

**Table S1****C1 Molecule**

[ moleculetype ]

; Name nrexcl

\_PF6 3

[ atoms ]

; nr type resnr resid atom cgnr charge mass

1	HC	1	_PF6	H30	1	0.192	1.0080
2	C	1	_PF6	CAR	2	-0.406	12.0110
3	HC	1	_PF6	H28	3	0.192	1.0080
4	HC	1	_PF6	H29	4	0.192	1.0080
5	NL	1	_PF6	NAQ	5	0.278	14.0067
6	C	1	_PF6	CAS	6	-0.406	12.0110
7	HC	1	_PF6	H22	7	0.192	1.0080
8	HC	1	_PF6	H23	8	0.192	1.0080
9	HC	1	_PF6	H24	9	0.192	1.0080
10	C	1	_PF6	CAT	10	-0.406	12.0110
11	HC	1	_PF6	H25	11	0.192	1.0080
12	HC	1	_PF6	H26	12	0.192	1.0080
13	HC	1	_PF6	H27	13	0.192	1.0080
14	C	1	_PF6	CAP	14	-0.312	12.0110
15	HC	1	_PF6	H20	15	0.160	1.0080
16	HC	1	_PF6	H21	16	0.160	1.0080
17	C	1	_PF6	CAO	17	0.112	12.0110
18	HC	1	_PF6	H18	18	0.024	1.0080
19	HC	1	_PF6	H19	19	0.024	1.0080
20	C	1	_PF6	CAN	20	0.006	12.0110
21	HC	1	_PF6	H16	21	0.020	1.0080
22	HC	1	_PF6	H17	22	0.020	1.0080
23	C	1	_PF6	CAM	23	-0.090	12.0110
24	HC	1	_PF6	H14	24	0.019	1.0080
25	HC	1	_PF6	H15	25	0.019	1.0080
26	C	1	_PF6	CAL	26	0.066	12.0110
27	HC	1	_PF6	H12	27	-0.012	1.0080
28	HC	1	_PF6	H13	28	-0.012	1.0080
29	C	1	_PF6	CAK	29	0.077	12.0110
30	HC	1	_PF6	H10	30	-0.018	1.0080
31	HC	1	_PF6	H11	31	-0.018	1.0080
32	C	1	_PF6	CAJ	32	-0.080	12.0110
33	HC	1	_PF6	H8	33	0.006	1.0080
34	HC	1	_PF6	H9	34	0.006	1.0080
35	C	1	_PF6	CAI	35	0.028	12.0110
36	HC	1	_PF6	H6	36	-0.006	1.0080
37	HC	1	_PF6	H7	37	-0.006	1.0080
38	C	1	_PF6	CAH	38	0.172	12.0110
39	HC	1	_PF6	H4	39	-0.027	1.0080
40	HC	1	_PF6	H5	40	-0.027	1.0080
41	C	1	_PF6	CAG	41	-0.309	12.0110

```

42 HC 1 _PF6 H1 42 0.070 1.0080
43 HC 1 _PF6 H2 43 0.070 1.0080
44 HC 1 _PF6 H3 44 0.070 1.0080
; total charge of the molecule: 1.000
[ bonds ]
; ai aj funct c0 c1
1 2 2 0.1090 1.2300e+07
2 3 2 0.1090 1.2300e+07
2 4 2 0.1090 1.2300e+07
2 5 2 0.1510 3.7279e+06
5 6 2 0.1510 3.7279e+06
5 10 2 0.1510 3.7279e+06
5 14 2 0.1530 7.1500e+06
6 7 2 0.1090 1.2300e+07
6 8 2 0.1090 1.2300e+07
6 9 2 0.1090 1.2300e+07
10 11 2 0.1090 1.2300e+07
10 12 2 0.1090 1.2300e+07
10 13 2 0.1090 1.2300e+07
14 15 2 0.1090 1.2300e+07
14 16 2 0.1090 1.2300e+07
14 17 2 0.1530 7.1500e+06
17 18 2 0.1090 1.2300e+07
17 19 2 0.1090 1.2300e+07
17 20 2 0.1540 4.2166e+06
20 21 2 0.1090 1.2300e+07
20 22 2 0.1090 1.2300e+07
20 23 2 0.1530 7.1500e+06
23 24 2 0.1090 1.2300e+07
23 25 2 0.1090 1.2300e+07
23 26 2 0.1530 7.1500e+06
26 27 2 0.1100 1.2100e+07
26 28 2 0.1100 1.2100e+07
26 29 2 0.1530 7.1500e+06
29 30 2 0.1100 1.2100e+07
29 31 2 0.1100 1.2100e+07
29 32 2 0.1530 7.1500e+06
32 33 2 0.1100 1.2100e+07
32 34 2 0.1100 1.2100e+07
32 35 2 0.1530 7.1500e+06
35 36 2 0.1100 1.2100e+07
35 37 2 0.1100 1.2100e+07
35 38 2 0.1530 7.1500e+06
38 39 2 0.1090 1.2300e+07
38 40 2 0.1090 1.2300e+07
38 41 2 0.1530 7.1500e+06
41 42 2 0.1090 1.2300e+07
41 43 2 0.1090 1.2300e+07
41 44 2 0.1090 1.2300e+07
[ pairs ]
; ai aj funct ; all 1-4 pairs but the ones excluded in GROMOS itp

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2 17 1  
3 6 1  
3 10 1  
3 14 1  
4 6 1  
4 10 1  
4 14 1  
5 18 1  
5 19 1  
5 20 1  
6 11 1  
6 12 1  
6 13 1  
6 15 1  
6 16 1  
6 17 1  
7 10 1  
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8 10 1  
8 14 1  
9 10 1  
9 14 1  
10 15 1  
10 16 1  
10 17 1  
11 14 1  
12 14 1  
13 14 1  
14 21 1  
14 22 1  
14 23 1  
15 18 1  
15 19 1  
15 20 1  
16 18 1  
16 19 1  
16 20 1  
17 24 1  
17 25 1  
17 26 1

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34	38	1

35 42 1  
35 43 1  
35 44 1  
36 39 1  
36 40 1  
36 41 1  
37 39 1  
37 40 1  
37 41 1  
39 42 1  
39 43 1  
39 44 1  
40 42 1  
40 43 1  
40 44 1

[ angles ]

```
; ai aj ak funct angle fc
1 2 3 2 110.30 524.00
1 2 4 2 110.30 524.00
1 2 5 2 108.53 443.00
3 2 4 2 110.30 524.00
3 2 5 2 108.53 443.00
4 2 5 2 108.53 443.00
2 5 6 2 109.60 450.00
2 5 10 2 109.60 450.00
2 5 14 2 111.00 530.00
6 5 10 2 109.60 450.00
6 5 14 2 111.00 530.00
10 5 14 2 111.00 530.00
5 6 7 2 108.53 443.00
5 6 8 2 108.53 443.00
5 6 9 2 108.53 443.00
7 6 8 2 110.30 524.00
7 6 9 2 110.30 524.00
8 6 9 2 110.30 524.00
5 10 11 2 108.53 443.00
5 10 12 2 108.53 443.00
5 10 13 2 108.53 443.00
11 10 12 2 110.30 524.00
11 10 13 2 110.30 524.00
12 10 13 2 110.30 524.00
5 14 15 2 106.00 1733.55
5 14 16 2 106.00 1733.55
5 14 17 2 115.00 610.00
15 14 16 2 108.00 465.00
15 14 17 2 111.00 530.00
16 14 17 2 111.00 530.00
14 17 18 2 111.00 530.00
14 17 19 2 111.00 530.00
14 17 20 2 109.50 520.00
18 17 19 2 107.57 484.00
```

18	17	20	2	108.53	443.00
19	17	20	2	108.53	443.00
17	20	21	2	109.60	450.00
17	20	22	2	109.60	450.00
17	20	23	2	111.00	530.00
21	20	22	2	106.75	503.00
21	20	23	2	109.00	1680.51
22	20	23	2	109.00	1680.51
20	23	24	2	109.00	1680.51
20	23	25	2	109.00	1680.51
20	23	26	2	111.00	530.00
24	23	25	2	106.00	1733.55
24	23	26	2	109.60	450.00
25	23	26	2	109.60	450.00
23	26	27	2	109.50	285.00
23	26	28	2	109.50	285.00
23	26	29	2	111.00	530.00
27	26	28	2	106.00	1733.55
27	26	29	2	109.50	285.00
28	26	29	2	109.50	285.00
26	29	30	2	109.00	1680.51
26	29	31	2	109.00	1680.51
26	29	32	2	111.00	530.00
30	29	31	2	106.00	1733.55
30	29	32	2	109.50	285.00
31	29	32	2	109.50	285.00
29	32	33	2	109.50	285.00
29	32	34	2	109.50	285.00
29	32	35	2	111.00	530.00
33	32	34	2	106.00	1733.55
33	32	35	2	109.00	1680.51
34	32	35	2	109.00	1680.51
32	35	36	2	109.50	285.00
32	35	37	2	109.50	285.00
32	35	38	2	111.00	530.00
36	35	37	2	106.00	1733.55
36	35	38	2	109.00	1680.51
37	35	38	2	109.00	1680.51
35	38	39	2	109.00	1680.51
35	38	40	2	109.00	1680.51
35	38	41	2	111.00	530.00
39	38	40	2	106.00	1733.55
39	38	41	2	109.50	285.00
40	38	41	2	109.50	285.00
38	41	42	2	111.40	532.00
38	41	43	2	111.40	532.00
38	41	44	2	111.40	532.00
42	41	43	2	107.57	484.00
42	41	44	2	107.57	484.00
43	41	44	2	107.57	484.00

[ dihedrals ]

```

; GROMOS improper dihedrals
; ai aj ak al funct angle fc
[ dihedrals ]
; ai aj ak al funct ph0 cp mult
  3 2 5 14 1 0.00 1.05 3
  5 14 17 20 1 0.00 5.92 3
  6 5 14 17 1 0.00 1.05 3
 14 5 6 7 1 0.00 1.05 3
 14 5 10 11 1 0.00 1.05 3
 14 17 20 23 1 0.00 5.92 3
 17 20 23 26 1 0.00 5.92 3
 20 23 26 29 1 0.00 5.92 3
 23 26 29 32 1 0.00 5.92 3
 26 29 32 35 1 0.00 5.92 3
 29 32 35 38 1 0.00 5.92 3
 32 35 38 41 1 0.00 5.92 3
 35 38 41 42 1 0.00 5.92 3
[ exclusions ]
; ai aj funct ; GROMOS 1-4 exclusions

```

**Table S2****C12 Molecule**

[ moleculetype ]

; Name nrexcl

4GGN 3

[ atoms ]

; nr type resnr resid atom cgnr charge mass

1	HC	1	4GGN	H50	1	0.073	1.0080
2	C	1	4GGN	C16	2	-0.319	12.0110
3	HC	1	4GGN	H48	3	0.073	1.0080
4	HC	1	4GGN	H49	4	0.073	1.0080
5	C	1	4GGN	C15	5	0.178	12.0110
6	HC	1	4GGN	H46	6	-0.028	1.0080
7	HC	1	4GGN	H47	7	-0.028	1.0080
8	C	1	4GGN	C14	8	0.011	12.0110
9	HC	1	4GGN	H44	9	-0.004	1.0080
10	HC	1	4GGN	H45	10	-0.004	1.0080
11	C	1	4GGN	C13	11	-0.063	12.0110
12	HC	1	4GGN	H42	12	0.001	1.0080
13	HC	1	4GGN	H43	13	0.001	1.0080
14	C	1	4GGN	C12	14	0.107	12.0110
15	HC	1	4GGN	H40	15	-0.028	1.0080
16	HC	1	4GGN	H41	16	-0.028	1.0080
17	C	1	4GGN	C11	17	0.011	12.0110
18	HC	1	4GGN	H38	18	-0.009	1.0080
19	HC	1	4GGN	H39	19	-0.009	1.0080
20	C	1	4GGN	C7	20	-0.016	12.0110
21	HC	1	4GGN	H27	21	-0.003	1.0080
22	HC	1	4GGN	H28	22	-0.003	1.0080
23	C	1	4GGN	C6	23	0.083	12.0110
24	HC	1	4GGN	H25	24	-0.018	1.0080
25	HC	1	4GGN	H26	25	-0.018	1.0080
26	C	1	4GGN	C5	26	-0.033	12.0110
27	HC	1	4GGN	H23	27	0.008	1.0080
28	HC	1	4GGN	H24	28	0.008	1.0080
29	C	1	4GGN	C4	29	-0.031	12.0110
30	HC	1	4GGN	H21	30	0.024	1.0080
31	HC	1	4GGN	H22	31	0.024	1.0080
32	C	1	4GGN	C3	32	0.117	12.0110
33	HC	1	4GGN	H19	33	0.021	1.0080
34	HC	1	4GGN	H20	34	0.021	1.0080
35	C	1	4GGN	C2	35	-0.281	12.0110
36	HC	1	4GGN	H17	36	0.155	1.0080
37	HC	1	4GGN	H18	37	0.155	1.0080
38	NL	1	4GGN	N1	38	0.251	14.0067
39	C	1	4GGN	C8	39	-0.406	12.0110
40	HC	1	4GGN	H33	40	0.194	1.0080
41	HC	1	4GGN	H34	41	0.194	1.0080



```

42 HC 1 4GGN H35 42 0.194 1.0080
43 C 1 4GGN C9 43 -0.406 12.0110
44 HC 1 4GGN H32 44 0.194 1.0080
45 HC 1 4GGN H36 45 0.194 1.0080
46 HC 1 4GGN H37 46 0.194 1.0080
47 C 1 4GGN C10 47 -0.406 12.0110
48 HC 1 4GGN H29 48 0.194 1.0080
49 HC 1 4GGN H30 49 0.194 1.0080
50 HC 1 4GGN H31 50 0.194 1.0080

```

; total charge of the molecule: 1.000

[ bonds ]

```

; ai aj funct c0 c1
1 2 2 0.1090 1.2300e+07
2 3 2 0.1090 1.2300e+07
2 4 2 0.1090 1.2300e+07
2 5 2 0.1530 7.1500e+06
5 6 2 0.1090 1.2300e+07
5 7 2 0.1090 1.2300e+07
5 8 2 0.1530 7.1500e+06
8 9 2 0.1100 1.2100e+07
8 10 2 0.1100 1.2100e+07
8 11 2 0.1530 7.1500e+06
11 12 2 0.1100 1.2100e+07
11 13 2 0.1100 1.2100e+07
11 14 2 0.1530 7.1500e+06
14 15 2 0.1100 1.2100e+07
14 16 2 0.1100 1.2100e+07
14 17 2 0.1530 7.1500e+06
17 18 2 0.1100 1.2100e+07
17 19 2 0.1100 1.2100e+07
17 20 2 0.1530 7.1500e+06
20 21 2 0.1100 1.2100e+07
20 22 2 0.1100 1.2100e+07
20 23 2 0.1530 7.1500e+06
23 24 2 0.1100 1.2100e+07
23 25 2 0.1100 1.2100e+07
23 26 2 0.1530 7.1500e+06
26 27 2 0.1090 1.2300e+07
26 28 2 0.1090 1.2300e+07
26 29 2 0.1530 7.1500e+06
29 30 2 0.1090 1.2300e+07
29 31 2 0.1090 1.2300e+07
29 32 2 0.1530 7.1500e+06
32 33 2 0.1090 1.2300e+07
32 34 2 0.1090 1.2300e+07
32 35 2 0.1530 7.1500e+06
35 36 2 0.1090 1.2300e+07
35 37 2 0.1090 1.2300e+07
35 38 2 0.1530 7.1500e+06
38 39 2 0.1510 3.7279e+06
38 43 2 0.1510 3.7279e+06

```

```
38 47 2 0.1510 3.7279e+06
39 40 2 0.1090 1.2300e+07
39 41 2 0.1090 1.2300e+07
39 42 2 0.1090 1.2300e+07
43 44 2 0.1090 1.2300e+07
43 45 2 0.1090 1.2300e+07
43 46 2 0.1090 1.2300e+07
47 48 2 0.1090 1.2300e+07
47 49 2 0.1090 1.2300e+07
47 50 2 0.1090 1.2300e+07
```

[ pairs ]

; ai aj funct ; all 1-4 pairs but the ones excluded in GROMOS itp

```
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1 7 1
1 8 1
2 9 1
2 10 1
2 11 1
3 6 1
3 7 1
3 8 1
4 6 1
4 7 1
4 8 1
5 12 1
5 13 1
5 14 1
6 9 1
6 10 1
6 11 1
7 9 1
7 10 1
7 11 1
8 15 1
8 16 1
8 17 1
9 12 1
9 13 1
9 14 1
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10 13 1
10 14 1
11 18 1
11 19 1
11 20 1
12 15 1
12 16 1
12 17 1
13 15 1
13 16 1
13 17 1
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14	23	1
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16	19	1
16	20	1
17	24	1
17	25	1
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30	35	1

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31 35 1  
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32 43 1  
32 47 1  
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33 38 1  
34 36 1  
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40 47 1  
41 43 1  
41 47 1  
42 43 1  
42 47 1  
43 48 1  
43 49 1  
43 50 1  
44 47 1  
45 47 1  
46 47 1

[ angles ]

; ai aj ak funct angle fc

1 2 3 2 107.57 484.00  
1 2 4 2 107.57 484.00  
1 2 5 2 111.40 532.00  
3 2 4 2 107.57 484.00

3	2	5	2	111.40	532.00
4	2	5	2	111.40	532.00
2	5	6	2	109.50	285.00
2	5	7	2	109.50	285.00
2	5	8	2	111.00	530.00
6	5	7	2	106.00	1733.55
6	5	8	2	109.00	1680.51
7	5	8	2	109.00	1680.51
5	8	9	2	109.00	1680.51
5	8	10	2	109.00	1680.51
5	8	11	2	111.00	530.00
9	8	10	2	106.00	1733.55
9	8	11	2	109.00	1680.51
10	8	11	2	109.00	1680.51
8	11	12	2	109.00	1680.51
8	11	13	2	109.00	1680.51
8	11	14	2	111.00	530.00
12	11	13	2	106.00	1733.55
12	11	14	2	109.50	285.00
13	11	14	2	109.50	285.00
11	14	15	2	109.00	1680.51
11	14	16	2	109.00	1680.51
11	14	17	2	111.00	530.00
15	14	16	2	106.00	1733.55
15	14	17	2	109.00	1680.51
16	14	17	2	109.00	1680.51
14	17	18	2	109.50	285.00
14	17	19	2	109.50	285.00
14	17	20	2	111.00	530.00
18	17	19	2	106.00	1733.55
18	17	20	2	109.50	285.00
19	17	20	2	109.50	285.00
17	20	21	2	109.00	1680.51
17	20	22	2	109.00	1680.51
17	20	23	2	111.00	530.00
21	20	22	2	106.00	1733.55
21	20	23	2	109.00	1680.51
22	20	23	2	109.00	1680.51
20	23	24	2	109.50	285.00
20	23	25	2	109.50	285.00
20	23	26	2	111.00	530.00
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25	23	26	2	109.50	285.00
23	26	27	2	109.50	285.00
23	26	28	2	109.50	285.00
23	26	29	2	111.00	530.00
27	26	28	2	106.00	1733.55
27	26	29	2	109.00	1680.51
28	26	29	2	109.00	1680.51
26	29	30	2	109.50	285.00

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31	29	32	2	109.50	285.00
29	32	33	2	109.00	1680.51
29	32	34	2	109.00	1680.51
29	32	35	2	111.00	530.00
33	32	34	2	107.57	484.00
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34	32	35	2	111.00	530.00
32	35	36	2	111.00	530.00
32	35	37	2	111.00	530.00
32	35	38	2	115.00	610.00
36	35	37	2	108.00	465.00
36	35	38	2	106.00	1733.55
37	35	38	2	106.00	1733.55
35	38	39	2	108.00	465.00
35	38	43	2	108.00	465.00
35	38	47	2	108.00	465.00
39	38	43	2	109.60	450.00
39	38	47	2	109.60	450.00
43	38	47	2	109.60	450.00
38	39	40	2	109.60	450.00
38	39	41	2	109.60	450.00
38	39	42	2	109.60	450.00
40	39	41	2	109.60	450.00
40	39	42	2	109.60	450.00
41	39	42	2	109.60	450.00
38	43	44	2	109.60	450.00
38	43	45	2	109.60	450.00
38	43	46	2	109.60	450.00
44	43	45	2	109.60	450.00
44	43	46	2	109.60	450.00
45	43	46	2	109.60	450.00
38	47	48	2	109.60	450.00
38	47	49	2	109.60	450.00
38	47	50	2	109.60	450.00
48	47	49	2	109.60	450.00
48	47	50	2	109.60	450.00
49	47	50	2	109.60	450.00

[ dihedrals ]

; GROMOS improper dihedrals

; ai aj ak al funct angle fc

[ dihedrals ]

; ai aj ak al funct ph0 cp mult

2 5 8 11 1 0.00 5.92 3

3 2 5 8 1 0.00 5.92 3

5 8 11 14 1 0.00 5.92 3

8 11 14 17 1 0.00 5.92 3

11 14 17 20 1 0.00 5.92 3

14	17	20	23	1	0.00	5.92	3
17	20	23	26	1	0.00	5.92	3
20	23	26	29	1	0.00	5.92	3
23	26	29	32	1	0.00	5.92	3
26	29	32	35	1	0.00	5.92	3
29	32	35	38	1	0.00	5.92	3
32	35	38	39	1	0.00	1.05	3
35	38	39	40	1	0.00	1.05	3
35	38	43	44	1	0.00	1.05	3
35	38	47	48	1	0.00	1.05	3

[ exclusions ]

; ai aj funct ; GROMOS 1-4 exclusions

**Table S3****C14 Molecule**

[ moleculetype ]

; Name nrexcl

SRVY 3

[ atoms ]

; nr type resnr resid atom cgnr charge mass

1	HC	1	SRVY	H38	1	0.074	1.0080
2	C	1	SRVY	C17	2	-0.211	12.0110
3	HC	1	SRVY	H36	3	0.074	1.0080
4	HC	1	SRVY	H37	4	0.074	1.0080
5	C	1	SRVY	C16	5	-0.159	12.0110
6	HC	1	SRVY	H34	6	0.078	1.0080
7	HC	1	SRVY	H35	7	0.078	1.0080
8	C	1	SRVY	C15	8	-0.158	12.0110
9	HC	1	SRVY	H32	9	0.079	1.0080
10	HC	1	SRVY	H33	10	0.079	1.0080
11	C	1	SRVY	C14	11	-0.158	12.0110
12	HC	1	SRVY	H30	12	0.080	1.0080
13	HC	1	SRVY	H31	13	0.080	1.0080
14	C	1	SRVY	C13	14	-0.158	12.0110
15	HC	1	SRVY	H28	15	0.080	1.0080
16	HC	1	SRVY	H29	16	0.080	1.0080
17	C	1	SRVY	C12	17	-0.158	12.0110
18	HC	1	SRVY	H26	18	0.080	1.0080
19	HC	1	SRVY	H27	19	0.080	1.0080
20	C	1	SRVY	C11	20	-0.158	12.0110
21	HC	1	SRVY	H24	21	0.080	1.0080
22	HC	1	SRVY	H25	22	0.080	1.0080
23	C	1	SRVY	C10	23	-0.158	12.0110
24	HC	1	SRVY	H22	24	0.082	1.0080
25	HC	1	SRVY	H23	25	0.082	1.0080
26	C	1	SRVY	C6	26	-0.158	12.0110
27	HC	1	SRVY	H11	27	0.082	1.0080
28	HC	1	SRVY	H12	28	0.082	1.0080
29	C	1	SRVY	C5	29	-0.158	12.0110
30	HC	1	SRVY	H9	30	0.085	1.0080
31	HC	1	SRVY	H10	31	0.085	1.0080
32	C	1	SRVY	C4	32	-0.158	12.0110
33	HC	1	SRVY	H7	33	0.087	1.0080
34	HC	1	SRVY	H8	34	0.087	1.0080
35	C	1	SRVY	C3	35	-0.159	12.0110
36	HC	1	SRVY	H5	36	0.094	1.0080
37	HC	1	SRVY	H6	37	0.094	1.0080
38	C	1	SRVY	C2	38	-0.182	12.0110
39	HC	1	SRVY	H3	39	0.104	1.0080
40	HC	1	SRVY	H4	40	0.104	1.0080
41	CPos	1	SRVY	C1	41	-0.123	12.0110



```

42 HC 1 SRVY H1 42 0.138 1.0080
43 HC 1 SRVY H2 43 0.138 1.0080
44 NL 1 SRVY N1 44 0.028 14.0067
45 CPos 1 SRVY C7 45 -0.187 12.0110
46 HC 1 SRVY H17 46 0.141 1.0080
47 HC 1 SRVY H18 47 0.141 1.0080
48 HC 1 SRVY H19 48 0.141 1.0080
49 CPos 1 SRVY C8 49 -0.187 12.0110
50 HC 1 SRVY H16 50 0.141 1.0080
51 HC 1 SRVY H20 51 0.141 1.0080
52 HC 1 SRVY H21 52 0.141 1.0080
53 CPos 1 SRVY C9 53 -0.187 12.0110
54 HC 1 SRVY H13 54 0.141 1.0080
55 HC 1 SRVY H14 55 0.141 1.0080
56 HC 1 SRVY H15 56 0.141 1.0080

```

; total charge of the molecule: 1.000

[ bonds ]

```

; ai aj funct c0 c1
1 2 2 0.1120 3.7000e+07
2 3 2 0.1120 3.7000e+07
2 4 2 0.1120 3.7000e+07
2 5 2 0.1510 3.7279e+06
5 6 2 0.1120 3.7000e+07
5 7 2 0.1120 3.7000e+07
5 8 2 0.1520 5.4300e+06
8 9 2 0.1120 3.7000e+07
8 10 2 0.1120 3.7000e+07
8 11 2 0.1520 5.4300e+06
11 12 2 0.1120 3.7000e+07
11 13 2 0.1120 3.7000e+07
11 14 2 0.1520 5.4300e+06
14 15 2 0.1120 3.7000e+07
14 16 2 0.1120 3.7000e+07
14 17 2 0.1520 5.4300e+06
17 18 2 0.1120 3.7000e+07
17 19 2 0.1120 3.7000e+07
17 20 2 0.1520 5.4300e+06
20 21 2 0.1120 3.7000e+07
20 22 2 0.1120 3.7000e+07
20 23 2 0.1520 5.4300e+06
23 24 2 0.1120 3.7000e+07
23 25 2 0.1120 3.7000e+07
23 26 2 0.1520 5.4300e+06
26 27 2 0.1120 3.7000e+07
26 28 2 0.1120 3.7000e+07
26 29 2 0.1520 5.4300e+06
29 30 2 0.1120 3.7000e+07
29 31 2 0.1120 3.7000e+07
29 32 2 0.1520 5.4300e+06
32 33 2 0.1120 3.7000e+07
32 34 2 0.1120 3.7000e+07

```

32	35	2	0.1520	5.4300e+06
35	36	2	0.1120	3.7000e+07
35	37	2	0.1120	3.7000e+07
35	38	2	0.1520	5.4300e+06
38	39	2	0.1120	3.7000e+07
38	40	2	0.1120	3.7000e+07
38	41	2	0.1520	5.4300e+06
41	42	2	0.1130	7.0483e+06
41	43	2	0.1130	7.0483e+06
41	44	2	0.1510	3.7279e+06
44	45	2	0.1490	1.4189e+07
44	49	2	0.1490	1.4189e+07
44	53	2	0.1490	1.4189e+07
45	46	2	0.1120	3.7000e+07
45	47	2	0.1120	3.7000e+07
45	48	2	0.1120	3.7000e+07
49	50	2	0.1120	3.7000e+07
49	51	2	0.1120	3.7000e+07
49	52	2	0.1120	3.7000e+07
53	54	2	0.1120	3.7000e+07
53	55	2	0.1120	3.7000e+07
53	56	2	0.1120	3.7000e+07

[ pairs ]

; ai aj funct ; all 1-4 pairs but the ones excluded in GROMOS itp

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

10	12	1
10	13	1
10	14	1
11	18	1
11	19	1
11	20	1
12	15	1
12	16	1
12	17	1
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26	35	1

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40	42	1
40	43	1
40	44	1
41	46	1
41	47	1
41	48	1
41	50	1
41	51	1
41	52	1
41	54	1
41	55	1
41	56	1

42 45 1  
 42 49 1  
 42 53 1  
 43 45 1  
 43 49 1  
 43 53 1  
 45 50 1  
 45 51 1  
 45 52 1  
 45 54 1  
 45 55 1  
 45 56 1  
 46 49 1  
 46 53 1  
 47 49 1  
 47 53 1  
 48 49 1  
 48 53 1  
 49 54 1  
 49 55 1  
 49 56 1  
 50 53 1  
 51 53 1  
 52 53 1

[angles]

```

; ai aj ak funct angle fc
  1  2  3  2 108.53 443.00
  1  2  4  2 108.53 443.00
  1  2  5  2 110.30 524.00
  3  2  4  2 108.53 443.00
  3  2  5  2 110.30 524.00
  4  2  5  2 110.30 524.00
  2  5  6  2 109.60 450.00
  2  5  7  2 109.60 450.00
  2  5  8  2 111.00 530.00
  6  5  7  2 107.00 2726.16
  6  5  8  2 109.50 285.00
  7  5  8  2 109.50 285.00
  5  8  9  2 109.50 285.00
  5  8 10  2 109.50 285.00
  5  8 11  2 111.00 530.00
  9  8 10  2 107.00 2726.16
  9  8 11  2 109.60 450.00
 10  8 11  2 109.60 450.00
  8 11 12  2 109.60 450.00
  8 11 13  2 109.60 450.00
  8 11 14  2 111.00 530.00
 12 11 13  2 107.00 2726.16
 12 11 14  2 109.60 450.00
 13 11 14  2 109.60 450.00
 11 14 15  2 109.60 450.00
  
```

11	14	16	2	109.60	450.00
11	14	17	2	111.00	530.00
15	14	16	2	107.00	2726.16
15	14	17	2	109.60	450.00
16	14	17	2	109.60	450.00
14	17	18	2	109.60	450.00
14	17	19	2	109.60	450.00
14	17	20	2	111.00	530.00
18	17	19	2	107.00	2726.16
18	17	20	2	109.60	450.00
19	17	20	2	109.60	450.00
17	20	21	2	109.60	450.00
17	20	22	2	109.60	450.00
17	20	23	2	111.00	530.00
21	20	22	2	107.00	2726.16
21	20	23	2	109.60	450.00
22	20	23	2	109.60	450.00
20	23	24	2	109.60	450.00
20	23	25	2	109.60	450.00
20	23	26	2	111.00	530.00
24	23	25	2	107.00	2726.16
24	23	26	2	109.60	450.00
25	23	26	2	109.60	450.00
23	26	27	2	109.60	450.00
23	26	28	2	109.60	450.00
23	26	29	2	111.00	530.00
27	26	28	2	107.00	2726.16
27	26	29	2	109.60	450.00
28	26	29	2	109.60	450.00
26	29	30	2	109.60	450.00
26	29	31	2	109.60	450.00
26	29	32	2	111.00	530.00
30	29	31	2	107.00	2726.16
30	29	32	2	109.60	450.00
31	29	32	2	109.60	450.00
29	32	33	2	109.60	450.00
29	32	34	2	109.60	450.00
29	32	35	2	111.00	530.00
33	32	34	2	107.57	484.00
33	32	35	2	109.60	450.00
34	32	35	2	109.60	450.00
32	35	36	2	109.50	285.00
32	35	37	2	109.50	285.00
32	35	38	2	111.00	530.00
36	35	37	2	107.57	484.00
36	35	38	2	110.00	285.00
37	35	38	2	110.00	285.00
35	38	39	2	109.00	1680.51
35	38	40	2	109.00	1680.51
35	38	41	2	109.50	520.00
39	38	40	2	108.00	465.00

39	38	41	2	111.00	530.00
40	38	41	2	111.00	530.00
38	41	42	2	109.50	285.00
38	41	43	2	109.50	285.00
38	41	44	2	115.00	610.00
42	41	43	2	108.53	443.00
42	41	44	2	107.00	2726.16
43	41	44	2	107.00	2726.16
41	44	45	2	110.30	524.00
41	44	49	2	110.30	524.00
41	44	53	2	110.30	524.00
45	44	49	2	109.00	1680.51
45	44	53	2	109.00	1680.51
49	44	53	2	109.00	1680.51
44	45	46	2	109.60	450.00
44	45	47	2	109.60	450.00
44	45	48	2	109.60	450.00
46	45	47	2	109.60	450.00
46	45	48	2	109.60	450.00
47	45	48	2	109.60	450.00
44	49	50	2	109.60	450.00
44	49	51	2	109.60	450.00
44	49	52	2	109.60	450.00
50	49	51	2	109.60	450.00
50	49	52	2	109.60	450.00
51	49	52	2	109.60	450.00
44	53	54	2	109.60	450.00
44	53	55	2	109.60	450.00
44	53	56	2	109.60	450.00
54	53	55	2	109.60	450.00
54	53	56	2	109.60	450.00
55	53	56	2	109.60	450.00

[ dihedrals ]

; GROMOS improper dihedrals

; ai aj ak al funct angle fc

[ dihedrals ]

; ai aj ak al funct ph0 cp mult

2	5	8	11	1	0.00	5.92	3
3	2	5	8	1	0.00	5.92	3
5	8	11	14	1	0.00	5.92	3
8	11	14	17	1	0.00	5.92	3
11	14	17	20	1	0.00	5.92	3
14	17	20	23	1	0.00	5.92	3
17	20	23	26	1	0.00	5.92	3
20	23	26	29	1	0.00	5.92	3
23	26	29	32	1	0.00	5.92	3
26	29	32	35	1	0.00	5.92	3
29	32	35	38	1	0.00	5.92	3
32	35	38	41	1	0.00	5.92	3
35	38	41	44	1	0.00	5.92	3
38	41	44	45	1	0.00	1.05	3

```
41 44 45 46 1 0.00 1.05 3
41 44 49 50 1 0.00 1.05 3
41 44 53 54 1 0.00 1.05 3
```

[ exclusions ]

; ai aj funct ; GROMOS 1-4 exclusions



**Table S4**

**C16 Molecule**

[ moleculetype ]

; Name nrexcl

AJFU 3

[ atoms ]

; nr type resnr resid atom cgnr charge mass

1	HC	1	AJFU	H62	1	0.073	1.0080
2	C	1	AJFU	C20	2	-0.211	12.0110
3	HC	1	AJFU	H60	3	0.073	1.0080
4	HC	1	AJFU	H61	4	0.073	1.0080
5	C	1	AJFU	C19	5	-0.159	12.0110
6	HC	1	AJFU	H58	6	0.078	1.0080
7	HC	1	AJFU	H59	7	0.078	1.0080
8	C	1	AJFU	C18	8	-0.158	12.0110
9	HC	1	AJFU	H56	9	0.079	1.0080
10	HC	1	AJFU	H57	10	0.079	1.0080
11	C	1	AJFU	C17	11	-0.158	12.0110
12	HC	1	AJFU	H54	12	0.079	1.0080
13	HC	1	AJFU	H55	13	0.079	1.0080
14	C	1	AJFU	C16	14	-0.158	12.0110
15	HC	1	AJFU	H52	15	0.079	1.0080
16	HC	1	AJFU	H53	16	0.079	1.0080
17	C	1	AJFU	C15	17	-0.158	12.0110
18	HC	1	AJFU	H50	18	0.080	1.0080
19	HC	1	AJFU	H51	19	0.080	1.0080
20	C	1	AJFU	C14	20	-0.158	12.0110
21	HC	1	AJFU	H48	21	0.080	1.0080
22	HC	1	AJFU	H49	22	0.080	1.0080
23	C	1	AJFU	C13	23	-0.158	12.0110
24	HC	1	AJFU	H46	24	0.080	1.0080
25	HC	1	AJFU	H47	25	0.080	1.0080
26	C	1	AJFU	C9	26	-0.158	12.0110
27	HC	1	AJFU	H35	27	0.080	1.0080
28	HC	1	AJFU	H36	28	0.080	1.0080
29	C	1	AJFU	C8	29	-0.158	12.0110
30	HC	1	AJFU	H33	30	0.082	1.0080
31	HC	1	AJFU	H34	31	0.082	1.0080
32	C	1	AJFU	C7	32	-0.158	12.0110
33	HC	1	AJFU	H31	33	0.082	1.0080
34	HC	1	AJFU	H32	34	0.082	1.0080
35	C	1	AJFU	C6	35	-0.158	12.0110
36	HC	1	AJFU	H29	36	0.085	1.0080
37	HC	1	AJFU	H30	37	0.085	1.0080
38	C	1	AJFU	C5	38	-0.158	12.0110
39	HC	1	AJFU	H27	39	0.087	1.0080
40	HC	1	AJFU	H28	40	0.087	1.0080
41	C	1	AJFU	C4	41	-0.159	12.0110

```

42 HC 1 AJFU H25 42 0.094 1.0080
43 HC 1 AJFU H26 43 0.094 1.0080
44 C 1 AJFU C3 44 -0.182 12.0110
45 HC 1 AJFU H23 45 0.104 1.0080
46 HC 1 AJFU H24 46 0.104 1.0080
47 CPos 1 AJFU C2 47 -0.123 12.0110
48 HC 1 AJFU H21 48 0.138 1.0080
49 HC 1 AJFU H22 49 0.138 1.0080
50 NL 1 AJFU N1 50 0.031 14.0067
51 CPos 1 AJFU C10 51 -0.187 12.0110
52 HC 1 AJFU H37 52 0.141 1.0080
53 HC 1 AJFU H38 53 0.141 1.0080
54 HC 1 AJFU H39 54 0.141 1.0080
55 CPos 1 AJFU C11 55 -0.187 12.0110
56 HC 1 AJFU H40 56 0.141 1.0080
57 HC 1 AJFU H41 57 0.141 1.0080
58 HC 1 AJFU H42 58 0.141 1.0080
59 CPos 1 AJFU C12 59 -0.187 12.0110
60 HC 1 AJFU H43 60 0.141 1.0080
61 HC 1 AJFU H44 61 0.141 1.0080
62 HC 1 AJFU H45 62 0.141 1.0080

```

; total charge of the molecule: 1.000

[ bonds ]

; ai aj funct c0 c1

```

1 2 2 0.1120 3.7000e+07
2 3 2 0.1120 3.7000e+07
2 4 2 0.1120 3.7000e+07
2 5 2 0.1510 3.7279e+06
5 6 2 0.1120 3.7000e+07
5 7 2 0.1120 3.7000e+07
5 8 2 0.1520 5.4300e+06
8 9 2 0.1120 3.7000e+07
8 10 2 0.1120 3.7000e+07
8 11 2 0.1520 5.4300e+06
11 12 2 0.1120 3.7000e+07
11 13 2 0.1120 3.7000e+07
11 14 2 0.1520 5.4300e+06
14 15 2 0.1120 3.7000e+07
14 16 2 0.1120 3.7000e+07
14 17 2 0.1520 5.4300e+06
17 18 2 0.1120 3.7000e+07
17 19 2 0.1120 3.7000e+07
17 20 2 0.1520 5.4300e+06
20 21 2 0.1120 3.7000e+07
20 22 2 0.1120 3.7000e+07
20 23 2 0.1520 5.4300e+06
23 24 2 0.1120 3.7000e+07
23 25 2 0.1120 3.7000e+07
23 26 2 0.1520 5.4300e+06
26 27 2 0.1120 3.7000e+07
26 28 2 0.1120 3.7000e+07

```

26	29	2	0.1520	5.4300e+06
29	30	2	0.1120	3.7000e+07
29	31	2	0.1120	3.7000e+07
29	32	2	0.1520	5.4300e+06
32	33	2	0.1120	3.7000e+07
32	34	2	0.1120	3.7000e+07
32	35	2	0.1520	5.4300e+06
35	36	2	0.1120	3.7000e+07
35	37	2	0.1120	3.7000e+07
35	38	2	0.1520	5.4300e+06
38	39	2	0.1120	3.7000e+07
38	40	2	0.1120	3.7000e+07
38	41	2	0.1520	5.4300e+06
41	42	2	0.1120	3.7000e+07
41	43	2	0.1120	3.7000e+07
41	44	2	0.1520	5.4300e+06
44	45	2	0.1120	3.7000e+07
44	46	2	0.1120	3.7000e+07
44	47	2	0.1520	5.4300e+06
47	48	2	0.1130	7.0483e+06
47	49	2	0.1130	7.0483e+06
47	50	2	0.1510	3.7279e+06
50	51	2	0.1490	1.4189e+07
50	55	2	0.1490	1.4189e+07
50	59	2	0.1490	1.4189e+07
51	52	2	0.1120	3.7000e+07
51	53	2	0.1120	3.7000e+07
51	54	2	0.1120	3.7000e+07
55	56	2	0.1120	3.7000e+07
55	57	2	0.1120	3.7000e+07
55	58	2	0.1120	3.7000e+07
59	60	2	0.1120	3.7000e+07
59	61	2	0.1120	3.7000e+07
59	62	2	0.1120	3.7000e+07

[ pairs ]

; ai aj funct ; all 1-4 pairs but the ones excluded in GROMOS itp

1	6	1
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2	10	1
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4	7	1
4	8	1
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5	14	1

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6 11 1  
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22 26 1

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51 61 1  
51 62 1  
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54 55 1  
54 59 1  
55 60 1  
55 61 1  
55 62 1

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57 59 1
58 59 1
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; ai aj ak funct angle fc
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1 2 4 2 108.53 443.00
1 2 5 2 110.30 524.00
3 2 4 2 108.53 443.00
3 2 5 2 110.30 524.00
4 2 5 2 110.30 524.00
2 5 6 2 109.60 450.00
2 5 7 2 109.60 450.00
2 5 8 2 111.00 530.00
6 5 7 2 107.00 2726.16
6 5 8 2 109.50 285.00
7 5 8 2 109.50 285.00
5 8 9 2 109.50 285.00
5 8 10 2 109.50 285.00
5 8 11 2 111.00 530.00
9 8 10 2 107.00 2726.16
9 8 11 2 109.60 450.00
10 8 11 2 109.60 450.00
8 11 12 2 109.60 450.00
8 11 13 2 109.60 450.00
8 11 14 2 111.00 530.00
12 11 13 2 107.00 2726.16
12 11 14 2 109.60 450.00
13 11 14 2 109.60 450.00
11 14 15 2 109.60 450.00
11 14 16 2 109.60 450.00
11 14 17 2 111.00 530.00
15 14 16 2 107.00 2726.16
15 14 17 2 109.60 450.00
16 14 17 2 109.60 450.00
14 17 18 2 109.60 450.00
14 17 19 2 109.60 450.00
14 17 20 2 111.00 530.00
18 17 19 2 107.00 2726.16
18 17 20 2 109.60 450.00
19 17 20 2 109.60 450.00
17 20 21 2 109.60 450.00
17 20 22 2 109.60 450.00
17 20 23 2 111.00 530.00
21 20 22 2 107.00 2726.16
21 20 23 2 109.60 450.00
22 20 23 2 109.60 450.00
20 23 24 2 109.60 450.00
20 23 25 2 109.60 450.00
20 23 26 2 111.00 530.00
24 23 25 2 107.00 2726.16

```

24	23	26	2	109.60	450.00
25	23	26	2	109.60	450.00
23	26	27	2	109.60	450.00
23	26	28	2	109.60	450.00
23	26	29	2	111.00	530.00
27	26	28	2	107.00	2726.16
27	26	29	2	109.60	450.00
28	26	29	2	109.60	450.00
26	29	30	2	109.60	450.00
26	29	31	2	109.60	450.00
26	29	32	2	111.00	530.00
30	29	31	2	107.00	2726.16
30	29	32	2	109.60	450.00
31	29	32	2	109.60	450.00
29	32	33	2	109.60	450.00
29	32	34	2	109.60	450.00
29	32	35	2	111.00	530.00
33	32	34	2	107.00	2726.16
33	32	35	2	109.60	450.00
34	32	35	2	109.60	450.00
32	35	36	2	109.60	450.00
32	35	37	2	109.60	450.00
32	35	38	2	111.00	530.00
36	35	37	2	107.00	2726.16
36	35	38	2	109.60	450.00
37	35	38	2	109.60	450.00
35	38	39	2	109.60	450.00
35	38	40	2	109.60	450.00
35	38	41	2	111.00	530.00
39	38	40	2	107.57	484.00
39	38	41	2	109.60	450.00
40	38	41	2	109.60	450.00
38	41	42	2	109.50	285.00
38	41	43	2	109.50	285.00
38	41	44	2	111.00	530.00
42	41	43	2	107.57	484.00
42	41	44	2	110.00	285.00
43	41	44	2	110.00	285.00
41	44	45	2	109.00	1680.51
41	44	46	2	109.00	1680.51
41	44	47	2	109.50	520.00
45	44	46	2	108.00	465.00
45	44	47	2	111.00	530.00
46	44	47	2	111.00	530.00
44	47	48	2	109.50	285.00
44	47	49	2	109.50	285.00
44	47	50	2	115.00	610.00
48	47	49	2	108.53	443.00
48	47	50	2	107.00	2726.16
49	47	50	2	107.00	2726.16
47	50	51	2	110.30	524.00



47	50	55	2	110.30	524.00
47	50	59	2	110.30	524.00
51	50	55	2	109.00	1680.51
51	50	59	2	109.00	1680.51
55	50	59	2	109.00	1680.51
50	51	52	2	109.60	450.00
50	51	53	2	109.60	450.00
50	51	54	2	109.60	450.00
52	51	53	2	109.50	285.00
52	51	54	2	109.50	285.00
53	51	54	2	109.50	285.00
50	55	56	2	109.60	450.00
50	55	57	2	109.60	450.00
50	55	58	2	109.60	450.00
56	55	57	2	109.50	285.00
56	55	58	2	109.50	285.00
57	55	58	2	109.50	285.00
50	59	60	2	109.60	450.00
50	59	61	2	109.60	450.00
50	59	62	2	109.60	450.00
60	59	61	2	109.50	285.00
60	59	62	2	109.50	285.00
61	59	62	2	109.50	285.00

[ dihedrals ]

; GROMOS improper dihedrals

; ai aj ak al funct angle fc

[ dihedrals ]

; ai aj ak al funct ph0 cp mult

2	5	8	11	1	0.00	5.92	3
3	2	5	8	1	0.00	5.92	3
5	8	11	14	1	0.00	5.92	3
8	11	14	17	1	0.00	5.92	3
11	14	17	20	1	0.00	5.92	3
14	17	20	23	1	0.00	5.92	3
17	20	23	26	1	0.00	5.92	3
20	23	26	29	1	0.00	5.92	3
23	26	29	32	1	0.00	5.92	3
26	29	32	35	1	0.00	5.92	3
29	32	35	38	1	0.00	5.92	3
32	35	38	41	1	0.00	5.92	3
35	38	41	44	1	0.00	5.92	3
38	41	44	47	1	0.00	5.92	3
41	44	47	50	1	0.00	5.92	3
44	47	50	51	1	0.00	1.05	3
47	50	51	52	1	0.00	1.05	3
47	50	55	56	1	0.00	1.05	3
47	50	59	60	1	0.00	1.05	3

[ exclusions ]

; ai aj funct ; GROMOS 1-4 exclusions

**Table S5**

**C18 Molecule**

[ moleculetype ]

; Name nrexcl

NZWE 3

[ atoms ]

; nr type resnr resid atom cgnr charge mass

1	HC	1	NZWE	H46	1	0.073	1.0080
2	C	1	NZWE	C21	2	-0.211	12.0110
3	HC	1	NZWE	H44	3	0.073	1.0080
4	HC	1	NZWE	H45	4	0.073	1.0080
5	C	1	NZWE	C20	5	-0.159	12.0110
6	HC	1	NZWE	H42	6	0.078	1.0080
7	HC	1	NZWE	H43	7	0.078	1.0080
8	C	1	NZWE	C19	8	-0.158	12.0110
9	HC	1	NZWE	H40	9	0.079	1.0080
10	HC	1	NZWE	H41	10	0.079	1.0080
11	C	1	NZWE	C18	11	-0.158	12.0110
12	HC	1	NZWE	H38	12	0.079	1.0080
13	HC	1	NZWE	H39	13	0.079	1.0080
14	C	1	NZWE	C17	14	-0.158	12.0110
15	HC	1	NZWE	H36	15	0.079	1.0080
16	HC	1	NZWE	H37	16	0.079	1.0080
17	C	1	NZWE	C16	17	-0.158	12.0110
18	HC	1	NZWE	H34	18	0.079	1.0080
19	HC	1	NZWE	H35	19	0.079	1.0080
20	C	1	NZWE	C15	20	-0.158	12.0110
21	HC	1	NZWE	H32	21	0.079	1.0080
22	HC	1	NZWE	H33	22	0.079	1.0080
23	C	1	NZWE	C14	23	-0.158	12.0110
24	HC	1	NZWE	H30	24	0.080	1.0080
25	HC	1	NZWE	H31	25	0.080	1.0080
26	C	1	NZWE	C13	26	-0.158	12.0110
27	HC	1	NZWE	H28	27	0.080	1.0080
28	HC	1	NZWE	H29	28	0.080	1.0080
29	C	1	NZWE	C12	29	-0.158	12.0110
30	HC	1	NZWE	H26	30	0.080	1.0080
31	HC	1	NZWE	H27	31	0.080	1.0080
32	C	1	NZWE	C11	32	-0.158	12.0110
33	HC	1	NZWE	H24	33	0.080	1.0080
34	HC	1	NZWE	H25	34	0.080	1.0080
35	C	1	NZWE	C10	35	-0.158	12.0110
36	HC	1	NZWE	H22	36	0.082	1.0080
37	HC	1	NZWE	H23	37	0.082	1.0080
38	C	1	NZWE	C9	38	-0.158	12.0110
39	HC	1	NZWE	H20	39	0.082	1.0080
40	HC	1	NZWE	H21	40	0.082	1.0080
41	C	1	NZWE	C8	41	-0.158	12.0110

```

42 HC 1 NZWE H18 42 0.085 1.0080
43 HC 1 NZWE H19 43 0.085 1.0080
44 C 1 NZWE C7 44 -0.158 12.0110
45 HC 1 NZWE H16 45 0.087 1.0080
46 HC 1 NZWE H17 46 0.087 1.0080
47 C 1 NZWE C6 47 -0.159 12.0110
48 HC 1 NZWE H14 48 0.094 1.0080
49 HC 1 NZWE H15 49 0.094 1.0080
50 C 1 NZWE C5 50 -0.182 12.0110
51 HC 1 NZWE H12 51 0.104 1.0080
52 HC 1 NZWE H13 52 0.104 1.0080
53 CPos 1 NZWE C4 53 -0.123 12.0110
54 HC 1 NZWE H10 54 0.138 1.0080
55 HC 1 NZWE H11 55 0.138 1.0080
56 NL 1 NZWE N1 56 0.031 14.0067
57 CPos 1 NZWE C1 57 -0.187 12.0110
58 HC 1 NZWE H1 58 0.141 1.0080
59 HC 1 NZWE H2 59 0.141 1.0080
60 HC 1 NZWE H3 60 0.141 1.0080
61 CPos 1 NZWE C2 61 -0.187 12.0110
62 HC 1 NZWE H4 62 0.141 1.0080
63 HC 1 NZWE H5 63 0.141 1.0080
64 HC 1 NZWE H6 64 0.141 1.0080
65 CPos 1 NZWE C3 65 -0.187 12.0110
66 HC 1 NZWE H7 66 0.141 1.0080
67 HC 1 NZWE H8 67 0.141 1.0080
68 HC 1 NZWE H9 68 0.141 1.0080

```

; total charge of the molecule: 1.000

[ bonds ]

```

; ai aj funct c0 c1
1 2 2 0.1120 3.7000e+07
2 3 2 0.1120 3.7000e+07
2 4 2 0.1120 3.7000e+07
2 5 2 0.1510 3.7279e+06
5 6 2 0.1120 3.7000e+07
5 7 2 0.1120 3.7000e+07
5 8 2 0.1520 5.4300e+06
8 9 2 0.1120 3.7000e+07
8 10 2 0.1120 3.7000e+07
8 11 2 0.1520 5.4300e+06
11 12 2 0.1120 3.7000e+07
11 13 2 0.1120 3.7000e+07
11 14 2 0.1520 5.4300e+06
14 15 2 0.1120 3.7000e+07
14 16 2 0.1120 3.7000e+07
14 17 2 0.1520 5.4300e+06
17 18 2 0.1120 3.7000e+07
17 19 2 0.1120 3.7000e+07
17 20 2 0.1520 5.4300e+06
20 21 2 0.1120 3.7000e+07
20 22 2 0.1120 3.7000e+07

```

20	23	2	0.1520	5.4300e+06
23	24	2	0.1120	3.7000e+07
23	25	2	0.1120	3.7000e+07
23	26	2	0.1520	5.4300e+06
26	27	2	0.1120	3.7000e+07
26	28	2	0.1120	3.7000e+07
26	29	2	0.1520	5.4300e+06
29	30	2	0.1120	3.7000e+07
29	31	2	0.1120	3.7000e+07
29	32	2	0.1520	5.4300e+06
32	33	2	0.1120	3.7000e+07
32	34	2	0.1120	3.7000e+07
32	35	2	0.1520	5.4300e+06
35	36	2	0.1120	3.7000e+07
35	37	2	0.1120	3.7000e+07
35	38	2	0.1520	5.4300e+06
38	39	2	0.1120	3.7000e+07
38	40	2	0.1120	3.7000e+07
38	41	2	0.1520	5.4300e+06
41	42	2	0.1120	3.7000e+07
41	43	2	0.1120	3.7000e+07
41	44	2	0.1520	5.4300e+06
44	45	2	0.1120	3.7000e+07
44	46	2	0.1120	3.7000e+07
44	47	2	0.1520	5.4300e+06
47	48	2	0.1120	3.7000e+07
47	49	2	0.1120	3.7000e+07
47	50	2	0.1520	5.4300e+06
50	51	2	0.1120	3.7000e+07
50	52	2	0.1120	3.7000e+07
50	53	2	0.1520	5.4300e+06
53	54	2	0.1130	7.0483e+06
53	55	2	0.1130	7.0483e+06
53	56	2	0.1510	3.7279e+06
56	57	2	0.1490	1.4189e+07
56	61	2	0.1490	1.4189e+07
56	65	2	0.1490	1.4189e+07
57	58	2	0.1120	3.7000e+07
57	59	2	0.1120	3.7000e+07
57	60	2	0.1120	3.7000e+07
61	62	2	0.1120	3.7000e+07
61	63	2	0.1120	3.7000e+07
61	64	2	0.1120	3.7000e+07
65	66	2	0.1120	3.7000e+07
65	67	2	0.1120	3.7000e+07
65	68	2	0.1120	3.7000e+07

[ pairs ]

; ai aj funct ; all 1-4 pairs but the ones excluded in GROMOS itp

1 6 1

1 7 1

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 53 60 1  
 53 62 1  
 53 63 1  
 53 64 1  
 53 66 1  
 53 67 1  
 53 68 1  
 54 57 1  
 54 61 1  
 54 65 1  
 55 57 1  
 55 61 1  
 55 65 1  
 57 62 1  
 57 63 1  
 57 64 1  
 57 66 1  
 57 67 1  
 57 68 1  
 58 61 1  
 58 65 1  
 59 61 1  
 59 65 1  
 60 61 1  
 60 65 1  
 61 66 1  
 61 67 1  
 61 68 1  
 62 65 1  
 63 65 1  
 64 65 1

[angles]

```

; ai aj ak funct angle fc
  1  2  3  2 108.53 443.00
  1  2  4  2 108.53 443.00
  1  2  5  2 110.30 524.00
  3  2  4  2 108.53 443.00
  3  2  5  2 110.30 524.00
  4  2  5  2 110.30 524.00
  2  5  6  2 109.60 450.00
  2  5  7  2 109.60 450.00
  2  5  8  2 111.00 530.00
  6  5  7  2 107.00 2726.16
  6  5  8  2 109.50 285.00
  7  5  8  2 109.50 285.00
  5  8  9  2 109.50 285.00
  5  8 10  2 109.50 285.00
  5  8 11  2 111.00 530.00
  9  8 10  2 107.00 2726.16
  
```



9	8	11	2	109.60	450.00
10	8	11	2	109.60	450.00
8	11	12	2	109.60	450.00
8	11	13	2	109.60	450.00
8	11	14	2	111.00	530.00
12	11	13	2	107.00	2726.16
12	11	14	2	109.60	450.00
13	11	14	2	109.60	450.00
11	14	15	2	109.60	450.00
11	14	16	2	109.60	450.00
11	14	17	2	111.00	530.00
15	14	16	2	107.00	2726.16
15	14	17	2	109.60	450.00
16	14	17	2	109.60	450.00
14	17	18	2	109.60	450.00
14	17	19	2	109.60	450.00
14	17	20	2	111.00	530.00
18	17	19	2	107.00	2726.16
18	17	20	2	109.60	450.00
19	17	20	2	109.60	450.00
17	20	21	2	109.60	450.00
17	20	22	2	109.60	450.00
17	20	23	2	111.00	530.00
21	20	22	2	107.00	2726.16
21	20	23	2	109.60	450.00
22	20	23	2	109.60	450.00
20	23	24	2	109.60	450.00
20	23	25	2	109.60	450.00
20	23	26	2	111.00	530.00
24	23	25	2	107.00	2726.16
24	23	26	2	109.60	450.00
25	23	26	2	109.60	450.00
23	26	27	2	109.60	450.00
23	26	28	2	109.60	450.00
23	26	29	2	111.00	530.00
27	26	28	2	107.00	2726.16
27	26	29	2	109.60	450.00
28	26	29	2	109.60	450.00
26	29	30	2	109.60	450.00
26	29	31	2	109.60	450.00
26	29	32	2	111.00	530.00
30	29	31	2	107.00	2726.16
30	29	32	2	109.60	450.00
31	29	32	2	109.60	450.00
29	32	33	2	109.60	450.00
29	32	34	2	109.60	450.00
29	32	35	2	111.00	530.00
33	32	34	2	107.00	2726.16
33	32	35	2	109.60	450.00
34	32	35	2	109.60	450.00
32	35	36	2	109.60	450.00

32	35	37	2	109.60	450.00
32	35	38	2	111.00	530.00
36	35	37	2	107.00	2726.16
36	35	38	2	109.60	450.00
37	35	38	2	109.60	450.00
35	38	39	2	109.60	450.00
35	38	40	2	109.60	450.00
35	38	41	2	111.00	530.00
39	38	40	2	107.00	2726.16
39	38	41	2	109.60	450.00
40	38	41	2	109.60	450.00
38	41	42	2	109.60	450.00
38	41	43	2	109.60	450.00
38	41	44	2	111.00	530.00
42	41	43	2	107.00	2726.16
42	41	44	2	109.60	450.00
43	41	44	2	109.60	450.00
41	44	45	2	109.60	450.00
41	44	46	2	109.60	450.00
41	44	47	2	111.00	530.00
45	44	46	2	107.57	484.00
45	44	47	2	109.60	450.00
46	44	47	2	109.60	450.00
44	47	48	2	109.50	285.00
44	47	49	2	109.50	285.00
44	47	50	2	111.00	530.00
48	47	49	2	107.57	484.00
48	47	50	2	110.00	285.00
49	47	50	2	110.00	285.00
47	50	51	2	109.00	1680.51
47	50	52	2	109.00	1680.51
47	50	53	2	109.50	520.00
51	50	52	2	108.00	465.00
51	50	53	2	111.00	530.00
52	50	53	2	111.00	530.00
50	53	54	2	109.50	285.00
50	53	55	2	109.50	285.00
50	53	56	2	115.00	610.00
54	53	55	2	108.53	443.00
54	53	56	2	107.00	2726.16
55	53	56	2	107.00	2726.16
53	56	57	2	110.30	524.00
53	56	61	2	110.30	524.00
53	56	65	2	110.30	524.00
57	56	61	2	109.00	1680.51
57	56	65	2	109.00	1680.51
61	56	65	2	109.00	1680.51
56	57	58	2	109.60	450.00
56	57	59	2	109.60	450.00
56	57	60	2	109.60	450.00
58	57	59	2	109.60	450.00

```

58 57 60 2 109.60 450.00
59 57 60 2 109.60 450.00
56 61 62 2 109.60 450.00
56 61 63 2 109.60 450.00
56 61 64 2 109.60 450.00
62 61 63 2 109.60 450.00
62 61 64 2 109.60 450.00
63 61 64 2 109.60 450.00
56 65 66 2 109.60 450.00
56 65 67 2 109.60 450.00
56 65 68 2 109.60 450.00
66 65 67 2 109.60 450.00
66 65 68 2 109.60 450.00
67 65 68 2 109.60 450.00

```

[ dihedrals ]

; GROMOS improper dihedrals

; ai aj ak al funct angle fc

[ dihedrals ]

; ai aj ak al funct ph0 cp mult

```

2 5 8 11 1 0.00 5.92 3
3 2 5 8 1 0.00 5.92 3
5 8 11 14 1 0.00 5.92 3
8 11 14 17 1 0.00 5.92 3
11 14 17 20 1 0.00 5.92 3
14 17 20 23 1 0.00 5.92 3
17 20 23 26 1 0.00 5.92 3
20 23 26 29 1 0.00 5.92 3
23 26 29 32 1 0.00 5.92 3
26 29 32 35 1 0.00 5.92 3
29 32 35 38 1 0.00 5.92 3
32 35 38 41 1 0.00 5.92 3
35 38 41 44 1 0.00 5.92 3
38 41 44 47 1 0.00 5.92 3
41 44 47 50 1 0.00 5.92 3
44 47 50 53 1 0.00 5.92 3
47 50 53 56 1 0.00 5.92 3
50 53 56 57 1 0.00 1.05 3
57 56 61 62 1 0.00 1.05 3
57 56 65 66 1 0.00 1.05 3
61 56 57 58 1 0.00 1.05 3

```

[ exclusions ]

; ai aj funct ; GROMOS 1-4 exclusions