Supporting information for: Molecular Cartography of A1 and A2 Asphaltens sub-fractions from classical molecular dynamic simulations

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1 Final snapshots of simulations with 160 models

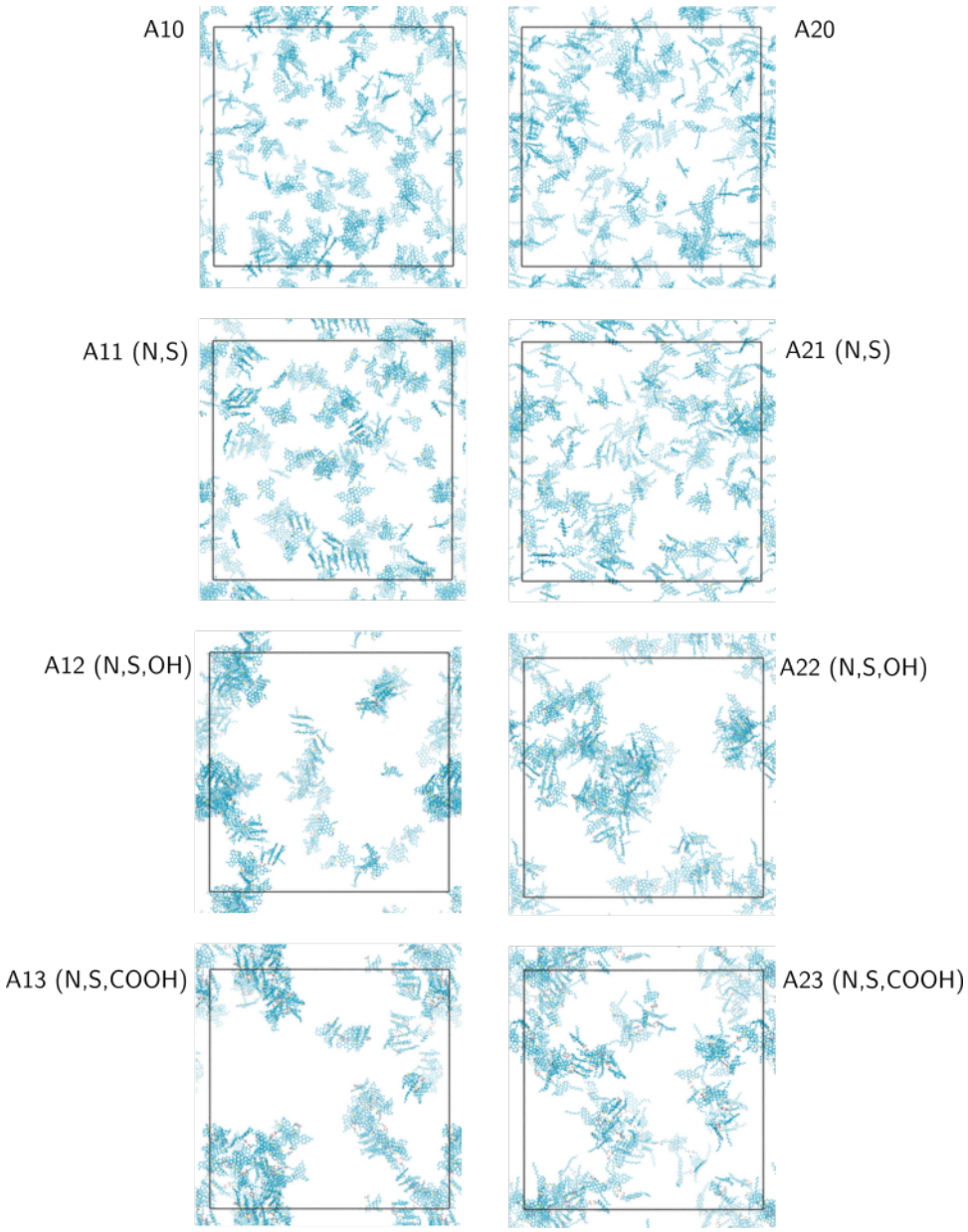

Figure S1: Final snapshots from simulations of systems containing 160 asphaltene models, the solvent molecules have been omitted for clarity

2 Radial distribution functions

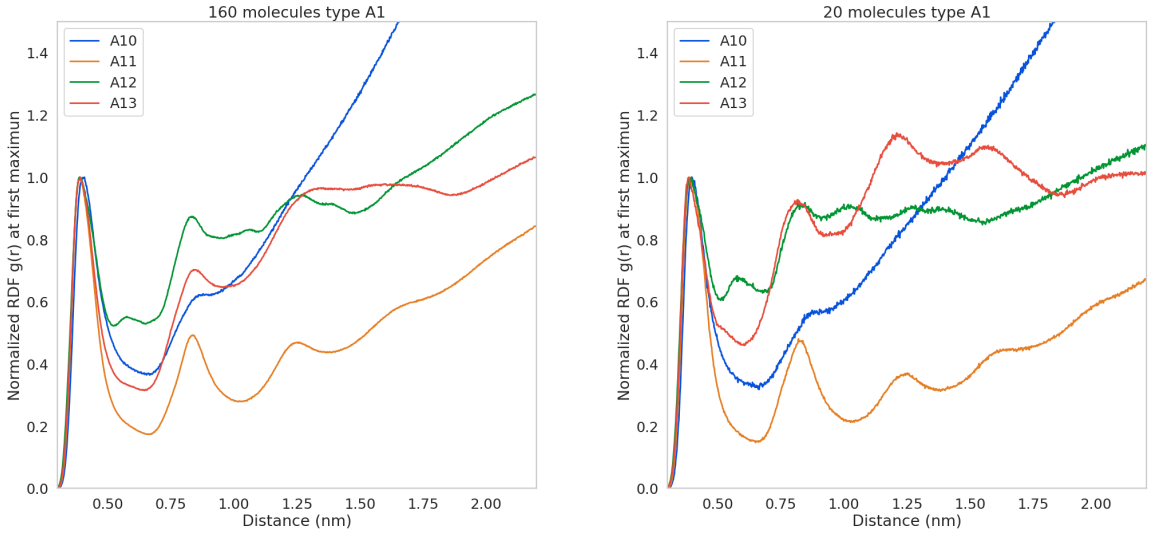

Figure S2: Radial distribution functions of systems of type A1 with 160 asphaltene models (left) and 20 asphaltene models (right).

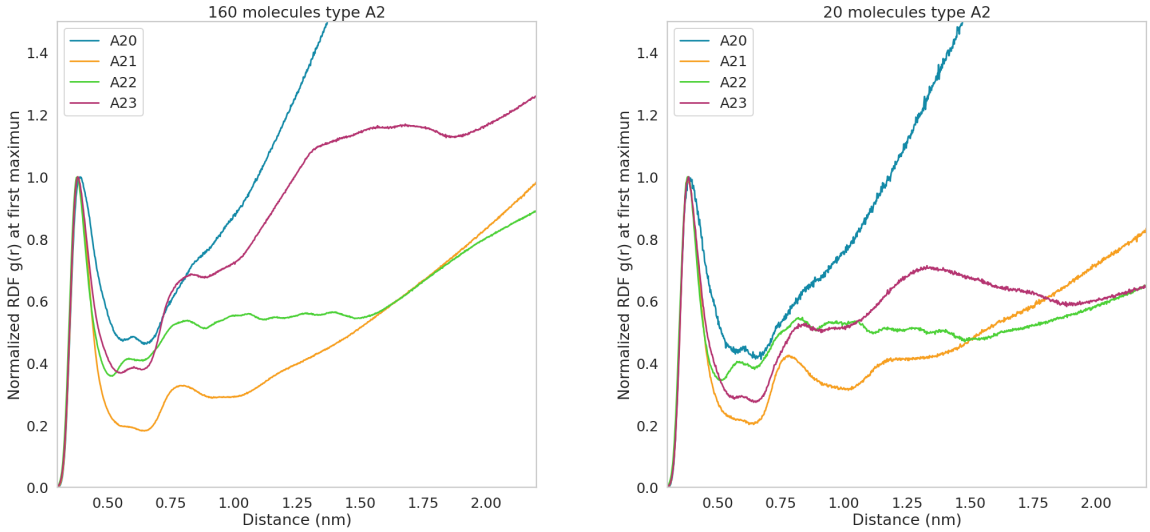

Figure S3: Radial distribution functions of systems of type A2 with 160 asphaltene models (left) and 20 asphaltene models (right).

3 Multiple trajectories

The figures below show a comparison between the radial distribution functions (RDF) obtained from the 4 independent simulations (gray lines) and the average over the 4 simulations (blue lines). One can see that the shape and the relative intensity between the short and long-distance regions in the RDF are similar over the 4 simulations which let us assume that the results do not depend on the initial conditions.

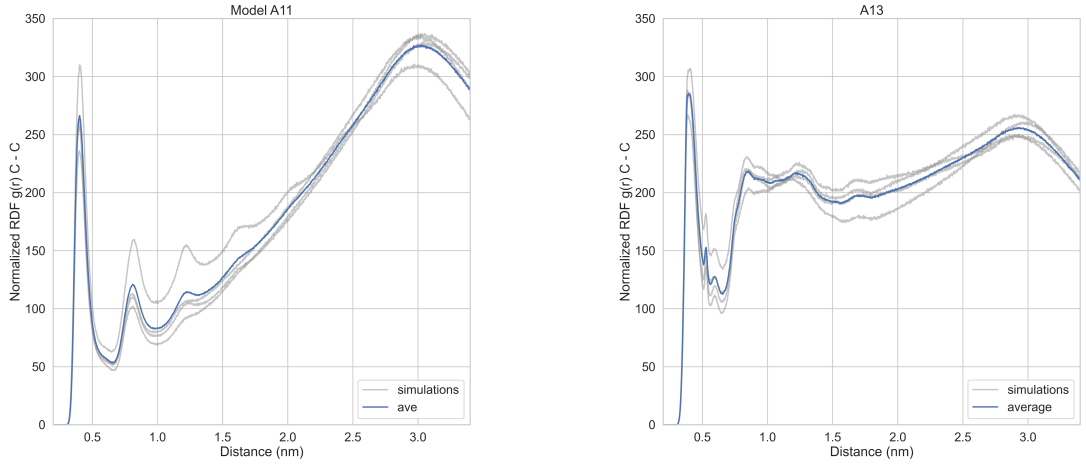

Figure S4: Radial distribution functions of 4 independent trajectories (in gray) and the average of the radial distribution functions (blue) for the A11 (left) and A13 (right) asphaltene molecules.

4 force field parameters

Hereafter are provided the topology files used with GROMACS, `itp` files, for all asphaltene models considered in this study as well as the topology file of the toluene molecule.

```
; This topology was generated by module mkitp in python
; Created by Orlando Villegas - 2019
; mail: orlando.villegas@univ-pau.fr
;------------------------------------------------------------
; Formula: C44H44
; MM: 572.836
; DBE: 23
; M. Dipolar: 1.869
; Forcefield gromos54a7


[ moleculetype ]
; name  nrexcl
A10     3

[ atoms ]
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     2      CR1    1     A10       C    1   0.071  12.011
     3      CR1    1     A10       C    1  -0.267  12.011
     4      CR1    1     A10       C    1  -0.093  12.011
     5      CR1    1     A10       C    1  -0.274  12.011
     6      CR1    1     A10       C    1   0.105  12.011
     7       HC    1     A10       H    1   0.126   1.008
     8       HC    1     A10       H    1   0.144   1.008
     9      CR1    1     A10       C    1  -0.253  12.011
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    15      CR1    1     A10       C    1   0.009  12.011
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```

```
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   15   25    2 gb_16
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26	30	31	32	2	gi_1

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   13   48   1
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   18   48   1
   18   49   1
   23   39   1
   28   43   1
   33   36   1
   33   42   1
   40   41   1
   44   47   1
   45   46   1
   47   49   1
```

```
; This topology was generated by module mkitp in python
; Created by Orlando Villegas - 2019
; mail: orlando.villegas@univ-pau.fr
;------------------------------------------------------------
; Formula: C42H41NS
; MM: 591.870
; DBE: 23
; M. Dipolar: 5.432
; Forcefield gromos54a7

#define gb_53        0.1710  3.4601e+06
#define ga_55        108.00      415.80

[ moleculetype ]
; name  nrexcl
A11     3

[ atoms ]
;   nr     type  resnr  residu    atom    cgnr  charge     mass
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     2      CR1    1     A11       C    1   0.424  12.011
     3      CR1    1     A11       C    1  -0.497  12.011
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     8       HC    1     A11       H    1   0.171   1.008
     9      CR1    1     A11       C    1   0.179  12.011
    10      CR1    1     A11       C    1  -0.107  12.011
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    15      CR1    1     A11       C    1  -0.095  12.011
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    18      CH1    1     A11       C    1   0.205  13.019
    19       HC    1     A11       H    1   0.123   1.008
    20      CR1    1     A11       C    1  -0.238  12.011
    21      CR1    1     A11       C    1  -0.365  12.011
    22      CR1    1     A11       C    1   0.342  12.011
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```

```
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    45      CH1    1     A11       C    1   0.276  13.019
    46      CH2    1     A11       C    1  -0.055  14.027
    47      CH2    1     A11       C    1   0.009  14.027
    48      CH2    1     A11       C    1  -0.069  14.027
    49      CH3    1     A11       C    1  -0.164  15.035

[ bonds ]
;  ai    aj funct
    1    2    2 gb_16
    1    6    2 gb_16
    1    9    2 gb_16
    2    3    2 gb_16
    2   12    2 gb_16
    3    4    2 gb_16
    3    8    2  gb_3
    4    5    2  gb_7
    4    7    2  gb_3
    5    6    2  gb_7
    6   24    2 gb_53
    9   10    2 gb_16
    9   20    2 gb_16
   10   11    2 gb_16
   10   14    2 gb_16
   11   12    2 gb_16
   11   17    2 gb_16
   12   13    2 gb_27
   13   44    2 gb_27
   14   15    2 gb_16
   14   21    2 gb_16
   15   16    2 gb_16
   15   25    2 gb_16
   16   17    2 gb_16
   16   19    2  gb_3
   17   18    2  gb_3
   18   44    2 gb_27
   18   46    2 gb_27
   20   22    2 gb_16
   20   24    2 gb_53
   21   22    2 gb_16
   21   27    2 gb_16
   22   23    2 gb_27
   23   37    2 gb_27
```

```
   25   26    2 gb_16
   25   29    2 gb_16
   26   27    2 gb_16
   26   30    2 gb_16
   27   28    2 gb_27
   28   40    2 gb_27
   29   32    2 gb_16
   29   34    2  gb_3
   30   31    2 gb_16
   30   33    2  gb_3
   31   32    2 gb_16
   31   36    2 gb_27
   32   35    2  gb_3
   33   40    2 gb_27
   33   43    2 gb_27
   36   41    2 gb_27
   37   38    2 gb_27
   38   39    2 gb_27
   41   42    2 gb_27
   41   43    2 gb_27
   44   45    2 gb_27
   45   48    2 gb_27
   45   49    2 gb_27
   46   47    2 gb_27
   47   48    2 gb_27

[ angles ]
;  ai    aj    ak funct
    1    2    3    2   ga_27
    1    2   12    2   ga_27
    1    6    5    2   ga_27
    1    6   24    2   ga_7
    1    9   10    2   ga_27
    1    9   20    2   ga_27
    2    1    6    2   ga_27
    2    1    9    2   ga_27
    2    3    4    2   ga_27
    2    3    8    2   ga_25
    2   12   11    2   ga_27
    2   12   13    2   ga_15
    3    2   12    2   ga_27
    3    4    5    2   ga_27
    3    4    7    2   ga_25
    4    3    8    2   ga_25
    4    5    6    2   ga_15
    5    4    7    2   ga_25
    5    6   24    2   ga_39
    6    1    9    2   ga_27
    6   24   20    2   ga_55
    9   10   11    2   ga_27
    9   10   14    2   ga_27
    9   20   22    2   ga_27
    9   20   24    2   ga_7
   10    9   20    2   ga_27
```

```
10   11   12    2   ga_27
10   11   17    2   ga_27
10   14   15    2   ga_27
10   14   21    2   ga_27
11   10   14    2   ga_27
11   12   13    2   ga_15
11   17   16    2   ga_27
11   17   18    2   ga_25
12   11   17    2   ga_27
12   13   44    2   ga_15
13   44   18    2   ga_15
13   44   45    2   ga_15
14   15   16    2   ga_27
14   15   25    2   ga_27
14   21   22    2   ga_27
14   21   27    2   ga_27
15   14   21    2   ga_27
15   16   17    2   ga_27
15   16   19    2   ga_25
15   25   26    2   ga_27
15   25   29    2   ga_27
16   15   25    2   ga_27
16   17   18    2   ga_25
17   16   19    2   ga_25
17   18   44    2   ga_15
17   18   46    2   ga_15
18   44   45    2   ga_15
18   46   47    2   ga_15
20   22   21    2   ga_27
20   22   23    2   ga_15
21   22   23    2   ga_15
21   27   26    2   ga_27
21   27   28    2   ga_15
22   20   24    2   ga_7
22   21   27    2   ga_27
22   23   37    2   ga_15
23   37   38    2   ga_15
25   26   27    2   ga_27
25   26   30    2   ga_27
25   29   32    2   ga_27
25   29   34    2   ga_25
26   25   29    2   ga_27
26   27   28    2   ga_15
26   30   31    2   ga_27
26   30   33    2   ga_25
27   26   30    2   ga_27
27   28   40    2   ga_15
28   40   33    2   ga_15
29   32   31    2   ga_27
29   32   35    2   ga_25
30   31   32    2   ga_27
30   31   36    2   ga_15
30   33   40    2   ga_15
30   33   43    2   ga_15
```

```
   31   30   33    2   ga_25
   31   32   35    2   ga_25
   31   36   41    2   ga_15
   32   29   34    2   ga_25
   32   31   36    2   ga_15
   33   43   41    2   ga_15
   36   41   42    2   ga_15
   36   41   43    2   ga_15
   37   38   39    2   ga_15
   40   33   43    2   ga_15
   42   41   43    2   ga_15
   44   18   46    2   ga_15
   44   45   48    2   ga_15
   44   45   49    2   ga_15
   45   48   47    2   ga_15
   46   47   48    2   ga_15
   48   45   49    2   ga_15

[ dihedrals ]
;  ai    aj    ak    al funct
    2   12   13   44    1   gd_40
   11   12   13   44    1   gd_40
   11   17   18   44    1   gd_40
   11   17   18   46    1   gd_40
   12   13   44   18    1   gd_10
   12   13   44   45    1   gd_10
   13   44   18   17    1   gd_10
   13   44   18   46    1   gd_10
   13   44   45   48    1   gd_10
   13   44   45   49    1   gd_10
   16   17   18   44    1   gd_40
   16   17   18   46    1   gd_40
   17   18   44   45    1   gd_10
   17   18   46   47    1   gd_10
   18   44   45   48    1   gd_10
   18   44   45   49    1   gd_10
   18   46   47   48    1   gd_10
   20   22   23   37    1   gd_40
   21   22   23   37    1   gd_40
   21   27   28   40    1   gd_40
   22   23   37   38    1   gd_10
   23   37   38   39    1   gd_10
   26   27   28   40    1   gd_40
   26   30   33   40    1   gd_40
   26   30   33   43    1   gd_40
   27   28   40   33    1   gd_10
   28   40   33   30    1   gd_10
   28   40   33   43    1   gd_10
   30   31   36   41    1   gd_40
   30   33   43   41    1   gd_10
   31   30   33   40    1   gd_40
   31   30   33   43    1   gd_40
   31   36   41   42    1   gd_10
   31   36   41   43    1   gd_10
```

32	31	36	41	1	gd_40
33	43	41	36	1	gd_10
33	43	41	42	1	gd_10
40	33	43	41	1	gd_10
44	18	46	47	1	gd_10
44	45	48	47	1	gd_10
45	44	18	46	1	gd_10
45	48	47	46	1	gd_10
47	48	45	49	1	gd_10
1	2	6	9	2	gi_1
2	1	3	12	2	gi_1
3	2	4	8	2	gi_1
4	3	5	7	2	gi_1
6	1	5	24	2	gi_1
9	1	10	20	2	gi_1
10	9	11	14	2	gi_1
11	10	12	17	2	gi_1
12	2	11	13	2	gi_1
14	10	15	21	2	gi_1
15	14	16	25	2	gi_1
16	15	17	19	2	gi_1
17	11	16	18	2	gi_1
18	17	44	46	2	gi_2
20	9	22	24	2	gi_1
21	14	22	27	2	gi_1
22	20	21	23	2	gi_1
25	15	26	29	2	gi_1
26	25	27	30	2	gi_1
27	21	26	28	2	gi_1
29	25	32	34	2	gi_1
30	26	31	33	2	gi_1
31	30	32	36	2	gi_1
32	29	31	35	2	gi_1
33	30	40	43	2	gi_2
41	36	42	43	2	gi_2
44	13	18	45	2	gi_2
45	44	48	49	2	gi_2
1	2	3	4	2	gi_1
1	2	12	11	2	gi_1
1	6	5	4	2	gi_1
1	6	24	20	2	gi_1
1	9	10	11	2	gi_1
1	9	10	14	2	gi_4
1	9	20	22	2	gi_4
1	9	20	24	2	gi_1
2	1	6	5	2	gi_1
2	1	6	24	2	gi_4
2	1	9	10	2	gi_1
2	1	9	20	2	gi_4
2	3	4	5	2	gi_1
2	12	11	10	2	gi_1
2	12	11	17	2	gi_4
3	2	1	6	2	gi_1
3	2	1	9	2	gi_4

3	2	12	11	2	gi_4
3	4	5	6	2	gi_1
4	3	2	12	2	gi_4
4	5	6	24	2	gi_4
5	6	1	9	2	gi_4
5	6	24	20	2	gi_4
6	1	2	12	2	gi_4
6	1	9	10	2	gi_4
6	1	9	20	2	gi_1
6	24	20	9	2	gi_1
6	24	20	22	2	gi_4
9	1	2	12	2	gi_1
9	1	6	24	2	gi_1
9	10	11	12	2	gi_1
9	10	11	17	2	gi_4
9	10	14	15	2	gi_4
9	10	14	21	2	gi_1
9	20	22	21	2	gi_1
10	9	20	22	2	gi_1
10	9	20	24	2	gi_4
10	11	17	16	2	gi_1
10	14	15	16	2	gi_1
10	14	15	25	2	gi_4
10	14	21	22	2	gi_1
10	14	21	27	2	gi_4
11	10	9	20	2	gi_4
11	10	14	15	2	gi_1
11	10	14	21	2	gi_4
11	17	16	15	2	gi_1
12	11	10	14	2	gi_4
12	11	17	16	2	gi_4
14	10	9	20	2	gi_1
14	10	11	17	2	gi_1
14	15	16	17	2	gi_1
14	15	25	26	2	gi_1
14	15	25	29	2	gi_4
14	21	22	20	2	gi_1
14	21	27	26	2	gi_1
15	14	21	22	2	gi_4
15	14	21	27	2	gi_1
15	25	26	27	2	gi_1
15	25	26	30	2	gi_4
15	25	29	32	2	gi_4
16	15	14	21	2	gi_4
16	15	25	26	2	gi_4
16	15	25	29	2	gi_1
17	16	15	25	2	gi_4
20	22	21	27	2	gi_4
21	14	15	25	2	gi_1
21	22	20	24	2	gi_4
21	27	26	25	2	gi_1
21	27	26	30	2	gi_4
22	21	27	26	2	gi_4
25	26	30	31	2	gi_1

```
   25   29   32   31    2   gi_1
   26   25   29   32    2   gi_1
   26   30   31   32    2   gi_1
   27   26   25   29    2   gi_4
   27   26   30   31    2   gi_4
   29   25   26   30    2   gi_1
   29   32   31   30    2   gi_1

[ pairs ]
;  ai    aj funct
   13   46   1
   13   48   1
   13   49   1
   18   48   1
   18   49   1
   23   39   1
   28   43   1
   33   36   1
   33   42   1
   40   41   1
   44   47   1
   45   46   1
   47   49   1
```

```
; This topology was generated by module mkitp in python
; Created by Orlando Villegas - 2019
; mail: orlando.villegas@univ-pau.fr
;------------------------------------------------------------
; Formula: C42H41NOS
; MM: 607.870
; DBE: 23
; M. Dipolar: 5.718
; Forcefield gromos54a7

#define gb_53        0.1710  3.4601e+06
#define ga_55        108.00      415.80

[ moleculetype ]
; name  nrexcl
A12     3

[ atoms ]
;   nr     type  resnr  residu    atom    cgnr  charge     mass
     1      CR1    1     A12       C    1  -0.390  12.011
     2      CR1    1     A12       C    1   0.440  12.011
     3      CR1    1     A12       C    1  -0.525  12.011
     4      CR1    1     A12       C    1   0.284  12.011
     5       NR    1     A12       N    1  -0.630  14.010
     6      CR1    1     A12       C    1   0.675  12.011
     7       HC    1     A12       H    1   0.078   1.008
     8       HC    1     A12       H    1   0.176   1.008
     9      CR1    1     A12       C    1   0.215  12.011
    10      CR1    1     A12       C    1  -0.161  12.011
    11      CR1    1     A12       C    1   0.214  12.011
    12      CR1    1     A12       C    1  -0.332  12.011
    13      CH2    1     A12       C    1   0.140  14.027
    14      CR1    1     A12       C    1   0.237  12.011
    15      CR1    1     A12       C    1  -0.114  12.011
    16      CR1    1     A12       C    1  -0.152  12.011
    17      CR1    1     A12       C    1  -0.192  12.011
    18      CH1    1     A12       C    1   0.239  13.019
    19       HC    1     A12       H    1   0.118   1.008
    20      CR1    1     A12       C    1  -0.248  12.011
    21      CR1    1     A12       C    1  -0.403  12.011
    22      CR1    1     A12       C    1   0.341  12.011
    23      CH2    1     A12       C    1  -0.097  14.027
    24        S    1     A12       S    1  -0.208  32.070
    25      CR1    1     A12       C    1   0.270  12.011
    26      CR1    1     A12       C    1  -0.140  12.011
    27      CR1    1     A12       C    1   0.159  12.011
    28      CH2    1     A12       C    1   0.186  14.027
    29      CR1    1     A12       C    1  -0.574  12.011
    30      CR1    1     A12       C    1  -0.180  12.011
    31      CR1    1     A12       C    1  -0.038  12.011
    32      CR1    1     A12       C    1   0.471  12.011
```

```
    33      CH1    1     A12       C    1   0.358  13.019
    34       HC    1     A12       H    1   0.206   1.008
    35       OA    1     A12       O    1  -0.649  16.000
    36      CH2    1     A12       C    1  -0.040  14.027
    37      CH2    1     A12       C    1   0.020  14.027
    38      CH2    1     A12       C    1   0.133  14.027
    39      CH3    1     A12       C    1  -0.096  15.035
    40      CH2    1     A12       C    1  -0.197  14.027
    41      CH1    1     A12       C    1   0.340  13.019
    42      CH3    1     A12       C    1  -0.144  15.035
    43      CH2    1     A12       C    1  -0.163  14.027
    44      CH1    1     A12       C    1  -0.060  13.019
    45      CH1    1     A12       C    1   0.280  13.019
    46      CH2    1     A12       C    1  -0.073  14.027
    47      CH2    1     A12       C    1   0.018  14.027
    48      CH2    1     A12       C    1  -0.074  14.027
    49      CH3    1     A12       C    1  -0.163  15.035
    50        H    1     A12       H    1   0.445   1.008

[ bonds ]
;  ai    aj funct
    1    2    2 gb_16
    1    6    2 gb_16
    1    9    2 gb_16
    2    3    2 gb_16
    2   12    2 gb_16
    3    4    2 gb_16
    3    8    2  gb_3
    4    5    2  gb_7
    4    7    2  gb_3
    5    6    2  gb_7
    6   24    2 gb_53
    9   10    2 gb_16
    9   20    2 gb_16
   10   11    2 gb_16
   10   14    2 gb_16
   11   12    2 gb_16
   11   17    2 gb_16
   12   13    2 gb_27
   13   44    2 gb_27
   14   15    2 gb_16
   14   21    2 gb_16
   15   16    2 gb_16
   15   25    2 gb_16
   16   17    2 gb_16
   16   19    2  gb_3
   17   18    2  gb_3
   18   44    2 gb_27
   18   46    2 gb_27
   20   22    2 gb_16
   20   24    2 gb_53
   21   22    2 gb_16
   21   27    2 gb_16
   22   23    2 gb_27
```

```
   23   37    2 gb_27
   25   26    2 gb_16
   25   29    2 gb_16
   26   27    2 gb_16
   26   30    2 gb_16
   27   28    2 gb_27
   28   40    2 gb_27
   29   32    2 gb_16
   29   34    2  gb_3
   30   31    2 gb_16
   30   33    2  gb_3
   31   32    2 gb_16
   31   36    2 gb_27
   32   35    2 gb_13
   33   40    2 gb_27
   33   43    2 gb_27
   35   50    2  gb_1
   36   41    2 gb_27
   37   38    2 gb_27
   38   39    2 gb_27
   41   42    2 gb_27
   41   43    2 gb_27
   44   45    2 gb_27
   45   48    2 gb_27
   45   49    2 gb_27
   46   47    2 gb_27
   47   48    2 gb_27

[ angles ]
;  ai    aj    ak funct
    1    2    3    2   ga_27
    1    2   12    2   ga_27
    1    6    5    2   ga_27
    1    6   24    2   ga_7
    1    9   10    2   ga_27
    1    9   20    2   ga_27
    2    1    6    2   ga_27
    2    1    9    2   ga_27
    2    3    4    2   ga_27
    2    3    8    2   ga_25
    2   12   11    2   ga_27
    2   12   13    2   ga_15
    3    2   12    2   ga_27
    3    4    5    2   ga_27
    3    4    7    2   ga_25
    4    3    8    2   ga_25
    4    5    6    2   ga_15
    5    4    7    2   ga_25
    5    6   24    2   ga_39
    6    1    9    2   ga_27
    6   24   20    2   ga_55
    9   10   11    2   ga_27
    9   10   14    2   ga_27
    9   20   22    2   ga_27
```

9	20	24	2	ga_7
10	9	20	2	ga_27
10	11	12	2	ga_27
10	11	17	2	ga_27
10	14	15	2	ga_27
10	14	21	2	ga_27
11	10	14	2	ga_27
11	12	13	2	ga_15
11	17	16	2	ga_27
11	17	18	2	ga_25
12	11	17	2	ga_27
12	13	44	2	ga_15
13	44	18	2	ga_15
13	44	45	2	ga_15
14	15	16	2	ga_27
14	15	25	2	ga_27
14	21	22	2	ga_27
14	21	27	2	ga_27
15	14	21	2	ga_27
15	16	17	2	ga_27
15	16	19	2	ga_25
15	25	26	2	ga_27
15	25	29	2	ga_27
16	15	25	2	ga_27
16	17	18	2	ga_25
17	16	19	2	ga_25
17	18	44	2	ga_15
17	18	46	2	ga_15
18	44	45	2	ga_15
18	46	47	2	ga_15
20	22	21	2	ga_27
20	22	23	2	ga_15
21	22	23	2	ga_15
21	27	26	2	ga_27
21	27	28	2	ga_15
22	20	24	2	ga_7
22	21	27	2	ga_27
22	23	37	2	ga_15
23	37	38	2	ga_15
25	26	27	2	ga_27
25	26	30	2	ga_27
25	29	32	2	ga_27
25	29	34	2	ga_25
26	25	29	2	ga_27
26	27	28	2	ga_15
26	30	31	2	ga_27
26	30	33	2	ga_25
27	26	30	2	ga_27
27	28	40	2	ga_15
28	40	33	2	ga_15
29	32	31	2	ga_27
29	32	35	2	ga_25
30	31	32	2	ga_27
30	31	36	2	ga_15

```
   30   33   40    2   ga_15
   30   33   43    2   ga_15
   31   30   33    2   ga_25
   31   32   35    2   ga_25
   31   36   41    2   ga_15
   32   29   34    2   ga_25
   32   31   36    2   ga_15
   32   35   50    2   ga_12
   33   43   41    2   ga_15
   36   41   42    2   ga_15
   36   41   43    2   ga_15
   37   38   39    2   ga_15
   40   33   43    2   ga_15
   42   41   43    2   ga_15
   44   18   46    2   ga_15
   44   45   48    2   ga_15
   44   45   49    2   ga_15
   45   48   47    2   ga_15
   46   47   48    2   ga_15
   48   45   49    2   ga_15

[ dihedrals ]
;  ai    aj    ak    al funct
    2   12   13   44    1   gd_40
   11   12   13   44    1   gd_40
   11   17   18   44    1   gd_40
   11   17   18   46    1   gd_40
   12   13   44   18    1   gd_10
   12   13   44   45    1   gd_10
   13   44   18   17    1   gd_10
   13   44   18   46    1   gd_10
   13   44   45   48    1   gd_10
   13   44   45   49    1   gd_10
   16   17   18   44    1   gd_40
   16   17   18   46    1   gd_40
   17   18   44   45    1   gd_10
   17   18   46   47    1   gd_10
   18   44   45   48    1   gd_10
   18   44   45   49    1   gd_10
   18   46   47   48    1   gd_10
   20   22   23   37    1   gd_40
   21   22   23   37    1   gd_40
   21   27   28   40    1   gd_40
   22   23   37   38    1   gd_10
   23   37   38   39    1   gd_10
   26   27   28   40    1   gd_40
   26   30   33   40    1   gd_40
   26   30   33   43    1   gd_40
   27   28   40   33    1   gd_10
   28   40   33   30    1   gd_10
   28   40   33   43    1   gd_10
   29   32   35   50    1   gd_23
   30   31   36   41    1   gd_40
   30   33   43   41    1   gd_10
```

31	30	33	40	1	gd_40
31	30	33	43	1	gd_40
31	32	35	50	1	gd_23
31	36	41	42	1	gd_10
31	36	41	43	1	gd_10
32	31	36	41	1	gd_40
33	43	41	36	1	gd_10
33	43	41	42	1	gd_10
40	33	43	41	1	gd_10
44	18	46	47	1	gd_10
44	45	48	47	1	gd_10
45	44	18	46	1	gd_10
45	48	47	46	1	gd_10
47	48	45	49	1	gd_10
1	2	6	9	2	gi_1
2	1	3	12	2	gi_1
3	2	4	8	2	gi_1
4	3	5	7	2	gi_1
6	1	5	24	2	gi_1
9	1	10	20	2	gi_1
10	9	11	14	2	gi_1
11	10	12	17	2	gi_1
12	2	11	13	2	gi_1
14	10	15	21	2	gi_1
15	14	16	25	2	gi_1
16	15	17	19	2	gi_1
17	11	16	18	2	gi_1
18	17	44	46	2	gi_2
20	9	22	24	2	gi_1
21	14	22	27	2	gi_1
22	20	21	23	2	gi_1
25	15	26	29	2	gi_1
26	25	27	30	2	gi_1
27	21	26	28	2	gi_1
29	25	32	34	2	gi_1
30	26	31	33	2	gi_1
31	30	32	36	2	gi_1
32	29	31	35	2	gi_1
33	30	40	43	2	gi_2
41	36	42	43	2	gi_2
44	13	18	45	2	gi_2
45	44	48	49	2	gi_2
1	2	3	4	2	gi_1
1	2	12	11	2	gi_1
1	6	5	4	2	gi_1
1	6	24	20	2	gi_1
1	9	10	11	2	gi_1
1	9	10	14	2	gi_4
1	9	20	22	2	gi_4
1	9	20	24	2	gi_1
2	1	6	5	2	gi_1
2	1	6	24	2	gi_4
2	1	9	10	2	gi_1
2	1	9	20	2	gi_4

2	3	4	5	2	gi_1
2	12	11	10	2	gi_1
2	12	11	17	2	gi_4
3	2	1	6	2	gi_1
3	2	1	9	2	gi_4
3	2	12	11	2	gi_4
3	4	5	6	2	gi_1
4	3	2	12	2	gi_4
4	5	6	24	2	gi_4
5	6	1	9	2	gi_4
5	6	24	20	2	gi_4
6	1	2	12	2	gi_4
6	1	9	10	2	gi_4
6	1	9	20	2	gi_1
6	24	20	9	2	gi_1
6	24	20	22	2	gi_4
9	1	2	12	2	gi_1
9	1	6	24	2	gi_1
9	10	11	12	2	gi_1
9	10	11	17	2	gi_4
9	10	14	15	2	gi_4
9	10	14	21	2	gi_1
9	20	22	21	2	gi_1
10	9	20	22	2	gi_1
10	9	20	24	2	gi_4
10	11	17	16	2	gi_1
10	14	15	16	2	gi_1
10	14	15	25	2	gi_4
10	14	21	22	2	gi_1
10	14	21	27	2	gi_4
11	10	9	20	2	gi_4
11	10	14	15	2	gi_1
11	10	14	21	2	gi_4
11	17	16	15	2	gi_1
12	11	10	14	2	gi_4
12	11	17	16	2	gi_4
14	10	9	20	2	gi_1
14	10	11	17	2	gi_1
14	15	16	17	2	gi_1
14	15	25	26	2	gi_1
14	15	25	29	2	gi_4
14	21	22	20	2	gi_1
14	21	27	26	2	gi_1
15	14	21	22	2	gi_4
15	14	21	27	2	gi_1
15	25	26	27	2	gi_1
15	25	26	30	2	gi_4
15	25	29	32	2	gi_4
16	15	14	21	2	gi_4
16	15	25	26	2	gi_4
16	15	25	29	2	gi_1
17	16	15	25	2	gi_4
20	22	21	27	2	gi_4
21	14	15	25	2	gi_1

```
   21   22   20   24    2   gi_4
   21   27   26   25    2   gi_1
   21   27   26   30    2   gi_4
   22   21   27   26    2   gi_4
   25   26   30   31    2   gi_1
   25   29   32   31    2   gi_1
   26   25   29   32    2   gi_1
   26   30   31   32    2   gi_1
   27   26   25   29    2   gi_4
   27   26   30   31    2   gi_4
   29   25   26   30    2   gi_1
   29   32   31   30    2   gi_1

[ pairs ]
;  ai    aj funct
   13   46   1
   13   48   1
   13   49   1
   18   48   1
   18   49   1
   23   39   1
   28   43   1
   33   36   1
   33   42   1
   40   41   1
   44   47   1
   45   46   1
   47   49   1
```

```
; This topology was generated by module mkitp in python
; Created by Orlando Villegas - 2019
; mail: orlando.villegas@univ-pau.fr
;------------------------------------------------------------
; Formula: C42H39NO2S
; MM: 621.854
; DBE: 24
; M. Dipolar: 5.038
; Forcefield gromos54a7

#define gb_53        0.1710  3.4601e+06
#define ga_55        108.00      415.80

[ moleculetype ]
; name  nrexcl
A13     3

[ atoms ]
;   nr     type  resnr  residu    atom    cgnr  charge     mass
     1      CR1    1     A13       C    1  -0.393  12.011
     2      CR1    1     A13       C    1   0.450  12.011
     3      CR1    1     A13       C    1  -0.543  12.011
     4      CR1    1     A13       C    1   0.318  12.011
     5       NR    1     A13       N    1  -0.634  14.010
     6      CR1    1     A13       C    1   0.676  12.011
     7       HC    1     A13       H    1   0.065   1.008
     8       HC    1     A13       H    1   0.176   1.008
     9      CR1    1     A13       C    1   0.213  12.011
    10      CR1    1     A13       C    1  -0.150  12.011
    11      CR1    1     A13       C    1   0.183  12.011
    12      CR1    1     A13       C    1  -0.347  12.011
    13      CH2    1     A13       C    1   0.196  14.027
    14      CR1    1     A13       C    1   0.178  12.011
    15      CR1    1     A13       C    1  -0.097  12.011
    16      CR1    1     A13       C    1  -0.163  12.011
    17      CR1    1     A13       C    1  -0.126  12.011
    18      CH1    1     A13       C    1   0.204  13.019
    19       HC    1     A13       H    1   0.105   1.008
    20      CR1    1     A13       C    1  -0.175  12.011
    21      CR1    1     A13       C    1  -0.260  12.011
    22      CR1    1     A13       C    1   0.213  12.011
    23      CH2    1     A13       C    1  -0.053  14.027
    24        S    1     A13       S    1  -0.226  32.070
    25      CR1    1     A13       C    1   0.168  12.011
    26      CR1    1     A13       C    1   0.010  12.011
    27      CR1    1     A13       C    1   0.021  12.011
    28      CH2    1     A13       C    1   0.168  14.027
    29      CR1    1     A13       C    1  -0.262  12.011
    30      CR1    1     A13       C    1  -0.214  12.011
    31      CR1    1     A13       C    1   0.229  12.011
    32      CR1    1     A13       C    1  -0.240  12.011
```

```
    33      CH1    1     A13       C    1   0.299  13.019
    34       HC    1     A13       H    1   0.173   1.008
    35       HC    1     A13       H    1   0.147   1.008
    36      CH2    1     A13       C    1  -0.193  14.027
    37      CH2    1     A13       C    1   0.127  14.027
    38      CH2    1     A13       C    1  -0.040  14.027
    39        C    1     A13       C    1   0.774  12.011
    40      CH2    1     A13       C    1  -0.146  14.027
    41      CH1    1     A13       C    1   0.416  13.019
    42      CH3    1     A13       C    1  -0.143  15.035
    43      CH2    1     A13       C    1  -0.206  14.027
    44      CH1    1     A13       C    1  -0.109  13.019
    45      CH1    1     A13       C    1   0.277  13.019
    46      CH2    1     A13       C    1  -0.049  14.027
    47      CH2    1     A13       C    1   0.015  14.027
    48      CH2    1     A13       C    1  -0.062  14.027
    49      CH3    1     A13       C    1  -0.160  15.035
    50        O    1     A13       O    1  -0.593  16.000
    51       OA    1     A13       O    1  -0.665  16.000
    52        H    1     A13       H    1   0.448   1.008

[ bonds ]
;  ai    aj funct
    1    2    2 gb_16
    1    6    2 gb_16
    1    9    2 gb_16
    2    3    2 gb_16
    2   12    2 gb_16
    3    4    2 gb_16
    3    8    2  gb_3
    4    5    2  gb_7
    4    7    2  gb_3
    5    6    2  gb_7
    6   24    2 gb_53
    9   10    2 gb_16
    9   20    2 gb_16
   10   11    2 gb_16
   10   14    2 gb_16
   11   12    2 gb_16
   11   17    2 gb_16
   12   13    2 gb_27
   13   44    2 gb_27
   14   15    2 gb_16
   14   21    2 gb_16
   15   16    2 gb_16
   15   25    2 gb_16
   16   17    2 gb_16
   16   19    2  gb_3
   17   18    2  gb_3
   18   44    2 gb_27
   18   46    2 gb_27
   20   22    2 gb_16
   20   24    2 gb_53
   21   22    2 gb_16
```

```
   21   27    2 gb_16
   22   23    2 gb_27
   23   37    2 gb_27
   25   26    2 gb_16
   25   29    2 gb_16
   26   27    2 gb_16
   26   30    2 gb_16
   27   28    2 gb_27
   28   40    2 gb_27
   29   32    2 gb_16
   29   34    2  gb_3
   30   31    2 gb_16
   30   33    2  gb_3
   31   32    2 gb_16
   31   36    2 gb_27
   32   35    2  gb_3
   33   40    2 gb_27
   33   43    2 gb_27
   36   41    2 gb_27
   37   38    2 gb_27
   38   39    2 gb_27
   39   50    2  gb_5
   39   51    2 gb_13
   41   42    2 gb_27
   41   43    2 gb_27
   44   45    2 gb_27
   45   48    2 gb_27
   45   49    2 gb_27
   46   47    2 gb_27
   47   48    2 gb_27
   51   52    2  gb_1

[ angles ]
;  ai    aj    ak funct
    1    2    3    2   ga_27
    1    2   12    2   ga_27
    1    6    5    2   ga_27
    1    6   24    2   ga_7
    1    9   10    2   ga_27
    1    9   20    2   ga_27
    2    1    6    2   ga_27
    2    1    9    2   ga_27
    2    3    4    2   ga_27
    2    3    8    2   ga_25
    2   12   11    2   ga_27
    2   12   13    2   ga_15
    3    2   12    2   ga_27
    3    4    5    2   ga_27
    3    4    7    2   ga_25
    4    3    8    2   ga_25
    4    5    6    2   ga_15
    5    4    7    2   ga_25
    5    6   24    2   ga_39
    6    1    9    2   ga_27
```

6	24	20	2	ga_55
9	10	11	2	ga_27
9	10	14	2	ga_27
9	20	22	2	ga_27
9	20	24	2	ga_7
10	9	20	2	ga_27
10	11	12	2	ga_27
10	11	17	2	ga_27
10	14	15	2	ga_27
10	14	21	2	ga_27
11	10	14	2	ga_27
11	12	13	2	ga_15
11	17	16	2	ga_27
11	17	18	2	ga_25
12	11	17	2	ga_27
12	13	44	2	ga_15
13	44	18	2	ga_15
13	44	45	2	ga_15
14	15	16	2	ga_27
14	15	25	2	ga_27
14	21	22	2	ga_27
14	21	27	2	ga_27
15	14	21	2	ga_27
15	16	17	2	ga_27
15	16	19	2	ga_25
15	25	26	2	ga_27
15	25	29	2	ga_27
16	15	25	2	ga_27
16	17	18	2	ga_25
17	16	19	2	ga_25
17	18	44	2	ga_15
17	18	46	2	ga_15
18	44	45	2	ga_15
18	46	47	2	ga_15
20	22	21	2	ga_27
20	22	23	2	ga_15
21	22	23	2	ga_15
21	27	26	2	ga_27
21	27	28	2	ga_15
22	20	24	2	ga_7
22	21	27	2	ga_27
22	23	37	2	ga_15
23	37	38	2	ga_15
25	26	27	2	ga_27
25	26	30	2	ga_27
25	29	32	2	ga_27
25	29	34	2	ga_25
26	25	29	2	ga_27
26	27	28	2	ga_15
26	30	31	2	ga_27
26	30	33	2	ga_25
27	26	30	2	ga_27
27	28	40	2	ga_15
28	40	33	2	ga_15

```
   29   32   31    2   ga_27
   29   32   35    2   ga_25
   30   31   32    2   ga_27
   30   31   36    2   ga_15
   30   33   40    2   ga_15
   30   33   43    2   ga_15
   31   30   33    2   ga_25
   31   32   35    2   ga_25
   31   36   41    2   ga_15
   32   29   34    2   ga_25
   32   31   36    2   ga_15
   33   43   41    2   ga_15
   36   41   42    2   ga_15
   36   41   43    2   ga_15
   37   38   39    2   ga_15
   38   39   50    2   ga_30
   38   39   51    2   ga_19
   39   51   52    2   ga_12
   40   33   43    2   ga_15
   42   41   43    2   ga_15
   44   18   46    2   ga_15
   44   45   48    2   ga_15
   44   45   49    2   ga_15
   45   48   47    2   ga_15
   46   47   48    2   ga_15
   48   45   49    2   ga_15
   50   39   51    2   ga_33

[ dihedrals ]
;  ai    aj    ak    al funct
    2   12   13   44    1   gd_40
   11   12   13   44    1   gd_40
   11   17   18   44    1   gd_40
   11   17   18   46    1   gd_40
   12   13   44   18    1   gd_10
   12   13   44   45    1   gd_10
   13   44   18   17    1   gd_10
   13   44   18   46    1   gd_10
   13   44   45   48    1   gd_10
   13   44   45   49    1   gd_10
   16   17   18   44    1   gd_40
   16   17   18   46    1   gd_40
   17   18   44   45    1   gd_10
   17   18   46   47    1   gd_10
   18   44   45   48    1   gd_10
   18   44   45   49    1   gd_10
   18   46   47   48    1   gd_10
   20   22   23   37    1   gd_40
   21   22   23   37    1   gd_40
   21   27   28   40    1   gd_40
   22   23   37   38    1   gd_10
   23   37   38   39    1   gd_10
   26   27   28   40    1   gd_40
   26   30   33   40    1   gd_40
```

26	30	33	43	1	gd_40
27	28	40	33	1	gd_10
28	40	33	30	1	gd_10
28	40	33	43	1	gd_10
30	31	36	41	1	gd_40
30	33	43	41	1	gd_10
31	30	33	40	1	gd_40
31	30	33	43	1	gd_40
31	36	41	42	1	gd_10
31	36	41	43	1	gd_10
32	31	36	41	1	gd_40
33	43	41	36	1	gd_10
33	43	41	42	1	gd_10
37	38	39	50	1	gd_29
37	38	39	51	1	gd_29
38	39	51	52	1	gd_12
40	33	43	41	1	gd_10
44	18	46	47	1	gd_10
44	45	48	47	1	gd_10
45	44	18	46	1	gd_10
45	48	47	46	1	gd_10
47	48	45	49	1	gd_10
50	39	51	52	1	gd_12
1	2	6	9	2	gi_1
2	1	3	12	2	gi_1
3	2	4	8	2	gi_1
4	3	5	7	2	gi_1
6	1	5	24	2	gi_1
9	1	10	20	2	gi_1
10	9	11	14	2	gi_1
11	10	12	17	2	gi_1
12	2	11	13	2	gi_1
14	10	15	21	2	gi_1
15	14	16	25	2	gi_1
16	15	17	19	2	gi_1
17	11	16	18	2	gi_1
18	17	44	46	2	gi_2
20	9	22	24	2	gi_1
21	14	22	27	2	gi_1
22	20	21	23	2	gi_1
25	15	26	29	2	gi_1
26	25	27	30	2	gi_1
27	21	26	28	2	gi_1
29	25	32	34	2	gi_1
30	26	31	33	2	gi_1
31	30	32	36	2	gi_1
32	29	31	35	2	gi_1
33	30	40	43	2	gi_2
39	38	50	51	2	gi_1
41	36	42	43	2	gi_2
44	13	18	45	2	gi_2
45	44	48	49	2	gi_2
1	2	3	4	2	gi_1
1	2	12	11	2	gi_1

1	6	5	4	2	gi_1
1	6	24	20	2	gi_1
1	9	10	11	2	gi_1
1	9	10	14	2	gi_4
1	9	20	22	2	gi_4
1	9	20	24	2	gi_1
2	1	6	5	2	gi_1
2	1	6	24	2	gi_4
2	1	9	10	2	gi_1
2	1	9	20	2	gi_4
2	3	4	5	2	gi_1
2	12	11	10	2	gi_1
2	12	11	17	2	gi_4
3	2	1	6	2	gi_1
3	2	1	9	2	gi_4
3	2	12	11	2	gi_4
3	4	5	6	2	gi_1
4	3	2	12	2	gi_4
4	5	6	24	2	gi_4
5	6	1	9	2	gi_4
5	6	24	20	2	gi_4
6	1	2	12	2	gi_4
6	1	9	10	2	gi_4
6	1	9	20	2	gi_1
6	24	20	9	2	gi_1
6	24	20	22	2	gi_4
9	1	2	12	2	gi_1
9	1	6	24	2	gi_1
9	10	11	12	2	gi_1
9	10	11	17	2	gi_4
9	10	14	15	2	gi_4
9	10	14	21	2	gi_1
9	20	22	21	2	gi_1
10	9	20	22	2	gi_1
10	9	20	24	2	gi_4
10	11	17	16	2	gi_1
10	14	15	16	2	gi_1
10	14	15	25	2	gi_4
10	14	21	22	2	gi_1
10	14	21	27	2	gi_4
11	10	9	20	2	gi_4
11	10	14	15	2	gi_1
11	10	14	21	2	gi_4
11	17	16	15	2	gi_1
12	11	10	14	2	gi_4
12	11	17	16	2	gi_4
14	10	9	20	2	gi_1
14	10	11	17	2	gi_1
14	15	16	17	2	gi_1
14	15	25	26	2	gi_1
14	15	25	29	2	gi_4
14	21	22	20	2	gi_1
14	21	27	26	2	gi_1
15	14	21	22	2	gi_4

```
   15   14   21   27    2   gi_1
   15   25   26   27    2   gi_1
   15   25   26   30    2   gi_4
   15   25   29   32    2   gi_4
   16   15   14   21    2   gi_4
   16   15   25   26    2   gi_4
   16   15   25   29    2   gi_1
   17   16   15   25    2   gi_4
   20   22   21   27    2   gi_4
   21   14   15   25    2   gi_1
   21   22   20   24    2   gi_4
   21   27   26   25    2   gi_1
   21   27   26   30    2   gi_4
   22   21   27   26    2   gi_4
   25   26   30   31    2   gi_1
   25   29   32   31    2   gi_1
   26   25   29   32    2   gi_1
   26   30   31   32    2   gi_1
   27   26   25   29    2   gi_4
   27   26   30   31    2   gi_4
   29   25   26   30    2   gi_1
   29   32   31   30    2   gi_1

[ pairs ]
;  ai    aj funct
   13   46   1
   13   48   1
   13   49   1
   18   48   1
   18   49   1
   23   39   1
   28   43   1
   33   36   1
   33   42   1
   37   50   1
   37   51   1
   38   52   1
   40   41   1
   44   47   1
   45   46   1
   47   49   1
   50   52   1
```

```
; This topology was generated by module mkitp in python
; Created by Orlando Villegas - 2019
; mail: orlando.villegas@univ-pau.fr
;------------------------------------------------------------
; Formula: C44H48
; MM: 576.868
; DBE: 21
; M. Dipolar: 1.685
; Forcefield gromos54a7


[ moleculetype ]
; name  nrexcl
A20     3

[ atoms ]
;   nr     type  resnr  residu    atom    cgnr  charge     mass
     1      CH3    1     A20       C    1  -0.111  15.035
     2      CH2    1     A20       C    1   0.133  14.027
     3      CH2    1     A20       C    1   0.013  14.027
     4      CH2    1     A20       C    1  -0.083  14.027
     5      CH2    1     A20       C    1   0.081  14.027
     6      CH2    1     A20       C    1  -0.023  14.027
     7      CH2    1     A20       C    1  -0.024  14.027
     8      CH2    1     A20       C    1   0.126  14.027
     9      CR1    1     A20       C    1  -0.320  12.011
    10      CR1    1     A20       C    1   0.235  12.011
    11      CR1    1     A20       C    1  -0.248  12.011
    12       HC    1     A20       H    1   0.182   1.008
    13      CR1    1     A20       C    1  -0.281  12.011
    14       HC    1     A20       H    1   0.159   1.008
    15      CR1    1     A20       C    1   0.181  12.011
    16      CR1    1     A20       C    1  -0.060  12.011
    17      CR1    1     A20       C    1   0.019  12.011
    18      CR1    1     A20       C    1  -0.221  12.011
    19      CR1    1     A20       C    1  -0.130  12.011
    20       HC    1     A20       H    1   0.130   1.008
    21      CR1    1     A20       C    1  -0.284  12.011
    22       HC    1     A20       H    1   0.154   1.008
    23      CR1    1     A20       C    1   0.225  12.011
    24      CH2    1     A20       C    1  -0.198  14.027
    25      CH1    1     A20       C    1   0.425  13.019
    26      CH3    1     A20       C    1  -0.149  15.035
    27      CH2    1     A20       C    1  -0.219  14.027
    28      CH1    1     A20       C    1   0.345  13.019
    29      CH2    1     A20       C    1  -0.168  14.027
    30      CH2    1     A20       C    1   0.179  14.027
    31      CR1    1     A20       C    1   0.026  12.011
    32      CR1    1     A20       C    1  -0.101  12.011
    33      CR1    1     A20       C    1  -0.017  12.011
    34      CR1    1     A20       C    1  -0.055  12.011
```

```
    35      CR1    1     A20       C    1  -0.046  12.011
    36      CR1    1     A20       C    1  -0.025  12.011
    37      CR1    1     A20       C    1   0.230  12.011
    38      CR1    1     A20       C    1  -0.320  12.011
    39       HC    1     A20       H    1   0.181   1.008
    40      CR1    1     A20       C    1  -0.087  12.011
    41       HC    1     A20       H    1   0.124   1.008
    42      CR1    1     A20       C    1  -0.264  12.011
    43       HC    1     A20       H    1   0.146   1.008
    44      CR1    1     A20       C    1   0.087  12.011
    45      CH2    1     A20       C    1   0.054  14.027
    46      CR1    1     A20       C    1   0.085  12.011
    47      CR1    1     A20       C    1  -0.093  12.011
    48      CH2    1     A20       C    1  -0.023  14.027
    49      CH2    1     A20       C    1   0.008  14.027
    50      CH2    1     A20       C    1   0.118  14.027
    51      CH3    1     A20       C    1  -0.096  15.035

[ bonds ]
;  ai    aj funct
    1    2    2 gb_27
    2    3    2 gb_27
    3    4    2 gb_27
    4    5    2 gb_27
    5    6    2 gb_27
    6    7    2 gb_27
    7    8    2 gb_27
    8    9    2 gb_27
    9   10    2 gb_16
    9   37    2 gb_16
   10   11    2 gb_16
   10   34    2 gb_16
   11   12    2  gb_3
   11   13    2 gb_16
   13   14    2  gb_3
   13   15    2 gb_16
   15   16    2 gb_16
   15   33    2 gb_16
   16   17    2 gb_16
   16   19    2 gb_16
   17   18    2 gb_16
   17   31    2 gb_16
   18   23    2 gb_16
   18   28    2  gb_3
   19   20    2  gb_3
   19   21    2 gb_16
   21   22    2  gb_3
   21   23    2 gb_16
   23   24    2 gb_27
   24   25    2 gb_27
   25   26    2 gb_27
   25   27    2 gb_27
   27   28    2 gb_27
   28   29    2 gb_27
```

```
   29   30    2 gb_27
   30   31    2 gb_27
   31   32    2 gb_16
   32   33    2 gb_16
   32   47    2 gb_16
   33   34    2 gb_16
   34   35    2 gb_16
   35   36    2 gb_16
   35   46    2 gb_16
   36   37    2 gb_16
   36   44    2 gb_16
   37   38    2 gb_16
   38   39    2  gb_3
   38   40    2 gb_16
   40   41    2  gb_3
   40   42    2 gb_16
   42   43    2  gb_3
   42   44    2 gb_16
   44   45    2 gb_27
   45   46    2 gb_27
   46   47    2 gb_16
   47   48    2 gb_27
   48   49    2 gb_27
   49   50    2 gb_27
   50   51    2 gb_27

[ angles ]
;  ai    aj    ak funct
    1    2    3    2   ga_15
    2    3    4    2   ga_15
    3    4    5    2   ga_15
    4    5    6    2   ga_15
    5    6    7    2   ga_15
    6    7    8    2   ga_15
    7    8    9    2   ga_15
    8    9   10    2   ga_15
    8    9   37    2   ga_15
    9   10   11    2   ga_27
    9   10   34    2   ga_27
    9   37   36    2   ga_27
    9   37   38    2   ga_27
   10    9   37    2   ga_27
   10   11   12    2   ga_25
   10   11   13    2   ga_27
   10   34   33    2   ga_27
   10   34   35    2   ga_27
   11   10   34    2   ga_27
   11   13   14    2   ga_25
   11   13   15    2   ga_27
   12   11   13    2   ga_25
   13   15   16    2   ga_27
   13   15   33    2   ga_27
   14   13   15    2   ga_25
   15   16   17    2   ga_27
```

```
15   16   19    2   ga_27
15   33   32    2   ga_27
15   33   34    2   ga_27
16   15   33    2   ga_27
16   17   18    2   ga_27
16   17   31    2   ga_27
16   19   20    2   ga_25
16   19   21    2   ga_27
17   16   19    2   ga_27
17   18   23    2   ga_27
17   18   28    2   ga_25
17   31   30    2   ga_15
17   31   32    2   ga_27
18   17   31    2   ga_27
18   23   21    2   ga_27
18   23   24    2   ga_15
18   28   27    2   ga_15
18   28   29    2   ga_15
19   21   22    2   ga_25
19   21   23    2   ga_27
20   19   21    2   ga_25
21   23   24    2   ga_15
22   21   23    2   ga_25
23   18   28    2   ga_25
23   24   25    2   ga_15
24   25   26    2   ga_15
24   25   27    2   ga_15
25   27   28    2   ga_15
26   25   27    2   ga_15
27   28   29    2   ga_15
28   29   30    2   ga_15
29   30   31    2   ga_15
30   31   32    2   ga_15
31   32   33    2   ga_27
31   32   47    2   ga_27
32   33   34    2   ga_27
32   47   46    2   ga_27
32   47   48    2   ga_15
33   32   47    2   ga_27
33   34   35    2   ga_27
34   35   36    2   ga_27
34   35   46    2   ga_27
35   36   37    2   ga_27
35   36   44    2   ga_27
35   46   45    2   ga_15
35   46   47    2   ga_27
36   35   46    2   ga_27
36   37   38    2   ga_27
36   44   42    2   ga_27
36   44   45    2   ga_15
37   36   44    2   ga_27
37   38   39    2   ga_25
37   38   40    2   ga_27
38   40   41    2   ga_25
```

```
   38   40   42    2   ga_27
   39   38   40    2   ga_25
   40   42   43    2   ga_25
   40   42   44    2   ga_27
   41   40   42    2   ga_25
   42   44   45    2   ga_15
   43   42   44    2   ga_25
   44   45   46    2   ga_15
   45   46   47    2   ga_15
   46   47   48    2   ga_15
   47   48   49    2   ga_15
   48   49   50    2   ga_15
   49   50   51    2   ga_15

[ dihedrals ]
;  ai    aj    ak    al funct
    1    2    3    4    1   gd_10
    2    3    4    5    1   gd_10
    3    4    5    6    1   gd_10
    4    5    6    7    1   gd_10
    5    6    7    8    1   gd_10
    6    7    8    9    1   gd_10
    7    8    9   10    1   gd_40
    7    8    9   37    1   gd_40
   17   18   28   27    1   gd_40
   17   18   28   29    1   gd_40
   17   31   30   29    1   gd_40
   18   23   24   25    1   gd_40
   18   28   27   25    1   gd_10
   18   28   29   30    1   gd_10
   21   23   24   25    1   gd_40
   23   18   28   27    1   gd_40
   23   18   28   29    1   gd_40
   23   24   25   26    1   gd_10
   23   24   25   27    1   gd_10
   24   25   27   28    1   gd_10
   25   27   28   29    1   gd_10
   26   25   27   28    1   gd_10
   27   28   29   30    1   gd_10
   28   29   30   31    1   gd_10
   29   30   31   32    1   gd_40
   32   47   48   49    1   gd_40
   35   46   45   44    1   gd_40
   36   44   45   46    1   gd_40
   42   44   45   46    1   gd_40
   44   45   46   47    1   gd_40
   46   47   48   49    1   gd_40
   47   48   49   50    1   gd_10
   48   49   50   51    1   gd_10
    9    8   10   37    2   gi_1
   10    9   11   34    2   gi_1
   11   10   12   13    2   gi_1
   13   11   14   15    2   gi_1
   15   13   16   33    2   gi_1
```

```
16   15   17   19    2   gi_1
17   16   18   31    2   gi_1
18   17   23   28    2   gi_1
19   16   20   21    2   gi_1
21   19   22   23    2   gi_1
23   18   21   24    2   gi_1
25   24   26   27    2   gi_2
28   18   27   29    2   gi_2
31   17   30   32    2   gi_1
32   31   33   47    2   gi_1
33   15   32   34    2   gi_1
34   10   33   35    2   gi_1
35   34   36   46    2   gi_1
36   35   37   44    2   gi_1
37    9   36   38    2   gi_1
38   37   39   40    2   gi_1
40   38   41   42    2   gi_1
42   40   43   44    2   gi_1
44   36   42   45    2   gi_1
46   35   45   47    2   gi_1
47   32   46   48    2   gi_1
 9   10   11   13    2   gi_4
 9   10   34   33    2   gi_4
 9   10   34   35    2   gi_1
 9   37   36   35    2   gi_1
 9   37   36   44    2   gi_4
 9   37   38   40    2   gi_4
10    9   37   36    2   gi_1
10    9   37   38    2   gi_4
10   11   13   15    2   gi_1
10   34   33   15    2   gi_1
10   34   33   32    2   gi_4
10   34   35   36    2   gi_1
10   34   35   46    2   gi_4
11   10    9   37    2   gi_4
11   10   34   33    2   gi_1
11   10   34   35    2   gi_4
11   13   15   16    2   gi_4
11   13   15   33    2   gi_1
13   11   10   34    2   gi_1
13   15   16   17    2   gi_4
13   15   16   19    2   gi_1
13   15   33   32    2   gi_4
13   15   33   34    2   gi_1
15   16   17   18    2   gi_4
15   16   17   31    2   gi_1
15   16   19   21    2   gi_4
15   33   32   31    2   gi_1
15   33   32   47    2   gi_4
15   33   34   35    2   gi_4
16   15   33   32    2   gi_1
16   15   33   34    2   gi_4
16   17   18   23    2   gi_1
16   17   31   32    2   gi_1
```

```
   16   19   21   23    2   gi_1
   17   16   15   33    2   gi_1
   17   16   19   21    2   gi_1
   17   18   23   21    2   gi_1
   17   31   32   33    2   gi_1
   17   31   32   47    2   gi_4
   18   17   16   19    2   gi_1
   18   17   31   32    2   gi_4
   18   23   21   19    2   gi_1
   19   16   15   33    2   gi_4
   19   16   17   31    2   gi_4
   23   18   17   31    2   gi_4
   31   32   33   34    2   gi_4
   31   32   47   46    2   gi_4
   32   33   34   35    2   gi_1
   32   47   46   35    2   gi_1
   33   32   47   46    2   gi_1
   33   34   35   36    2   gi_4
   33   34   35   46    2   gi_1
   34   10    9   37    2   gi_1
   34   33   32   47    2   gi_1
   34   35   36   37    2   gi_1
   34   35   36   44    2   gi_4
   34   35   46   47    2   gi_1
   35   36   37   38    2   gi_4
   35   36   44   42    2   gi_4
   36   35   46   47    2   gi_4
   36   37   38   40    2   gi_1
   36   44   42   40    2   gi_1
   37   36   35   46    2   gi_4
   37   36   44   42    2   gi_1
   37   38   40   42    2   gi_1
   38   37   36   44    2   gi_1
   38   40   42   44    2   gi_1
   44   36   35   46    2   gi_1

[ pairs ]
;  ai    aj funct
    1    4   1
    2    5   1
    3    6   1
    4    7   1
    5    8   1
   24   28   1
   25   29   1
   26   28   1
   27   30   1
   48   51   1
```

```
; This topology was generated by module mkitp in python
; Created by Orlando Villegas - 2019
; mail: orlando.villegas@univ-pau.fr
;------------------------------------------------------------
; Formula: C42H45NS
; MM: 595.902
; DBE: 21
; M. Dipolar: 5.271
; Forcefield gromos54a7

#define gb_53        0.1710  3.4601e+06
#define ga_55        108.00      415.80

[ moleculetype ]
; name  nrexcl
A21     3

[ atoms ]
;   nr     type  resnr  residu    atom    cgnr  charge     mass
     1      CR1    1     A21       C    1  -0.530  12.011
     2      CR1    1     A21       C    1   0.617  12.011
     3      CR1    1     A21       C    1  -0.616  12.011
     4      CR1    1     A21       C    1   0.321  12.011
     5       NR    1     A21       N    1  -0.640  14.010
     6      CR1    1     A21       C    1   0.700  12.011
     7       HC    1     A21       H    1   0.067   1.008
     8       HC    1     A21       H    1   0.223   1.008
     9      CR1    1     A21       C    1   0.396  12.011
    10      CR1    1     A21       C    1  -0.294  12.011
    11      CR1    1     A21       C    1   0.374  12.011
    12      CR1    1     A21       C    1  -0.518  12.011
    13      CH2    1     A21       C    1   0.183  14.027
    14      CR1    1     A21       C    1   0.184  12.011
    15      CR1    1     A21       C    1   0.088  12.011
    16      CR1    1     A21       C    1  -0.245  12.011
    17      CR1    1     A21       C    1  -0.266  12.011
    18       HC    1     A21       H    1   0.155   1.008
    19      CR1    1     A21       C    1  -0.309  12.011
    20      CR1    1     A21       C    1  -0.405  12.011
    21      CR1    1     A21       C    1   0.400  12.011
    22      CH2    1     A21       C    1  -0.150  14.027
    23        S    1     A21       S    1  -0.203  32.070
    24      CR1    1     A21       C    1   0.005  12.011
    25      CR1    1     A21       C    1  -0.020  12.011
    26      CR1    1     A21       C    1   0.167  12.011
    27      CH2    1     A21       C    1   0.148  14.027
    28      CR1    1     A21       C    1  -0.178  12.011
    29      CR1    1     A21       C    1  -0.207  12.011
    30      CR1    1     A21       C    1   0.200  12.011
    31      CR1    1     A21       C    1  -0.244  12.011
    32      CH1    1     A21       C    1   0.312  13.019
```

```
    33       HC    1     A21       H    1   0.144   1.008
    34       HC    1     A21       H    1   0.149   1.008
    35      CH2    1     A21       C    1  -0.168  14.027
    36      CH2    1     A21       C    1   0.058  14.027
    37      CH2    1     A21       C    1   0.121  14.027
    38      CH3    1     A21       C    1  -0.094  15.035
    39      CH2    1     A21       C    1  -0.149  14.027
    40      CH1    1     A21       C    1   0.414  13.019
    41      CH3    1     A21       C    1  -0.151  15.035
    42      CH2    1     A21       C    1  -0.201  14.027
    43       HC    1     A21       H    1   0.188   1.008
    44      CH2    1     A21       C    1  -0.046  14.027
    45      CH2    1     A21       C    1  -0.025  14.027
    46      CH2    1     A21       C    1   0.101  14.027
    47      CH2    1     A21       C    1  -0.096  14.027
    48      CH2    1     A21       C    1   0.018  14.027
    49      CH2    1     A21       C    1   0.133  14.027
    50      CH3    1     A21       C    1  -0.111  15.035

[ bonds ]
;  ai    aj funct
    1    2    2 gb_16
    1    6    2 gb_16
    1    9    2 gb_16
    2    3    2 gb_16
    2   12    2 gb_16
    3    4    2 gb_16
    3    8    2  gb_3
    4    5    2  gb_7
    4    7    2  gb_3
    5    6    2  gb_7
    6   23    2 gb_53
    9   10    2 gb_16
    9   19    2 gb_16
   10   11    2 gb_16
   10   14    2 gb_16
   11   12    2 gb_16
   11   17    2 gb_16
   12   13    2 gb_27
   13   44    2 gb_27
   14   15    2 gb_16
   14   20    2 gb_16
   15   16    2 gb_16
   15   24    2 gb_16
   16   17    2 gb_16
   16   18    2  gb_3
   17   43    2  gb_3
   19   21    2 gb_16
   19   23    2 gb_53
   20   21    2 gb_16
   20   26    2 gb_16
   21   22    2 gb_27
   22   36    2 gb_27
   24   25    2 gb_16
```

```
   24   28    2 gb_16
   25   26    2 gb_16
   25   29    2 gb_16
   26   27    2 gb_27
   27   39    2 gb_27
   28   31    2 gb_16
   28   33    2  gb_3
   29   30    2 gb_16
   29   32    2  gb_3
   30   31    2 gb_16
   30   35    2 gb_27
   31   34    2  gb_3
   32   39    2 gb_27
   32   42    2 gb_27
   35   40    2 gb_27
   36   37    2 gb_27
   37   38    2 gb_27
   40   41    2 gb_27
   40   42    2 gb_27
   44   45    2 gb_27
   45   46    2 gb_27
   46   47    2 gb_27
   47   48    2 gb_27
   48   49    2 gb_27
   49   50    2 gb_27

[ angles ]
;  ai    aj    ak funct
    1    2    3    2   ga_27
    1    2   12    2   ga_27
    1    6    5    2   ga_27
    1    6   23    2   ga_7
    1    9   10    2   ga_27
    1    9   19    2   ga_27
    2    1    6    2   ga_27
    2    1    9    2   ga_27
    2    3    4    2   ga_27
    2    3    8    2   ga_25
    2   12   11    2   ga_27
    2   12   13    2   ga_15
    3    2   12    2   ga_27
    3    4    5    2   ga_27
    3    4    7    2   ga_25
    4    3    8    2   ga_25
    4    5    6    2   ga_15
    5    4    7    2   ga_25
    5    6   23    2   ga_39
    6    1    9    2   ga_27
    6   23   19    2   ga_55
    9   10   11    2   ga_27
    9   10   14    2   ga_27
    9   19   21    2   ga_27
    9   19   23    2   ga_7
   10    9   19    2   ga_27
```

10	11	12	2	ga_27
10	11	17	2	ga_27
10	14	15	2	ga_27
10	14	20	2	ga_27
11	10	14	2	ga_27
11	12	13	2	ga_15
11	17	16	2	ga_27
11	17	43	2	ga_25
12	11	17	2	ga_27
12	13	44	2	ga_15
13	44	45	2	ga_15
14	15	16	2	ga_27
14	15	24	2	ga_27
14	20	21	2	ga_27
14	20	26	2	ga_27
15	14	20	2	ga_27
15	16	17	2	ga_27
15	16	18	2	ga_25
15	24	25	2	ga_27
15	24	28	2	ga_27
16	15	24	2	ga_27
16	17	43	2	ga_25
17	16	18	2	ga_25
19	21	20	2	ga_27
19	21	22	2	ga_15
20	21	22	2	ga_15
20	26	25	2	ga_27
20	26	27	2	ga_15
21	19	23	2	ga_7
21	20	26	2	ga_27
21	22	36	2	ga_15
22	36	37	2	ga_15
24	25	26	2	ga_27
24	25	29	2	ga_27
24	28	31	2	ga_27
24	28	33	2	ga_25
25	24	28	2	ga_27
25	26	27	2	ga_15
25	29	30	2	ga_27
25	29	32	2	ga_25
26	25	29	2	ga_27
26	27	39	2	ga_15
27	39	32	2	ga_15
28	31	30	2	ga_27
28	31	34	2	ga_25
29	30	31	2	ga_27
29	30	35	2	ga_15
29	32	39	2	ga_15
29	32	42	2	ga_15
30	29	32	2	ga_25
30	31	34	2	ga_25
30	35	40	2	ga_15
31	28	33	2	ga_25
31	30	35	2	ga_15

```
   32   42   40    2   ga_15
   35   40   41    2   ga_15
   35   40   42    2   ga_15
   36   37   38    2   ga_15
   39   32   42    2   ga_15
   41   40   42    2   ga_15
   44   45   46    2   ga_15
   45   46   47    2   ga_15
   46   47   48    2   ga_15
   47   48   49    2   ga_15
   48   49   50    2   ga_15

[ dihedrals ]
;  ai    aj    ak    al funct
    2   12   13   44    1   gd_40
   11   12   13   44    1   gd_40
   12   13   44   45    1   gd_10
   13   44   45   46    1   gd_10
   19   21   22   36    1   gd_40
   20   21   22   36    1   gd_40
   20   26   27   39    1   gd_40
   21   22   36   37    1   gd_10
   22   36   37   38    1   gd_10
   25   26   27   39    1   gd_40
   25   29   32   39    1   gd_40
   25   29   32   42    1   gd_40
   26   27   39   32    1   gd_10
   27   39   32   29    1   gd_10
   27   39   32   42    1   gd_10
   29   30   35   40    1   gd_40
   29   32   42   40    1   gd_10
   30   29   32   39    1   gd_40
   30   29   32   42    1   gd_40
   30   35   40   41    1   gd_10
   30   35   40   42    1   gd_10
   31   30   35   40    1   gd_40
   32   42   40   35    1   gd_10
   32   42   40   41    1   gd_10
   39   32   42   40    1   gd_10
   44   45   46   47    1   gd_10
   45   46   47   48    1   gd_10
   46   47   48   49    1   gd_10
   47   48   49   50    1   gd_10
    1    2    6    9    2   gi_1
    2    1    3   12    2   gi_1
    3    2    4    8    2   gi_1
    4    3    5    7    2   gi_1
    6    1    5   23    2   gi_1
    9    1   10   19    2   gi_1
   10    9   11   14    2   gi_1
   11   10   12   17    2   gi_1
   12    2   11   13    2   gi_1
   14   10   15   20    2   gi_1
   15   14   16   24    2   gi_1
```

16	15	17	18	2	gi_1
17	11	16	43	2	gi_1
19	9	21	23	2	gi_1
20	14	21	26	2	gi_1
21	19	20	22	2	gi_1
24	15	25	28	2	gi_1
25	24	26	29	2	gi_1
26	20	25	27	2	gi_1
28	24	31	33	2	gi_1
29	25	30	32	2	gi_1
30	29	31	35	2	gi_1
31	28	30	34	2	gi_1
32	29	39	42	2	gi_2
40	35	41	42	2	gi_2
1	2	3	4	2	gi_1
1	2	12	11	2	gi_1
1	6	5	4	2	gi_1
1	6	23	19	2	gi_1
1	9	10	11	2	gi_1
1	9	10	14	2	gi_4
1	9	19	21	2	gi_4
1	9	19	23	2	gi_1
2	1	6	5	2	gi_1
2	1	6	23	2	gi_4
2	1	9	10	2	gi_1
2	1	9	19	2	gi_4
2	3	4	5	2	gi_1
2	12	11	10	2	gi_1
2	12	11	17	2	gi_4
3	2	1	6	2	gi_1
3	2	1	9	2	gi_4
3	2	12	11	2	gi_4
3	4	5	6	2	gi_1
4	3	2	12	2	gi_4
4	5	6	23	2	gi_4
5	6	1	9	2	gi_4
5	6	23	19	2	gi_4
6	1	2	12	2	gi_4
6	1	9	10	2	gi_4
6	1	9	19	2	gi_1
6	23	19	9	2	gi_1
6	23	19	21	2	gi_4
9	1	2	12	2	gi_1
9	1	6	23	2	gi_1
9	10	11	12	2	gi_1
9	10	11	17	2	gi_4
9	10	14	15	2	gi_4
9	10	14	20	2	gi_1
9	19	21	20	2	gi_1
10	9	19	21	2	gi_1
10	9	19	23	2	gi_4
10	11	17	16	2	gi_1
10	14	15	16	2	gi_1
10	14	15	24	2	gi_4

```
   10   14   20   21    2   gi_1
   10   14   20   26    2   gi_4
   11   10    9   19    2   gi_4
   11   10   14   15    2   gi_1
   11   10   14   20    2   gi_4
   11   17   16   15    2   gi_1
   12   11   10   14    2   gi_4
   12   11   17   16    2   gi_4
   14   10    9   19    2   gi_1
   14   10   11   17    2   gi_1
   14   15   16   17    2   gi_1
   14   15   24   25    2   gi_1
   14   15   24   28    2   gi_4
   14   20   21   19    2   gi_1
   14   20   26   25    2   gi_1
   15   14   20   21    2   gi_4
   15   14   20   26    2   gi_1
   15   24   25   26    2   gi_1
   15   24   25   29    2   gi_4
   15   24   28   31    2   gi_4
   16   15   14   20    2   gi_4
   16   15   24   25    2   gi_4
   16   15   24   28    2   gi_1
   17   16   15   24    2   gi_4
   19   21   20   26    2   gi_4
   20   14   15   24    2   gi_1
   20   21   19   23    2   gi_4
   20   26   25   24    2   gi_1
   20   26   25   29    2   gi_4
   21   20   26   25    2   gi_4
   24   25   29   30    2   gi_1
   24   28   31   30    2   gi_1
   25   24   28   31    2   gi_1
   25   29   30   31    2   gi_1
   26   25   24   28    2   gi_4
   26   25   29   30    2   gi_4
   28   24   25   29    2   gi_1
   28   31   30   29    2   gi_1

[ pairs ]
;  ai    aj funct
   13   46   1
   22   38   1
   27   42   1
   32   35   1
   32   41   1
   39   40   1
   44   47   1
   45   48   1
   46   49   1
   47   50   1
```

```
; This topology was generated by module mkitp in python
; Created by Orlando Villegas - 2019
; mail: orlando.villegas@univ-pau.fr
;------------------------------------------------------------
; Formula: C42H45NOS
; MM: 611.902
; DBE: 21
; M. Dipolar: 5.196
; Forcefield gromos54a7

#define gb_53        0.1710  3.4601e+06
#define ga_55        108.00      415.80

[ moleculetype ]
; name  nrexcl
A22     3

[ atoms ]
;   nr     type  resnr  residu    atom    cgnr  charge     mass
     1      CR1    1     A22       C    1  -0.566  12.011
     2      CR1    1     A22       C    1   0.634  12.011
     3      CR1    1     A22       C    1  -0.625  12.011
     4      CR1    1     A22       C    1   0.330  12.011
     5       NR    1     A22       N    1  -0.650  14.010
     6      CR1    1     A22       C    1   0.718  12.011
     7       HC    1     A22       H    1   0.066   1.008
     8       HC    1     A22       H    1   0.223   1.008
     9      CR1    1     A22       C    1   0.479  12.011
    10      CR1    1     A22       C    1  -0.350  12.011
    11      CR1    1     A22       C    1   0.417  12.011
    12      CR1    1     A22       C    1  -0.549  12.011
    13      CH2    1     A22       C    1   0.196  14.027
    14      CR1    1     A22       C    1   0.161  12.011
    15      CR1    1     A22       C    1   0.147  12.011
    16      CR1    1     A22       C    1  -0.211  12.011
    17      CR1    1     A22       C    1  -0.317  12.011
    18       HC    1     A22       H    1   0.146   1.008
    19      CR1    1     A22       C    1  -0.382  12.011
    20      CR1    1     A22       C    1  -0.385  12.011
    21      CR1    1     A22       C    1   0.438  12.011
    22      CH2    1     A22       C    1  -0.156  14.027
    23        S    1     A22       S    1  -0.201  32.070
    24      CR1    1     A22       C    1  -0.005  12.011
    25      CR1    1     A22       C    1  -0.027  12.011
    26      CR1    1     A22       C    1   0.132  12.011
    27      CH2    1     A22       C    1   0.170  14.027
    28      CR1    1     A22       C    1  -0.442  12.011
    29      CR1    1     A22       C    1  -0.207  12.011
    30      CR1    1     A22       C    1   0.017  12.011
    31      CR1    1     A22       C    1   0.422  12.011
    32      CH1    1     A22       C    1   0.360  13.019
```

```
    33       HC    1     A22       H    1   0.170   1.008
    34      CH2    1     A22       C    1  -0.064  14.027
    35      CH2    1     A22       C    1   0.059  14.027
    36      CH2    1     A22       C    1   0.128  14.027
    37      CH3    1     A22       C    1  -0.098  15.035
    38      CH2    1     A22       C    1  -0.169  14.027
    39      CH1    1     A22       C    1   0.375  13.019
    40      CH3    1     A22       C    1  -0.150  15.035
    41      CH2    1     A22       C    1  -0.203  14.027
    42       HC    1     A22       H    1   0.195   1.008
    43      CH2    1     A22       C    1  -0.046  14.027
    44      CH2    1     A22       C    1  -0.036  14.027
    45      CH2    1     A22       C    1   0.117  14.027
    46      CH2    1     A22       C    1  -0.106  14.027
    47      CH2    1     A22       C    1   0.022  14.027
    48      CH2    1     A22       C    1   0.134  14.027
    49      CH3    1     A22       C    1  -0.113  15.035
    50       OA    1     A22       O    1  -0.645  16.000
    51        H    1     A22       H    1   0.447   1.008

[ bonds ]
;  ai    aj funct
    1    2    2 gb_16
    1    6    2 gb_16
    1    9    2 gb_16
    2    3    2 gb_16
    2   12    2 gb_16
    3    4    2 gb_16
    3    8    2  gb_3
    4    5    2  gb_7
    4    7    2  gb_3
    5    6    2  gb_7
    6   23    2 gb_53
    9   10    2 gb_16
    9   19    2 gb_16
   10   11    2 gb_16
   10   14    2 gb_16
   11   12    2 gb_16
   11   17    2 gb_16
   12   13    2 gb_27
   13   43    2 gb_27
   14   15    2 gb_16
   14   20    2 gb_16
   15   16    2 gb_16
   15   24    2 gb_16
   16   17    2 gb_16
   16   18    2  gb_3
   17   42    2  gb_3
   19   21    2 gb_16
   19   23    2 gb_53
   20   21    2 gb_16
   20   26    2 gb_16
   21   22    2 gb_27
   22   35    2 gb_27
```

```
   24   25    2 gb_16
   24   28    2 gb_16
   25   26    2 gb_16
   25   29    2 gb_16
   26   27    2 gb_27
   27   38    2 gb_27
   28   31    2 gb_16
   28   33    2  gb_3
   29   30    2 gb_16
   29   32    2  gb_3
   30   31    2 gb_16
   30   34    2 gb_27
   31   50    2 gb_13
   32   38    2 gb_27
   32   41    2 gb_27
   34   39    2 gb_27
   35   36    2 gb_27
   36   37    2 gb_27
   39   40    2 gb_27
   39   41    2 gb_27
   43   44    2 gb_27
   44   45    2 gb_27
   45   46    2 gb_27
   46   47    2 gb_27
   47   48    2 gb_27
   48   49    2 gb_27
   50   51    2  gb_1

[ angles ]
;  ai    aj    ak funct
    1    2    3    2   ga_27
    1    2   12    2   ga_27
    1    6    5    2   ga_27
    1    6   23    2   ga_7
    1    9   10    2   ga_27
    1    9   19    2   ga_27
    2    1    6    2   ga_27
    2    1    9    2   ga_27
    2    3    4    2   ga_27
    2    3    8    2   ga_25
    2   12   11    2   ga_27
    2   12   13    2   ga_15
    3    2   12    2   ga_27
    3    4    5    2   ga_27
    3    4    7    2   ga_25
    4    3    8    2   ga_25
    4    5    6    2   ga_15
    5    4    7    2   ga_25
    5    6   23    2   ga_39
    6    1    9    2   ga_27
    6   23   19    2   ga_55
    9   10   11    2   ga_27
    9   10   14    2   ga_27
    9   19   21    2   ga_27
```

9	19	23	2	ga_7
10	9	19	2	ga_27
10	11	12	2	ga_27
10	11	17	2	ga_27
10	14	15	2	ga_27
10	14	20	2	ga_27
11	10	14	2	ga_27
11	12	13	2	ga_15
11	17	16	2	ga_27
11	17	42	2	ga_25
12	11	17	2	ga_27
12	13	43	2	ga_15
13	43	44	2	ga_15
14	15	16	2	ga_27
14	15	24	2	ga_27
14	20	21	2	ga_27
14	20	26	2	ga_27
15	14	20	2	ga_27
15	16	17	2	ga_27
15	16	18	2	ga_25
15	24	25	2	ga_27
15	24	28	2	ga_27
16	15	24	2	ga_27
16	17	42	2	ga_25
17	16	18	2	ga_25
19	21	20	2	ga_27
19	21	22	2	ga_15
20	21	22	2	ga_15
20	26	25	2	ga_27
20	26	27	2	ga_15
21	19	23	2	ga_7
21	20	26	2	ga_27
21	22	35	2	ga_15
22	35	36	2	ga_15
24	25	26	2	ga_27
24	25	29	2	ga_27
24	28	31	2	ga_27
24	28	33	2	ga_25
25	24	28	2	ga_27
25	26	27	2	ga_15
25	29	30	2	ga_27
25	29	32	2	ga_25
26	25	29	2	ga_27
26	27	38	2	ga_15
27	38	32	2	ga_15
28	31	30	2	ga_27
28	31	50	2	ga_25
29	30	31	2	ga_27
29	30	34	2	ga_15
29	32	38	2	ga_15
29	32	41	2	ga_15
30	29	32	2	ga_25
30	31	50	2	ga_25
30	34	39	2	ga_15

```
   31   28   33    2   ga_25
   31   30   34    2   ga_15
   31   50   51    2   ga_12
   32   41   39    2   ga_15
   34   39   40    2   ga_15
   34   39   41    2   ga_15
   35   36   37    2   ga_15
   38   32   41    2   ga_15
   40   39   41    2   ga_15
   43   44   45    2   ga_15
   44   45   46    2   ga_15
   45   46   47    2   ga_15
   46   47   48    2   ga_15
   47   48   49    2   ga_15

[ dihedrals ]
;  ai    aj    ak    al funct
    2   12   13   43    1   gd_40
   11   12   13   43    1   gd_40
   12   13   43   44    1   gd_10
   13   43   44   45    1   gd_10
   19   21   22   35    1   gd_40
   20   21   22   35    1   gd_40
   20   26   27   38    1   gd_40
   21   22   35   36    1   gd_10
   22   35   36   37    1   gd_10
   25   26   27   38    1   gd_40
   25   29   32   38    1   gd_40
   25   29   32   41    1   gd_40
   26   27   38   32    1   gd_10
   27   38   32   29    1   gd_10
   27   38   32   41    1   gd_10
   28   31   50   51    1   gd_23
   29   30   34   39    1   gd_40
   29   32   41   39    1   gd_10
   30   29   32   38    1   gd_40
   30   29   32   41    1   gd_40
   30   31   50   51    1   gd_23
   30   34   39   40    1   gd_10
   30   34   39   41    1   gd_10
   31   30   34   39    1   gd_40
   32   41   39   34    1   gd_10
   32   41   39   40    1   gd_10
   38   32   41   39    1   gd_10
   43   44   45   46    1   gd_10
   44   45   46   47    1   gd_10
   45   46   47   48    1   gd_10
   46   47   48   49    1   gd_10
    1    2    6    9    2   gi_1
    2    1    3   12    2   gi_1
    3    2    4    8    2   gi_1
    4    3    5    7    2   gi_1
    6    1    5   23    2   gi_1
    9    1   10   19    2   gi_1
```

10	9	11	14	2	gi_1
11	10	12	17	2	gi_1
12	2	11	13	2	gi_1
14	10	15	20	2	gi_1
15	14	16	24	2	gi_1
16	15	17	18	2	gi_1
17	11	16	42	2	gi_1
19	9	21	23	2	gi_1
20	14	21	26	2	gi_1
21	19	20	22	2	gi_1
24	15	25	28	2	gi_1
25	24	26	29	2	gi_1
26	20	25	27	2	gi_1
28	24	31	33	2	gi_1
29	25	30	32	2	gi_1
30	29	31	34	2	gi_1
31	28	30	50	2	gi_1
32	29	38	41	2	gi_2
39	34	40	41	2	gi_2
1	2	3	4	2	gi_1
1	2	12	11	2	gi_1
1	6	5	4	2	gi_1
1	6	23	19	2	gi_1
1	9	10	11	2	gi_1
1	9	10	14	2	gi_4
1	9	19	21	2	gi_4
1	9	19	23	2	gi_1
2	1	6	5	2	gi_1
2	1	6	23	2	gi_4
2	1	9	10	2	gi_1
2	1	9	19	2	gi_4
2	3	4	5	2	gi_1
2	12	11	10	2	gi_1
2	12	11	17	2	gi_4
3	2	1	6	2	gi_1
3	2	1	9	2	gi_4
3	2	12	11	2	gi_4
3	4	5	6	2	gi_1
4	3	2	12	2	gi_4
4	5	6	23	2	gi_4
5	6	1	9	2	gi_4
5	6	23	19	2	gi_4
6	1	2	12	2	gi_4
6	1	9	10	2	gi_4
6	1	9	19	2	gi_1
6	23	19	9	2	gi_1
6	23	19	21	2	gi_4
9	1	2	12	2	gi_1
9	1	6	23	2	gi_1
9	10	11	12	2	gi_1
9	10	11	17	2	gi_4
9	10	14	15	2	gi_4
9	10	14	20	2	gi_1
9	19	21	20	2	gi_1

```
   10    9   19   21    2   gi_1
   10    9   19   23    2   gi_4
   10   11   17   16    2   gi_1
   10   14   15   16    2   gi_1
   10   14   15   24    2   gi_4
   10   14   20   21    2   gi_1
   10   14   20   26    2   gi_4
   11   10    9   19    2   gi_4
   11   10   14   15    2   gi_1
   11   10   14   20    2   gi_4
   11   17   16   15    2   gi_1
   12   11   10   14    2   gi_4
   12   11   17   16    2   gi_4
   14   10    9   19    2   gi_1
   14   10   11   17    2   gi_1
   14   15   16   17    2   gi_1
   14   15   24   25    2   gi_1
   14   15   24   28    2   gi_4
   14   20   21   19    2   gi_1
   14   20   26   25    2   gi_1
   15   14   20   21    2   gi_4
   15   14   20   26    2   gi_1
   15   24   25   26    2   gi_1
   15   24   25   29    2   gi_4
   15   24   28   31    2   gi_4
   16   15   14   20    2   gi_4
   16   15   24   25    2   gi_4
   16   15   24   28    2   gi_1
   17   16   15   24    2   gi_4
   19   21   20   26    2   gi_4
   20   14   15   24    2   gi_1
   20   21   19   23    2   gi_4
   20   26   25   24    2   gi_1
   20   26   25   29    2   gi_4
   21   20   26   25    2   gi_4
   24   25   29   30    2   gi_1
   24   28   31   30    2   gi_1
   25   24   28   31    2   gi_1
   25   29   30   31    2   gi_1
   26   25   24   28    2   gi_4
   26   25   29   30    2   gi_4
   28   24   25   29    2   gi_1
   28   31   30   29    2   gi_1

[ pairs ]
;  ai    aj funct
   13   45   1
   22   37   1
   27   41   1
   32   34   1
   32   40   1
   38   39   1
   43   46   1
   44   47   1
```

```
45   48   1
46   49   1
```

```
; This topology was generated by module mkitp in python
; Created by Orlando Villegas - 2019
; mail: orlando.villegas@univ-pau.fr
;------------------------------------------------------------
; Formula: C42H43NO2S
; MM: 625.886
; DBE: 22
; M. Dipolar: 4.846
; Forcefield gromos54a7

#define gb_53        0.1710  3.4601e+06
#define ga_55        108.00      415.80

[ moleculetype ]
; name  nrexcl
A23     3

[ atoms ]
;   nr     type  resnr  residu    atom    cgnr  charge     mass
     1      CR1    1     A23       C    1  -0.426  12.011
     2      CR1    1     A23       C    1   0.567  12.011
     3      CR1    1     A23       C    1  -0.557  12.011
     4      CR1    1     A23       C    1   0.239  12.011
     5       NR    1     A23       N    1  -0.601  14.010
     6      CR1    1     A23       C    1   0.670  12.011
     7       HC    1     A23       H    1   0.090   1.008
     8       HC    1     A23       H    1   0.217   1.008
     9      CR1    1     A23       C    1   0.186  12.011
    10      CR1    1     A23       C    1  -0.094  12.011
    11      CR1    1     A23       C    1   0.297  12.011
    12      CR1    1     A23       C    1  -0.467  12.011
    13      CH2    1     A23       C    1   0.124  14.027
    14      CR1    1     A23       C    1   0.086  12.011
    15      CR1    1     A23       C    1   0.128  12.011
    16      CR1    1     A23       C    1  -0.272  12.011
    17      CR1    1     A23       C    1  -0.241  12.011
    18       HC    1     A23       H    1   0.157   1.008
    19      CR1    1     A23       C    1  -0.215  12.011
    20      CR1    1     A23       C    1  -0.403  12.011
    21      CR1    1     A23       C    1   0.360  12.011
    22      CH2    1     A23       C    1  -0.125  14.027
    23        S    1     A23       S    1  -0.213  32.070
    24      CR1    1     A23       C    1   0.026  12.011
    25      CR1    1     A23       C    1  -0.012  12.011
    26      CR1    1     A23       C    1   0.145  12.011
    27      CH2    1     A23       C    1   0.153  14.027
    28      CR1    1     A23       C    1  -0.214  12.011
    29      CR1    1     A23       C    1  -0.202  12.011
    30      CR1    1     A23       C    1   0.203  12.011
    31      CR1    1     A23       C    1  -0.227  12.011
    32      CH1    1     A23       C    1   0.313  13.019
```

```
    33       HC    1     A23       H    1   0.154   1.008
    34       HC    1     A23       H    1   0.146   1.008
    35      CH2    1     A23       C    1  -0.178  14.027
    36      CH2    1     A23       C    1   0.199  14.027
    37      CH2    1     A23       C    1  -0.098  14.027
    38        C    1     A23       C    1   0.748  12.011
    39      CH2    1     A23       C    1  -0.140  14.027
    40      CH1    1     A23       C    1   0.398  13.019
    41      CH3    1     A23       C    1  -0.142  15.035
    42      CH2    1     A23       C    1  -0.194  14.027
    43       HC    1     A23       H    1   0.186   1.008
    44      CH2    1     A23       C    1  -0.003  14.027
    45      CH2    1     A23       C    1  -0.025  14.027
    46      CH2    1     A23       C    1   0.069  14.027
    47      CH2    1     A23       C    1  -0.050  14.027
    48      CH2    1     A23       C    1  -0.019  14.027
    49      CH2    1     A23       C    1   0.144  14.027
    50      CH3    1     A23       C    1  -0.109  15.035
    51        O    1     A23       O    1  -0.583  16.000
    52       OA    1     A23       O    1  -0.635  16.000
    53        H    1     A23       H    1   0.440   1.008

[ bonds ]
;  ai    aj funct
    1    2    2 gb_16
    1    6    2 gb_16
    1    9    2 gb_16
    2    3    2 gb_16
    2   12    2 gb_16
    3    4    2 gb_16
    3    8    2  gb_3
    4    5    2  gb_7
    4    7    2  gb_3
    5    6    2  gb_7
    6   23    2 gb_53
    9   10    2 gb_16
    9   19    2 gb_16
   10   11    2 gb_16
   10   14    2 gb_16
   11   12    2 gb_16
   11   17    2 gb_16
   12   13    2 gb_27
   13   44    2 gb_27
   14   15    2 gb_16
   14   20    2 gb_16
   15   16    2 gb_16
   15   24    2 gb_16
   16   17    2 gb_16
   16   18    2  gb_3
   17   43    2  gb_3
   19   21    2 gb_16
   19   23    2 gb_53
   20   21    2 gb_16
   20   26    2 gb_16
```

```
   21   22    2 gb_27
   22   36    2 gb_27
   24   25    2 gb_16
   24   28    2 gb_16
   25   26    2 gb_16
   25   29    2 gb_16
   26   27    2 gb_27
   27   39    2 gb_27
   28   31    2 gb_16
   28   33    2  gb_3
   29   30    2 gb_16
   29   32    2  gb_3
   30   31    2 gb_16
   30   35    2 gb_27
   31   34    2  gb_3
   32   39    2 gb_27
   32   42    2 gb_27
   35   40    2 gb_27
   36   37    2 gb_27
   37   38    2 gb_27
   38   51    2  gb_5
   38   52    2 gb_13
   40   41    2 gb_27
   40   42    2 gb_27
   44   45    2 gb_27
   45   46    2 gb_27
   46   47    2 gb_27
   47   48    2 gb_27
   48   49    2 gb_27
   49   50    2 gb_27
   52   53    2  gb_1

[ angles ]
;  ai    aj    ak funct
    1    2    3    2   ga_27
    1    2   12    2   ga_27
    1    6    5    2   ga_27
    1    6   23    2   ga_7
    1    9   10    2   ga_27
    1    9   19    2   ga_27
    2    1    6    2   ga_27
    2    1    9    2   ga_27
    2    3    4    2   ga_27
    2    3    8    2   ga_25
    2   12   11    2   ga_27
    2   12   13    2   ga_15
    3    2   12    2   ga_27
    3    4    5    2   ga_27
    3    4    7    2   ga_25
    4    3    8    2   ga_25
    4    5    6    2   ga_15
    5    4    7    2   ga_25
    5    6   23    2   ga_39
    6    1    9    2   ga_27
```

6	23	19	2	ga_55
9	10	11	2	ga_27
9	10	14	2	ga_27
9	19	21	2	ga_27
9	19	23	2	ga_7
10	9	19	2	ga_27
10	11	12	2	ga_27
10	11	17	2	ga_27
10	14	15	2	ga_27
10	14	20	2	ga_27
11	10	14	2	ga_27
11	12	13	2	ga_15
11	17	16	2	ga_27
11	17	43	2	ga_25
12	11	17	2	ga_27
12	13	44	2	ga_15
13	44	45	2	ga_15
14	15	16	2	ga_27
14	15	24	2	ga_27
14	20	21	2	ga_27
14	20	26	2	ga_27
15	14	20	2	ga_27
15	16	17	2	ga_27
15	16	18	2	ga_25
15	24	25	2	ga_27
15	24	28	2	ga_27
16	15	24	2	ga_27
16	17	43	2	ga_25
17	16	18	2	ga_25
19	21	20	2	ga_27
19	21	22	2	ga_15
20	21	22	2	ga_15
20	26	25	2	ga_27
20	26	27	2	ga_15
21	19	23	2	ga_7
21	20	26	2	ga_27
21	22	36	2	ga_15
22	36	37	2	ga_15
24	25	26	2	ga_27
24	25	29	2	ga_27
24	28	31	2	ga_27
24	28	33	2	ga_25
25	24	28	2	ga_27
25	26	27	2	ga_15
25	29	30	2	ga_27
25	29	32	2	ga_25
26	25	29	2	ga_27
26	27	39	2	ga_15
27	39	32	2	ga_15
28	31	30	2	ga_27
28	31	34	2	ga_25
29	30	31	2	ga_27
29	30	35	2	ga_15
29	32	39	2	ga_15

```
   29   32   42    2   ga_15
   30   29   32    2   ga_25
   30   31   34    2   ga_25
   30   35   40    2   ga_15
   31   28   33    2   ga_25
   31   30   35    2   ga_15
   32   42   40    2   ga_15
   35   40   41    2   ga_15
   35   40   42    2   ga_15
   36   37   38    2   ga_15
   37   38   51    2   ga_30
   37   38   52    2   ga_19
   38   52   53    2   ga_12
   39   32   42    2   ga_15
   41   40   42    2   ga_15
   44   45   46    2   ga_15
   45   46   47    2   ga_15
   46   47   48    2   ga_15
   47   48   49    2   ga_15
   48   49   50    2   ga_15
   51   38   52    2   ga_33

[ dihedrals ]
;  ai    aj    ak    al funct
    2   12   13   44    1   gd_40
   11   12   13   44    1   gd_40
   12   13   44   45    1   gd_10
   13   44   45   46    1   gd_10
   19   21   22   36    1   gd_40
   20   21   22   36    1   gd_40
   20   26   27   39    1   gd_40
   21   22   36   37    1   gd_10
   22   36   37   38    1   gd_10
   25   26   27   39    1   gd_40
   25   29   32   39    1   gd_40
   25   29   32   42    1   gd_40
   26   27   39   32    1   gd_10
   27   39   32   29    1   gd_10
   27   39   32   42    1   gd_10
   29   30   35   40    1   gd_40
   29   32   42   40    1   gd_10
   30   29   32   39    1   gd_40
   30   29   32   42    1   gd_40
   30   35   40   41    1   gd_10
   30   35   40   42    1   gd_10
   31   30   35   40    1   gd_40
   32   42   40   35    1   gd_10
   32   42   40   41    1   gd_10
   36   37   38   51    1   gd_29
   36   37   38   52    1   gd_29
   37   38   52   53    1   gd_12
   39   32   42   40    1   gd_10
   44   45   46   47    1   gd_10
   45   46   47   48    1   gd_10
```

46	47	48	49	1	gd_10
47	48	49	50	1	gd_10
51	38	52	53	1	gd_12
1	2	6	9	2	gi_1
2	1	3	12	2	gi_1
3	2	4	8	2	gi_1
4	3	5	7	2	gi_1
6	1	5	23	2	gi_1
9	1	10	19	2	gi_1
10	9	11	14	2	gi_1
11	10	12	17	2	gi_1
12	2	11	13	2	gi_1
14	10	15	20	2	gi_1
15	14	16	24	2	gi_1
16	15	17	18	2	gi_1
17	11	16	43	2	gi_1
19	9	21	23	2	gi_1
20	14	21	26	2	gi_1
21	19	20	22	2	gi_1
24	15	25	28	2	gi_1
25	24	26	29	2	gi_1
26	20	25	27	2	gi_1
28	24	31	33	2	gi_1
29	25	30	32	2	gi_1
30	29	31	35	2	gi_1
31	28	30	34	2	gi_1
32	29	39	42	2	gi_2
38	37	51	52	2	gi_1
40	35	41	42	2	gi_2
1	2	3	4	2	gi_1
1	2	12	11	2	gi_1
1	6	5	4	2	gi_1
1	6	23	19	2	gi_1
1	9	10	11	2	gi_1
1	9	10	14	2	gi_4
1	9	19	21	2	gi_4
1	9	19	23	2	gi_1
2	1	6	5	2	gi_1
2	1	6	23	2	gi_4
2	1	9	10	2	gi_1
2	1	9	19	2	gi_4
2	3	4	5	2	gi_1
2	12	11	10	2	gi_1
2	12	11	17	2	gi_4
3	2	1	6	2	gi_1
3	2	1	9	2	gi_4
3	2	12	11	2	gi_4
3	4	5	6	2	gi_1
4	3	2	12	2	gi_4
4	5	6	23	2	gi_4
5	6	1	9	2	gi_4
5	6	23	19	2	gi_4
6	1	2	12	2	gi_4
6	1	9	10	2	gi_4

6	1	9	19	2	gi_1
6	23	19	9	2	gi_1
6	23	19	21	2	gi_4
9	1	2	12	2	gi_1
9	1	6	23	2	gi_1
9	10	11	12	2	gi_1
9	10	11	17	2	gi_4
9	10	14	15	2	gi_4
9	10	14	20	2	gi_1
9	19	21	20	2	gi_1
10	9	19	21	2	gi_1
10	9	19	23	2	gi_4
10	11	17	16	2	gi_1
10	14	15	16	2	gi_1
10	14	15	24	2	gi_4
10	14	20	21	2	gi_1
10	14	20	26	2	gi_4
11	10	9	19	2	gi_4
11	10	14	15	2	gi_1
11	10	14	20	2	gi_4
11	17	16	15	2	gi_1
12	11	10	14	2	gi_4
12	11	17	16	2	gi_4
14	10	9	19	2	gi_1
14	10	11	17	2	gi_1
14	15	16	17	2	gi_1
14	15	24	25	2	gi_1
14	15	24	28	2	gi_4
14	20	21	19	2	gi_1
14	20	26	25	2	gi_1
15	14	20	21	2	gi_4
15	14	20	26	2	gi_1
15	24	25	26	2	gi_1
15	24	25	29	2	gi_4
15	24	28	31	2	gi_4
16	15	14	20	2	gi_4
16	15	24	25	2	gi_4
16	15	24	28	2	gi_1
17	16	15	24	2	gi_4
19	21	20	26	2	gi_4
20	14	15	24	2	gi_1
20	21	19	23	2	gi_4
20	26	25	24	2	gi_1
20	26	25	29	2	gi_4
21	20	26	25	2	gi_4
24	25	29	30	2	gi_1
24	28	31	30	2	gi_1
25	24	28	31	2	gi_1
25	29	30	31	2	gi_1
26	25	24	28	2	gi_4
26	25	29	30	2	gi_4
28	24	25	29	2	gi_1
28	31	30	29	2	gi_1

```
[ pairs ]
;  ai    aj funct
   13   46   1
   22   38   1
   27   42   1
   32   35   1
   32   41   1
   36   51   1
   36   52   1
   37   53   1
   39   40   1
   44   47   1
   45   48   1
   46   49   1
   47   50   1
   51   53   1
```

Toluene

```
; This topology was generated by module mkitp in python
; Created by Orlando Villegas - 2020
; mail: orlando.villegas@univ-pau.fr
;------------------------------------------------------------
; Formula: C7H8
; MM: 92.141
; DBE: 4
; M. Dipolar: 0.737
; Forcefield Gromos 54a7


[ moleculetype ]
; name  nrexcl
TOL     3

[ atoms ]
;   nr     type  resnr  residu    atom    cgnr  charge     mass
     1        C    1     TOL       C    1  -0.140  12.011
     2        C    1     TOL       C    2  -0.140  12.011
     3        C    1     TOL       C    3  -0.140  12.011
     4        C    1     TOL       C    4  -0.140  12.011
     5        C    1     TOL       C    5  -0.140  12.011
     6        C    1     TOL       C    6   0.000  12.011
     7      CH3    1     TOL       C    7   0.000  15.035
     8       HC    1     TOL       H    8   0.140   1.008
     9       HC    1     TOL       H    9   0.140   1.008
    10       HC    1     TOL       H   10   0.140   1.008
    11       HC    1     TOL       H   11   0.140   1.008
    12       HC    1     TOL       H   12   0.140   1.008

[ bonds ]
;  ai    aj    ak funct
    1    2    2     gb_16
    1    6    2     gb_16
    1    8    2      gb_3
    2    3    2     gb_16
    2    9    2      gb_3
    3    4    2     gb_16
    3   10    2      gb_3
    4    5    2     gb_16
    4   11    2      gb_3
    5    6    2     gb_16
    5   12    2      gb_3
    6    7    2     gb_27

[ angles ]
;  ai    aj    ak funct
    1    2    3    2     ga_27
    1    2    9    2     ga_25
    1    6    5    2     ga_27
    1    6    7    2     ga_25
```

```
    2    1    6    2     ga_27
    2    1    8    2     ga_25
    2    3    4    2     ga_27
    2    3   10    2     ga_25
    3    2    9    2     ga_25
    3    4    5    2     ga_27
    3    4   11    2     ga_25
    4    3   10    2     ga_25
    4    5    6    2     ga_27
    4    5   12    2     ga_25
    5    4   11    2     ga_25
    5    6    7    2     ga_25
    6    1    8    2     ga_25
    6    5   12    2     ga_25

[ dihedrals ]
;  ai    aj    ak    al funct
    1    2    6    8    2      gi_1
    2    1    3    9    2      gi_1
    3    2    4   10    2      gi_1
    4    3    5   11    2      gi_1
    5    4    6   12    2      gi_1
    6    1    5    7    2      gi_1
    1    2    3    4    2      gi_1
    1    6    5    4    2      gi_1
    2    1    6    5    2      gi_1
    2    3    4    5    2      gi_1
    3    2    1    6    2      gi_1
    3    4    5    6    2      gi_1
```
