

Supplementary Information

The impact of lipid oxidation on functioning of a lung surfactant model

Anna Stachowicz-Kuśnierz,^{*a} Lukasz Cwiklik,^b Jacek Korchowiec,^a Ewa Rogalska,^c and
Beata Korchowiec,^{*c}

^a *Department of Theoretical Chemistry, Faculty of Chemistry, Jagiellonian University,
Gronostajowa 2, 30-387, Krakow, Poland*

^b *J. Heyrovský Institute of Physical Chemistry, Academy of Sciences of the Czech Republic,
v.v.i., Dolejškova 3, 18223 Prague 8, Czech Republic*

^c *Structure et Réactivité des Systèmes Moléculaires Complexes, BP 239, CNRS/Université de
Lorraine, 54506 Vandoeuvre-lès-Nancy cedex, France*

^d *Department of Physical Chemistry and Electrochemistry, Faculty of Chemistry, Jagiellonian
University, Gronostajowa 2, 30-387, Krakow, Poland*

^{*} Corresponding author. (BK) E-mail: bkorch@chemia.uj.edu.pl. Telephone: +48 (12) 663 22 51. Fax: +48 (12) 634 05 15. (ASK) E-mail: stachowa@chemia.uj.edu.pl. Telephone: +48 (12) 663 20 27. Fax: +48 (12) 634 05 15.

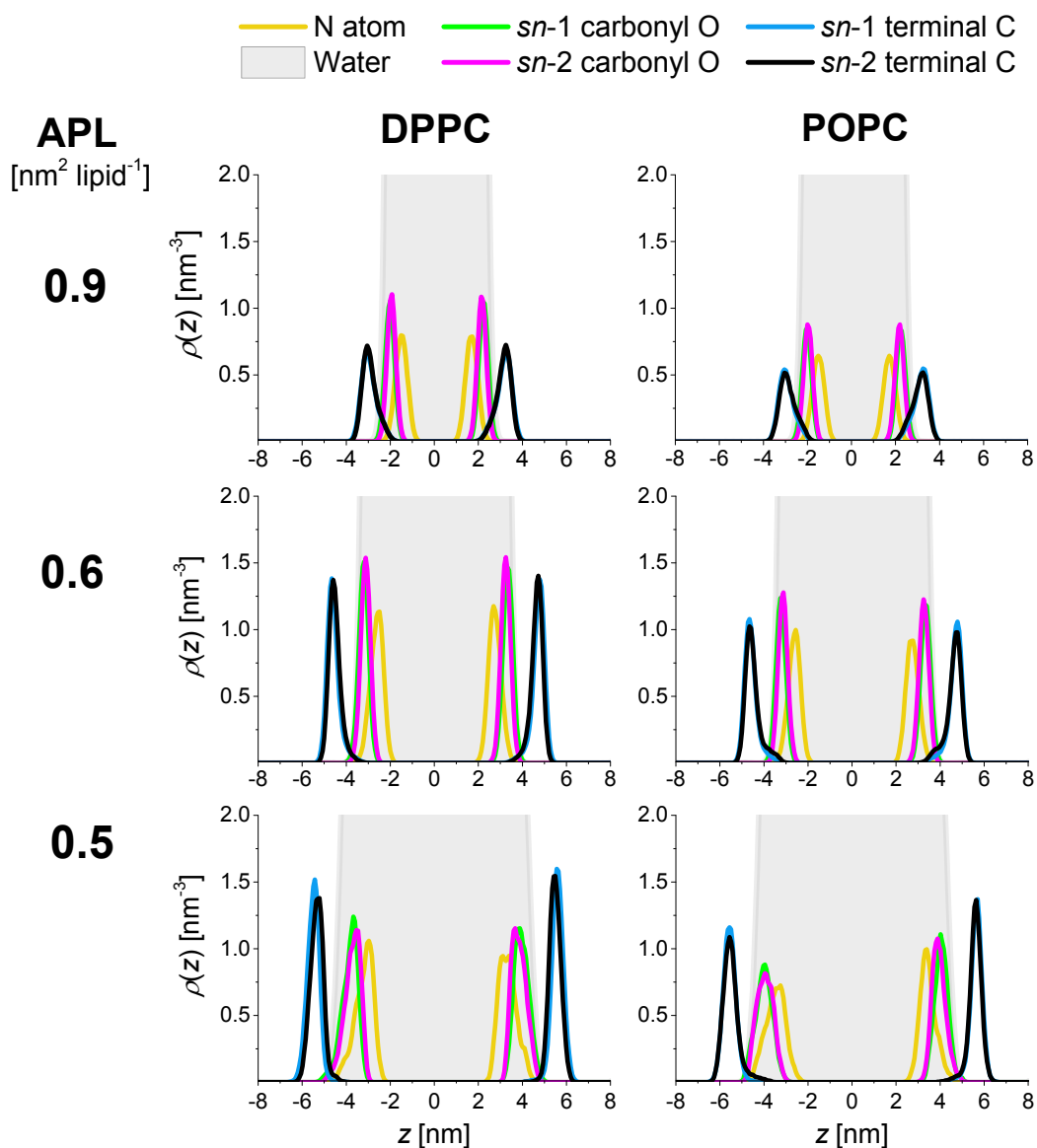


Fig. S.1 Number density profiles along monolayer normal for selected atoms in DPPC and POPC at APL equal to 0.9, 0.6, and 0.5 nm² lipid⁻¹. Densities of choline nitrogen (yellow), ester carbonyl O atoms (magenta and green), and chain terminal C atoms (blue and black) are presented.

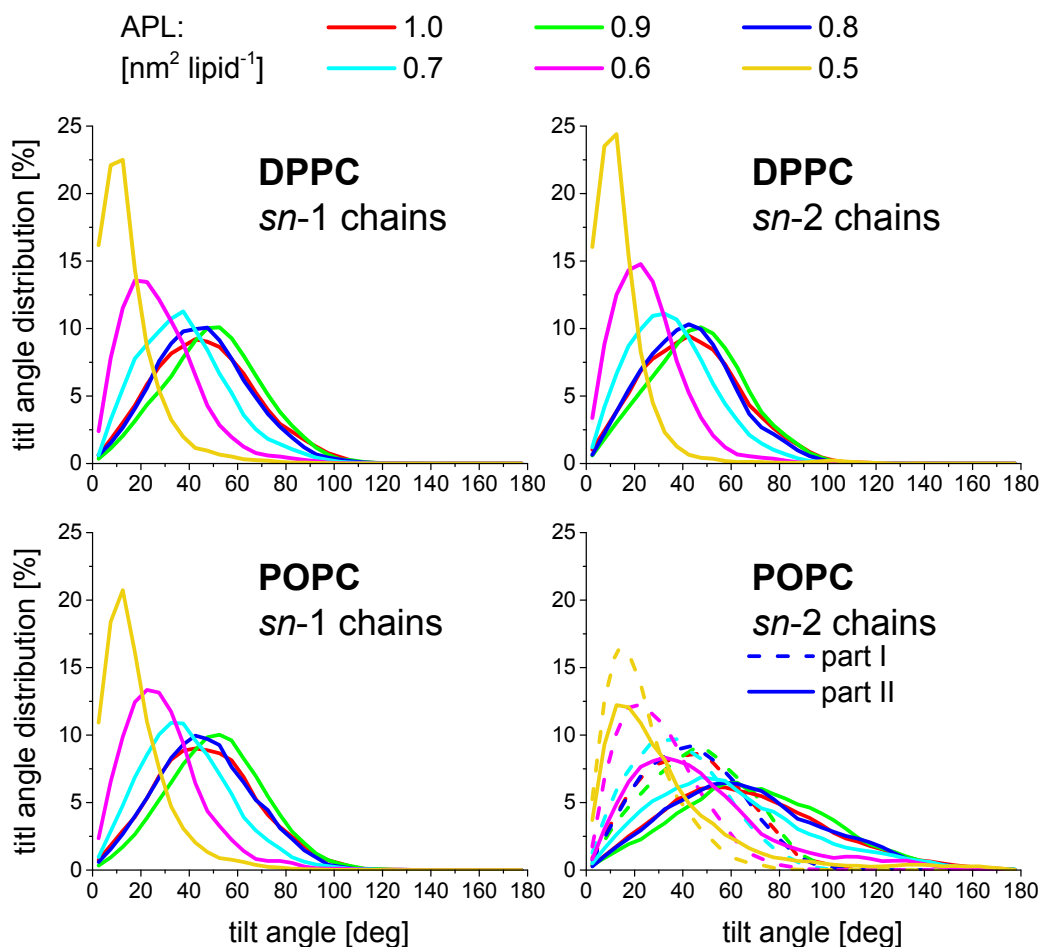


Fig. S.2 Distributions of tilt angles between lipid chains of DPPC and POPC and monolayer normal at various APL. In *sn*-2 chains of POPC ‘part I’ refers to atoms from C1 to C9 (before the double bond), and ‘part II’ refers to atoms from C10 to C18 (after the double bond); atom numbering starts from ester carbon. The curves have been subject to signal smoothing procedure for clarity.

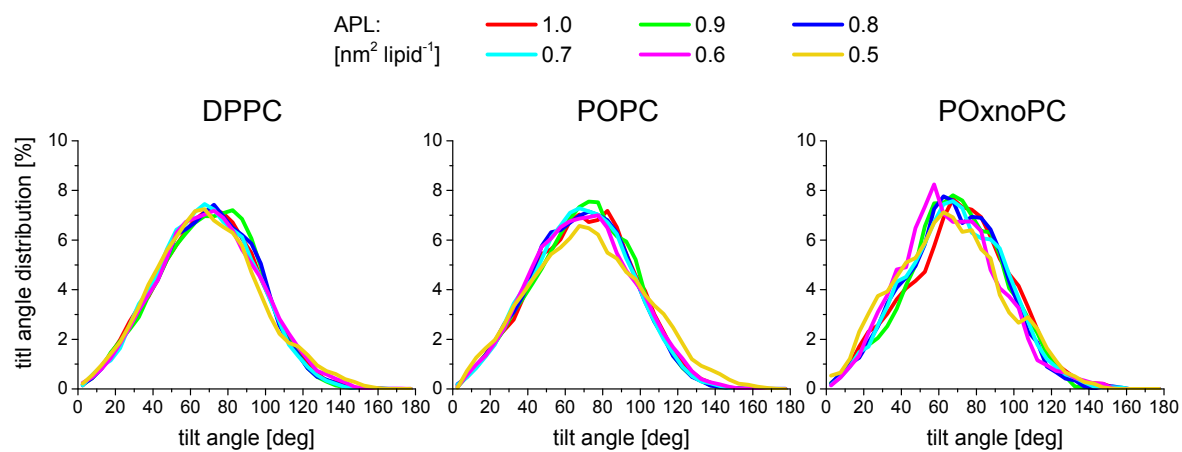


Fig. S.3 Distributions of tilt angles between lipid headgroups and monolayer normal at various APL. The curves have been subject to signal smoothing procedure for clarity.

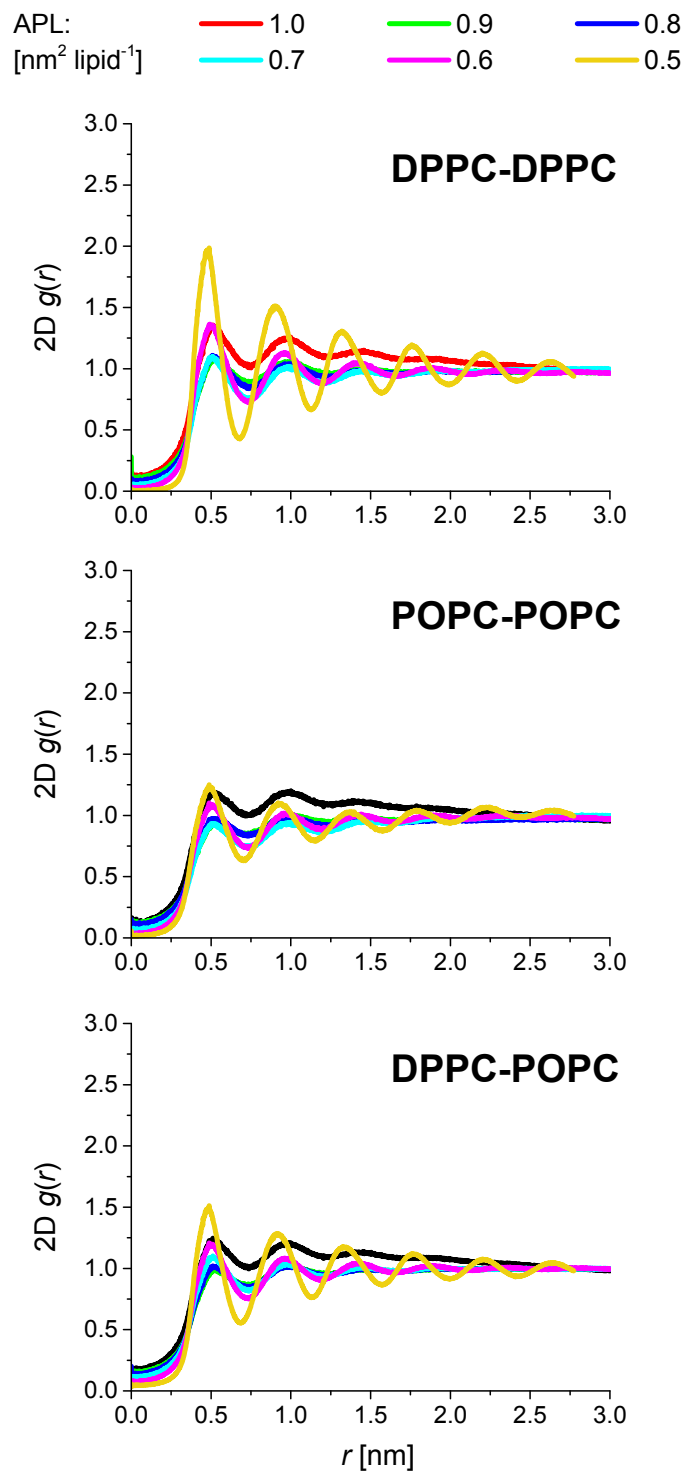


Fig. S.4 Lipid-lipid two dimensional radial pair distribution functions at various APL. The plots are calculated between four central atoms in each chain of DPPC (top), POPC (middle), or both DPPC and POPC molecules (bottom).

poxnopc.itp file:

; PoxnoPC in Slipids

; by Lukasz Cwiklik, 2015

; cwiklik[at]gmail.com

[moleculetype]

; Name nrexcl

POXN 3

[atoms]

; nr	type	resnr	residue	atom	cgnr	charge	mass
1	NTL	1	POXN	N	1	0.20	14.007
2	CTL2	1	POXN	C12	14	-0.20	12.011
3	CTL5	1	POXN	C13	2	-0.38	12.011
4	CTL5	1	POXN	C14	6	-0.38	12.011
5	CTL5	1	POXN	C15	10	-0.38	12.011
6	HL	1	POXN	H12A	15	0.09	1.008
7	HL	1	POXN	H12B	16	0.09	1.008
8	HL	1	POXN	H13A	3	0.19	1.008
9	HL	1	POXN	H13B	4	0.19	1.008
10	HL	1	POXN	H13C	5	0.19	1.008
11	HL	1	POXN	H14A	7	0.19	1.008
12	HL	1	POXN	H14B	8	0.19	1.008
13	HL	1	POXN	H14C	9	0.19	1.008
14	HL	1	POXN	H15A	11	0.19	1.008
15	HL	1	POXN	H15B	12	0.19	1.008
16	HL	1	POXN	H15C	13	0.19	1.008
17	CTL2	1	POXN	C11	17	0.17	12.011

18	HAL2	1	POXN	H11A	18	0.03	1.008
19	HAL2	1	POXN	H11B	19	0.03	1.008
20	PL	1	POXN	P	20	1.58	30.974
21	O2L	1	POXN	O13	21	-0.86	15.9994
22	O2L	1	POXN	O14	22	-0.86	15.9994
23	OSLP	1	POXN	O12	23	-0.49	15.9994
24	OSLP	1	POXN	O11	24	-0.49	15.9994
25	CTL2	1	POXN	C1	25	-0.11	12.011
26	HAL2	1	POXN	HA	26	0.07	1.008
27	HAL2	1	POXN	HB	27	0.07	1.008
28	CTL1	1	POXN	C2	28	0.48	12.011
29	HAL1	1	POXN	HS	29	0.04	1.008
30	OSL	1	POXN	O21	30	-0.47	15.9994
31	CL	1	POXN	C21	31	0.79	12.011
32	OBL	1	POXN	O22	32	-0.65	15.9994
33	CTL2	1	POXN	C22	33	-0.06	12.011
34	HAL2	1	POXN	H2R	34	0.03	1.008
35	HAL2	1	POXN	H2S	35	0.03	1.008
36	CTL2	1	POXN	C3	36	0.13	12.011
37	HAL2	1	POXN	HX	37	0.06	1.008
38	HAL2	1	POXN	HY	38	0.06	1.008
39	OSL	1	POXN	O31	39	-0.47	15.9994
40	CL	1	POXN	C31	40	0.79	12.011
41	OBL	1	POXN	O32	41	-0.65	15.9994
42	CTL2	1	POXN	C32	42	-0.06	12.011
43	HAL2	1	POXN	H2X	43	0.03	1.008
44	HAL2	1	POXN	H2Y	44	0.03	1.008
45	CTL2	1	POXN	C23	45	0.00	12.011
46	HAL2	1	POXN	H3R	46	0.00	1.008

47	HAL2	1	POXN	H3S	47	0.00	1.008	
48	CTL2	1	POXN	C24	48	0.00	12.011	
49	HAL2	1	POXN	H4R	49	0.00	1.008	
50	HAL2	1	POXN	H4S	50	0.00	1.008	
51	CTL2	1	POXN	C25	51	0.00	12.011	
52	HAL2	1	POXN	H5R	52	0.00	1.008	
53	HAL2	1	POXN	H5S	53	0.00	1.008	
54	CTL2	1	POXN	C26	54	0.00	12.011	
55	HAL2	1	POXN	H6R	55	0.00	1.008	
56	HAL2	1	POXN	H6S	56	0.00	1.008	
57	CTL2	1	POXN	C27	57	0.00	12.011	
58	HAL2	1	POXN	H7R	58	0.00	1.008	
59	HAL2	1	POXN	H7S	59	0.00	1.008	
60	CTL2	1	POXN	C28	60	0.09	12.011	;tzv: RESP charge
61	HAL2	1	POXN	H8R	61	-0.01	1.008	;tzv: RESP charge
62	HAL2	1	POXN	H8S	62	-0.01	1.008	;tzv: RESP charge
63	CFO	1	POXN	C	63	0.44	12.011	;tzv: RESP charge, new type and name
64	HFO	1	POXN	H	64	-0.03	1.008	;tzv: RESP charge, new type and name
65	OFO	1	POXN	O	65	-0.48	12.011	;tzv: RESP charge, new type and name
66	CTL2	1	POXN	C33	66	0.00	12.011	
67	HAL2	1	POXN	H3X	67	0.00	1.008	
68	HAL2	1	POXN	H3Y	68	0.00	1.008	
69	CTL2	1	POXN	C34	69	0.00	12.011	
70	HAL2	1	POXN	H4X	70	0.00	1.008	
71	HAL2	1	POXN	H4Y	71	0.00	1.008	
72	CTL2	1	POXN	C35	72	0.00	12.011	
73	HAL2	1	POXN	H5X	73	0.00	1.008	

74	HAL2	1	POXN	H5Y	74	0.00	1.008
75	CTL2	1	POXN	C36	75	0.00	12.011
76	HAL2	1	POXN	H6X	76	0.00	1.008
77	HAL2	1	POXN	H6Y	77	0.00	1.008
78	CTL2	1	POXN	C37	78	0.00	12.011
79	HAL2	1	POXN	H7X	79	0.00	1.008
80	HAL2	1	POXN	H7Y	80	0.00	1.008
81	CTL2	1	POXN	C38	81	0.00	12.011
82	HAL2	1	POXN	H8X	82	0.00	1.008
83	HAL2	1	POXN	H8Y	83	0.00	1.008
84	CTL2	1	POXN	C39	84	0.00	12.011
85	HAL2	1	POXN	H9X	85	0.00	1.008
86	HAL2	1	POXN	H9Y	86	0.00	1.008
87	CTL2	1	POXN	C310	87	0.00	12.011
88	HAL2	1	POXN	H10X	88	0.00	1.008
89	HAL2	1	POXN	H10Y	89	0.00	1.008
90	CTL2	1	POXN	C311	90	0.00	12.011
91	HAL2	1	POXN	H11X	91	0.00	1.008
92	HAL2	1	POXN	H11Y	92	0.00	1.008
93	CTL2	1	POXN	C312	93	0.00	12.011
94	HAL2	1	POXN	H12X	94	0.00	1.008
95	HAL2	1	POXN	H12Y	95	0.00	1.008
96	CTL2	1	POXN	C313	96	0.00	12.011
97	HAL2	1	POXN	H13X	97	0.00	1.008
98	HAL2	1	POXN	H13Y	98	0.00	1.008
99	CTL2	1	POXN	C314	99	0.00	12.011
100	HAL2	1	POXN	H14X	100	0.00	1.008
101	HAL2	1	POXN	H14Y	101	0.00	1.008
102	CTL2	1	POXN	C315	102	0.047	12.011

103	HAL2	1	POXN	H15X	103	-0.007	1.008
104	HAL2	1	POXN	H15Y	104	-0.007	1.008
105	CTL3	1	POXN	C316	105	-0.081	12.011
106	HAL3	1	POXN	H16X	106	0.016	1.008
107	HAL3	1	POXN	H16Y	107	0.016	1.008
108	HAL3	1	POXN	H16Z	108	0.016	1.008

[bonds]

	ai	aj	funct	c0	c1	c2	c3
	1	2	1				
	1	3	1				
	1	4	1				
	1	5	1				
	2	6	1				
	2	7	1				
	2	17	1				
	3	8	1				
	3	9	1				
	3	10	1				
	4	11	1				
	4	12	1				
	4	13	1				
	5	14	1				
	5	15	1				
	5	16	1				
	17	18	1				
	17	19	1				
	17	23	1				
	20	21	1				

20	22	1
20	23	1
20	24	1
24	25	1
25	26	1
25	27	1
25	28	1
28	29	1
28	30	1
28	36	1
30	31	1
31	32	1
31	33	1
33	34	1
33	35	1
33	45	1
36	37	1
36	38	1
36	39	1
39	40	1
40	41	1
40	42	1
42	43	1
42	44	1
42	66	1 ;tzv
45	46	1
45	47	1
45	48	1
48	49	1

48	50	1	
48	51	1	
51	52	1	
51	53	1	
51	54	1	
54	55	1	
54	56	1	
54	57	1	
57	58	1	
57	59	1	
57	60	1	
60	61	1	
60	62	1	
60	63	1	1.5080e-01 2.7472e+05 ;tzv: from GAFF
63	64	1	1.1123e-01 2.5983e+05 ;tzv: from GAFF
63	65	1	1.2140e-01 5.4225e+05 ;tzv: from GAFF
66	67	1	
66	68	1	
66	69	1	
69	70	1	
69	71	1	
69	72	1	
72	73	1	
72	74	1	
72	75	1	
75	76	1	
75	77	1	
75	78	1	
78	79	1	

78 80 1
78 81 1
81 82 1
81 83 1
81 84 1
84 85 1
84 86 1
84 87 1
87 88 1
87 89 1
87 90 1
90 91 1
90 92 1
90 93 1
93 94 1
93 95 1
93 96 1
96 97 1
96 98 1
96 99 1
99 100 1
99 101 1
99 102 1
102 103 1
102 104 1
102 105 1
105 106 1
105 107 1
105 108 1

[pairs]

	ai	aj	funct	c0	c1	c2	c3
	1	18	1				
	1	19	1				
	1	23	1				
	2	8	1				
	2	9	1				
	2	10	1				
	2	11	1				
	2	12	1				
	2	13	1				
	2	14	1				
	2	15	1				
	2	16	1				
	2	20	1				
	3	6	1				
	3	7	1				
	3	11	1				
	3	12	1				
	3	13	1				
	3	14	1				
	3	15	1				
	3	16	1				
	3	17	1				
	4	6	1				
	4	7	1				
	4	8	1				
	4	9	1				

4	10	1
4	14	1
4	15	1
4	16	1
4	17	1
5	6	1
5	7	1
5	8	1
5	9	1
5	10	1
5	11	1
5	12	1
5	13	1
5	17	1
6	18	1
6	19	1
6	23	1
7	18	1
7	19	1
7	23	1
17	21	1
17	22	1
17	24	1
18	20	1
19	20	1
20	26	1
20	27	1
20	28	1
21	25	1

22	25	1
23	25	1
24	29	1
24	30	1
24	36	1
25	31	1
25	37	1
25	38	1
25	39	1
26	29	1
26	30	1
26	36	1
27	29	1
27	30	1
27	36	1
28	32	1
28	33	1
28	40	1
29	31	1
29	37	1
29	38	1
29	39	1
30	34	1
30	35	1
30	37	1
30	38	1
30	39	1
30	45	1
31	36	1

31	46	1
31	47	1
31	48	1
32	34	1
32	35	1
32	45	1
33	49	1
33	50	1
33	51	1
34	46	1
34	47	1
34	48	1
35	46	1
35	47	1
35	48	1
36	41	1
36	42	1
37	40	1
38	40	1
39	43	1
39	44	1
39	66	1
40	67	1
40	68	1
40	69	1
41	43	1
41	44	1
41	66	1
42	70	1

42	71	1
42	72	1
43	67	1
43	68	1
43	69	1
44	67	1
44	68	1
44	69	1
45	52	1
45	53	1
45	54	1
46	49	1
46	50	1
46	51	1
47	49	1
47	50	1
47	51	1
48	55	1
48	56	1
48	57	1
49	52	1
49	53	1
49	54	1
50	52	1
50	53	1
50	54	1
51	58	1
51	59	1
51	60	1

52	55	1
52	56	1
52	57	1
53	55	1
53	56	1
53	57	1
54	61	1
54	62	1
54	63	1
55	58	1
55	59	1
55	60	1
56	58	1
56	59	1
56	60	1
57	64	1
57	65	1
58	61	1
58	62	1
58	63	1
59	61	1
59	62	1
59	63	1
66	73	1
66	74	1
66	75	1
67	70	1
67	71	1
67	72	1

68 70	1
68 71	1
68 72	1
69 76	1
69 77	1
69 78	1
70 73	1
70 74	1
70 75	1
71 73	1
71 74	1
71 75	1
72 79	1
72 80	1
72 81	1
73 76	1
73 77	1
73 78	1
74 76	1
74 77	1
74 78	1
75 82	1
75 83	1
75 84	1
76 79	1
76 80	1
76 81	1
77 79	1
77 80	1

77 81	1
78 85	1
78 86	1
78 87	1
79 82	1
79 83	1
79 84	1
80 82	1
80 83	1
80 84	1
81 88	1
81 89	1
81 90	1
82 85	1
82 86	1
82 87	1
83 85	1
83 86	1
83 87	1
84 91	1
84 92	1
84 93	1
85 88	1
85 89	1
85 90	1
86 88	1
86 89	1
86 90	1
87 94	1

87 95	1
87 96	1
88 91	1
88 92	1
88 93	1
89 91	1
89 92	1
89 93	1
90 97	1
90 98	1
90 99	1
91 94	1
91 95	1
91 96	1
92 94	1
92 95	1
92 96	1
93 100	1
93 101	1
93 102	1
94 97	1
94 98	1
94 99	1
95 97	1
95 98	1
95 99	1
96 103	1
96 104	1
96 105	1

97 100 1
 97 101 1
 97 102 1
 98 100 1
 98 101 1
 98 102 1
 99 106 1
 99 107 1
 99 108 1
 100 103 1
 100 104 1
 100 105 1
 101 103 1
 101 104 1
 101 105 1
 103 106 1
 103 107 1
 103 108 1
 104 106 1
 104 107 1
 104 108 1

[angles]

	ai	aj	ak	funct	c0	c1	c2	c3
	2	1	3	5				
	2	1	4	5				
	2	1	5	5				
	3	1	4	5				
	3	1	5	5				

4	1	5	5
1	2	6	5
1	2	7	5
1	2	17	5
6	2	7	5
6	2	17	5
7	2	17	5
1	3	8	5
1	3	9	5
1	3	10	5
8	3	9	5
8	3	10	5
9	3	10	5
1	4	11	5
1	4	12	5
1	4	13	5
11	4	12	5
11	4	13	5
12	4	13	5
1	5	14	5
1	5	15	5
1	5	16	5
14	5	15	5
14	5	16	5
15	5	16	5
2	17	18	5
2	17	19	5
2	17	23	5
18	17	19	5

18	17	23	5
19	17	23	5
21	20	22	5
21	20	23	5
21	20	24	5
22	20	23	5
22	20	24	5
23	20	24	5
17	23	20	5
20	24	25	5
24	25	26	5
24	25	27	5
24	25	28	5
26	25	27	5
26	25	28	5
27	25	28	5
25	28	29	5
25	28	30	5
25	28	36	5
29	28	30	5
29	28	36	5
30	28	36	5
28	30	31	5
30	31	32	5
30	31	33	5
32	31	33	5
31	33	34	5
31	33	35	5
31	33	45	5

34	33	35	5
34	33	45	5
35	33	45	5
28	36	37	5
28	36	38	5
28	36	39	5
37	36	38	5
37	36	39	5
38	36	39	5
36	39	40	5
39	40	41	5
39	40	42	5
41	40	42	5
40	42	43	5
40	42	44	5
40	42	66	5
43	42	44	5
43	42	66	5
44	42	66	5
33	45	46	5
33	45	47	5
33	45	48	5
46	45	47	5
46	45	48	5
47	45	48	5
45	48	49	5
45	48	50	5
45	48	51	5
49	48	50	5

49	48	51	5		
50	48	51	5		
48	51	52	5		
48	51	53	5		
48	51	54	5		
52	51	53	5		
52	51	54	5		
53	51	54	5		
51	54	55	5		
51	54	56	5		
51	54	57	5		
55	54	56	5		
55	54	57	5		
56	54	57	5		
54	57	58	5		
54	57	59	5		
54	57	60	5		
58	57	59	5		
58	57	60	5		
59	57	60	5		
57	60	61	5		
57	60	62	5		
57	60	63	1	1.1053e+02	5.3379e+02 ; tzv: from GAFF
61	60	62	5		
61	60	63	1	1.0968e+02	3.9497e+02 ; tzv: from GAFF
62	60	63	1	1.0968e+02	3.9497e+02 ; tzv: from GAFF
60	63	64	1	1.1440e+02	3.8585e+02 ; tzv: from GAFF
60	63	65	1	1.2311e+02	5.6928e+02 ; tzv: from GAFF
64	63	65	1	1.2093e+02	4.5422e+02 ; tzv: from GAFF

42	66	67	5
42	66	68	5
42	66	69	5
67	66	68	5
67	66	69	5
68	66	69	5
66	69	70	5
66	69	71	5
66	69	72	5
70	69	71	5
70	69	72	5
71	69	72	5
69	72	73	5
69	72	74	5
69	72	75	5
73	72	74	5
73	72	75	5
74	72	75	5
72	75	76	5
72	75	77	5
72	75	78	5
76	75	77	5
76	75	78	5
77	75	78	5
75	78	79	5
75	78	80	5
75	78	81	5
79	78	80	5
79	78	81	5

80 78 81	5
78 81 82	5
78 81 83	5
78 81 84	5
82 81 83	5
82 81 84	5
83 81 84	5
81 84 85	5
81 84 86	5
81 84 87	5
85 84 86	5
85 84 87	5
86 84 87	5
84 87 88	5
84 87 89	5
84 87 90	5
88 87 89	5
88 87 90	5
89 87 90	5
87 90 91	5
87 90 92	5
87 90 93	5
91 90 92	5
91 90 93	5
92 90 93	5
90 93 94	5
90 93 95	5
90 93 96	5
94 93 95	5

94 93 96 5
 95 93 96 5
 93 96 97 5
 93 96 98 5
 93 96 99 5
 97 96 98 5
 97 96 99 5
 98 96 99 5
 96 99 100 5
 96 99 101 5
 96 99 102 5
 100 99 101 5
 100 99 102 5
 101 99 102 5
 99 102 103 5
 99 102 104 5
 99 102 105 5
 103 102 104 5
 103 102 105 5
 104 102 105 5
 102 105 106 5
 102 105 107 5
 102 105 108 5
 106 105 107 5
 106 105 108 5
 107 105 108 5

[dihedrals]

; ai aj ak al funct c0 c1 c2 c3 c4 c5

3	1	2	6	9
3	1	2	7	9
3	1	2	17	9
4	1	2	6	9
4	1	2	7	9
4	1	2	17	9
5	1	2	6	9
5	1	2	7	9
5	1	2	17	9
2	1	3	8	9
2	1	3	9	9
2	1	3	10	9
4	1	3	8	9
4	1	3	9	9
4	1	3	10	9
5	1	3	8	9
5	1	3	9	9
5	1	3	10	9
2	1	4	11	9
2	1	4	12	9
2	1	4	13	9
3	1	4	11	9
3	1	4	12	9
3	1	4	13	9
5	1	4	11	9
5	1	4	12	9
5	1	4	13	9
2	1	5	14	9
2	1	5	15	9

2	1	5	16	9
3	1	5	14	9
3	1	5	15	9
3	1	5	16	9
4	1	5	14	9
4	1	5	15	9
4	1	5	16	9
1	2	17	18	9
1	2	17	19	9
1	2	17	23	9
6	2	17	18	9
6	2	17	19	9
6	2	17	23	9
7	2	17	18	9
7	2	17	19	9
7	2	17	23	9
2	17	23	20	9
18	17	23	20	9
19	17	23	20	9
21	20	23	17	9
22	20	23	17	9
24	20	23	17	9
21	20	24	25	9
22	20	24	25	9
23	20	24	25	9
20	24	25	26	9
20	24	25	27	9
20	24	25	28	9
24	25	28	29	9

24	25	28	30	9
24	25	28	36	9
26	25	28	29	9
26	25	28	30	9
26	25	28	36	9
27	25	28	29	9
27	25	28	30	9
27	25	28	36	9
25	28	30	31	9
29	28	30	31	9
36	28	30	31	9
25	28	36	37	9
25	28	36	38	9
25	28	36	39	9
29	28	36	37	9
29	28	36	38	9
29	28	36	39	9
30	28	36	37	9
30	28	36	38	9
30	28	36	39	9
28	30	31	32	9
28	30	31	33	9
30	31	33	34	9
30	31	33	35	9
30	31	33	45	9
32	31	33	34	9
32	31	33	35	9
32	31	33	45	9
31	33	45	46	9

31	33	45	47	9
31	33	45	48	9
34	33	45	46	9
34	33	45	47	9
34	33	45	48	9
35	33	45	46	9
35	33	45	47	9
35	33	45	48	9
28	36	39	40	9
37	36	39	40	9
38	36	39	40	9
36	39	40	41	9
36	39	40	42	9
39	40	42	43	9
39	40	42	44	9
39	40	42	66	9
41	40	42	43	9
41	40	42	44	9
41	40	42	66	9
40	42	66	67	9
40	42	66	68	9
40	42	66	69	9
43	42	66	67	9
43	42	66	68	9
43	42	66	69	9
44	42	66	67	9
44	42	66	68	9
44	42	66	69	9
33	45	48	49	9

33	45	48	50	9
33	45	48	51	9
46	45	48	49	9
46	45	48	50	9
46	45	48	51	9
47	45	48	49	9
47	45	48	50	9
47	45	48	51	9
45	48	51	52	9
45	48	51	53	9
45	48	51	54	9
49	48	51	52	9
49	48	51	53	9
49	48	51	54	9
50	48	51	52	9
50	48	51	53	9
50	48	51	54	9
48	51	54	55	9
48	51	54	56	9
48	51	54	57	9
52	51	54	55	9
52	51	54	56	9
52	51	54	57	9
53	51	54	55	9
53	51	54	56	9
53	51	54	57	9
51	54	57	58	9
51	54	57	59	9
51	54	57	60	9

55	54	57	58	9							
55	54	57	59	9							
55	54	57	60	9							
56	54	57	58	9							
56	54	57	59	9							
56	54	57	60	9							
54	57	60	61	9							
54	57	60	62	9							
54	57	60	63	9	; tzv: left from Slipids						
58	57	60	61	9							
58	57	60	62	9							
58	57	60	63	9	; tzv: left from Slipids						
59	57	60	61	9	; tzv: left from Slipids						
59	57	60	62	9							
59	57	60	63	9	; tzv: left from Slipids						
57	60	63	64	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	; tzv: from GAFF
57	60	63	65	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	
61	60	63	64	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	
61	60	63	65	3	3.68192	-4.35136	0.00000	1.33888	0.00000	0.00000	; tzv: from GAFF
62	60	63	64	3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	
62	60	63	65	3	3.68192	-4.35136	0.00000	1.33888	0.00000	0.00000	
42	66	69	70	9							
42	66	69	71	9							
42	66	69	72	9							
67	66	69	70	9							

67 66 69 71	9
67 66 69 72	9
68 66 69 70	9
68 66 69 71	9
68 66 69 72	9
66 69 72 73	9
66 69 72 74	9
66 69 72 75	9
70 69 72 73	9
70 69 72 74	9
70 69 72 75	9
71 69 72 73	9
71 69 72 74	9
71 69 72 75	9
69 72 75 76	9
69 72 75 77	9
69 72 75 78	9
73 72 75 76	9
73 72 75 77	9
73 72 75 78	9
74 72 75 76	9
74 72 75 77	9
74 72 75 78	9
72 75 78 79	9
72 75 78 80	9
72 75 78 81	9
76 75 78 79	9
76 75 78 80	9
76 75 78 81	9

77 75 78 79	9
77 75 78 80	9
77 75 78 81	9
75 78 81 82	9
75 78 81 83	9
75 78 81 84	9
79 78 81 82	9
79 78 81 83	9
79 78 81 84	9
80 78 81 82	9
80 78 81 83	9
80 78 81 84	9
78 81 84 85	9
78 81 84 86	9
78 81 84 87	9
82 81 84 85	9
82 81 84 86	9
82 81 84 87	9
83 81 84 85	9
83 81 84 86	9
83 81 84 87	9
81 84 87 88	9
81 84 87 89	9
81 84 87 90	9
85 84 87 88	9
85 84 87 89	9
85 84 87 90	9
86 84 87 88	9
86 84 87 89	9

86 84 87 90	9
84 87 90 91	9
84 87 90 92	9
84 87 90 93	9
88 87 90 91	9
88 87 90 92	9
88 87 90 93	9
89 87 90 91	9
89 87 90 92	9
89 87 90 93	9
87 90 93 94	9
87 90 93 95	9
87 90 93 96	9
91 90 93 94	9
91 90 93 95	9
91 90 93 96	9
92 90 93 94	9
92 90 93 95	9
92 90 93 96	9
90 93 96 97	9
90 93 96 98	9
90 93 96 99	9
94 93 96 97	9
94 93 96 98	9
94 93 96 99	9
95 93 96 97	9
95 93 96 98	9
95 93 96 99	9
93 96 99 100	9

93 96 99 101 9
 93 96 99 102 9
 97 96 99 100 9
 97 96 99 101 9
 97 96 99 102 9
 98 96 99 100 9
 98 96 99 101 9
 98 96 99 102 9
 96 99 102 103 9
 96 99 102 104 9
 96 99 102 105 9
 100 99 102 103 9
 100 99 102 104 9
 100 99 102 105 9
 101 99 102 103 9
 101 99 102 104 9
 101 99 102 105 9
 99 102 105 106 9
 99 102 105 107 9
 99 102 105 108 9
 103 102 105 106 9
 103 102 105 107 9
 103 102 105 108 9
 104 102 105 106 9
 104 102 105 107 9
 104 102 105 108 9

[dihedrals]

; ai aj ak al funct c0 c1 c2 c3

31 30 33 32 2

40 39 42 41 2

60 64 63 65 1 180.00 43.93200 2 ; tzv: from GAFF