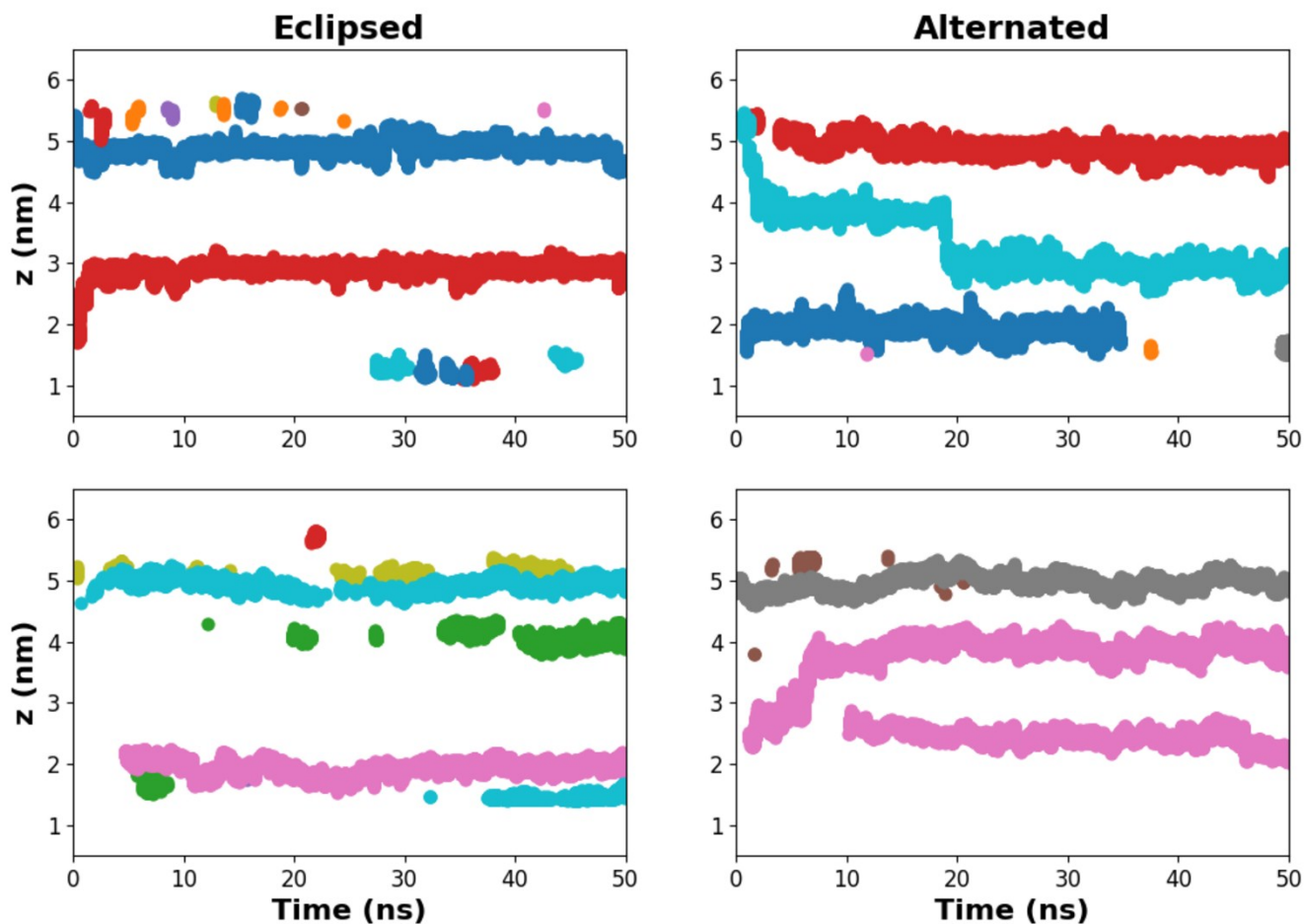




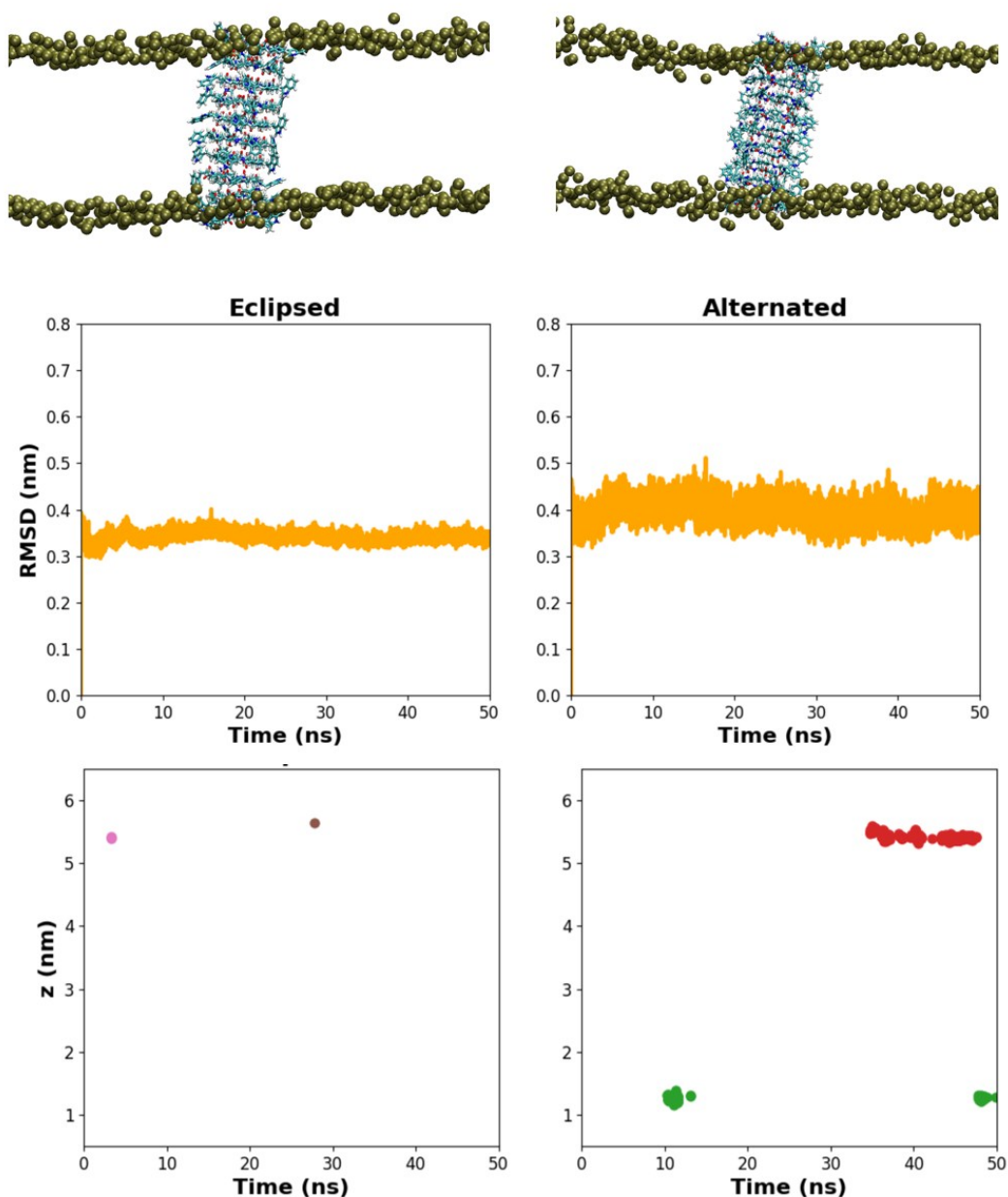
**Figure S9:** Snapshots of the four simulated SCPNs composed of CPs decorated with just 2 COOH or COO<sup>-</sup> groups, in NaCl 0.5M, after 50 ns of simulation. Lipids, water and external ions have been removed for clarity. Brown spheres correspond to the phosphorous from the lipids and black circles are the corresponding ions.



**Figure S10:** RMSD for the two nanotube models **SCPN<sub>2</sub>COOH** (top) and **SCPN<sub>2</sub>COO<sup>-</sup>** (bottom), in eclipsed or alternated conformations, simulated in NaCl 0.5M for 50 ns and considering all atoms of the SCPN.



**Figure S11:** Z-coordinate for each of the cations inside the simulated peptide nanotubes  $\text{SCPN}_{2\text{COOH}}$  (top) and  $\text{SCPN}_{2\text{COO}^-}$  (bottom), in eclipsed or alternated conformations, simulated in NaCl 0.5M along the 50 ns trajectory. The nanotube z-region is comprehended between the region  $\approx 1\text{--}6$  nm. Each color corresponds to a different ion.



**Figure S12:** Top: Snapshots of SCPN<sub>2</sub>COOH in eclipsed or alternated conformations, simulated in CaCl<sub>2</sub> 0.5M, after 50 ns of simulation. Lipids, water and external ions have been removed for clarity. Brown spheres correspond to the phosphorous from the lipids. Medium: RMSD for those systems considering all atoms of the SCPN. Bottom: Z-coordinate for each of the cations (Ca<sup>2+</sup>) near the edges of the simulated systems. The nanotube z-region is comprehended between the region  $\approx 1-6$  nm. Each color corresponds to a different ion.

# Gromacs itp files for the cyclic peptides CP<sub>4</sub>COOH and CP<sub>4</sub>COO<sup>-</sup>:

## CP<sub>4</sub>COOH:

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MOL             3

[ atoms ]
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4        ca     1      MOL      C3    4     -0.22162    12.000000
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8        ha     1      MOL      H79   8     0.14627     1.000000
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38       hc     1      MOL      H9    38    0.14042     1.000000
39       hc     1      MOL      H8    39    0.01950     1.000000
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45       hn     1      MOL      H     45    0.35252     1.000000
46       o      1      MOL      O7    46    -0.50462    16.000000
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[ bonds ]

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11	12	1	1.0830e-01	2.9296e+05	
16	17	1	1.0920e-01	2.8225e+05	
16	18	1	1.0920e-01	2.8225e+05	
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21	45	1	1.0090e-01	3.4326e+05	
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30	35	1	1.0920e-01	2.8225e+05
31	32	1	1.0920e-01	2.8225e+05
31	33	1	1.0920e-01	2.8225e+05
41	42	1	9.7400e-02	3.0928e+05
48	49	1	1.0090e-01	3.4326e+05
52	59	1	1.0920e-01	2.8225e+05
53	58	1	1.0920e-01	2.8225e+05
55	56	1	9.7400e-02	3.0928e+05
60	61	1	1.0920e-01	2.8225e+05
60	62	1	1.0920e-01	2.8225e+05
63	64	1	1.0920e-01	2.8225e+05
63	65	1	1.0920e-01	2.8225e+05
66	67	1	1.0920e-01	2.8225e+05
66	68	1	1.0920e-01	2.8225e+05
69	70	1	1.0930e-01	2.8108e+05
71	72	1	1.0090e-01	3.4326e+05
75	94	1	1.0930e-01	2.8108e+05
76	92	1	1.0920e-01	2.8225e+05
76	93	1	1.0920e-01	2.8225e+05
78	91	1	1.0830e-01	2.9296e+05
79	90	1	1.0110e-01	3.4024e+05
82	89	1	1.0870e-01	2.8811e+05
83	88	1	1.0870e-01	2.8811e+05
84	87	1	1.0870e-01	2.8811e+05
85	86	1	1.0870e-01	2.8811e+05
95	96	1	1.0090e-01	3.4326e+05
99	106	1	1.0920e-01	2.8225e+05
100	105	1	1.0920e-01	2.8225e+05
102	103	1	9.7400e-02	3.0928e+05
107	108	1	1.0920e-01	2.8225e+05
107	109	1	1.0920e-01	2.8225e+05
110	111	1	1.0920e-01	2.8225e+05
110	112	1	1.0920e-01	2.8225e+05
113	114	1	1.0920e-01	2.8225e+05
113	115	1	1.0920e-01	2.8225e+05
116	117	1	1.0930e-01	2.8108e+05
118	119	1	1.0090e-01	3.4326e+05
122	141	1	1.0930e-01	2.8108e+05
123	139	1	1.0920e-01	2.8225e+05
123	140	1	1.0920e-01	2.8225e+05
125	138	1	1.0830e-01	2.9296e+05
126	137	1	1.0110e-01	3.4024e+05
129	136	1	1.0870e-01	2.8811e+05
130	135	1	1.0870e-01	2.8811e+05
131	134	1	1.0870e-01	2.8811e+05
132	133	1	1.0870e-01	2.8811e+05
142	143	1	1.0090e-01	3.4326e+05
146	153	1	1.0920e-01	2.8225e+05
147	152	1	1.0920e-01	2.8225e+05
149	150	1	9.7400e-02	3.0928e+05
154	155	1	1.0920e-01	2.8225e+05
154	156	1	1.0920e-01	2.8225e+05
157	158	1	1.0920e-01	2.8225e+05
157	159	1	1.0920e-01	2.8225e+05
160	161	1	1.0920e-01	2.8225e+05
160	162	1	1.0920e-01	2.8225e+05
163	164	1	1.0930e-01	2.8108e+05
165	166	1	1.0090e-01	3.4326e+05
169	170	1	1.0930e-01	2.8108e+05
171	172	1	1.0920e-01	2.8225e+05
171	173	1	1.0920e-01	2.8225e+05
175	176	1	1.0830e-01	2.9296e+05
177	178	1	1.0110e-01	3.4024e+05
181	182	1	1.0870e-01	2.8811e+05
183	184	1	1.0870e-01	2.8811e+05
185	186	1	1.0870e-01	2.8811e+05
187	188	1	1.0870e-01	2.8811e+05
1	2	1	1.3870e-01	4.0033e+05
1	9	1	1.3870e-01	4.0033e+05
2	3	1	1.3870e-01	4.0033e+05
3	4	1	1.3870e-01	4.0033e+05
4	14	1	1.3870e-01	4.0033e+05
9	10	1	1.3500e-01	3.9355e+05
9	14	1	1.3870e-01	4.0033e+05
10	11	1	1.3710e-01	3.6719e+05
11	15	1	1.3710e-01	4.2175e+05
14	15	1	1.4340e-01	3.4451e+05
15	16	1	1.4990e-01	2.8225e+05
16	19	1	1.5350e-01	2.5363e+05
19	20	1	1.5080e-01	2.7472e+05
19	48	1	1.4600e-01	2.7665e+05
20	21	1	1.3450e-01	4.0016e+05
20	46	1	1.2140e-01	5.4225e+05
21	22	1	1.4600e-01	2.7665e+05
22	23	1	1.5350e-01	2.5363e+05
22	31	1	1.5350e-01	2.5363e+05
23	24	1	1.5350e-01	2.5363e+05
23	40	1	1.5080e-01	2.7472e+05
24	25	1	1.5080e-01	2.7472e+05
24	29	1	1.5350e-01	2.5363e+05
25	26	1	1.3450e-01	4.0016e+05
25	28	1	1.2140e-01	5.4225e+05
26	169	1	1.4600e-01	2.7665e+05
29	30	1	1.5350e-01	2.5363e+05
30	31	1	1.5350e-01	2.5363e+05
40	41	1	1.3060e-01	3.9028e+05
40	43	1	1.2140e-01	5.4225e+05
48	50	1	1.3450e-01	4.0016e+05
50	51	1	1.2140e-01	5.4225e+05
50	52	1	1.5080e-01	2.7472e+05
52	53	1	1.5350e-01	2.5363e+05
52	60	1	1.5350e-01	2.5363e+05
53	54	1	1.5080e-01	2.7472e+05
53	69	1	1.5350e-01	2.5363e+05
54	55	1	1.3060e-01	3.9028e+05
54	57	1	1.2140e-01	5.4225e+05
60	63	1	1.5350e-01	2.5363e+05
63	66	1	1.5350e-01	2.5363e+05
66	69	1	1.5350e-01	2.5363e+05
69	71	1	1.4600e-01	2.7665e+05
71	73	1	1.3450e-01	4.0016e+05
73	74	1	1.2140e-01	5.4225e+05

73	75	1	1.5080e-01	2.7472e+05
75	76	1	1.5350e-01	2.5363e+05
75	95	1	1.4600e-01	2.7665e+05
76	77	1	1.4990e-01	2.8225e+05
77	78	1	1.3710e-01	4.2175e+05
77	81	1	1.4340e-01	3.4451e+05
78	79	1	1.3710e-01	3.6719e+05
79	80	1	1.3500e-01	3.9355e+05
80	81	1	1.3870e-01	4.0033e+05
80	85	1	1.3870e-01	4.0033e+05
81	82	1	1.3870e-01	4.0033e+05
82	83	1	1.3870e-01	4.0033e+05
83	84	1	1.3870e-01	4.0033e+05
84	85	1	1.3870e-01	4.0033e+05
95	97	1	1.3450e-01	4.0016e+05
97	98	1	1.2140e-01	5.4225e+05
97	99	1	1.5080e-01	2.7472e+05
99	100	1	1.5350e-01	2.5363e+05
99	107	1	1.5350e-01	2.5363e+05
100	101	1	1.5080e-01	2.7472e+05
100	116	1	1.5350e-01	2.5363e+05
101	102	1	1.3060e-01	3.9028e+05
101	104	1	1.2140e-01	5.4225e+05
107	110	1	1.5350e-01	2.5363e+05
110	113	1	1.5350e-01	2.5363e+05
113	116	1	1.5350e-01	2.5363e+05
116	118	1	1.4600e-01	2.7665e+05
118	120	1	1.3450e-01	4.0016e+05
120	121	1	1.2140e-01	5.4225e+05
120	122	1	1.5080e-01	2.7472e+05
122	123	1	1.5350e-01	2.5363e+05
122	142	1	1.4600e-01	2.7665e+05
123	124	1	1.4990e-01	2.8225e+05
124	125	1	1.3710e-01	4.2175e+05
124	128	1	1.4340e-01	3.4451e+05
125	126	1	1.3710e-01	3.6719e+05
126	127	1	1.3500e-01	3.9355e+05
127	128	1	1.3870e-01	4.0033e+05
127	132	1	1.3870e-01	4.0033e+05
128	129	1	1.3870e-01	4.0033e+05
129	130	1	1.3870e-01	4.0033e+05
130	131	1	1.3870e-01	4.0033e+05
131	132	1	1.3870e-01	4.0033e+05
142	144	1	1.3450e-01	4.0016e+05
144	145	1	1.2140e-01	5.4225e+05
144	146	1	1.5080e-01	2.7472e+05
146	147	1	1.5350e-01	2.5363e+05
146	154	1	1.5350e-01	2.5363e+05
147	148	1	1.5080e-01	2.7472e+05
147	163	1	1.5350e-01	2.5363e+05
148	149	1	1.3060e-01	3.9028e+05
148	151	1	1.2140e-01	5.4225e+05
154	157	1	1.5350e-01	2.5363e+05
157	160	1	1.5350e-01	2.5363e+05
160	163	1	1.5350e-01	2.5363e+05
163	165	1	1.4600e-01	2.7665e+05
165	167	1	1.3450e-01	4.0016e+05
167	168	1	1.2140e-01	5.4225e+05
167	169	1	1.5080e-01	2.7472e+05
169	171	1	1.5350e-01	2.5363e+05
171	174	1	1.4990e-01	2.8225e+05
174	175	1	1.3710e-01	4.2175e+05
174	180	1	1.4340e-01	3.4451e+05
175	177	1	1.3710e-01	3.6719e+05
177	179	1	1.3500e-01	3.9355e+05
179	180	1	1.3870e-01	4.0033e+05
179	187	1	1.3870e-01	4.0033e+05
180	181	1	1.3870e-01	4.0033e+05
181	183	1	1.3870e-01	4.0033e+05
183	185	1	1.3870e-01	4.0033e+05
185	187	1	1.3870e-01	4.0033e+05

[ pairs ]  
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[ angles ]

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	2	3	6	1	1.2001e+02	4.0551e+02
	3	2	7	1	1.2001e+02	4.0551e+02
	3	4	5	1	1.2001e+02	4.0551e+02
	4	3	6	1	1.2001e+02	4.0551e+02
	5	4	14	1	1.2001e+02	4.0551e+02
	8	1	9	1	1.2001e+02	4.0551e+02
	9	10	13	1	1.2559e+02	3.9857e+02
	10	11	12	1	1.1966e+02	4.2024e+02
	11	10	13	1	1.2522e+02	3.9388e+02
	12	11	15	1	1.2911e+02	3.9489e+02
	15	16	17	1	1.1086e+02	3.9497e+02
	15	16	18	1	1.1086e+02	3.9497e+02
	16	19	47	1	1.1007e+02	3.8794e+02
	17	16	18	1	1.0835e+02	3.2995e+02
	17	16	19	1	1.1005e+02	3.8802e+02
	18	16	19	1	1.1005e+02	3.8802e+02
	19	48	49	1	1.1678e+02	3.8526e+02
	20	19	47	1	1.0766e+02	3.9857e+02
	20	21	45	1	1.1846e+02	4.1179e+02
	21	22	44	1	1.0932e+02	4.1689e+02
	22	21	45	1	1.1678e+02	3.8526e+02
	22	23	39	1	1.1005e+02	3.8802e+02
	22	31	32	1	1.1005e+02	3.8802e+02
	22	31	33	1	1.1005e+02	3.8802e+02
	23	22	44	1	1.1007e+02	3.8794e+02
	23	24	38	1	1.1005e+02	3.8802e+02
	24	23	39	1	1.1005e+02	3.8802e+02
	24	29	36	1	1.1005e+02	3.8802e+02
	24	29	37	1	1.1005e+02	3.8802e+02
	25	24	38	1	1.0968e+02	3.9497e+02
	25	26	27	1	1.1846e+02	4.1179e+02
	26	169	170	1	1.0932e+02	4.1689e+02
	27	26	169	1	1.1678e+02	3.8526e+02
	29	24	38	1	1.1005e+02	3.8802e+02
	29	30	34	1	1.1005e+02	3.8802e+02
	29	30	35	1	1.1005e+02	3.8802e+02
	30	29	36	1	1.1005e+02	3.8802e+02
	30	29	37	1	1.1005e+02	3.8802e+02
	30	31	32	1	1.1005e+02	3.8802e+02
	30	31	33	1	1.1005e+02	3.8802e+02
	31	30	34	1	1.1005e+02	3.8802e+02
	31	30	35	1	1.1005e+02	3.8802e+02
	31	22	44	1	1.1007e+02	3.8794e+02
	32	31	33	1	1.0835e+02	3.2995e+02
	34	30	35	1	1.0835e+02	3.2995e+02
	36	29	37	1	1.0835e+02	3.2995e+02
	39	23	40	1	1.0968e+02	3.9497e+02

40	41	42	1	1.0737e+02	4.2836e+02
47	19	48	1	1.0932e+02	4.1689e+02
49	48	50	1	1.1846e+02	4.1179e+02
50	52	59	1	1.0968e+02	3.9497e+02
52	53	58	1	1.1005e+02	3.8802e+02
52	60	61	1	1.1005e+02	3.8802e+02
52	60	62	1	1.1005e+02	3.8802e+02
53	52	59	1	1.1005e+02	3.8802e+02
53	69	70	1	1.1007e+02	3.8794e+02
54	53	58	1	1.0968e+02	3.9497e+02
54	55	56	1	1.0737e+02	4.2836e+02
58	53	69	1	1.1005e+02	3.8802e+02
59	52	60	1	1.1005e+02	3.8802e+02
60	63	64	1	1.1005e+02	3.8802e+02
60	63	65	1	1.1005e+02	3.8802e+02
61	60	62	1	1.0835e+02	3.2995e+02
61	60	63	1	1.1005e+02	3.8802e+02
62	60	63	1	1.1005e+02	3.8802e+02
63	66	67	1	1.1005e+02	3.8802e+02
63	66	68	1	1.1005e+02	3.8802e+02
64	63	65	1	1.0835e+02	3.2995e+02
64	63	66	1	1.1005e+02	3.8802e+02
65	63	66	1	1.1005e+02	3.8802e+02
66	69	70	1	1.1007e+02	3.8794e+02
67	66	68	1	1.0835e+02	3.2995e+02
67	66	69	1	1.1005e+02	3.8802e+02
68	66	69	1	1.1005e+02	3.8802e+02
69	71	72	1	1.1678e+02	3.8526e+02
70	69	71	1	1.0932e+02	4.1689e+02
72	71	73	1	1.1846e+02	4.1179e+02
73	75	94	1	1.0766e+02	3.9857e+02
75	76	92	1	1.1005e+02	3.8802e+02
75	76	93	1	1.1005e+02	3.8802e+02
75	95	96	1	1.1678e+02	3.8526e+02
76	75	94	1	1.1007e+02	3.8794e+02
77	76	92	1	1.1086e+02	3.9497e+02
77	76	93	1	1.1086e+02	3.9497e+02
77	78	91	1	1.2911e+02	3.9489e+02
78	79	90	1	1.2522e+02	3.9388e+02
79	78	91	1	1.1966e+02	4.2024e+02
80	79	90	1	1.2559e+02	3.9857e+02
80	85	86	1	1.2001e+02	4.0551e+02
81	82	89	1	1.2001e+02	4.0551e+02
82	83	88	1	1.2001e+02	4.0551e+02
83	82	89	1	1.2001e+02	4.0551e+02
83	84	87	1	1.2001e+02	4.0551e+02
84	83	88	1	1.2001e+02	4.0551e+02
84	85	86	1	1.2001e+02	4.0551e+02
85	84	87	1	1.2001e+02	4.0551e+02
92	76	93	1	1.0835e+02	3.2995e+02
94	75	95	1	1.0932e+02	4.1689e+02
96	95	97	1	1.1846e+02	4.1179e+02
97	99	106	1	1.0968e+02	3.9497e+02
99	100	105	1	1.1005e+02	3.8802e+02
99	107	108	1	1.1005e+02	3.8802e+02
99	107	109	1	1.1005e+02	3.8802e+02
100	99	106	1	1.1005e+02	3.8802e+02
100	116	117	1	1.1007e+02	3.8794e+02
101	100	105	1	1.0968e+02	3.9497e+02
101	102	103	1	1.0737e+02	4.2836e+02
105	100	116	1	1.1005e+02	3.8802e+02
106	99	107	1	1.1005e+02	3.8802e+02
107	110	111	1	1.1005e+02	3.8802e+02
107	110	112	1	1.1005e+02	3.8802e+02
108	107	109	1	1.0835e+02	3.2995e+02
108	107	110	1	1.1005e+02	3.8802e+02
109	107	110	1	1.1005e+02	3.8802e+02
110	113	114	1	1.1005e+02	3.8802e+02
110	113	115	1	1.1005e+02	3.8802e+02
111	110	112	1	1.0835e+02	3.2995e+02
111	110	113	1	1.1005e+02	3.8802e+02
112	110	113	1	1.1005e+02	3.8802e+02
113	116	117	1	1.1007e+02	3.8794e+02
114	113	115	1	1.0835e+02	3.2995e+02
114	113	116	1	1.1005e+02	3.8802e+02
115	113	116	1	1.1005e+02	3.8802e+02
116	118	119	1	1.1678e+02	3.8526e+02
117	116	118	1	1.0932e+02	4.1689e+02
119	118	120	1	1.1846e+02	4.1179e+02
120	122	141	1	1.0766e+02	3.9857e+02
122	123	139	1	1.1005e+02	3.8802e+02
122	123	140	1	1.1005e+02	3.8802e+02
122	142	143	1	1.1678e+02	3.8526e+02
123	122	141	1	1.1007e+02	3.8794e+02
124	123	139	1	1.1086e+02	3.9497e+02
124	123	140	1	1.1086e+02	3.9497e+02
124	125	138	1	1.2911e+02	3.9489e+02
125	126	137	1	1.2522e+02	3.9388e+02
126	125	138	1	1.1966e+02	4.2024e+02
127	126	137	1	1.2559e+02	3.9857e+02
127	132	133	1	1.2001e+02	4.0551e+02
128	129	136	1	1.2001e+02	4.0551e+02
129	130	135	1	1.2001e+02	4.0551e+02
130	129	136	1	1.2001e+02	4.0551e+02
130	131	134	1	1.2001e+02	4.0551e+02
131	130	135	1	1.2001e+02	4.0551e+02
131	132	133	1	1.2001e+02	4.0551e+02
132	131	134	1	1.2001e+02	4.0551e+02
139	123	140	1	1.0835e+02	3.2995e+02
141	122	142	1	1.0932e+02	4.1689e+02
143	142	144	1	1.1846e+02	4.1179e+02
144	146	153	1	1.0968e+02	3.9497e+02
146	147	152	1	1.1005e+02	3.8802e+02
146	154	155	1	1.1005e+02	3.8802e+02
146	154	156	1	1.1005e+02	3.8802e+02
147	146	153	1	1.1005e+02	3.8802e+02
147	163	164	1	1.1007e+02	3.8794e+02
148	147	152	1	1.0968e+02	3.9497e+02
148	149	150	1	1.0737e+02	4.2836e+02
152	147	163	1	1.1005e+02	3.8802e+02
153	146	154	1	1.1005e+02	3.8802e+02
154	157	158	1	1.1005e+02	3.8802e+02
154	157	159	1	1.1005e+02	3.8802e+02

155	154	156	1	1.0835e+02	3.2995e+02
155	154	157	1	1.1005e+02	3.8802e+02
156	154	157	1	1.1005e+02	3.8802e+02
157	160	161	1	1.1005e+02	3.8802e+02
157	160	162	1	1.1005e+02	3.8802e+02
158	157	159	1	1.0835e+02	3.2995e+02
158	157	160	1	1.1005e+02	3.8802e+02
159	157	160	1	1.1005e+02	3.8802e+02
160	163	164	1	1.1007e+02	3.8794e+02
161	160	162	1	1.0835e+02	3.2995e+02
161	160	163	1	1.1005e+02	3.8802e+02
162	160	163	1	1.1005e+02	3.8802e+02
163	165	166	1	1.1678e+02	3.8526e+02
164	163	165	1	1.0932e+02	4.1689e+02
166	165	167	1	1.1846e+02	4.1179e+02
167	169	170	1	1.0766e+02	3.9857e+02
169	171	172	1	1.1005e+02	3.8802e+02
169	171	173	1	1.1005e+02	3.8802e+02
170	169	171	1	1.1007e+02	3.8794e+02
172	171	173	1	1.0835e+02	3.2995e+02
172	171	174	1	1.1086e+02	3.9497e+02
173	171	174	1	1.1086e+02	3.9497e+02
174	175	176	1	1.2911e+02	3.9489e+02
175	177	178	1	1.2522e+02	3.9388e+02
176	175	177	1	1.1966e+02	4.2024e+02
178	177	179	1	1.2559e+02	3.9857e+02
179	187	188	1	1.2001e+02	4.0551e+02
180	181	182	1	1.2001e+02	4.0551e+02
181	183	184	1	1.2001e+02	4.0551e+02
182	181	183	1	1.2001e+02	4.0551e+02
183	185	186	1	1.2001e+02	4.0551e+02
184	183	185	1	1.2001e+02	4.0551e+02
185	187	188	1	1.2001e+02	4.0551e+02
186	185	187	1	1.2001e+02	4.0551e+02
1	2	3	1	1.1997e+02	5.6216e+02
1	9	10	1	1.1834e+02	5.8752e+02
1	9	14	1	1.1997e+02	5.6216e+02
2	1	9	1	1.1997e+02	5.6216e+02
2	3	4	1	1.1997e+02	5.6216e+02
3	4	14	1	1.1997e+02	5.6216e+02
4	14	9	1	1.1997e+02	5.6216e+02
4	14	15	1	1.2010e+02	5.5220e+02
9	10	11	1	1.1315e+02	5.7287e+02
9	14	15	1	1.2010e+02	5.5220e+02
10	9	14	1	1.1834e+02	5.8752e+02
10	11	15	1	1.0942e+02	6.1011e+02
11	15	14	1	1.1351e+02	5.7095e+02
11	15	16	1	1.1945e+02	5.4233e+02
14	15	16	1	1.2643e+02	5.1739e+02
15	16	19	1	1.1192e+02	5.3195e+02
16	19	20	1	1.1053e+02	5.3379e+02
16	19	48	1	1.1213e+02	5.5103e+02
19	20	21	1	1.1515e+02	5.6785e+02
19	20	46	1	1.2311e+02	5.6928e+02
19	48	50	1	1.2135e+02	5.3488e+02
20	19	48	1	1.1156e+02	5.5789e+02
20	21	22	1	1.2135e+02	5.3488e+02
21	20	46	1	1.2203e+02	6.3455e+02
21	22	23	1	1.1213e+02	5.5103e+02
21	22	31	1	1.1213e+02	5.5103e+02
22	23	24	1	1.1063e+02	5.2894e+02
22	23	40	1	1.1053e+02	5.3379e+02
22	31	30	1	1.1063e+02	5.2894e+02
23	22	31	1	1.1063e+02	5.2894e+02
23	24	25	1	1.1053e+02	5.3379e+02
23	24	29	1	1.1063e+02	5.2894e+02
23	40	41	1	1.1220e+02	5.8442e+02
23	40	43	1	1.2311e+02	5.6928e+02
24	23	40	1	1.1053e+02	5.3379e+02
24	25	26	1	1.1515e+02	5.6785e+02
24	25	28	1	1.2311e+02	5.6928e+02
24	29	30	1	1.1063e+02	5.2894e+02
25	24	29	1	1.1053e+02	5.3379e+02
25	26	169	1	1.2135e+02	5.3488e+02
26	25	28	1	1.2203e+02	6.3455e+02
26	169	167	1	1.1156e+02	5.5789e+02
26	169	171	1	1.1213e+02	5.5103e+02
29	30	31	1	1.1063e+02	5.2894e+02
41	40	43	1	1.2288e+02	6.4752e+02
48	50	51	1	1.2203e+02	6.3455e+02
48	50	52	1	1.1515e+02	5.6785e+02
50	52	53	1	1.1053e+02	5.3379e+02
50	52	60	1	1.1053e+02	5.3379e+02
51	50	52	1	1.2311e+02	5.6928e+02
52	53	54	1	1.1053e+02	5.3379e+02
52	53	69	1	1.1063e+02	5.2894e+02
52	60	63	1	1.1063e+02	5.2894e+02
53	52	60	1	1.1063e+02	5.2894e+02
53	54	55	1	1.1220e+02	5.8442e+02
53	54	57	1	1.2311e+02	5.6928e+02
53	69	66	1	1.1063e+02	5.2894e+02
53	69	71	1	1.1213e+02	5.5103e+02
54	53	69	1	1.1053e+02	5.3379e+02
55	54	57	1	1.2288e+02	6.4752e+02
60	63	66	1	1.1063e+02	5.2894e+02
63	66	69	1	1.1063e+02	5.2894e+02
66	69	71	1	1.1213e+02	5.5103e+02
69	71	73	1	1.2135e+02	5.3488e+02
71	73	74	1	1.2203e+02	6.3455e+02
71	73	75	1	1.1515e+02	5.6785e+02
73	75	76	1	1.1053e+02	5.3379e+02
73	75	95	1	1.1156e+02	5.5789e+02
74	73	75	1	1.2311e+02	5.6928e+02
75	76	77	1	1.1192e+02	5.3195e+02
75	95	97	1	1.2135e+02	5.3488e+02
76	75	95	1	1.1213e+02	5.5103e+02
76	77	78	1	1.1945e+02	5.4233e+02
76	77	81	1	1.2643e+02	5.1739e+02
77	78	79	1	1.0942e+02	6.1011e+02
77	81	80	1	1.2010e+02	5.5220e+02
77	81	82	1	1.2010e+02	5.5220e+02
78	77	81	1	1.1351e+02	5.7095e+02
78	79	80	1	1.1315e+02	5.7287e+02

79	80	81	1	1.1834e+02	5.8752e+02
79	80	85	1	1.1834e+02	5.8752e+02
80	81	82	1	1.1997e+02	5.6216e+02
80	85	84	1	1.1997e+02	5.6216e+02
81	80	85	1	1.1997e+02	5.6216e+02
81	82	83	1	1.1997e+02	5.6216e+02
82	83	84	1	1.1997e+02	5.6216e+02
83	84	85	1	1.1997e+02	5.6216e+02
95	97	98	1	1.2203e+02	6.3455e+02
95	97	99	1	1.1515e+02	5.6785e+02
97	99	100	1	1.1053e+02	5.3379e+02
97	99	107	1	1.1053e+02	5.3379e+02
98	97	99	1	1.2311e+02	5.6928e+02
99	100	101	1	1.1053e+02	5.3379e+02
99	100	116	1	1.1063e+02	5.2894e+02
99	107	110	1	1.1063e+02	5.2894e+02
100	99	107	1	1.1063e+02	5.2894e+02
100	101	102	1	1.1220e+02	5.8442e+02
100	101	104	1	1.2311e+02	5.6928e+02
100	116	113	1	1.1063e+02	5.2894e+02
100	116	118	1	1.1213e+02	5.5103e+02
101	100	116	1	1.1053e+02	5.3379e+02
102	101	104	1	1.2288e+02	6.4752e+02
107	110	113	1	1.1063e+02	5.2894e+02
110	113	116	1	1.1063e+02	5.2894e+02
113	116	118	1	1.1213e+02	5.5103e+02
116	118	120	1	1.2135e+02	5.3488e+02
118	120	121	1	1.2203e+02	6.3455e+02
118	120	122	1	1.1515e+02	5.6785e+02
120	122	123	1	1.1053e+02	5.3379e+02
120	122	142	1	1.1156e+02	5.5789e+02
121	120	122	1	1.2311e+02	5.6928e+02
122	123	124	1	1.1192e+02	5.3195e+02
122	142	144	1	1.2135e+02	5.3488e+02
123	122	142	1	1.1213e+02	5.5103e+02
123	124	125	1	1.1945e+02	5.4233e+02
123	124	128	1	1.2643e+02	5.1739e+02
124	125	126	1	1.0942e+02	6.1011e+02
124	128	127	1	1.2010e+02	5.5220e+02
124	128	129	1	1.2010e+02	5.5220e+02
125	124	128	1	1.1351e+02	5.7095e+02
125	126	127	1	1.1315e+02	5.7287e+02
126	127	128	1	1.1834e+02	5.8752e+02
126	127	132	1	1.1834e+02	5.8752e+02
127	128	129	1	1.1997e+02	5.6216e+02
127	132	131	1	1.1997e+02	5.6216e+02
128	127	132	1	1.1997e+02	5.6216e+02
128	129	130	1	1.1997e+02	5.6216e+02
129	130	131	1	1.1997e+02	5.6216e+02
130	131	132	1	1.1997e+02	5.6216e+02
142	144	145	1	1.2203e+02	6.3455e+02
142	144	146	1	1.1515e+02	5.6785e+02
144	146	147	1	1.1053e+02	5.3379e+02
144	146	154	1	1.1053e+02	5.3379e+02
145	144	146	1	1.2311e+02	5.6928e+02
146	147	148	1	1.1053e+02	5.3379e+02
146	147	163	1	1.1063e+02	5.2894e+02
146	154	157	1	1.1063e+02	5.2894e+02
147	146	154	1	1.1063e+02	5.2894e+02
147	148	149	1	1.1220e+02	5.8442e+02
147	148	151	1	1.2311e+02	5.6928e+02
147	163	160	1	1.1063e+02	5.2894e+02
147	163	165	1	1.1213e+02	5.5103e+02
148	147	163	1	1.1053e+02	5.3379e+02
149	148	151	1	1.2288e+02	6.4752e+02
154	157	160	1	1.1063e+02	5.2894e+02
157	160	163	1	1.1063e+02	5.2894e+02
160	163	165	1	1.1213e+02	5.5103e+02
163	165	167	1	1.2135e+02	5.3488e+02
165	167	168	1	1.2203e+02	6.3455e+02
165	167	169	1	1.1515e+02	5.6785e+02
167	169	171	1	1.1053e+02	5.3379e+02
168	167	169	1	1.2311e+02	5.6928e+02
169	171	174	1	1.1192e+02	5.3195e+02
171	174	175	1	1.1945e+02	5.4233e+02
171	174	180	1	1.2643e+02	5.1739e+02
174	175	177	1	1.0942e+02	6.1011e+02
174	180	179	1	1.2010e+02	5.5220e+02
174	180	181	1	1.2010e+02	5.5220e+02
175	174	180	1	1.1351e+02	5.7095e+02
175	177	179	1	1.1315e+02	5.7287e+02
177	179	180	1	1.1834e+02	5.8752e+02
177	179	187	1	1.1834e+02	5.8752e+02
179	180	181	1	1.1997e+02	5.6216e+02
179	187	185	1	1.1997e+02	5.6216e+02
180	179	187	1	1.1997e+02	5.6216e+02
180	181	183	1	1.1997e+02	5.6216e+02
181	183	185	1	1.1997e+02	5.6216e+02
183	185	187	1	1.1997e+02	5.6216e+02

[ dihedrals ]

i	j	k	l	func	C0	...	C5					
1	2	3	6	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	0.00000	;
1	9	10	13	3	2.51040	0.00000	-2.51040	0.00000	0.00000	0.00000	0.00000	;
2	3	4	5	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	0.00000	;
8	1	2	3	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	0.00000	;
4	3	2	7	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	0.00000	;
5	4	3	6	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	0.00000	;
5	4	14	9	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	0.00000	;
5	4	14	15	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	0.00000	;
6	3	2	7	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	0.00000	;
6	3	4	14	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	0.00000	;
8	1	2	7	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	0.00000	;
9	1	2	7	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	0.00000	;
8	1	9	10	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	0.00000	;
8	1	9	14	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	0.00000	;
9	10	11	12	3	14.22560	0.00000	-14.22560	0.00000	0.00000	0.00000	0.00000	;
11	15	16	17	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
11	15	16	18	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
12	11	10	13	3	14.22560	0.00000	-14.22560	0.00000	0.00000	0.00000	0.00000	;
12	11	15	14	3	33.47200	0.00000	-33.47200	0.00000	0.00000	0.00000	0.00000	;
12	11	15	16	3	33.47200	0.00000	-33.47200	0.00000	0.00000	0.00000	0.00000	;
13	10	9	14	3	2.51040	0.00000	-2.51040	0.00000	0.00000	0.00000	0.00000	;















30	c3	1	MOL	C21	30	0.69685	12.000000
31	c3	1	MOL	C22	31	0.11793	12.000000
32	c3	1	MOL	C23	32	-0.11613	12.000000
33	c3	1	MOL	C24	33	0.14940	12.000000
34	c3	1	MOL	C25	34	-0.23588	12.000000
35	c	1	MOL	C26	35	0.84521	12.000000
36	c3	1	MOL	C27	36	-0.03162	12.000000
37	c	1	MOL	C28	37	0.65821	12.000000
38	o	1	MOL	O6	38	-0.59402	16.000000
39	n	1	MOL	N5	39	-0.80485	14.000000
40	c3	1	MOL	C29	40	0.54224	12.000000
41	c3	1	MOL	C30	41	-0.07259	12.000000
42	cc	1	MOL	C31	42	-0.27795	12.000000
43	cd	1	MOL	C32	43	-0.00954	12.000000
44	na	1	MOL	N6	44	-0.53217	14.000000
45	ca	1	MOL	C33	45	0.28712	12.000000
46	ca	1	MOL	C34	46	0.19418	12.000000
47	ca	1	MOL	C35	47	-0.18687	12.000000
48	ca	1	MOL	C36	48	-0.22699	12.000000
49	ca	1	MOL	C37	49	-0.13743	12.000000
50	ca	1	MOL	C38	50	-0.33869	12.000000
51	c	1	MOL	C39	51	0.57875	12.000000
52	o	1	MOL	O7	52	-0.61087	16.000000
53	n	1	MOL	N7	53	-0.87894	14.000000
54	c3	1	MOL	C40	54	0.69685	12.000000
55	c3	1	MOL	C41	55	0.11793	12.000000
56	c3	1	MOL	C42	56	-0.11613	12.000000
57	c3	1	MOL	C43	57	0.14940	12.000000
58	c3	1	MOL	C44	58	-0.23588	12.000000
59	c	1	MOL	C45	59	0.84521	12.000000
60	o	1	MOL	O8	60	-0.77692	16.000000
61	o	1	MOL	O9	61	-0.77692	16.000000
62	c3	1	MOL	C46	62	-0.03162	12.000000
63	c	1	MOL	C47	63	0.65821	12.000000
64	o	1	MOL	O10	64	-0.59402	16.000000
65	n	1	MOL	N8	65	-0.80485	14.000000
66	c3	1	MOL	C48	66	0.54224	12.000000
67	c3	1	MOL	C49	67	-0.07259	12.000000
68	cc	1	MOL	C50	68	-0.27795	12.000000
69	cd	1	MOL	C51	69	-0.00954	12.000000
70	na	1	MOL	N9	70	-0.53217	14.000000
71	ca	1	MOL	C52	71	0.28712	12.000000
72	ca	1	MOL	C53	72	0.19418	12.000000
73	ca	1	MOL	C54	73	-0.18687	12.000000
74	ca	1	MOL	C55	74	-0.22699	12.000000
75	ca	1	MOL	C56	75	-0.13743	12.000000
76	ca	1	MOL	C57	76	-0.33869	12.000000
77	c	1	MOL	C58	77	0.57875	12.000000
78	o	1	MOL	O11	78	-0.61087	16.000000
79	n	1	MOL	N10	79	-0.87894	14.000000
80	c3	1	MOL	C59	80	0.69685	12.000000
81	c3	1	MOL	C60	81	0.11793	12.000000
82	c3	1	MOL	C61	82	-0.11613	12.000000
83	c3	1	MOL	C62	83	0.14940	12.000000
84	c3	1	MOL	C63	84	-0.23588	12.000000
85	c	1	MOL	C64	85	0.84521	12.000000
86	c3	1	MOL	C65	86	-0.03162	12.000000
87	c	1	MOL	C66	87	0.65821	12.000000
88	o	1	MOL	O12	88	-0.59402	16.000000
89	n	1	MOL	N11	89	-0.80485	14.000000
90	c3	1	MOL	C67	90	0.54224	12.000000
91	c3	1	MOL	C68	91	-0.07259	12.000000
92	cc	1	MOL	C69	92	-0.27795	12.000000
93	cd	1	MOL	C70	93	-0.00954	12.000000
94	na	1	MOL	N12	94	-0.53217	14.000000
95	ca	1	MOL	C71	95	0.28712	12.000000
96	ca	1	MOL	C72	96	0.19418	12.000000
97	ca	1	MOL	C73	97	-0.18687	12.000000
98	ca	1	MOL	C74	98	-0.22699	12.000000
99	ca	1	MOL	C75	99	-0.13743	12.000000
100	ca	1	MOL	C76	100	-0.33869	12.000000
101	o	1	MOL	O13	101	-0.77692	16.000000
102	o	1	MOL	O14	102	-0.77692	16.000000
103	o	1	MOL	O15	103	-0.77692	16.000000
104	o	1	MOL	O16	104	-0.77692	16.000000
105	h1	1	MOL	H1	105	-0.00142	1.000000
106	hn	1	MOL	H2	106	0.41341	1.000000
107	hc	1	MOL	H3	107	0.02251	1.000000
108	hc	1	MOL	H4	108	0.06142	1.000000
109	h1	1	MOL	H5	109	-0.07891	1.000000
110	hn	1	MOL	H6	110	0.37592	1.000000
111	hc	1	MOL	H7	111	-0.05800	1.000000
112	hc	1	MOL	H8	112	-0.05800	1.000000
113	hc	1	MOL	H9	113	-0.01891	1.000000
114	hc	1	MOL	H10	114	-0.01891	1.000000
115	hc	1	MOL	H11	115	-0.06332	1.000000
116	hc	1	MOL	H12	116	-0.06332	1.000000
117	hc	1	MOL	H13	117	0.02049	1.000000
118	hc	1	MOL	H14	118	0.02049	1.000000
119	h4	1	MOL	H15	119	0.14034	1.000000
120	hn	1	MOL	H16	120	0.35889	1.000000
121	ha	1	MOL	H17	121	0.13930	1.000000
122	ha	1	MOL	H18	122	0.11665	1.000000
123	ha	1	MOL	H19	123	0.09061	1.000000
124	ha	1	MOL	H20	124	0.13926	1.000000
125	hn	1	MOL	H21	125	0.37592	1.000000
126	h1	1	MOL	H22	126	-0.07891	1.000000
127	hc	1	MOL	H23	127	-0.05800	1.000000
128	hc	1	MOL	H24	128	-0.05800	1.000000
129	hc	1	MOL	H25	129	-0.01891	1.000000
130	hc	1	MOL	H26	130	-0.01891	1.000000
131	hc	1	MOL	H27	131	-0.06332	1.000000
132	hc	1	MOL	H28	132	-0.06332	1.000000
133	hc	1	MOL	H29	133	0.06142	1.000000
134	hc	1	MOL	H30	134	0.02251	1.000000
135	hn	1	MOL	H31	135	0.41341	1.000000
136	h1	1	MOL	H32	136	-0.00142	1.000000
137	hc	1	MOL	H33	137	0.02049	1.000000
138	hc	1	MOL	H34	138	0.02049	1.000000
139	h4	1	MOL	H35	139	0.14034	1.000000
140	hn	1	MOL	H36	140	0.35889	1.000000
141	ha	1	MOL	H37	141	0.13930	1.000000
142	ha	1	MOL	H38	142	0.11665	1.000000

143	ha	1	MOL	H39	143	0.09061	1.000000
144	ha	1	MOL	H40	144	0.13926	1.000000
145	hn	1	MOL	H41	145	0.37592	1.000000
146	hl	1	MOL	H42	146	-0.07891	1.000000
147	hc	1	MOL	H43	147	-0.05800	1.000000
148	hc	1	MOL	H44	148	-0.05800	1.000000
149	hc	1	MOL	H45	149	-0.01891	1.000000
150	hc	1	MOL	H46	150	-0.01891	1.000000
151	hc	1	MOL	H47	151	-0.06332	1.000000
152	hc	1	MOL	H48	152	-0.06332	1.000000
153	hc	1	MOL	H49	153	0.06142	1.000000
154	hc	1	MOL	H50	154	0.02251	1.000000
155	hn	1	MOL	H51	155	0.41341	1.000000
156	hl	1	MOL	H52	156	-0.00142	1.000000
157	hc	1	MOL	H53	157	0.02049	1.000000
158	hc	1	MOL	H54	158	0.02049	1.000000
159	h4	1	MOL	H55	159	0.14034	1.000000
160	hn	1	MOL	H56	160	0.35889	1.000000
161	ha	1	MOL	H57	161	0.13930	1.000000
162	ha	1	MOL	H58	162	0.11665	1.000000
163	ha	1	MOL	H59	163	0.09061	1.000000
164	ha	1	MOL	H60	164	0.13926	1.000000
165	hn	1	MOL	H61	165	0.37592	1.000000
166	hl	1	MOL	H62	166	-0.07891	1.000000
167	hc	1	MOL	H63	167	-0.05800	1.000000
168	hc	1	MOL	H64	168	-0.05800	1.000000
169	hc	1	MOL	H65	169	-0.01891	1.000000
170	hc	1	MOL	H66	170	-0.01891	1.000000
171	hc	1	MOL	H67	171	-0.06332	1.000000
172	hc	1	MOL	H68	172	-0.06332	1.000000
173	hc	1	MOL	H69	173	0.06142	1.000000
174	hc	1	MOL	H70	174	0.02251	1.000000
175	hn	1	MOL	H71	175	0.41341	1.000000
176	hl	1	MOL	H72	176	-0.00142	1.000000
177	hc	1	MOL	H73	177	0.02049	1.000000
178	hc	1	MOL	H74	178	0.02049	1.000000
179	h4	1	MOL	H75	179	0.14034	1.000000
180	hn	1	MOL	H76	180	0.35889	1.000000
181	ha	1	MOL	H77	181	0.13930	1.000000
182	ha	1	MOL	H78	182	0.11665	1.000000
183	ha	1	MOL	H79	183	0.09061	1.000000
184	ha	1	MOL	H80	184	0.13926	1.000000

[ bonds ]

;	ai	aj	funct	r	k
	1	105	1	1.0970e-01	2.7665e+05
	2	106	1	1.0130e-01	3.3740e+05
	4	107	1	1.0970e-01	2.7665e+05
	5	108	1	1.0970e-01	2.7665e+05
	6	109	1	1.0970e-01	2.7665e+05
	7	110	1	1.0130e-01	3.3740e+05
	10	111	1	1.0970e-01	2.7665e+05
	10	112	1	1.0970e-01	2.7665e+05
	11	113	1	1.0970e-01	2.7665e+05
	11	114	1	1.0970e-01	2.7665e+05
	12	115	1	1.0970e-01	2.7665e+05
	12	116	1	1.0970e-01	2.7665e+05
	17	117	1	1.0970e-01	2.7665e+05
	17	118	1	1.0970e-01	2.7665e+05
	19	119	1	1.0820e-01	2.9455e+05
	20	120	1	1.0100e-01	3.4175e+05
	23	121	1	1.0860e-01	2.8937e+05
	24	122	1	1.0860e-01	2.8937e+05
	25	123	1	1.0860e-01	2.8937e+05
	26	124	1	1.0860e-01	2.8937e+05
	29	125	1	1.0130e-01	3.3740e+05
	30	126	1	1.0970e-01	2.7665e+05
	31	127	1	1.0970e-01	2.7665e+05
	31	128	1	1.0970e-01	2.7665e+05
	32	129	1	1.0970e-01	2.7665e+05
	32	130	1	1.0970e-01	2.7665e+05
	33	131	1	1.0970e-01	2.7665e+05
	33	132	1	1.0970e-01	2.7665e+05
	34	133	1	1.0970e-01	2.7665e+05
	36	134	1	1.0970e-01	2.7665e+05
	39	135	1	1.0130e-01	3.3740e+05
	40	136	1	1.0970e-01	2.7665e+05
	41	137	1	1.0970e-01	2.7665e+05
	41	138	1	1.0970e-01	2.7665e+05
	43	139	1	1.0820e-01	2.9455e+05
	44	140	1	1.0100e-01	3.4175e+05
	47	141	1	1.0860e-01	2.8937e+05
	48	142	1	1.0860e-01	2.8937e+05
	49	143	1	1.0860e-01	2.8937e+05
	50	144	1	1.0860e-01	2.8937e+05
	53	145	1	1.0130e-01	3.3740e+05
	54	146	1	1.0970e-01	2.7665e+05
	55	147	1	1.0970e-01	2.7665e+05
	55	148	1	1.0970e-01	2.7665e+05
	56	149	1	1.0970e-01	2.7665e+05
	56	150	1	1.0970e-01	2.7665e+05
	57	151	1	1.0970e-01	2.7665e+05
	57	152	1	1.0970e-01	2.7665e+05
	58	153	1	1.0970e-01	2.7665e+05
	62	154	1	1.0970e-01	2.7665e+05
	65	155	1	1.0130e-01	3.3740e+05
	66	156	1	1.0970e-01	2.7665e+05
	67	157	1	1.0970e-01	2.7665e+05
	67	158	1	1.0970e-01	2.7665e+05
	69	159	1	1.0820e-01	2.9455e+05
	70	160	1	1.0100e-01	3.4175e+05
	73	161	1	1.0860e-01	2.8937e+05
	74	162	1	1.0860e-01	2.8937e+05
	75	163	1	1.0860e-01	2.8937e+05
	76	164	1	1.0860e-01	2.8937e+05
	79	165	1	1.0130e-01	3.3740e+05
	80	166	1	1.0970e-01	2.7665e+05
	81	167	1	1.0970e-01	2.7665e+05
	81	168	1	1.0970e-01	2.7665e+05
	82	169	1	1.0970e-01	2.7665e+05
	82	170	1	1.0970e-01	2.7665e+05
	83	171	1	1.0970e-01	2.7665e+05
	83	172	1	1.0970e-01	2.7665e+05

84	173	1	1.0970e-01	2.7665e+05
86	174	1	1.0970e-01	2.7665e+05
89	175	1	1.0130e-01	3.3740e+05
90	176	1	1.0970e-01	2.7665e+05
91	177	1	1.0970e-01	2.7665e+05
91	178	1	1.0970e-01	2.7665e+05
93	179	1	1.0820e-01	2.9455e+05
94	180	1	1.0100e-01	3.4175e+05
97	181	1	1.0860e-01	2.8937e+05
98	182	1	1.0860e-01	2.8937e+05
99	183	1	1.0860e-01	2.8937e+05
100	184	1	1.0860e-01	2.8937e+05
1	2	1	1.4620e-01	2.7506e+05
1	17	1	1.5380e-01	2.5179e+05
1	27	1	1.5240e-01	2.6192e+05
2	3	1	1.3790e-01	3.5782e+05
3	4	1	1.5240e-01	2.6192e+05
3	16	1	1.2180e-01	5.3363e+05
4	5	1	1.5380e-01	2.5179e+05
4	12	1	1.5380e-01	2.5179e+05
5	6	1	1.5380e-01	2.5179e+05
5	13	1	1.5240e-01	2.6192e+05
6	7	1	1.4620e-01	2.7506e+05
6	10	1	1.5380e-01	2.5179e+05
7	8	1	1.3790e-01	3.5782e+05
8	9	1	1.2180e-01	5.3363e+05
8	90	1	1.5240e-01	2.6192e+05
10	11	1	1.5380e-01	2.5179e+05
11	12	1	1.5380e-01	2.5179e+05
13	14	1	1.2180e-01	5.3363e+05
13	15	1	1.2180e-01	5.3363e+05
17	18	1	1.5020e-01	2.8016e+05
18	19	1	1.3730e-01	4.1915e+05
18	22	1	1.4560e-01	3.2225e+05
19	20	1	1.3800e-01	3.5631e+05
20	21	1	1.3840e-01	3.5187e+05
21	22	1	1.3980e-01	3.8585e+05
21	26	1	1.3980e-01	3.8585e+05
22	23	1	1.3980e-01	3.8585e+05
23	24	1	1.3980e-01	3.8585e+05
24	25	1	1.3980e-01	3.8585e+05
25	26	1	1.3980e-01	3.8585e+05
27	28	1	1.2180e-01	5.3363e+05
27	29	1	1.3790e-01	3.5782e+05
29	30	1	1.4620e-01	2.7506e+05
30	31	1	1.5380e-01	2.5179e+05
30	34	1	1.5380e-01	2.5179e+05
31	32	1	1.5380e-01	2.5179e+05
32	33	1	1.5380e-01	2.5179e+05
33	36	1	1.5380e-01	2.5179e+05
34	35	1	1.5240e-01	2.6192e+05
34	36	1	1.5380e-01	2.5179e+05
35	101	1	1.2180e-01	5.3363e+05
35	103	1	1.2180e-01	5.3363e+05
36	37	1	1.5240e-01	2.6192e+05
37	38	1	1.2180e-01	5.3363e+05
37	39	1	1.3790e-01	3.5782e+05
39	40	1	1.4620e-01	2.7506e+05
40	41	1	1.5380e-01	2.5179e+05
40	51	1	1.5240e-01	2.6192e+05
41	42	1	1.5020e-01	2.8016e+05
42	43	1	1.3730e-01	4.1915e+05
42	46	1	1.4560e-01	3.2225e+05
43	44	1	1.3800e-01	3.5631e+05
44	45	1	1.3840e-01	3.5187e+05
45	46	1	1.3980e-01	3.8585e+05
45	50	1	1.3980e-01	3.8585e+05
46	47	1	1.3980e-01	3.8585e+05
47	48	1	1.3980e-01	3.8585e+05
48	49	1	1.3980e-01	3.8585e+05
49	50	1	1.3980e-01	3.8585e+05
51	52	1	1.2180e-01	5.3363e+05
51	53	1	1.3790e-01	3.5782e+05
53	54	1	1.4620e-01	2.7506e+05
54	55	1	1.5380e-01	2.5179e+05
54	58	1	1.5380e-01	2.5179e+05
55	56	1	1.5380e-01	2.5179e+05
56	57	1	1.5380e-01	2.5179e+05
57	62	1	1.5380e-01	2.5179e+05
58	59	1	1.5240e-01	2.6192e+05
58	62	1	1.5380e-01	2.5179e+05
59	60	1	1.2180e-01	5.3363e+05
59	61	1	1.2180e-01	5.3363e+05
62	63	1	1.5240e-01	2.6192e+05
63	64	1	1.2180e-01	5.3363e+05
63	65	1	1.3790e-01	3.5782e+05
65	66	1	1.4620e-01	2.7506e+05
66	67	1	1.5380e-01	2.5179e+05
66	77	1	1.5240e-01	2.6192e+05
67	68	1	1.5020e-01	2.8016e+05
68	69	1	1.3730e-01	4.1915e+05
68	72	1	1.4560e-01	3.2225e+05
69	70	1	1.3800e-01	3.5631e+05
70	71	1	1.3840e-01	3.5187e+05
71	72	1	1.3980e-01	3.8585e+05
71	76	1	1.3980e-01	3.8585e+05
72	73	1	1.3980e-01	3.8585e+05
73	74	1	1.3980e-01	3.8585e+05
74	75	1	1.3980e-01	3.8585e+05
75	76	1	1.3980e-01	3.8585e+05
77	78	1	1.2180e-01	5.3363e+05
77	79	1	1.3790e-01	3.5782e+05
79	80	1	1.4620e-01	2.7506e+05
80	81	1	1.5380e-01	2.5179e+05
80	84	1	1.5380e-01	2.5179e+05
81	82	1	1.5380e-01	2.5179e+05
82	83	1	1.5380e-01	2.5179e+05
83	86	1	1.5380e-01	2.5179e+05
84	85	1	1.5240e-01	2.6192e+05
84	86	1	1.5380e-01	2.5179e+05
85	102	1	1.2180e-01	5.3363e+05
85	104	1	1.2180e-01	5.3363e+05
86	87	1	1.5240e-01	2.6192e+05



87	88	1	1.2180e-01	5.3363e+05
87	89	1	1.3790e-01	3.5782e+05
89	90	1	1.4620e-01	2.7506e+05
90	91	1	1.5380e-01	2.5179e+05
91	92	1	1.5020e-01	2.8016e+05
92	93	1	1.3730e-01	4.1915e+05
92	96	1	1.4560e-01	3.2225e+05
93	94	1	1.3800e-01	3.5631e+05
94	95	1	1.3840e-01	3.5187e+05
95	96	1	1.3980e-01	3.8585e+05
95	100	1	1.3980e-01	3.8585e+05
96	97	1	1.3980e-01	3.8585e+05
97	98	1	1.3980e-01	3.8585e+05
98	99	1	1.3980e-01	3.8585e+05
99	100	1	1.3980e-01	3.8585e+05

[ pairs ]

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```
[ angles ]
; ai aj ak funct theta cth
```

1	2	106	1	1.1768e+02	3.8325e+02
1	17	117	1	1.0980e+02	3.8777e+02
1	17	118	1	1.0980e+02	3.8777e+02
2	1	105	1	1.0888e+02	4.1706e+02
3	2	106	1	1.1755e+02	4.0443e+02
3	4	107	1	1.0877e+02	3.9271e+02
4	5	108	1	1.0980e+02	3.8777e+02
4	12	115	1	1.0980e+02	3.8777e+02
4	12	116	1	1.0980e+02	3.8777e+02
5	4	107	1	1.0980e+02	3.8777e+02
5	6	109	1	1.0956e+02	3.8819e+02
6	5	108	1	1.0980e+02	3.8777e+02
6	7	110	1	1.1768e+02	3.8325e+02
6	10	111	1	1.0980e+02	3.8777e+02
6	10	112	1	1.0980e+02	3.8777e+02
7	6	109	1	1.0888e+02	4.1706e+02
8	7	110	1	1.1755e+02	4.0443e+02
8	90	176	1	1.0822e+02	3.9363e+02
10	6	109	1	1.0956e+02	3.8819e+02
10	11	113	1	1.0980e+02	3.8777e+02
10	11	114	1	1.0980e+02	3.8777e+02
11	10	111	1	1.0980e+02	3.8777e+02
11	10	112	1	1.0980e+02	3.8777e+02
11	12	115	1	1.0980e+02	3.8777e+02
11	12	116	1	1.0980e+02	3.8777e+02
12	4	107	1	1.0980e+02	3.8777e+02
12	11	113	1	1.0980e+02	3.8777e+02
12	11	114	1	1.0980e+02	3.8777e+02
13	5	108	1	1.0877e+02	3.9271e+02
17	1	105	1	1.0956e+02	3.8819e+02
18	17	117	1	1.1049e+02	3.9480e+02
18	17	118	1	1.1049e+02	3.9480e+02
18	19	119	1	1.2848e+02	3.9556e+02
19	20	120	1	1.2550e+02	3.9120e+02
20	19	119	1	1.2053e+02	4.1664e+02
21	20	120	1	1.2554e+02	3.9020e+02
21	26	124	1	1.1988e+02	4.0317e+02
22	23	121	1	1.1988e+02	4.0317e+02
23	24	122	1	1.1988e+02	4.0317e+02
24	23	121	1	1.1988e+02	4.0317e+02
24	25	123	1	1.1988e+02	4.0317e+02
25	24	122	1	1.1988e+02	4.0317e+02
25	26	124	1	1.1988e+02	4.0317e+02
26	25	123	1	1.1988e+02	4.0317e+02
27	1	105	1	1.0822e+02	3.9363e+02
27	29	125	1	1.1755e+02	4.0443e+02
29	30	126	1	1.0888e+02	4.1706e+02
30	29	125	1	1.1768e+02	3.8325e+02
30	31	127	1	1.0980e+02	3.8777e+02
30	31	128	1	1.0980e+02	3.8777e+02
30	34	133	1	1.0980e+02	3.8777e+02
31	30	126	1	1.0956e+02	3.8819e+02
31	32	129	1	1.0980e+02	3.8777e+02
31	32	130	1	1.0980e+02	3.8777e+02
32	31	127	1	1.0980e+02	3.8777e+02
32	31	128	1	1.0980e+02	3.8777e+02
32	33	131	1	1.0980e+02	3.8777e+02
32	33	132	1	1.0980e+02	3.8777e+02
33	32	129	1	1.0980e+02	3.8777e+02
33	32	130	1	1.0980e+02	3.8777e+02
33	36	134	1	1.0980e+02	3.8777e+02
34	30	126	1	1.0956e+02	3.8819e+02
34	36	134	1	1.0980e+02	3.8777e+02
35	34	133	1	1.0877e+02	3.9271e+02
36	33	131	1	1.0980e+02	3.8777e+02
36	33	132	1	1.0980e+02	3.8777e+02
36	34	133	1	1.0980e+02	3.8777e+02
37	36	134	1	1.0877e+02	3.9271e+02
37	39	135	1	1.1755e+02	4.0443e+02
39	40	136	1	1.0888e+02	4.1706e+02
40	39	135	1	1.1768e+02	3.8325e+02
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40	41	138	1	1.0980e+02	3.8777e+02
41	40	136	1	1.0956e+02	3.8819e+02
42	41	137	1	1.1049e+02	3.9480e+02
42	41	138	1	1.1049e+02	3.9480e+02
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45	44	140	1	1.2554e+02	3.9020e+02
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47	48	142	1	1.1988e+02	4.0317e+02
48	47	141	1	1.1988e+02	4.0317e+02
48	49	143	1	1.1988e+02	4.0317e+02
49	48	142	1	1.1988e+02	4.0317e+02
49	50	144	1	1.1988e+02	4.0317e+02
50	49	143	1	1.1988e+02	4.0317e+02
51	40	136	1	1.0822e+02	3.9363e+02
51	53	145	1	1.1755e+02	4.0443e+02
53	54	146	1	1.0888e+02	4.1706e+02
54	53	145	1	1.1768e+02	3.8325e+02
54	55	147	1	1.0980e+02	3.8777e+02
54	55	148	1	1.0980e+02	3.8777e+02
54	58	153	1	1.0980e+02	3.8777e+02
55	54	146	1	1.0956e+02	3.8819e+02
55	56	149	1	1.0980e+02	3.8777e+02
55	56	150	1	1.0980e+02	3.8777e+02
56	55	147	1	1.0980e+02	3.8777e+02
56	55	148	1	1.0980e+02	3.8777e+02
56	57	151	1	1.0980e+02	3.8777e+02
56	57	152	1	1.0980e+02	3.8777e+02
57	56	149	1	1.0980e+02	3.8777e+02
57	56	150	1	1.0980e+02	3.8777e+02
57	62	154	1	1.0980e+02	3.8777e+02
58	54	146	1	1.0956e+02	3.8819e+02
58	62	154	1	1.0980e+02	3.8777e+02
59	58	153	1	1.0877e+02	3.9271e+02
62	57	151	1	1.0980e+02	3.8777e+02
62	57	152	1	1.0980e+02	3.8777e+02
62	58	153	1	1.0980e+02	3.8777e+02
63	62	154	1	1.0877e+02	3.9271e+02
63	65	155	1	1.1755e+02	4.0443e+02

65	66	156	1	1.0888e+02	4.1706e+02
66	65	155	1	1.1768e+02	3.8325e+02
66	67	157	1	1.0980e+02	3.8777e+02
66	67	158	1	1.0980e+02	3.8777e+02
67	66	156	1	1.0956e+02	3.8819e+02
68	67	157	1	1.1049e+02	3.9480e+02
68	67	158	1	1.1049e+02	3.9480e+02
68	69	159	1	1.2848e+02	3.9556e+02
69	70	160	1	1.2550e+02	3.9120e+02
70	69	159	1	1.2053e+02	4.1664e+02
71	70	160	1	1.2554e+02	3.9020e+02
71	76	164	1	1.1988e+02	4.0317e+02
72	73	161	1	1.1988e+02	4.0317e+02
73	74	162	1	1.1988e+02	4.0317e+02
74	73	161	1	1.1988e+02	4.0317e+02
74	75	163	1	1.1988e+02	4.0317e+02
75	74	162	1	1.1988e+02	4.0317e+02
75	76	164	1	1.1988e+02	4.0317e+02
76	75	163	1	1.1988e+02	4.0317e+02
77	66	156	1	1.0822e+02	3.9363e+02
77	79	165	1	1.1755e+02	4.0443e+02
79	80	166	1	1.0888e+02	4.1706e+02
80	79	165	1	1.1768e+02	3.8325e+02
80	81	167	1	1.0980e+02	3.8777e+02
80	81	168	1	1.0980e+02	3.8777e+02
80	84	173	1	1.0980e+02	3.8777e+02
81	80	166	1	1.0956e+02	3.8819e+02
81	82	169	1	1.0980e+02	3.8777e+02
81	82	170	1	1.0980e+02	3.8777e+02
82	81	167	1	1.0980e+02	3.8777e+02
82	81	168	1	1.0980e+02	3.8777e+02
82	83	171	1	1.0980e+02	3.8777e+02
82	83	172	1	1.0980e+02	3.8777e+02
83	82	169	1	1.0980e+02	3.8777e+02
83	82	170	1	1.0980e+02	3.8777e+02
83	86	174	1	1.0980e+02	3.8777e+02
84	80	166	1	1.0956e+02	3.8819e+02
84	86	174	1	1.0980e+02	3.8777e+02
85	84	173	1	1.0877e+02	3.9271e+02
86	83	171	1	1.0980e+02	3.8777e+02
86	83	172	1	1.0980e+02	3.8777e+02
86	84	173	1	1.0980e+02	3.8777e+02
87	86	174	1	1.0877e+02	3.9271e+02
87	89	175	1	1.1755e+02	4.0443e+02
89	90	176	1	1.0888e+02	4.1706e+02
90	89	175	1	1.1768e+02	3.8325e+02
90	91	177	1	1.0980e+02	3.8777e+02
90	91	178	1	1.0980e+02	3.8777e+02
91	90	176	1	1.0956e+02	3.8819e+02
92	91	177	1	1.1049e+02	3.9480e+02
92	91	178	1	1.1049e+02	3.9480e+02
92	93	179	1	1.2848e+02	3.9556e+02
93	94	180	1	1.2550e+02	3.9120e+02
94	93	179	1	1.2053e+02	4.1664e+02
95	94	180	1	1.2554e+02	3.9020e+02
95	100	184	1	1.1988e+02	4.0317e+02
96	97	181	1	1.1988e+02	4.0317e+02
97	98	182	1	1.1988e+02	4.0317e+02
98	97	181	1	1.1988e+02	4.0317e+02
98	99	183	1	1.1988e+02	4.0317e+02
99	98	182	1	1.1988e+02	4.0317e+02
99	100	184	1	1.1988e+02	4.0317e+02
100	99	183	1	1.1988e+02	4.0317e+02
111	10	112	1	1.0758e+02	3.2970e+02
113	11	114	1	1.0758e+02	3.2970e+02
115	12	116	1	1.0758e+02	3.2970e+02
117	17	118	1	1.0758e+02	3.2970e+02
127	31	128	1	1.0758e+02	3.2970e+02
129	32	130	1	1.0758e+02	3.2970e+02
131	33	132	1	1.0758e+02	3.2970e+02
137	41	138	1	1.0758e+02	3.2970e+02
147	55	148	1	1.0758e+02	3.2970e+02
149	56	150	1	1.0758e+02	3.2970e+02
151	57	152	1	1.0758e+02	3.2970e+02
157	67	158	1	1.0758e+02	3.2970e+02
167	81	168	1	1.0758e+02	3.2970e+02
169	82	170	1	1.0758e+02	3.2970e+02
171	83	172	1	1.0758e+02	3.2970e+02
177	91	178	1	1.0758e+02	3.2970e+02
1	2	3	1	1.2069e+02	5.3045e+02
1	17	18	1	1.1193e+02	5.3112e+02
1	27	28	1	1.2320e+02	5.6400e+02
1	27	29	1	1.1518e+02	5.5890e+02
2	1	17	1	1.1161e+02	5.5153e+02
2	1	27	1	1.0906e+02	5.6066e+02
2	3	4	1	1.1518e+02	5.5890e+02
2	3	16	1	1.2305e+02	6.2107e+02
3	4	5	1	1.1104e+02	5.2944e+02
3	4	12	1	1.1104e+02	5.2944e+02
4	3	16	1	1.2320e+02	5.6400e+02
4	5	6	1	1.1151e+02	5.2601e+02
4	5	13	1	1.1104e+02	5.2944e+02
4	12	11	1	1.1151e+02	5.2601e+02
5	4	12	1	1.1151e+02	5.2601e+02
5	6	7	1	1.1161e+02	5.5153e+02
5	6	10	1	1.1151e+02	5.2601e+02
5	13	14	1	1.2320e+02	5.6400e+02
5	13	15	1	1.2320e+02	5.6400e+02
6	5	13	1	1.1104e+02	5.2944e+02
6	7	8	1	1.2069e+02	5.3045e+02
6	10	11	1	1.1151e+02	5.2601e+02
7	6	10	1	1.1161e+02	5.5153e+02
7	8	9	1	1.2305e+02	6.2107e+02
7	8	90	1	1.1518e+02	5.5890e+02
8	90	89	1	1.0906e+02	5.6066e+02
8	90	91	1	1.1104e+02	5.2944e+02
9	8	90	1	1.2320e+02	5.6400e+02
10	11	12	1	1.1151e+02	5.2601e+02
14	13	15	1	1.3025e+02	6.5220e+02
17	1	27	1	1.1104e+02	5.2944e+02
17	18	19	1	1.1945e+02	5.4149e+02
17	18	22	1	1.2652e+02	5.1329e+02
18	19	20	1	1.0699e+02	6.1446e+02

18	22	21	1	1.2079e+02	5.4409e+02
18	22	23	1	1.2079e+02	5.4409e+02
19	18	22	1	1.1351e+02	5.6584e+02
19	20	21	1	1.1315e+02	5.6400e+02
20	21	22	1	1.1834e+02	5.7806e+02
20	21	26	1	1.1834e+02	5.7806e+02
21	22	23	1	1.2002e+02	5.5748e+02
21	26	25	1	1.2002e+02	5.5748e+02
22	21	26	1	1.2002e+02	5.5748e+02
22	23	24	1	1.2002e+02	5.5748e+02
23	24	25	1	1.2002e+02	5.5748e+02
24	25	26	1	1.2002e+02	5.5748e+02
27	29	30	1	1.2069e+02	5.3045e+02
28	27	29	1	1.2305e+02	6.2107e+02
29	30	31	1	1.1161e+02	5.5153e+02
29	30	34	1	1.1161e+02	5.5153e+02
30	31	32	1	1.1151e+02	5.2601e+02
30	34	35	1	1.1104e+02	5.2944e+02
30	34	36	1	1.1151e+02	5.2601e+02
31	30	34	1	1.1151e+02	5.2601e+02
31	32	33	1	1.1151e+02	5.2601e+02
32	33	36	1	1.1151e+02	5.2601e+02
33	36	34	1	1.1151e+02	5.2601e+02
33	36	37	1	1.1104e+02	5.2944e+02
34	35	101	1	1.2320e+02	5.6400e+02
34	35	103	1	1.2320e+02	5.6400e+02
34	36	37	1	1.1104e+02	5.2944e+02
35	34	36	1	1.1104e+02	5.2944e+02
36	37	38	1	1.2320e+02	5.6400e+02
36	37	39	1	1.1518e+02	5.5890e+02
37	39	40	1	1.2069e+02	5.3045e+02
38	37	39	1	1.2305e+02	6.2107e+02
39	40	41	1	1.1161e+02	5.5153e+02
39	40	51	1	1.0906e+02	5.6066e+02
40	41	42	1	1.1193e+02	5.3112e+02
40	51	52	1	1.2320e+02	5.6400e+02
40	51	53	1	1.1518e+02	5.5890e+02
41	40	51	1	1.1104e+02	5.2944e+02
41	42	43	1	1.1945e+02	5.4149e+02
41	42	46	1	1.2652e+02	5.1329e+02
42	43	44	1	1.0699e+02	6.1446e+02
42	46	45	1	1.2079e+02	5.4409e+02
42	46	47	1	1.2079e+02	5.4409e+02
43	42	46	1	1.1351e+02	5.6584e+02
43	44	45	1	1.1315e+02	5.6400e+02
44	45	46	1	1.1834e+02	5.7806e+02
44	45	50	1	1.1834e+02	5.7806e+02
45	46	47	1	1.2002e+02	5.5748e+02
45	50	49	1	1.2002e+02	5.5748e+02
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47	48	49	1	1.2002e+02	5.5748e+02
48	49	50	1	1.2002e+02	5.5748e+02
51	53	54	1	1.2069e+02	5.3045e+02
52	51	53	1	1.2305e+02	6.2107e+02
53	54	55	1	1.1161e+02	5.5153e+02
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54	55	56	1	1.1151e+02	5.2601e+02
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57	62	63	1	1.1104e+02	5.2944e+02
58	59	60	1	1.2320e+02	5.6400e+02
58	59	61	1	1.2320e+02	5.6400e+02
58	62	63	1	1.1104e+02	5.2944e+02
59	58	62	1	1.1104e+02	5.2944e+02
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62	63	64	1	1.2320e+02	5.6400e+02
62	63	65	1	1.1518e+02	5.5890e+02
63	65	66	1	1.2069e+02	5.3045e+02
64	63	65	1	1.2305e+02	6.2107e+02
65	66	67	1	1.1161e+02	5.5153e+02
65	66	77	1	1.0906e+02	5.6066e+02
66	67	68	1	1.1193e+02	5.3112e+02
66	77	78	1	1.2320e+02	5.6400e+02
66	77	79	1	1.1518e+02	5.5890e+02
67	66	77	1	1.1104e+02	5.2944e+02
67	68	69	1	1.1945e+02	5.4149e+02
67	68	72	1	1.2652e+02	5.1329e+02
68	69	70	1	1.0699e+02	6.1446e+02
68	72	71	1	1.2079e+02	5.4409e+02
68	72	73	1	1.2079e+02	5.4409e+02
69	68	72	1	1.1351e+02	5.6584e+02
69	70	71	1	1.1315e+02	5.6400e+02
70	71	72	1	1.1834e+02	5.7806e+02
70	71	76	1	1.1834e+02	5.7806e+02
71	72	73	1	1.2002e+02	5.5748e+02
71	76	75	1	1.2002e+02	5.5748e+02
72	71	76	1	1.2002e+02	5.5748e+02
72	73	74	1	1.2002e+02	5.5748e+02
73	74	75	1	1.2002e+02	5.5748e+02
74	75	76	1	1.2002e+02	5.5748e+02
77	79	80	1	1.2069e+02	5.3045e+02
78	77	79	1	1.2305e+02	6.2107e+02
79	80	81	1	1.1161e+02	5.5153e+02
79	80	84	1	1.1161e+02	5.5153e+02
80	81	82	1	1.1151e+02	5.2601e+02
80	84	85	1	1.1104e+02	5.2944e+02
80	84	86	1	1.1151e+02	5.2601e+02
81	80	84	1	1.1151e+02	5.2601e+02
81	82	83	1	1.1151e+02	5.2601e+02
82	83	86	1	1.1151e+02	5.2601e+02
83	86	84	1	1.1151e+02	5.2601e+02
83	86	87	1	1.1104e+02	5.2944e+02
84	85	102	1	1.2320e+02	5.6400e+02
84	85	104	1	1.2320e+02	5.6400e+02
84	86	87	1	1.1104e+02	5.2944e+02
85	84	86	1	1.1104e+02	5.2944e+02
86	87	88	1	1.2320e+02	5.6400e+02
86	87	89	1	1.1518e+02	5.5890e+02



```

87 89 90 1 1.2069e+02 5.3045e+02
88 87 89 1 1.2305e+02 6.2107e+02
89 90 91 1 1.1161e+02 5.5153e+02
90 91 92 1 1.1193e+02 5.3112e+02
91 92 93 1 1.1945e+02 5.4149e+02
91 92 96 1 1.2652e+02 5.1329e+02
92 93 94 1 1.0699e+02 6.1446e+02
92 96 95 1 1.2079e+02 5.4409e+02
92 96 97 1 1.2079e+02 5.4409e+02
93 92 96 1 1.1351e+02 5.6584e+02
93 94 95 1 1.1315e+02 5.6400e+02
94 95 96 1 1.1834e+02 5.7806e+02
94 95 100 1 1.1834e+02 5.7806e+02
95 96 97 1 1.2002e+02 5.5748e+02
95 100 99 1 1.2002e+02 5.5748e+02
96 95 100 1 1.2002e+02 5.5748e+02
96 97 98 1 1.2002e+02 5.5748e+02
97 98 99 1 1.2002e+02 5.5748e+02
98 99 100 1 1.2002e+02 5.5748e+02
101 35 103 1 1.3025e+02 6.5220e+02
102 85 104 1 1.3025e+02 6.5220e+02

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[ dihedrals ]
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2 3 4 107 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ;
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8 7 6 109 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ;
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9 8 7 110 3 29.28800 -8.36800 -20.92000 0.00000 0.00000 0.00000 ;
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17 1 2 106 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ;
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105 1 17 18 3 0.65270 1.95811 0.00000 -2.61082 0.00000 0.00000 ;
18 19 20 120 3 14.22560 0.00000 -14.22560 0.00000 0.00000 0.00000 ;
18 22 23 121 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ;
19 18 17 117 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ;
19 18 17 118 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ;
20 21 26 124 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ;
21 20 19 119 3 14.22560 0.00000 -14.22560 0.00000 0.00000 0.00000 ;
21 22 23 121 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ;
21 26 25 123 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ;
22 18 17 117 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ;
22 18 17 118 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ;
22 18 19 119 3 33.47200 0.00000 -33.47200 0.00000 0.00000 0.00000 ;
22 21 20 120 3 2.51040 0.00000 -2.51040 0.00000 0.00000 0.00000 ;
22 21 26 124 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ;
22 23 24 122 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ;
23 24 25 123 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ;
24 25 26 124 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ;
25 24 23 121 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ;
26 21 20 120 3 2.51040 0.00000 -2.51040 0.00000 0.00000 0.00000 ;
26 25 24 122 3 30.33400 0.00000 -30.33400 0.00000 0.00000 0.00000 ;
27 1 2 106 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ;
27 1 17 117 3 0.65270 1.95811 0.00000 -2.61082 0.00000 0.00000 ;
27 1 17 118 3 0.65270 1.95811 0.00000 -2.61082 0.00000 0.00000 ;
27 29 30 126 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ;
105 1 27 28 3 3.68192 -4.35136 0.00000 1.33888 0.00000 0.00000 ;
28 27 29 125 3 29.28800 -8.36800 -20.92000 0.00000 0.00000 0.00000 ;
105 1 27 29 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ;
29 30 31 127 3 0.65270 1.95811 0.00000 -2.61082 0.00000 0.00000 ;
29 30 31 128 3 0.65270 1.95811 0.00000 -2.61082 0.00000 0.00000 ;
29 30 34 133 3 0.65270 1.95811 0.00000 -2.61082 0.00000 0.00000 ;
30 31 32 129 3 0.66944 2.00832 0.00000 -2.67776 0.00000 0.00000 ;
30 31 32 130 3 0.66944 2.00832 0.00000 -2.67776 0.00000 0.00000 ;
30 34 36 134 3 0.66944 2.00832 0.00000 -2.67776 0.00000 0.00000 ;
31 30 29 125 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 ;
31 30 34 133 3 0.66944 2.00832 0.00000 -2.67776 0.00000 0.00000 ;
31 32 33 131 3 0.66944 2.00832 0.00000 -2.67776 0.00000 0.00000 ;
31 32 33 132 3 0.66944 2.00832 0.00000 -2.67776 0.00000 0.00000 ;
32 31 30 126 3 0.65270 1.95811 0.00000 -2.61082 0.00000 0.00000 ;
32 33 36 134 3 0.66944 2.00832 0.00000 -2.67776 0.00000 0.00000 ;
33 32 31 127 3 0.66944 2.00832 0.00000 -2.67776 0.00000 0.00000 ;
33 32 31 128 3 0.66944 2.00832 0.00000 -2.67776 0.00000 0.00000 ;
33 36 34 133 3 0.66944 2.00832 0.00000 -2.67776 0.00000 0.00000 ;

```

34	30	29	125	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
34	30	31	127	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	;
34	30	31	128	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	;
34	36	33	131	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	;
34	36	33	132	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	;
35	34	30	126	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
35	34	36	134	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
36	33	32	129	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	;
36	33	32	130	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	;
36	34	30	126	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
36	37	39	135	3	20.92000	0.00000	-20.92000	0.00000	0.00000	0.00000	;
37	36	33	131	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
37	36	33	132	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
37	36	34	133	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
37	39	40	136	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
38	37	36	134	3	3.68192	-4.35136	0.00000	1.33888	0.00000	0.00000	;
38	37	39	135	3	29.28800	-8.36800	-20.92000	0.00000	0.00000	0.00000	;
39	37	36	134	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
39	40	41	137	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
39	40	41	138	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
40	51	53	145	3	20.92000	0.00000	-20.92000	0.00000	0.00000	0.00000	;
41	40	39	135	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
41	42	43	139	3	33.47200	0.00000	-33.47200	0.00000	0.00000	0.00000	;
42	41	40	136	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
42	43	44	140	3	14.22560	0.00000	-14.22560	0.00000	0.00000	0.00000	;
42	46	47	141	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
43	42	41	137	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
43	42	41	138	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
44	45	50	144	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
45	44	43	139	3	14.22560	0.00000	-14.22560	0.00000	0.00000	0.00000	;
45	46	47	141	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
45	50	49	143	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
46	42	41	137	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
46	42	41	138	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
46	42	43	139	3	33.47200	0.00000	-33.47200	0.00000	0.00000	0.00000	;
46	45	44	140	3	2.51040	0.00000	-2.51040	0.00000	0.00000	0.00000	;
46	45	50	144	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
46	47	48	142	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
47	48	49	143	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
48	49	50	144	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
49	48	47	141	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
50	45	44	140	3	2.51040	0.00000	-2.51040	0.00000	0.00000	0.00000	;
50	49	48	142	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
51	40	39	135	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
51	40	41	137	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
51	40	41	138	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
51	53	54	146	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
52	51	40	136	3	3.68192	-4.35136	0.00000	1.33888	0.00000	0.00000	;
52	51	53	145	3	29.28800	-8.36800	-20.92000	0.00000	0.00000	0.00000	;
53	51	40	136	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
53	54	55	147	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
53	54	55	148	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
53	54	58	153	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
54	55	56	149	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	;
54	55	56	150	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	;
54	58	62	154	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	;
55	54	53	145	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
55	54	58	153	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	;
55	56	57	151	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	;
55	56	57	152	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	;
56	55	54	146	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
56	57	62	154	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	;
57	56	55	147	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	;
57	56	55	148	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	;
57	62	58	153	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	;
58	54	53	145	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
58	54	55	147	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	;
58	54	55	148	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	;
58	62	57	151	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	;
58	62	57	152	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	;
59	58	54	146	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
59	58	62	154	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
60	59	58	153	3	3.68192	-4.35136	0.00000	1.33888	0.00000	0.00000	;
61	59	58	153	3	3.68192	-4.35136	0.00000	1.33888	0.00000	0.00000	;
62	57	56	149	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	;
62	57	56	150	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	;
62	58	54	146	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
62	63	65	155	3	20.92000	0.00000	-20.92000	0.00000	0.00000	0.00000	;
63	62	57	151	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
63	62	57	152	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
63	62	58	153	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
63	65	66	156	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
64	63	62	154	3	3.68192	-4.35136	0.00000	1.33888	0.00000	0.00000	;
64	63	65	155	3	29.28800	-8.36800	-20.92000	0.00000	0.00000	0.00000	;
65	63	62	154	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
65	66	67	157	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
65	66	67	158	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
66	77	79	165	3	20.92000	0.00000	-20.92000	0.00000	0.00000	0.00000	;
67	66	65	155	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
67	68	69	159	3	33.47200	0.00000	-33.47200	0.00000	0.00000	0.00000	;
68	67	66	156	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
68	69	70	160	3	14.22560	0.00000	-14.22560	0.00000	0.00000	0.00000	;
68	72	73	161	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
69	68	67	157	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
69	68	67	158	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
70	71	76	164	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
71	70	69	159	3	14.22560	0.00000	-14.22560	0.00000	0.00000	0.00000	;
71	72	73	161	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
71	76	75	163	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
72	68	67	157	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
72	68	67	158	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
72	68	69	159	3	33.47200	0.00000	-33.47200	0.00000	0.00000	0.00000	;
72	71	70	160	3	2.51040	0.00000	-2.51040	0.00000	0.00000	0.00000	;
72	71	76	164	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
72	73	74	162	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
73	74	75	163	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	

77	79	80	166	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
78	77	66	156	3	3.68192	-4.35136	0.00000	1.33888	0.00000	0.00000	;
78	77	79	165	3	29.28800	-8.36800	-20.92000	0.00000	0.00000	0.00000	;
79	77	66	156	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
79	80	81	167	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
79	80	81	168	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
79	80	84	173	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
80	81	82	169	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	;
80	81	82	170	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	;
80	84	86	174	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	;
81	80	79	165	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
81	80	84	173	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	;
81	82	83	171	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	;
81	82	83	172	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	;
82	81	80	166	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
82	83	86	174	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	;
83	82	81	167	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	;
83	82	81	168	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	;
83	86	84	173	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	;
84	80	79	165	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
84	80	81	167	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	;
84	80	81	168	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	;
84	86	83	171	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	;
84	86	83	172	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	;
85	84	80	166	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
85	84	86	174	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
86	83	82	169	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	;
86	83	82	170	3	0.66944	2.00832	0.00000	-2.67776	0.00000	0.00000	;
86	84	80	166	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
86	87	89	175	3	20.92000	0.00000	-20.92000	0.00000	0.00000	0.00000	;
87	86	83	171	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
87	86	83	172	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
87	86	84	173	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
87	89	90	176	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
88	87	86	174	3	3.68192	-4.35136	0.00000	1.33888	0.00000	0.00000	;
88	87	89	175	3	29.28800	-8.36800	-20.92000	0.00000	0.00000	0.00000	;
89	87	86	174	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
89	90	91	177	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
89	90	91	178	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
90	8	7	110	3	20.92000	0.00000	-20.92000	0.00000	0.00000	0.00000	;
91	90	89	175	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
91	92	93	179	3	33.47200	0.00000	-33.47200	0.00000	0.00000	0.00000	;
92	91	90	176	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
92	93	94	180	3	14.22560	0.00000	-14.22560	0.00000	0.00000	0.00000	;
92	96	97	181	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
93	92	91	177	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
93	92	91	178	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
94	95	100	184	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
95	94	93	179	3	14.22560	0.00000	-14.22560	0.00000	0.00000	0.00000	;
95	96	97	181	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
95	100	99	183	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
96	92	91	177	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
96	92	91	178	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
96	92	93	179	3	33.47200	0.00000	-33.47200	0.00000	0.00000	0.00000	;
96	95	94	180	3	2.51040	0.00000	-2.51040	0.00000	0.00000	0.00000	;
96	95	100	184	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
96	97	98	182	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
97	98	99	183	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
98	99	100	184	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
99	98	97	181	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
100	95	94	180	3	2.51040	0.00000	-2.51040	0.00000	0.00000	0.00000	;
100	99	98	182	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
101	35	34	133	3	3.68192	-4.35136	0.00000	1.33888	0.00000	0.00000	;
102	85	84	173	3	3.68192	-4.35136	0.00000	1.33888	0.00000	0.00000	;
103	35	34	133	3	3.68192	-4.35136	0.00000	1.33888	0.00000	0.00000	;
104	85	84	173	3	3.68192	-4.35136	0.00000	1.33888	0.00000	0.00000	;
105	1	2	106	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
105	1	17	117	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
105	1	17	118	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
107	4	5	108	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000	;
107	4	12	115	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000	;
107	4	12	116	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000	;
108	5	6	109	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
109	6	7	110	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
109	6	10	111	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
109	6	10	112	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
111	10	11	113	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000	;
111	10	11	114	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000	;
112	10	11	113	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000	;
112	10	11	114	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000	;
113	11	12	115	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000	;
113	11	12	116	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000	;
114	11	12	115	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000	;
114	11	12	116	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000	;
119	19	20	120	3	14.22560	0.00000	-14.22560	0.00000	0.00000	0.00000	;
121	23	24	122	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
122	24	25	123	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
123	25	26	124	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
125	29	30	126	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
126	30	31	127	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
126	30	31	128	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
126	30	34	133	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
127	31	32	129	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000	;
127	31	32	130	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000	;
128	31	32	129	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000	;
128	31	32	130	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000	;
129	32	33	131	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000	;
129	32	33	132	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000	;
130	32	33	131	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000	;
130	32	33	132	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000	;
131	33	36	134	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000	;
132	33	36	134	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000	;
133	34	36	134	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000	;
135	39	40	136	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
136	40	41	137	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.	

146	54	58	153	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
147	55	56	149	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000	;
147	55	56	150	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000	;
148	55	56	149	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000	;
148	55	56	150	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000	;
149	56	57	151	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000	;
149	56	57	152	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000	;
150	56	57	151	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000	;
150	56	57	152	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000	;
151	57	62	154	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000	;
152	57	62	154	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000	;
153	58	62	154	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000	;
155	65	66	156	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
156	66	67	157	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
156	66	67	158	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
159	69	70	160	3	14.22560	0.00000	-14.22560	0.00000	0.00000	0.00000	;
161	73	74	162	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
162	74	75	163	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
163	75	76	164	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
165	79	80	166	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
166	80	81	167	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
166	80	81	168	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
166	80	84	173	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
167	81	82	169	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000	;
167	81	82	170	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000	;
168	81	82	169	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000	;
168	81	82	170	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000	;
169	82	83	171	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000	;
169	82	83	172	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000	;
170	82	83	171	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000	;
170	82	83	172	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000	;
171	83	86	174	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000	;
172	83	86	174	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000	;
173	84	86	174	3	0.62760	1.88280	0.00000	-2.51040	0.00000	0.00000	;
175	89	90	176	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
176	90	91	177	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
176	90	91	178	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
179	93	94	180	3	14.22560	0.00000	-14.22560	0.00000	0.00000	0.00000	;
181	97	98	182	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
182	98	99	183	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
183	99	100	184	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
3	1	2	106	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
8	6	7	110	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
18	119	19	20	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
21	19	20	120	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
22	24	23	121	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
23	25	24	122	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
24	26	25	123	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
21	25	26	124	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
27	30	29	125	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
37	40	39	135	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
42	139	43	44	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
45	43	44	140	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
46	48	47	141	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
47	49	48	142	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
48	50	49	143	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
45	49	50	144	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
51	54	53	145	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
63	66	65	155	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
68	159	69	70	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
71	69	70	160	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
72	74	73	161	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
73	75	74	162	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
74	76	75	163	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
71	75	76	164	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
77	80	79	165	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
87	90	89	175	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
92	179	93	94	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
95	93	94	180	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
96	98	97	181	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
97	99	98	182	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
98	100	99	183	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
95	99	100	184	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
1	2	3	4	3	6.27600	6.27600	0.00000	0.00000	0.00000	0.00000	;
1	2	3	16	3	20.92000	0.00000	-20.92000	0.00000	0.00000	0.00000	;
1	17	18	19	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
1	17	18	22	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
1	27	29	30	3	6.27600	6.27600	0.00000	0.00000	0.00000	0.00000	;
2	1	17	18	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
2	1	27	28	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
2	1	27	29	3	23.84880	7.11280	-16.73600	0.00000	0.00000	0.00000	;
2	3	4	5	3	0.83680	0.00000	-2.76144	0.00000	3.34720	0.00000	;
2	3	4	12	3	0.83680	0.00000	-2.76144	0.00000	3.34720	0.00000	;
17	1	2	3	3	2.84512	-4.10032	16.73600	2.51040	-16.73600	0.00000	;
27	1	2	3	3	10.46000	-3.34720	0.00000	0.00000	0.00000	0.00000	;
3	4	5	6	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
3	4	5	13	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
3	4	12	11	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
4	5	6	7	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
4	5	6	10	3	3.68192	3.09616	-2.09200	-3.01248	0.00000	0.00000	;
4	5	13	14	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
4	5	13	15	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
4	12	11	10	3	3.68192	3.09616	-2.09200	-3.01248	0.00000	0.00000	;
5	4	3	16	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
5	4	12	11	3	3.68192	3.09616	-2.09200	-3.01248	0.00000	0.00000	;
5	6	7	8	3	2.84512	-4.10032	16.73600	2.51040	-16.73600	0.00000	;
5	6	10	11	3	3.68192	3.09616	-2.09200	-3.01248	0.00000	0.00000	;
6	5	4	12	3	3.68192	3.09616	-2.09200	-3.01248	0.00000	0.00000	;
6	5	13	14	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
6	5	13	15	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
6	7	8	9	3	20.92000	0.00000	-20.92000	0.00000	0.00000	0.00000	;
6	7	8	90	3	6.27600	6.27600	0.00000	0.00000	0.00000	0.00000	;
6	10	11	12	3	3.68192	3.09616	-2.09200	-3.01248	0.00000	0.00000	;
7	6	5	13	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
7	6	10	11	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
7	8	90	89	3	23.84880	7.11280	-16.73600	0.00000	0.00000	0.00000	

12	4	3	16	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
12	4	5	13	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
17	1	27	28	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
17	1	27	29	3	0.83680	0.00000	-2.76144	0.00000	3.34720	0.00000	;
17	18	19	20	3	33.47200	0.00000	-33.47200	0.00000	0.00000	0.00000	;
17	18	22	21	3	5.85760	0.00000	-5.85760	0.00000	0.00000	0.00000	;
17	18	22	23	3	5.85760	0.00000	-5.85760	0.00000	0.00000	0.00000	;
27	1	17	18	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
18	19	20	21	3	14.22560	0.00000	-14.22560	0.00000	0.00000	0.00000	;
18	22	21	20	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
18	22	21	26	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
18	22	23	24	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
19	18	22	21	3	5.85760	0.00000	-5.85760	0.00000	0.00000	0.00000	;
19	18	22	23	3	5.85760	0.00000	-5.85760	0.00000	0.00000	0.00000	;
19	20	21	22	3	2.51040	0.00000	-2.51040	0.00000	0.00000	0.00000	;
19	20	21	26	3	2.51040	0.00000	-2.51040	0.00000	0.00000	0.00000	;
20	19	18	22	3	33.47200	0.00000	-33.47200	0.00000	0.00000	0.00000	;
20	21	22	23	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
20	21	26	25	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
21	22	23	24	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
21	26	25	24	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
22	21	26	25	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
22	23	24	25	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
23	22	21	26	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
23	24	25	26	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
27	29	30	31	3	2.84512	-4.10032	16.73600	2.51040	-16.73600	0.00000	;
27	29	30	34	3	2.84512	-4.10032	16.73600	2.51040	-16.73600	0.00000	;
28	27	29	30	3	20.92000	0.00000	-20.92000	0.00000	0.00000	0.00000	;
29	30	31	32	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
29	30	34	35	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
29	30	34	36	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
30	31	32	33	3	3.68192	3.09616	-2.09200	-3.01248	0.00000	0.00000	;
30	34	35	101	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
30	34	35	103	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
30	34	36	33	3	3.68192	3.09616	-2.09200	-3.01248	0.00000	0.00000	;
30	34	36	37	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
31	30	34	35	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
31	30	34	36	3	3.68192	3.09616	-2.09200	-3.01248	0.00000	0.00000	;
31	32	33	36	3	3.68192	3.09616	-2.09200	-3.01248	0.00000	0.00000	;
32	31	30	34	3	3.68192	3.09616	-2.09200	-3.01248	0.00000	0.00000	;
32	33	36	34	3	3.68192	3.09616	-2.09200	-3.01248	0.00000	0.00000	;
32	33	36	37	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
33	36	34	35	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
33	36	37	38	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
33	36	37	39	3	0.83680	0.00000	-2.76144	0.00000	3.34720	0.00000	;
34	36	37	38	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
34	36	37	39	3	0.83680	0.00000	-2.76144	0.00000	3.34720	0.00000	;
35	34	36	37	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
36	34	35	101	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
36	34	35	103	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
36	37	39	40	3	6.27600	6.27600	0.00000	0.00000	0.00000	0.00000	;
37	39	40	41	3	2.84512	-4.10032	16.73600	2.51040	-16.73600	0.00000	;
37	39	40	51	3	10.46000	-3.34720	0.00000	0.00000	0.00000	0.00000	;
38	37	39	40	3	20.92000	0.00000	-20.92000	0.00000	0.00000	0.00000	;
39	40	41	42	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
39	40	51	52	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
39	40	51	53	3	23.84880	7.11280	-16.73600	0.00000	0.00000	0.00000	;
40	41	42	43	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
40	41	42	46	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
40	51	53	54	3	6.27600	6.27600	0.00000	0.00000	0.00000	0.00000	;
41	40	51	52	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
41	40	51	53	3	0.83680	0.00000	-2.76144	0.00000	3.34720	0.00000	;
41	42	43	44	3	33.47200	0.00000	-33.47200	0.00000	0.00000	0.00000	;
41	42	46	45	3	5.85760	0.00000	-5.85760	0.00000	0.00000	0.00000	;
41	42	46	47	3	5.85760	0.00000	-5.85760	0.00000	0.00000	0.00000	;
42	41	40	51	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
42	43	44	45	3	14.22560	0.00000	-14.22560	0.00000	0.00000	0.00000	;
42	46	45	44	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
42	46	45	50	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
42	46	47	48	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
43	42	46	45	3	5.85760	0.00000	-5.85760	0.00000	0.00000	0.00000	;
43	42	46	47	3	5.85760	0.00000	-5.85760	0.00000	0.00000	0.00000	;
43	44	45	46	3	2.51040	0.00000	-2.51040	0.00000	0.00000	0.00000	;
43	44	45	50	3	2.51040	0.00000	-2.51040	0.00000	0.00000	0.00000	;
44	43	42	46	3	33.47200	0.00000	-33.47200	0.00000	0.00000	0.00000	;
44	45	46	47	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
44	45	50	49	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
45	46	47	48	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
45	50	49	48	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
46	45	50	49	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
46	47	48	49	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
47	46	45	50	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
47	48	49	50	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
51	53	54	55	3	2.84512	-4.10032	16.73600	2.51040	-16.73600	0.00000	;
51	53	54	58	3	2.84512	-4.10032	16.73600	2.51040	-16.73600	0.00000	;
52	51	53	54	3	20.92000	0.00000	-20.92000	0.00000	0.00000	0.00000	;
53	54	55	56	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
53	54	58	59	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
53	54	58	62	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
54	55	56	57	3	3.68192	3.09616	-2.09200	-3.01248	0.00000	0.00000	;
54	58	59	60	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
54	58	59	61	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
54	58	62	57	3	3.68192	3.09616	-2.09200	-3.01248	0.00000	0.00000	;
54	58	62	63	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
55	54	58	59	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
55	54	58	62	3	3.68192	3.09616	-2.09200	-3.01248	0.00000	0.00000	;
55	56	57	62	3	3.68192	3.09616	-2.09200	-3.01248	0.00000	0.00000	;
56	55	54	58	3	3.68192	3.09616	-2.09200	-3.01248	0.00000	0.00000	;
56	57	62	58	3	3.68192	3.09616	-2.09200	-3.01248	0.00000	0.00000	;
56	57	62	63	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
57	62	58	59	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
57	62	63	64	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
57	62	63	65	3	0.83680	0.00000	-2.76144	0.00000	3.34720	0.00000	;
58	62	63	64	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
58	62	63	65	3	0.83680	0.00000	-2.76144	0.00000	3.34720	0.00000	;
59	58	62	63	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
60	59	58	62	3	0.00000	0.00000	0.00000	0.00000	0.00		

65	66	77	78	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
65	66	77	79	3	23.84880	7.11280	-16.73600	0.00000	0.00000	0.00000	;
66	67	68	69	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
66	67	68	72	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
66	77	79	80	3	6.27600	6.27600	0.00000	0.00000	0.00000	0.00000	;
67	66	77	78	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
67	66	77	79	3	0.83680	0.00000	-2.76144	0.00000	3.34720	0.00000	;
67	68	69	70	3	33.47200	0.00000	-33.47200	0.00000	0.00000	0.00000	;
67	68	72	71	3	5.85760	0.00000	-5.85760	0.00000	0.00000	0.00000	;
67	68	72	73	3	5.85760	0.00000	-5.85760	0.00000	0.00000	0.00000	;
68	67	66	77	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
68	69	70	71	3	14.22560	0.00000	-14.22560	0.00000	0.00000	0.00000	;
68	72	71	70	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
68	72	71	76	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
68	72	73	74	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
69	68	72	71	3	5.85760	0.00000	-5.85760	0.00000	0.00000	0.00000	;
69	68	72	73	3	5.85760	0.00000	-5.85760	0.00000	0.00000	0.00000	;
69	70	71	72	3	2.51040	0.00000	-2.51040	0.00000	0.00000	0.00000	;
69	70	71	76	3	2.51040	0.00000	-2.51040	0.00000	0.00000	0.00000	;
70	69	68	72	3	33.47200	0.00000	-33.47200	0.00000	0.00000	0.00000	;
70	71	72	73	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
70	71	76	75	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
71	72	73	74	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
71	76	75	74	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
72	71	76	75	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
72	73	74	75	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
73	72	71	76	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
73	74	75	76	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
77	79	80	81	3	2.84512	-4.10032	16.73600	2.51040	-16.73600	0.00000	;
77	79	80	84	3	2.84512	-4.10032	16.73600	2.51040	-16.73600	0.00000	;
78	77	79	80	3	20.92000	0.00000	-20.92000	0.00000	0.00000	0.00000	;
79	80	81	82	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
79	80	84	85	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
79	80	84	86	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
80	81	82	83	3	3.68192	3.09616	-2.09200	-3.01248	0.00000	0.00000	;
80	84	85	102	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
80	84	85	104	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
80	84	86	83	3	3.68192	3.09616	-2.09200	-3.01248	0.00000	0.00000	;
80	84	86	87	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
81	80	84	85	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
81	80	84	86	3	3.68192	3.09616	-2.09200	-3.01248	0.00000	0.00000	;
81	82	83	86	3	3.68192	3.09616	-2.09200	-3.01248	0.00000	0.00000	;
82	81	80	84	3	3.68192	3.09616	-2.09200	-3.01248	0.00000	0.00000	;
82	83	86	84	3	3.68192	3.09616	-2.09200	-3.01248	0.00000	0.00000	;
82	83	86	87	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
83	86	84	85	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
83	86	87	88	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
83	86	87	89	3	0.83680	0.00000	-2.76144	0.00000	3.34720	0.00000	;
84	86	87	88	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
84	86	87	89	3	0.83680	0.00000	-2.76144	0.00000	3.34720	0.00000	;
85	84	86	87	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
86	84	85	102	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
86	84	85	104	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
86	87	89	90	3	6.27600	6.27600	0.00000	0.00000	0.00000	0.00000	;
87	89	90	91	3	2.84512	-4.10032	16.73600	2.51040	-16.73600	0.00000	;
88	87	89	90	3	20.92000	0.00000	-20.92000	0.00000	0.00000	0.00000	;
89	90	91	92	3	0.65270	1.95811	0.00000	-2.61082	0.00000	0.00000	;
90	91	92	93	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
90	91	92	96	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	;
91	92	93	94	3	33.47200	0.00000	-33.47200	0.00000	0.00000	0.00000	;
91	92	96	95	3	5.85760	0.00000	-5.85760	0.00000	0.00000	0.00000	;
91	92	96	97	3	5.85760	0.00000	-5.85760	0.00000	0.00000	0.00000	;
92	93	94	95	3	14.22560	0.00000	-14.22560	0.00000	0.00000	0.00000	;
92	96	95	94	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
92	96	95	100	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
92	96	97	98	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
93	92	96	95	3	5.85760	0.00000	-5.85760	0.00000	0.00000	0.00000	;
93	92	96	97	3	5.85760	0.00000	-5.85760	0.00000	0.00000	0.00000	;
93	94	95	96	3	2.51040	0.00000	-2.51040	0.00000	0.00000	0.00000	;
93	94	95	100	3	2.51040	0.00000	-2.51040	0.00000	0.00000	0.00000	;
94	93	92	96	3	33.47200	0.00000	-33.47200	0.00000	0.00000	0.00000	;
94	95	96	97	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
94	95	100	99	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
95	96	97	98	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
95	100	99	98	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
96	95	100	99	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
96	97	98	99	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
97	96	95	100	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
97	98	99	100	3	30.33400	0.00000	-30.33400	0.00000	0.00000	0.00000	;
4	2	3	16	3	87.86400	0.00000	-87.86400	0.00000	0.00000	0.00000	;
90	7	8	9	3	87.86400	0.00000	-87.86400	0.00000	0.00000	0.00000	;
5	14	13	15	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
17	22	18	19	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
22	26	21	20	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
21	23	22	18	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
1	29	27	28	3	87.86400	0.00000	-87.86400	0.00000	0.00000	0.00000	;
34	101	35	103	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
36	39	37	38	3	87.86400	0.00000	-87.86400	0.00000	0.00000	0.00000	;
41	46	42	43	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
46	50	45	44	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
45	47	46	42	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
40	53	51	52	3	87.86400	0.00000	-87.86400	0.00000	0.00000	0.00000	;
58	60	59	61	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
62	65	63	64	3	87.86400	0.00000	-87.86400	0.00000	0.00000	0.00000	;
67	72	68	69	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
72	76	71	70	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
71	73	72	68	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
66	79	77	78	3	87.86400	0.00000	-87.86400	0.00000	0.00000	0.00000	;
84	102	85	104	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
86	89	87	88	3	87.86400	0.00000	-87.86400	0.00000	0.00000	0.00000	;
91	96	92	93	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
96	100	95	94	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;
95	97	96	92	3	9.20480	0.00000	-9.20480	0.00000	0.00000	0.00000	;