Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Content

1. Gromacs topologies with all force field parameters used
2. Coordinates in Gromacs format (*.gro)

Attention: The topologies built with the amb2gmx.pl script. All parameters all from GAFF. The membrane was modeled with the Slipids force field (available for free at http://people.su.se/~jjm, where you also can find coordinates for pre-equilibrated lipid bilayers).

1. Gromacs topologies

1,3,5 trichlorobenzene (gas phase charges)

```
[ moleculetype ]
; Name            nrexcl
135trichlorobenzene 3

[ atoms ]
;   nr       type  resnr residue  atom   cgnr     charge       mass  typeB    chargeB
     1         ca      1     LIG     C1      1    0.1646  12.000000
     2         ha      1     LIG     H2      2    0.1044   1.000000
     3         ca      1     LIG     C3      3   -0.2043  12.000000
     4         ca      1     LIG     C4      4    0.1646  12.000000
     5         ha      1     LIG     H5      5    0.1044   1.000000
     6         ca      1     LIG     C6      6   -0.2043  12.000000
     7         ca      1     LIG     C7      7    0.1646  12.000000
     8         ha      1     LIG     H8      8    0.1044   1.000000
     9         ca      1     LIG     C9      9   -0.2043  12.000000
    10         cl      1     LIG   CL1     10   -0.0647  35.500000
    11         cl      1     LIG   CL2     11   -0.0647  35.500000
    12         cl      1     LIG   CL3     12   -0.0647  35.500000

[ bonds ]
;  ai    aj funct  r  k
    1     2     1  1.0870e-01  2.8811e+05
    4     5     1  1.0870e-01  2.8811e+05
    7     8     1  1.0870e-01  2.8811e+05
    1     3     1  1.3870e-01  4.0033e+05
    1     9     1  1.3870e-01  4.0033e+05
    3     4     1  1.3870e-01  4.0033e+05
    3    12     1  1.7290e-01  2.7012e+05
    4     6     1  1.3870e-01  4.0033e+05
    6     7     1  1.3870e-01  4.0033e+05
    6    11     1  1.7290e-01  2.7012e+05
    7     9     1  1.3870e-01  4.0033e+05
    9    10     1  1.7290e-01  2.7012e+05

[ pairs ]
;  ai    aj funct
     1     5      1
     1     8      1
     2     4      1
     2    12      1
     2     7      1
     2    10      1
     4     8      1
     5    12      1
     5     7      1
     5    11      1
     8    11      1
     8    10      1
     1     6      1
     3     7      1
     3    10      1
     3    11      1
     9     4      1
     6    12      1
     6    10      1
     9    12      1
     9    11      1

[ angles ]
;  ai    aj    ak funct  theta   cth
    2     1     3     1  1.2001e+02  4.0551e+02
    2     1     9     1  1.2001e+02  4.0551e+02
    3     4     5     1  1.2001e+02  4.0551e+02
    5     4     6     1  1.2001e+02  4.0551e+02
    6     7     8     1  1.2001e+02  4.0551e+02
    8     7     9     1  1.2001e+02  4.0551e+02
    1     3     4     1  1.1997e+02  5.6216e+02
    1     3    12     1  1.1940e+02  5.2651e+02
    1     9     7     1  1.1997e+02  5.6216e+02
    1     9    10     1  1.1940e+02  5.2651e+02
    3     1     9     1  1.1997e+02  5.6216e+02
    3     4     6     1  1.1997e+02  5.6216e+02
    4     3    12     1  1.1940e+02  5.2651e+02
    4     6     7     1  1.1997e+02  5.6216e+02
    4     6    11     1  1.1940e+02  5.2651e+02
    6     7     9     1  1.1997e+02  5.6216e+02
    7     6    11     1  1.1940e+02  5.2651e+02
    7     9    10     1  1.1940e+02  5.2651e+02

[ dihedrals ]
;i  j   k  l      func    C0  ...  C5
    1    3    4    5      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    1    9    7    8      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
```

```
    2    1    3    4      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    2    1    3    12     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    2    1    9    7      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    2    1    9    10     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    4    6    7    8      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    5    4    3    12     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    5    4    6    7      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    5    4    6    11     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    8    7    6    11     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    8    7    9    10     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    2    1    9    3      3     9.20480     0.00000    -9.20480     0.00000     0.00000     0.00000  ;
    3    6    4    5      3     9.20480     0.00000    -9.20480     0.00000     0.00000     0.00000  ;
    6    9    7    8      3     9.20480     0.00000    -9.20480     0.00000     0.00000     0.00000  ;
    1    3    4    6      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    1    9    7    6      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    3    1    9    7      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    3    1    9    10     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    3    4    6    7      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    3    4    6    11     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    9    1    3    4      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    4    6    7    9      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    6    4    3    12     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    6    7    9    10     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    9    1    3    12     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    9    7    6    11     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    1    4    3    12     3     9.20480     0.00000    -9.20480     0.00000     0.00000     0.00000  ;
    4    7    6    11     3     9.20480     0.00000    -9.20480     0.00000     0.00000     0.00000  ;
    1    7    9    10     3     9.20480     0.00000    -9.20480     0.00000     0.00000     0.00000  ;

end----------------------------------------------------------------------------------------------------------------------------
```

1,3,5 trichlorobenzene (polarized charges, water)

```
[ moleculetype ]
; Name            nrexcl
135trichlorobenzene 3

[ atoms ]
;   nr       type  resnr residue  atom   cgnr     charge       mass  typeB    chargeB
     1         ca      1      LIG     C1      1    0.16220  12.000000
     2         ha      1      LIG     H2      2    0.11750   1.000000
     3         ca      1      LIG     C3      3   -0.20170  12.000000
     4         ca      1      LIG     C4      4    0.16220  12.000000
     5         ha      1      LIG     H5      5    0.11750   1.000000
     6         ca      1      LIG     C6      6   -0.20170  12.000000
     7         ca      1      LIG     C7      7    0.16220  12.000000
     8         ha      1      LIG     H8      8    0.11750   1.000000
     9         ca      1      LIG     C9      9   -0.20170  12.000000
    10         cl      1      LIG    CL1     10   -0.07800  35.500000
    11         cl      1      LIG    CL2     11   -0.07800  35.500000
    12         cl      1      LIG    CL3     12   -0.07800  35.500000

[ bonds ]
;  ai    aj funct  r  k
    1     2     1  1.0870e-01  2.8811e+05
    4     5     1  1.0870e-01  2.8811e+05
    7     8     1  1.0870e-01  2.8811e+05
    1     3     1  1.3870e-01  4.0033e+05
    1     9     1  1.3870e-01  4.0033e+05
    3     4     1  1.3870e-01  4.0033e+05
    3    12     1  1.7290e-01  2.7012e+05
    4     6     1  1.3870e-01  4.0033e+05
    6     7     1  1.3870e-01  4.0033e+05
    6    11     1  1.7290e-01  2.7012e+05
    7     9     1  1.3870e-01  4.0033e+05
    9    10     1  1.7290e-01  2.7012e+05

[ pairs ]
;  ai    aj funct
     1     5      1
     1     8      1
     2     4      1
     2    12      1
     2     7      1
     2    10      1
     4     8      1
     5    12      1
     5     7      1
     5    11      1
     8    11      1
     8    10      1
     1     6      1
     3     7      1
     3    10      1
     3    11      1
     9     4      1
     6    12      1
     6    10      1
     9    12      1
     9    11      1
```

```
[ angles ]
;  ai    aj    ak funct   theta   cth
    2     1     3     1  1.2001e+02  4.0551e+02
    2     1     9     1  1.2001e+02  4.0551e+02
    3     4     5     1  1.2001e+02  4.0551e+02
    5     4     6     1  1.2001e+02  4.0551e+02
    6     7     8     1  1.2001e+02  4.0551e+02
    8     7     9     1  1.2001e+02  4.0551e+02
    1     3     4     1  1.1997e+02  5.6216e+02
    1     3    12     1  1.1940e+02  5.2651e+02
    1     9     7     1  1.1997e+02  5.6216e+02
    1     9    10     1  1.1940e+02  5.2651e+02
    3     1     9     1  1.1997e+02  5.6216e+02
    3     4     6     1  1.1997e+02  5.6216e+02
    4     3    12     1  1.1940e+02  5.2651e+02
    4     6     7     1  1.1997e+02  5.6216e+02
    4     6    11     1  1.1940e+02  5.2651e+02
    6     7     9     1  1.1997e+02  5.6216e+02
    7     6    11     1  1.1940e+02  5.2651e+02
    7     9    10     1  1.1940e+02  5.2651e+02

[ dihedrals ]
;i  j   k  l      func    C0  ...  C5
    1    3    4    5      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    1    9    7    8      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    2    1    3    4      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    2    1    3   12      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    2    1    9    7      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    2    1    9   10      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    4    6    7    8      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    5    4    3   12      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    5    4    6    7      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    5    4    6   11      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    8    7    6   11      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    8    7    9   10      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    2    1    9    3      3     9.20480     0.00000    -9.20480     0.00000     0.00000     0.00000  ;
    3    6    4    5      3     9.20480     0.00000    -9.20480     0.00000     0.00000     0.00000  ;
    6    9    7    8      3     9.20480     0.00000    -9.20480     0.00000     0.00000     0.00000  ;
    1    3    4    6      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    1    9    7    6      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    3    1    9    7      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    3    1    9   10      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    3    4    6    7      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    3    4    6   11      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    9    1    3    4      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    4    6    7    9      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    6    4    3   12      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    6    7    9   10      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    9    1    3   12      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    9    7    6   11      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    1    4    3   12      3     9.20480     0.00000    -9.20480     0.00000     0.00000     0.00000  ;
    4    7    6   11      3     9.20480     0.00000    -9.20480     0.00000     0.00000     0.00000  ;
    1    7    9   10      3     9.20480     0.00000    -9.20480     0.00000     0.00000     0.00000  ;

end----------------------------------------------------------------------------------------------------------------------------
```

1,3,5 trichlorobenzene (polarized charges, hexadecane)

```
[ moleculetype ]
; Name            nrexcl
C1X               3

[ atoms ]
;   nr       type  resnr residue  atom   cgnr     charge       mass  typeB    chargeB
     1         ca      1      LIG     C1      1     0.1634  12.000000
     2         ha      1      LIG     H2      2     0.1099   1.000000
     3         ca      1      LIG     C3      3    -0.2028  12.000000
     4         ca      1      LIG     C4      4     0.1634  12.000000
     5         ha      1      LIG     H5      5     0.1099   1.000000
     6         ca      1      LIG     C6      6    -0.2028  12.000000
     7         ca      1      LIG     C7      7     0.1634  12.000000
     8         ha      1      LIG     H8      8     0.1099   1.000000
     9         ca      1      LIG     C9      9    -0.2028  12.000000
    10         cl      1      LIG    CL1     10    -0.0705  35.500000
    11         cl      1      LIG    CL2     11    -0.0705  35.500000
    12         cl      1      LIG    CL3     12    -0.0705  35.500000

[ bonds ]
;  ai    aj funct  r  k
    1     2     1  1.0870e-01  2.8811e+05
    4     5     1  1.0870e-01  2.8811e+05
    7     8     1  1.0870e-01  2.8811e+05
    1     3     1  1.3870e-01  4.0033e+05
    1     9     1  1.3870e-01  4.0033e+05
    3     4     1  1.3870e-01  4.0033e+05
    3    12     1  1.7290e-01  2.7012e+05
    4     6     1  1.3870e-01  4.0033e+05
    6     7     1  1.3870e-01  4.0033e+05
    6    11     1  1.7290e-01  2.7012e+05
    7     9     1  1.3870e-01  4.0033e+05
    9    10     1  1.7290e-01  2.7012e+05
```

```
[ pairs ]
;  ai    aj funct
     1     5      1
     1     8      1
     2     4      1
     2    12      1
     2     7      1
     2    10      1
     4     8      1
     5    12      1
     5     7      1
     5    11      1
     8    11      1
     8    10      1
     1     6      1
     3     7      1
     3    10      1
     3    11      1
     9     4      1
     6    12      1
     6    10      1
     9    12      1
     9    11      1

[ angles ]
;  ai    aj    ak funct  theta   cth
    2     1     3     1  1.2001e+02  4.0551e+02
    2     1     9     1  1.2001e+02  4.0551e+02
    3     4     5     1  1.2001e+02  4.0551e+02
    5     4     6     1  1.2001e+02  4.0551e+02
    6     7     8     1  1.2001e+02  4.0551e+02
    8     7     9     1  1.2001e+02  4.0551e+02
    1     3     4     1  1.1997e+02  5.6216e+02
    1     3    12     1  1.1940e+02  5.2651e+02
    1     9     7     1  1.1997e+02  5.6216e+02
    1     9    10     1  1.1940e+02  5.2651e+02
    3     1     9     1  1.1997e+02  5.6216e+02
    3     4     6     1  1.1997e+02  5.6216e+02
    4     3    12     1  1.1940e+02  5.2651e+02
    4     6     7     1  1.1997e+02  5.6216e+02
    4     6    11     1  1.1940e+02  5.2651e+02
    6     7     9     1  1.1997e+02  5.6216e+02
    7     6    11     1  1.1940e+02  5.2651e+02
    7     9    10     1  1.1940e+02  5.2651e+02

[ dihedrals ]
;i  j   k  l      func    C0  ...  C5
    1    3    4    5      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    1    9    7    8      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    2    1    3    4      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    2    1    3    12     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    2    1    9    7      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    2    1    9    10     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    4    6    7    8      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    5    4    3    12     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    5    4    6    7      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    5    4    6    11     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    8    7    6    11     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    8    7    9    10     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    2    1    9    3      3     9.20480     0.00000    -9.20480     0.00000     0.00000     0.00000  ;
    3    6    4    5      3     9.20480     0.00000    -9.20480     0.00000     0.00000     0.00000  ;
    6    9    7    8      3     9.20480     0.00000    -9.20480     0.00000     0.00000     0.00000  ;
    1    3    4    6      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    1    9    7    6      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    3    1    9    7      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    3    1    9    10     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    3    4    6    7      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    3    4    6    11     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    9    1    3    4      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    4    6    7    9      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    6    4    3    12     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    6    7    9    10     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    9    1    3    12     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    9    7    6    11     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    1    4    3    12     3     9.20480     0.00000    -9.20480     0.00000     0.00000     0.00000  ;
    4    7    6    11     3     9.20480     0.00000    -9.20480     0.00000     0.00000     0.00000  ;
    1    7    9    10     3     9.20480     0.00000    -9.20480     0.00000     0.00000     0.00000  ;

end----------------------------------------------------------------------------------------------------------------------
```

Chlorobenzene (gas phase charges)

```
[ moleculetype ]
; Name            nrexcl
Chlorobenzene     3

[ atoms ]
;   nr       type  resnr residue  atom   cgnr     charge       mass  typeB    chargeB
     1         ca      1    LIG      C      1   -0.0781  12.000000
     2         ha      1    LIG      H      2    0.1266   1.000000
     3         ca      1    LIG     C1      3   -0.1503  12.000000
     4         ha      1    LIG     H1      4    0.1454   1.000000
     5         ca      1    LIG     C2      5   -0.1519  12.000000
     6         ha      1    LIG     H2      6    0.1464   1.000000
     7         ca      1    LIG     C3      7   -0.1519  12.000000
     8         ha      1    LIG     H3      8    0.1464   1.000000
     9         ca      1    LIG     C4      9   -0.0781  12.000000
    10         ha      1    LIG     H4     10    0.1266   1.000000
    11         ca      1    LIG     C5     11    0.0489  12.000000
    12         cl      1    LIG     CL     12   -0.1300  35.500000

[ bonds ]
;  ai    aj funct  r  k
    1     2     1  1.0870e-01  2.8811e+05
    3     4     1  1.0870e-01  2.8811e+05
    5     6     1  1.0870e-01  2.8811e+05
    7     8     1  1.0870e-01  2.8811e+05
    9    10     1  1.0870e-01  2.8811e+05
    1     3     1  1.3870e-01  4.0033e+05
    1    11     1  1.3870e-01  4.0033e+05
    3     5     1  1.3870e-01  4.0033e+05
    5     7     1  1.3870e-01  4.0033e+05
    7     9     1  1.3870e-01  4.0033e+05
    9    11     1  1.3870e-01  4.0033e+05
   11    12     1  1.7290e-01  2.7012e+05

[ pairs ]
;  ai    aj funct
     1     6      1
     1    10      1
     2     4      1
     2     5      1
     2     9      1
     2    12      1
     3     8      1
    11     4      1
     4     6      1
     4     7      1
     5    10      1
     6     8      1
     6     9      1
     8    10      1
     8    11      1
    10    12      1
     1     7      1
     3     9      1
     3    12      1
    11     5      1
     7    12      1

[ angles ]
;  ai    aj    ak funct  theta   cth
    1     3     4     1  1.2001e+02  4.0551e+02
    2     1     3     1  1.2001e+02  4.0551e+02
    2     1    11     1  1.2001e+02  4.0551e+02
    3     5     6     1  1.2001e+02  4.0551e+02
    4     3     5     1  1.2001e+02  4.0551e+02
    5     7     8     1  1.2001e+02  4.0551e+02
    6     5     7     1  1.2001e+02  4.0551e+02
    7     9    10     1  1.2001e+02  4.0551e+02
    8     7     9     1  1.2001e+02  4.0551e+02
   10     9    11     1  1.2001e+02  4.0551e+02
    1     3     5     1  1.1997e+02  5.6216e+02
    1    11     9     1  1.1997e+02  5.6216e+02
    1    11    12     1  1.1940e+02  5.2651e+02
    3     1    11     1  1.1997e+02  5.6216e+02
    3     5     7     1  1.1997e+02  5.6216e+02
    5     7     9     1  1.1997e+02  5.6216e+02
    7     9    11     1  1.1997e+02  5.6216e+02
    9    11    12     1  1.1940e+02  5.2651e+02

[ dihedrals ]
;i  j   k  l      func    C0  ...  C5
    1    3    5    6      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    1   11    9   10      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    2    1    3    4      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    2    1    3    5      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    2    1   11    9      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    2    1   11   12      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    3    5    7    8      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
   11    1    3    4      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
```

```
    4    3    5    6      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    4    3    5    7      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    5    7    9   10      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    6    5    7    8      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    6    5    7    9      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    8    7    9   10      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    8    7    9   11      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
   10    9   11   12      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    2    1   11    3      3     9.20480     0.00000    -9.20480     0.00000     0.00000     0.00000  ;
    1    5    3    4      3     9.20480     0.00000    -9.20480     0.00000     0.00000     0.00000  ;
    3    7    5    6      3     9.20480     0.00000    -9.20480     0.00000     0.00000     0.00000  ;
    5    9    7    8      3     9.20480     0.00000    -9.20480     0.00000     0.00000     0.00000  ;
    7   11    9   10      3     9.20480     0.00000    -9.20480     0.00000     0.00000     0.00000  ;
    1    3    5    7      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    1   11    9    7      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    3    1   11    9      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    3    1   11   12      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    3    5    7    9      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
   11    1    3    5      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    5    7    9   11      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    7    9   11   12      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    1    9   11   12      3     9.20480     0.00000    -9.20480     0.00000     0.00000     0.00000  ;

end----------------------------------------------------------------------------------------------------------------------------
```

Chlorobenzene (polarized charges, water)

```
[ moleculetype ]
; Name            nrexcl
Chlorobenzene     3

[ atoms ]
;   nr       type  resnr residue  atom   cgnr     charge       mass  typeB    chargeB
     1         ca      1    LIG      C      1   -0.09190  12.000000
     2         ha      1    LIG      H      2    0.14220   1.000000
     3         ca      1    LIG     C1      3   -0.16130  12.000000
     4         ha      1    LIG     H1      4    0.16390   1.000000
     5         ca      1    LIG     C2      5   -0.16260  12.000000
     6         ha      1    LIG     H2      6    0.16490   1.000000
     7         ca      1    LIG     C3      7   -0.16260  12.000000
     8         ha      1    LIG     H3      8    0.16470   1.000000
     9         ca      1    LIG     C4      9   -0.09190  12.000000
    10         ha      1    LIG     H4     10    0.14220   1.000000
    11         ca      1    LIG     C5     11    0.04540  12.000000
    12         cl      1    LIG     CL     12   -0.15300  35.500000

[ bonds ]
;  ai    aj funct  r  k
    1     2     1  1.0870e-01  2.8811e+05
    3     4     1  1.0870e-01  2.8811e+05
    5     6     1  1.0870e-01  2.8811e+05
    7     8     1  1.0870e-01  2.8811e+05
    9    10     1  1.0870e-01  2.8811e+05
    1     3     1  1.3870e-01  4.0033e+05
    1    11     1  1.3870e-01  4.0033e+05
    3     5     1  1.3870e-01  4.0033e+05
    5     7     1  1.3870e-01  4.0033e+05
    7     9     1  1.3870e-01  4.0033e+05
    9    11     1  1.3870e-01  4.0033e+05
   11    12     1  1.7290e-01  2.7012e+05

[ pairs ]
;  ai    aj funct
     1     6      1
     1    10      1
     2     4      1
     2     5      1
     2     9      1
     2    12      1
     3     8      1
    11     4      1
     4     6      1
     4     7      1
     5    10      1
     6     8      1
     6     9      1
     8    10      1
     8    11      1
    10    12      1
     1     7      1
     3     9      1
     3    12      1
    11     5      1
     7    12      1

[ angles ]
;  ai    aj    ak funct  theta   cth
    1     3     4     1  1.2001e+02  4.0551e+02
    2     1     3     1  1.2001e+02  4.0551e+02
    2     1    11     1  1.2001e+02  4.0551e+02
    3     5     6     1  1.2001e+02  4.0551e+02
```

```
    4     3     5     1  1.2001e+02  4.0551e+02
    5     7     8     1  1.2001e+02  4.0551e+02
    6     5     7     1  1.2001e+02  4.0551e+02
    7     9    10     1  1.2001e+02  4.0551e+02
    8     7     9     1  1.2001e+02  4.0551e+02
   10     9    11     1  1.2001e+02  4.0551e+02
    1     3     5     1  1.1997e+02  5.6216e+02
    1    11     9     1  1.1997e+02  5.6216e+02
    1    11    12     1  1.1940e+02  5.2651e+02
    3     1    11     1  1.1997e+02  5.6216e+02
    3     5     7     1  1.1997e+02  5.6216e+02
    5     7     9     1  1.1997e+02  5.6216e+02
    7     9    11     1  1.1997e+02  5.6216e+02
    9    11    12     1  1.1940e+02  5.2651e+02

[ dihedrals ]
;i   j    k   l      func    C0   ...   C5
    1    3    5    6      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    1   11    9   10      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    2    1    3    4      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    2    1    3    5      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    2    1   11    9      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    2    1   11   12      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    3    5    7    8      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
   11    1    3    4      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    4    3    5    6      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    4    3    5    7      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    5    7    9   10      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    6    5    7    8      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    6    5    7    9      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    8    7    9   10      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    8    7    9   11      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
   10    9   11   12      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    2    1   11    3      3     9.20480     0.00000    -9.20480     0.00000     0.00000     0.00000  ;
    1    5    3    4      3     9.20480     0.00000    -9.20480     0.00000     0.00000     0.00000  ;
    3    7    5    6      3     9.20480     0.00000    -9.20480     0.00000     0.00000     0.00000  ;
    5    9    7    8      3     9.20480     0.00000    -9.20480     0.00000     0.00000     0.00000  ;
    7   11    9   10      3     9.20480     0.00000    -9.20480     0.00000     0.00000     0.00000  ;
    1    3    5    7      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    1   11    9    7      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    3    1   11    9      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    3    1   11   12      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    3    5    7    9      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
   11    1    3    5      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    5    7    9   11      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    7    9   11   12      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    1    9   11   12      3     9.20480     0.00000    -9.20480     0.00000     0.00000     0.00000  ;

end----------------------------------------------------------------------------------------------------------------------------
```

Chlorobenzene (polarized charges, hexadecane)

```
[ moleculetype ]
; Name            nrexcl
Chlorobenzene     3

[ atoms ]
;   nr       type  resnr residue  atom   cgnr     charge       mass  typeB    chargeB
     1         ca      1    LIG      C      1   -0.0836  12.000000
     2         ha      1    LIG      H      2    0.1326   1.000000
     3         ca      1    LIG     C1      3   -0.1542  12.000000
     4         ha      1    LIG     H1      4    0.1521   1.000000
     5         ca      1    LIG     C2      5   -0.1556  12.000000
     6         ha      1    LIG     H2      6    0.1531   1.000000
     7         ca      1    LIG     C3      7   -0.1556  12.000000
     8         ha      1    LIG     H3      8    0.1531   1.000000
     9         ca      1    LIG     C4      9   -0.0836  12.000000
    10         ha      1    LIG     H4     10    0.1326   1.000000
    11         ca      1    LIG     C5     11    0.0499  12.000000
    12         cl      1    LIG     CL     12   -0.1408  35.500000

[ bonds ]
;  ai    aj funct  r  k
    1     2     1  1.0870e-01  2.8811e+05
    3     4     1  1.0870e-01  2.8811e+05
    5     6     1  1.0870e-01  2.8811e+05
    7     8     1  1.0870e-01  2.8811e+05
    9    10     1  1.0870e-01  2.8811e+05
    1     3     1  1.3870e-01  4.0033e+05
    1    11     1  1.3870e-01  4.0033e+05
    3     5     1  1.3870e-01  4.0033e+05
    5     7     1  1.3870e-01  4.0033e+05
    7     9     1  1.3870e-01  4.0033e+05
    9    11     1  1.3870e-01  4.0033e+05
   11    12     1  1.7290e-01  2.7012e+05

[ pairs ]
;  ai    aj funct
     1     6      1
     1    10      1
     2     4      1
```

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

[ angles ]
;  ai    aj    ak funct   theta   cth
    1     3     4     1  1.2001e+02  4.0551e+02
    2     1     3     1  1.2001e+02  4.0551e+02
    2     1    11     1  1.2001e+02  4.0551e+02
    3     5     6     1  1.2001e+02  4.0551e+02
    4     3     5     1  1.2001e+02  4.0551e+02
    5     7     8     1  1.2001e+02  4.0551e+02
    6     5     7     1  1.2001e+02  4.0551e+02
    7     9    10     1  1.2001e+02  4.0551e+02
    8     7     9     1  1.2001e+02  4.0551e+02
   10     9    11     1  1.2001e+02  4.0551e+02
    1     3     5     1  1.1997e+02  5.6216e+02
    1    11     9     1  1.1997e+02  5.6216e+02
    1    11    12     1  1.1940e+02  5.2651e+02
    3     1    11     1  1.1997e+02  5.6216e+02
    3     5     7     1  1.1997e+02  5.6216e+02
    5     7     9     1  1.1997e+02  5.6216e+02
    7     9    11     1  1.1997e+02  5.6216e+02
    9    11    12     1  1.1940e+02  5.2651e+02

[ dihedrals ]
;i  j   k  l      func    C0  ...  C5
    1    3    5    6      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    1   11    9   10      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    2    1    3    4      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    2    1    3    5      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    2    1   11    9      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    2    1   11   12      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    3    5    7    8      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
   11    1    3    4      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    4    3    5    6      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    4    3    5    7      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    5    7    9   10      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    6    5    7    8      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    6    5    7    9      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    8    7    9   10      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    8    7    9   11      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
   10    9   11   12      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    2    1   11    3      3     9.20480     0.00000    -9.20480     0.00000     0.00000     0.00000  ;
    1    5    3    4      3     9.20480     0.00000    -9.20480     0.00000     0.00000     0.00000  ;
    3    7    5    6      3     9.20480     0.00000    -9.20480     0.00000     0.00000     0.00000  ;
    5    9    7    8      3     9.20480     0.00000    -9.20480     0.00000     0.00000     0.00000  ;
    7   11    9   10      3     9.20480     0.00000    -9.20480     0.00000     0.00000     0.00000  ;
    1    3    5    7      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    1   11    9    7      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    3    1   11    9      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    3    1   11   12      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    3    5    7    9      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
   11    1    3    5      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    5    7    9   11      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    7    9   11   12      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    1    9   11   12      3     9.20480     0.00000    -9.20480     0.00000     0.00000     0.00000  ;

end--------------------------------------------------------------------------------------------------------------------------
```

Chloroform (gas phase charges)

```
[ moleculetype ]
; Name            nrexcl
C1X               3

[ atoms ]
;   nr       type  resnr residue  atom   cgnr     charge       mass  typeB    chargeB
     1         c3      1    LIG      C      1   -0.5151  12.000000
     2         h3      1    LIG      H      2    0.3303   1.000000
     3         cl      1    LIG     CL      3    0.0616  35.500000
     4         cl      1    LIG    Cl1      4    0.0616  35.500000
     5         cl      1    LIG    Cl2      5    0.0616  35.500000

[ bonds ]
;  ai    aj funct  r  k
    1     2     1  1.0950e-01  2.7899e+05
    1     3     1  1.7860e-01  2.3347e+05
    1     4     1  1.7860e-01  2.3347e+05
    1     5     1  1.7860e-01  2.3347e+05

[ pairs ]
;  ai    aj funct

[ angles ]
;  ai    aj    ak funct  theta   cth
    2     1     3     1  1.0765e+02  3.6284e+02
    2     1     4     1  1.0765e+02  3.6284e+02
    2     1     5     1  1.0765e+02  3.6284e+02
    3     1     4     1  1.1103e+02  5.2467e+02
    3     1     5     1  1.1103e+02  5.2467e+02
    4     1     5     1  1.1103e+02  5.2467e+02

end----------------------------------------------------------------------------------------------------------------------------
```

Chloroform (polarized charges, water)

```
[ moleculetype ]
; Name            nrexcl
Chloroform            3

[ atoms ]
;   nr       type  resnr residue  atom   cgnr     charge       mass  typeB    chargeB
     1         c3      1    LIG      C      1   -0.5699  12.000000
     2         h3      1    LIG      H      2    0.3935   1.000000
     3         cl      1    LIG     CL      3    0.0588  35.500000
     4         cl      1    LIG    Cl1      4    0.0588  35.500000
     5         cl      1    LIG    Cl2      5    0.0588  35.500000

[ bonds ]
;  ai    aj funct  r  k
    1     2     1  1.0950e-01  2.7899e+05
    1     3     1  1.7860e-01  2.3347e+05
    1     4     1  1.7860e-01  2.3347e+05
    1     5     1  1.7860e-01  2.3347e+05

[ pairs ]
;  ai    aj funct

[ angles ]
;  ai    aj    ak funct  theta   cth
    2     1     3     1  1.0765e+02  3.6284e+02
    2     1     4     1  1.0765e+02  3.6284e+02
    2     1     5     1  1.0765e+02  3.6284e+02
    3     1     4     1  1.1103e+02  5.2467e+02
    3     1     5     1  1.1103e+02  5.2467e+02
    4     1     5     1  1.1103e+02  5.2467e+02

end----------------------------------------------------------------------------------------------------------------------------
```

Chloroform (polarized charges, hexadecane)

```
[ moleculetype ]
; Name            nrexcl
Chloroform            3

[ atoms ]
;   nr       type  resnr residue  atom   cgnr     charge       mass  typeB    chargeB
     1         c3      1    LIG      C      1   -0.5308  12.000000
     2         h3      1    LIG      H      2    0.3508   1.000000
     3         cl      1    LIG     CL      3    0.0600  35.500000
     4         cl      1    LIG    Cl1      4    0.0600  35.500000
     5         cl      1    LIG    Cl2      5    0.0600  35.500000

[ bonds ]
;  ai    aj funct  r  k
    1     2     1  1.0950e-01  2.7899e+05
    1     3     1  1.7860e-01  2.3347e+05
    1     4     1  1.7860e-01  2.3347e+05
    1     5     1  1.7860e-01  2.3347e+05
```

```
[ pairs ]
;  ai    aj funct

[ angles ]
;  ai    aj    ak funct  theta   cth
    2     1     3     1  1.0765e+02  3.6284e+02
    2     1     4     1  1.0765e+02  3.6284e+02
    2     1     5     1  1.0765e+02  3.6284e+02
    3     1     4     1  1.1103e+02  5.2467e+02
    3     1     5     1  1.1103e+02  5.2467e+02
    4     1     5     1  1.1103e+02  5.2467e+02

end----------------------------------------------------------------------------------------------------------------------------
```

2,4,5 trichloroaniline (gas phase charges)

```
[ moleculetype ]
; Name            nrexcl
245trichloroaniline            3

[ atoms ]
;   nr       type  resnr residue  atom   cgnr     charge       mass  typeB    chargeB
     1         ca      1    LIG      C      1   -0.1303  12.000000
     2         ca      1    LIG     C1      2    0.0901  12.000000
     3         ha      1    LIG      H      3    0.1381   1.000000
     4         ca      1    LIG     C2      4   -0.2955  12.000000
     5         ca      1    LIG     C3      5    0.7206  12.000000
     6         ca      1    LIG     C4      6   -0.4350  12.000000
     7         ha      1    LIG     H1      7    0.1985   1.000000
     8         ca      1    LIG     C5      8    0.1510  12.000000
     9         cl      1    LIG     CL      9   -0.0792  35.500000
    10         cl      1    LIG    Cl1     10   -0.0775  35.500000
    11         cl      1    LIG    Cl2     11   -0.0789  35.500000
    12         nh      1    LIG      N     12   -1.1448  14.000000
    13         hn      1    LIG     H2     13    0.4714   1.000000
    14         hn      1    LIG     H3     14    0.4714   1.000000

[ bonds ]
;  ai    aj funct  r  k
    2     3     1  1.0870e-01  2.8811e+05
    6     7     1  1.0870e-01  2.8811e+05
   12    13     1  1.0140e-01  3.3572e+05
   12    14     1  1.0140e-01  3.3572e+05
    1     2     1  1.3870e-01  4.0033e+05
    1     8     1  1.3870e-01  4.0033e+05
    1     9     1  1.7290e-01  2.7012e+05
    2     4     1  1.3870e-01  4.0033e+05
    4     5     1  1.3870e-01  4.0033e+05
    4    11     1  1.7290e-01  2.7012e+05
    5     6     1  1.3870e-01  4.0033e+05
    5    12     1  1.3640e-01  3.7572e+05
    6     8     1  1.3870e-01  4.0033e+05
    8    10     1  1.7290e-01  2.7012e+05

[ pairs ]
;  ai    aj funct
     1     7     1
     8     3     1
     9     3     1
     3     5     1
     3    11     1
     4     7     1
     4    13     1
     4    14     1
     6    13     1
     6    14     1
     7    12     1
     7    10     1
     1     5     1
     1    11     1
     2     6     1
     2    10     1
     2    12     1
     8     4     1
     9     4     1
     5    10     1
     6    11     1
     9     6     1
     8    12     1
     9    10     1
    11    12     1

[ angles ]
;  ai    aj    ak funct  theta   cth
    1     2     3     1  1.2001e+02  4.0551e+02
    3     2     4     1  1.2001e+02  4.0551e+02
    5     6     7     1  1.2001e+02  4.0551e+02
    5    12    13     1  1.1613e+02  4.1070e+02
    5    12    14     1  1.1613e+02  4.1070e+02
    7     6     8     1  1.2001e+02  4.0551e+02
   13    12    14     1  1.1485e+02  3.3514e+02
    1     2     4     1  1.1997e+02  5.6216e+02
    1     8     6     1  1.1997e+02  5.6216e+02
    1     8    10     1  1.1940e+02  5.2651e+02
    2     1     8     1  1.1997e+02  5.6216e+02
    2     1     9     1  1.1940e+02  5.2651e+02
    2     4     5     1  1.1997e+02  5.6216e+02
    2     4    11     1  1.1940e+02  5.2651e+02
    4     5     6     1  1.1997e+02  5.6216e+02
    4     5    12     1  1.2013e+02  5.8024e+02
    5     4    11     1  1.1940e+02  5.2651e+02
    5     6     8     1  1.1997e+02  5.6216e+02
    6     5    12     1  1.2013e+02  5.8024e+02
    6     8    10     1  1.1940e+02  5.2651e+02
    8     1     9     1  1.1940e+02  5.2651e+02
```

```
[ dihedrals ]
;i  j   k  l      func    C0  ...  C5
    1    8    6    7      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    8    1    2    3      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    9    1    2    3      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    3    2    4    5      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    3    2    4   11      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    4    5    6    7      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    4    5   12   13      3     8.78640     0.00000    -8.78640     0.00000     0.00000     0.00000  ;
    4    5   12   14      3     8.78640     0.00000    -8.78640     0.00000     0.00000     0.00000  ;
    6    5   12   13      3     8.78640     0.00000    -8.78640     0.00000     0.00000     0.00000  ;
    6    5   12   14      3     8.78640     0.00000    -8.78640     0.00000     0.00000     0.00000  ;
    7    6    5   12      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    7    6    8   10      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    1    4    2    3      3     9.20480     0.00000    -9.20480     0.00000     0.00000     0.00000  ;
    5    8    6    7      3     9.20480     0.00000    -9.20480     0.00000     0.00000     0.00000  ;
    5   13   12   14      3     9.20480     0.00000    -9.20480     0.00000     0.00000     0.00000  ;
    1    2    4    5      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    1    2    4   11      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    1    8    6    5      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    2    1    8    6      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    2    1    8   10      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    2    4    5    6      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    2    4    5   12      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    8    1    2    4      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    9    1    2    4      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    4    5    6    8      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    5    6    8   10      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    6    5    4   11      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    9    1    8    6      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    8    6    5   12      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    9    1    8   10      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
   11    4    5   12      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    9    1    8    2      3     9.20480     0.00000    -9.20480     0.00000     0.00000     0.00000  ;
    2    5    4   11      3     9.20480     0.00000    -9.20480     0.00000     0.00000     0.00000  ;
    4    6    5   12      3     9.20480     0.00000    -9.20480     0.00000     0.00000     0.00000  ;
    1    6    8   10      3     9.20480     0.00000    -9.20480     0.00000     0.00000     0.00000  ;

end----------------------------------------------------------------------------------------------------------------------------------
```

2,4,5 trichloroaniline (polarized charges, water)

```
[ moleculetype ]
; Name            nrexcl
C1X               3

[ atoms ]
;   nr       type  resnr residue  atom   cgnr     charge       mass  typeB    chargeB
     1         ca      1    LIG      C      1   -0.13550  12.000000
     2         ca      1    LIG     C1      2    0.09760  12.000000
     3         ha      1    LIG      H      3    0.14930   1.000000
     4         ca      1    LIG     C2      4   -0.31550  12.000000
     5         ca      1    LIG     C3      5    0.73590  12.000000
     6         ca      1    LIG     C4      6   -0.43780  12.000000
     7         ha      1    LIG     H1      7    0.22190   1.000000
     8         ca      1    LIG     C5      8    0.14170  12.000000
     9         cl      1    LIG     CL      9   -0.10130  35.500000
    10         cl      1    LIG    Cl1     10   -0.09310  35.500000
    11         cl      1    LIG    Cl2     11   -0.08520  35.500000
    12         nh      1    LIG      N     12   -1.16050  14.000000
    13         hn      1    LIG     H2     13    0.49130   1.000000
    14         hn      1    LIG     H3     14    0.49130   1.000000

[ bonds ]
;  ai    aj funct  r  k
    2     3     1  1.0870e-01  2.8811e+05
    6     7     1  1.0870e-01  2.8811e+05
   12    13     1  1.0140e-01  3.3572e+05
   12    14     1  1.0140e-01  3.3572e+05
    1     2     1  1.3870e-01  4.0033e+05
    1     8     1  1.3870e-01  4.0033e+05
    1     9     1  1.7290e-01  2.7012e+05
    2     4     1  1.3870e-01  4.0033e+05
    4     5     1  1.3870e-01  4.0033e+05
    4    11     1  1.7290e-01  2.7012e+05
    5     6     1  1.3870e-01  4.0033e+05
    5    12     1  1.3640e-01  3.7572e+05
    6     8     1  1.3870e-01  4.0033e+05
    8    10     1  1.7290e-01  2.7012e+05

[ pairs ]
;  ai    aj funct
     1     7     1
     8     3     1
     9     3     1
     3     5     1
     3    11     1
     4     7     1
     4    13     1
     4    14     1
```

```
     6     13      1
     6     14      1
     7     12      1
     7     10      1
     1      5      1
     1     11      1
     2      6      1
     2     10      1
     2     12      1
     8      4      1
     9      4      1
     5     10      1
     6     11      1
     9      6      1
     8     12      1
     9     10      1
    11     12      1

[ angles ]
;  ai    aj    ak funct  theta   cth
    1     2     3     1  1.2001e+02  4.0551e+02
    3     2     4     1  1.2001e+02  4.0551e+02
    5     6     7     1  1.2001e+02  4.0551e+02
    5    12    13     1  1.1613e+02  4.1070e+02
    5    12    14     1  1.1613e+02  4.1070e+02
    7     6     8     1  1.2001e+02  4.0551e+02
   13    12    14     1  1.1485e+02  3.3514e+02
    1     2     4     1  1.1997e+02  5.6216e+02
    1     8     6     1  1.1997e+02  5.6216e+02
    1     8    10     1  1.1940e+02  5.2651e+02
    2     1     8     1  1.1997e+02  5.6216e+02
    2     1     9     1  1.1940e+02  5.2651e+02
    2     4     5     1  1.1997e+02  5.6216e+02
    2     4    11     1  1.1940e+02  5.2651e+02
    4     5     6     1  1.1997e+02  5.6216e+02
    4     5    12     1  1.2013e+02  5.8024e+02
    5     4    11     1  1.1940e+02  5.2651e+02
    5     6     8     1  1.1997e+02  5.6216e+02
    6     5    12     1  1.2013e+02  5.8024e+02
    6     8    10     1  1.1940e+02  5.2651e+02
    8     1     9     1  1.1940e+02  5.2651e+02

[ dihedrals ]
;i  j   k  l      func    C0  ...  C5
    1    8    6    7     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    8    1    2    3     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    9    1    2    3     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    3    2    4    5     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    3    2    4   11     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    4    5    6    7     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    4    5   12   13     3     8.78640     0.00000    -8.78640     0.00000     0.00000     0.00000  ;
    4    5   12   14     3     8.78640     0.00000    -8.78640     0.00000     0.00000     0.00000  ;
    6    5   12   13     3     8.78640     0.00000    -8.78640     0.00000     0.00000     0.00000  ;
    6    5   12   14     3     8.78640     0.00000    -8.78640     0.00000     0.00000     0.00000  ;
    7    6    5   12     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    7    6    8   10     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    1    4    2    3     3     9.20480     0.00000    -9.20480     0.00000     0.00000     0.00000  ;
    5    8    6    7     3     9.20480     0.00000    -9.20480     0.00000     0.00000     0.00000  ;
    5   13   12   14     3     9.20480     0.00000    -9.20480     0.00000     0.00000     0.00000  ;
    1    2    4    5     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    1    2    4   11     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    1    8    6    5     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    2    1    8    6     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    2    1    8   10     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    2    4    5    6     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    2    4    5   12     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    8    1    2    4     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    9    1    2    4     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    4    5    6    8     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    5    6    8   10     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    6    5    4   11     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    9    1    8    6     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    8    6    5   12     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    9    1    8   10     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
   11    4    5   12     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    9    1    8    2     3     9.20480     0.00000    -9.20480     0.00000     0.00000     0.00000  ;
    2    5    4   11     3     9.20480     0.00000    -9.20480     0.00000     0.00000     0.00000  ;
    4    6    5   12     3     9.20480     0.00000    -9.20480     0.00000     0.00000     0.00000  ;
    1    6    8   10     3     9.20480     0.00000    -9.20480     0.00000     0.00000     0.00000  ;

end----------------------------------------------------------------------------------------------------------------------------------
```

2,4,5 trichloroaniline (polarized charges, hexadecane)

```
[ moleculetype ]
; Name            nrexcl
C1X               3

[ atoms ]
;   nr       type  resnr residue  atom   cgnr     charge       mass  typeB    chargeB
     1         ca      1    LIG      C      1   -0.1313  12.000000
```

```
     2         ca      1    LIG     C1      2    0.0919  12.000000
     3         ha      1    LIG      H      3    0.1428   1.000000
     4         ca      1    LIG     C2      4   -0.3018  12.000000
     5         ca      1    LIG     C3      5    0.7270  12.000000
     6         ca      1    LIG     C4      6   -0.4372  12.000000
     7         ha      1    LIG     H1      7    0.2074   1.000000
     8         ca      1    LIG     C5      8    0.1483  12.000000
     9         cl      1    LIG     CL      9   -0.0884  35.500000
    10         cl      1    LIG    Cl1     10   -0.0842  35.500000
    11         cl      1    LIG    Cl2     11   -0.0824  35.500000
    12         nh      1    LIG      N     12   -1.1511  14.000000
    13         hn      1    LIG     H2     13    0.4795   1.000000
    14         hn      1    LIG     H3     14    0.4795   1.000000

[ bonds ]
;  ai    aj funct  r  k
    2     3     1  1.0870e-01  2.8811e+05
    6     7     1  1.0870e-01  2.8811e+05
   12    13     1  1.0140e-01  3.3572e+05
   12    14     1  1.0140e-01  3.3572e+05
    1     2     1  1.3870e-01  4.0033e+05
    1     8     1  1.3870e-01  4.0033e+05
    1     9     1  1.7290e-01  2.7012e+05
    2     4     1  1.3870e-01  4.0033e+05
    4     5     1  1.3870e-01  4.0033e+05
    4    11     1  1.7290e-01  2.7012e+05
    5     6     1  1.3870e-01  4.0033e+05
    5    12     1  1.3640e-01  3.7572e+05
    6     8     1  1.3870e-01  4.0033e+05
    8    10     1  1.7290e-01  2.7012e+05

[ pairs ]
;  ai    aj funct
     1     7     1
     8     3     1
     9     3     1
     3     5     1
     3    11     1
     4     7     1
     4    13     1
     4    14     1
     6    13     1
     6    14     1
     7    12     1
     7    10     1
     1     5     1
     1    11     1
     2     6     1
     2    10     1
     2    12     1
     8     4     1
     9     4     1
     5    10     1
     6    11     1
     9     6     1
     8    12     1
     9    10     1
    11    12     1

[ angles ]
;  ai    aj    ak funct  theta   cth
    1     2     3     1  1.2001e+02  4.0551e+02
    3     2     4     1  1.2001e+02  4.0551e+02
    5     6     7     1  1.2001e+02  4.0551e+02
    5    12    13     1  1.1613e+02  4.1070e+02
    5    12    14     1  1.1613e+02  4.1070e+02
    7     6     8     1  1.2001e+02  4.0551e+02
   13    12    14     1  1.1485e+02  3.3514e+02
    1     2     4     1  1.1997e+02  5.6216e+02
    1     8     6     1  1.1997e+02  5.6216e+02
    1     8    10     1  1.1940e+02  5.2651e+02
    2     1     8     1  1.1997e+02  5.6216e+02
    2     1     9     1  1.1940e+02  5.2651e+02
    2     4     5     1  1.1997e+02  5.6216e+02
    2     4    11     1  1.1940e+02  5.2651e+02
    4     5     6     1  1.1997e+02  5.6216e+02
    4     5    12     1  1.2013e+02  5.8024e+02
    5     4    11     1  1.1940e+02  5.2651e+02
    5     6     8     1  1.1997e+02  5.6216e+02
    6     5    12     1  1.2013e+02  5.8024e+02
    6     8    10     1  1.1940e+02  5.2651e+02
    8     1     9     1  1.1940e+02  5.2651e+02

[ dihedrals ]
;i  j   k  l      func    C0  ...  C5
    1    8    6    7      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    8    1    2    3      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    9    1    2    3      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    3    2    4    5      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    3    2    4    11     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    4    5    6    7      3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
```

```
    4    5   12   13    3     8.78640    0.00000   -8.78640    0.00000    0.00000    0.00000  ;
    4    5   12   14    3     8.78640    0.00000   -8.78640    0.00000    0.00000    0.00000  ;
    6    5   12   13    3     8.78640    0.00000   -8.78640    0.00000    0.00000    0.00000  ;
    6    5   12   14    3     8.78640    0.00000   -8.78640    0.00000    0.00000    0.00000  ;
    7    6    5   12    3    30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000  ;
    7    6    8   10    3    30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000  ;
    1    4    2    3    3     9.20480    0.00000   -9.20480    0.00000    0.00000    0.00000  ;
    5    8    6    7    3     9.20480    0.00000   -9.20480    0.00000    0.00000    0.00000  ;
    5   13   12   14    3     9.20480    0.00000   -9.20480    0.00000    0.00000    0.00000  ;
    1    2    4    5    3    30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000  ;
    1    2    4   11    3    30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000  ;
    1    8    6    5    3    30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000  ;
    2    1    8    6    3    30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000  ;
    2    1    8   10    3    30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000  ;
    2    4    5    6    3    30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000  ;
    2    4    5   12    3    30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000  ;
    8    1    2    4    3    30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000  ;
    9    1    2    4    3    30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000  ;
    4    5    6    8    3    30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000  ;
    5    6    8   10    3    30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000  ;
    6    5    4   11    3    30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000  ;
    9    1    8    6    3    30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000  ;
    8    6    5   12    3    30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000  ;
    9    1    8   10    3    30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000  ;
   11    4    5   12    3    30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000  ;
    9    1    8    2    3     9.20480    0.00000   -9.20480    0.00000    0.00000    0.00000  ;
    2    5    4   11    3     9.20480    0.00000   -9.20480    0.00000    0.00000    0.00000  ;
    4    6    5   12    3     9.20480    0.00000   -9.20480    0.00000    0.00000    0.00000  ;
    1    6    8   10    3     9.20480    0.00000   -9.20480    0.00000    0.00000    0.00000  ;

end-------------------------------------------------------------------------------------------------------------------------------
```

Lidocaine (gas phase charges)

```
[ moleculetype ]
; Name            nrexcl
Lidocaine             3

[ atoms ]
;   nr       type  resnr residue  atom   cgnr     charge       mass  typeB    chargeB
     1         ca      1    LIG      C      1   -0.3589  12.000000
     2         ha      1    LIG      H      2    0.1836   1.000000
     3         ca      1    LIG     C1      3   -0.0887  12.000000
     4         ha      1    LIG     H1      4    0.1549   1.000000
     5         ca      1    LIG     C2      5   -0.3589  12.000000
     6         ha      1    LIG     H2      6    0.1836   1.000000
     7         ca      1    LIG     C3      7    0.2389  12.000000
     8         ca      1    LIG     C4      8   -0.0235  12.000000
     9         ca      1    LIG     C5      9    0.2445  12.000000
    10         c3      1    LIG     C6     10   -0.3112  12.000000
    11         hc      1    LIG     H3     11    0.0898   1.000000
    12         hc      1    LIG     H4     12    0.0898   1.000000
    13         hc      1    LIG     H5     13    0.0898   1.000000
    14         c3      1    LIG     C7     14   -0.3112  12.000000
    15         hc      1    LIG     H6     15    0.0898   1.000000
    16         hc      1    LIG     H7     16    0.0898   1.000000
    17         hc      1    LIG     H8     17    0.0898   1.000000
    18          n      1    LIG      N     18   -0.4654  14.000000
    19         hn      1    LIG     H9     19    0.3223   1.000000
    20          c      1    LIG     C8     20    0.6026  12.000000
    21          o      1    LIG      O     21   -0.6336  16.000000
    22         c3      1    LIG     C9     22    0.1477  12.000000
    23         h1      1    LIG    H10     23   -0.0093   1.000000
    24         h1      1    LIG    H11     24   -0.0093   1.000000
    25         n3      1    LIG     N1     25   -0.1523  14.000000
    26         c3      1    LIG    C10     26   -0.0178  12.000000
    27         h1      1    LIG    H12     27    0.0456   1.000000
    28         h1      1    LIG    H13     28    0.0456   1.000000
    29         c3      1    LIG    C11     29   -0.1914  12.000000
    30         hc      1    LIG    H14     30    0.0569   1.000000
    31         hc      1    LIG    H15     31    0.0569   1.000000
    32         hc      1    LIG    H16     32    0.0569   1.000000
    33         c3      1    LIG    C12     33   -0.0178  12.000000
    34         h1      1    LIG    H17     34    0.0456   1.000000
    35         h1      1    LIG    H18     35    0.0456   1.000000
    36         c3      1    LIG    C13     36   -0.1914  12.000000
    37         hc      1    LIG    H19     37    0.0569   1.000000
    38         hc      1    LIG    H20     38    0.0569   1.000000
    39         hc      1    LIG    H21     39    0.0569   1.000000

[ bonds ]
;  ai    aj funct  r  k
    1     2     1  1.0870e-01  2.8811e+05
    3     4     1  1.0870e-01  2.8811e+05
    5     6     1  1.0870e-01  2.8811e+05
   10    11     1  1.0920e-01  2.8225e+05
   10    12     1  1.0920e-01  2.8225e+05
   10    13     1  1.0920e-01  2.8225e+05
   14    15     1  1.0920e-01  2.8225e+05
   14    16     1  1.0920e-01  2.8225e+05
   14    17     1  1.0920e-01  2.8225e+05
   18    19     1  1.0090e-01  3.4326e+05
   22    23     1  1.0930e-01  2.8108e+05
   22    24     1  1.0930e-01  2.8108e+05
   26    27     1  1.0930e-01  2.8108e+05
   26    28     1  1.0930e-01  2.8108e+05
   29    30     1  1.0920e-01  2.8225e+05
   29    31     1  1.0920e-01  2.8225e+05
   29    32     1  1.0920e-01  2.8225e+05
   33    34     1  1.0930e-01  2.8108e+05
   33    35     1  1.0930e-01  2.8108e+05
   36    37     1  1.0920e-01  2.8225e+05
   36    38     1  1.0920e-01  2.8225e+05
   36    39     1  1.0920e-01  2.8225e+05
    1     3     1  1.3870e-01  4.0033e+05
    1     9     1  1.3870e-01  4.0033e+05
    3     5     1  1.3870e-01  4.0033e+05
    5     7     1  1.3870e-01  4.0033e+05
    7     8     1  1.3870e-01  4.0033e+05
    7    14     1  1.5130e-01  2.7070e+05
    8     9     1  1.3870e-01  4.0033e+05
    8    18     1  1.4220e-01  3.1154e+05
    9    10     1  1.5130e-01  2.7070e+05
   18    20     1  1.3450e-01  4.0016e+05
   20    21     1  1.2140e-01  5.4225e+05
   20    22     1  1.5080e-01  2.7472e+05
   22    25     1  1.4700e-01  2.6828e+05
   25    26     1  1.4700e-01  2.6828e+05
   25    33     1  1.4700e-01  2.6828e+05
   26    29     1  1.5350e-01  2.5363e+05
   33    36     1  1.5350e-01  2.5363e+05

[ pairs ]
```

```
;  ai    aj funct
     1     6      1
     1    11      1
     1    12      1
     1    13      1
     2     4      1
     2     5      1
     2     8      1
     2    10      1
     9     4      1
     4     6      1
     4     7      1
     5    15      1
     5    16      1
     5    17      1
     6     8      1
     6    14      1
     7    19      1
     8    15      1
     8    16      1
     8    17      1
     8    11      1
     8    12      1
     8    13      1
     9    19      1
    18    23      1
    18    24      1
    19    21      1
    19    22      1
    21    23      1
    21    24      1
    22    27      1
    22    28      1
    22    34      1
    22    35      1
    23    26      1
    23    33      1
    24    26      1
    24    33      1
    25    30      1
    25    31      1
    25    32      1
    25    37      1
    25    38      1
    25    39      1
    26    34      1
    26    35      1
    27    33      1
    27    30      1
    27    31      1
    27    32      1
    28    33      1
    28    30      1
    28    31      1
    28    32      1
    34    37      1
    34    38      1
    34    39      1
    35    37      1
    35    38      1
    35    39      1
     1     7      1
     1    18      1
     3     8      1
     3    10      1
     3    14      1
     9     5      1
     5    18      1
     7    10      1
     7    20      1
     8    21      1
     8    22      1
     9    14      1
     9    20      1
    10    18      1
    14    18      1
    18    25      1
    20    26      1
    20    33      1
    21    25      1
    22    29      1
    22    36      1
    26    36      1
    29    33      1

[ angles ]
;  ai    aj    ak funct  theta   cth
    1     3     4     1  1.2001e+02  4.0551e+02
    2     1     3     1  1.2001e+02  4.0551e+02
    2     1     9     1  1.2001e+02  4.0551e+02
    3     5     6     1  1.2001e+02  4.0551e+02
```

```
     4     3     5     1  1.2001e+02  4.0551e+02
     6     5     7     1  1.2001e+02  4.0551e+02
     7    14    15     1  1.1015e+02  3.9296e+02
     7    14    16     1  1.1015e+02  3.9296e+02
     7    14    17     1  1.1015e+02  3.9296e+02
     8    18    19     1  1.1594e+02  3.9631e+02
     9    10    11     1  1.1015e+02  3.9296e+02
     9    10    12     1  1.1015e+02  3.9296e+02
     9    10    13     1  1.1015e+02  3.9296e+02
    11    10    12     1  1.0835e+02  3.2995e+02
    11    10    13     1  1.0835e+02  3.2995e+02
    12    10    13     1  1.0835e+02  3.2995e+02
    15    14    16     1  1.0835e+02  3.2995e+02
    15    14    17     1  1.0835e+02  3.2995e+02
    16    14    17     1  1.0835e+02  3.2995e+02
    19    18    20     1  1.1846e+02  4.1179e+02
    20    22    23     1  1.0766e+02  3.9857e+02
    20    22    24     1  1.0766e+02  3.9857e+02
    23    22    24     1  1.0955e+02  3.2786e+02
    23    22    25     1  1.0992e+02  4.1330e+02
    24    22    25     1  1.0992e+02  4.1330e+02
    25    26    27     1  1.0992e+02  4.1330e+02
    25    26    28     1  1.0992e+02  4.1330e+02
    25    33    34     1  1.0992e+02  4.1330e+02
    25    33    35     1  1.0992e+02  4.1330e+02
    26    29    30     1  1.1005e+02  3.8802e+02
    26    29    31     1  1.1005e+02  3.8802e+02
    26    29    32     1  1.1005e+02  3.8802e+02
    27    26    28     1  1.0955e+02  3.2786e+02
    27    26    29     1  1.1007e+02  3.8794e+02
    28    26    29     1  1.1007e+02  3.8794e+02
    30    29    31     1  1.0835e+02  3.2995e+02
    30    29    32     1  1.0835e+02  3.2995e+02
    31    29    32     1  1.0835e+02  3.2995e+02
    33    36    37     1  1.1005e+02  3.8802e+02
    33    36    38     1  1.1005e+02  3.8802e+02
    33    36    39     1  1.1005e+02  3.8802e+02
    34    33    35     1  1.0955e+02  3.2786e+02
    34    33    36     1  1.1007e+02  3.8794e+02
    35    33    36     1  1.1007e+02  3.8794e+02
    37    36    38     1  1.0835e+02  3.2995e+02
    37    36    39     1  1.0835e+02  3.2995e+02
    38    36    39     1  1.0835e+02  3.2995e+02
     1     3     5     1  1.1997e+02  5.6216e+02
     1     9     8     1  1.1997e+02  5.6216e+02
     1     9    10     1  1.2063e+02  5.3421e+02
     3     1     9     1  1.1997e+02  5.6216e+02
     3     5     7     1  1.1997e+02  5.6216e+02
     5     7     8     1  1.1997e+02  5.6216e+02
     5     7    14     1  1.2063e+02  5.3421e+02
     7     8     9     1  1.1997e+02  5.6216e+02
     7     8    18     1  1.1989e+02  5.6877e+02
     8     7    14     1  1.2063e+02  5.3421e+02
     8     9    10     1  1.2063e+02  5.3421e+02
     8    18    20     1  1.2371e+02  5.3798e+02
     9     8    18     1  1.1989e+02  5.6877e+02
    18    20    21     1  1.2203e+02  6.3455e+02
    18    20    22     1  1.1515e+02  5.6785e+02
    20    22    25     1  1.1114e+02  5.5723e+02
    21    20    22     1  1.2311e+02  5.6928e+02
    22    25    26     1  1.1090e+02  5.3564e+02
    22    25    33     1  1.1090e+02  5.3564e+02
    25    26    29     1  1.1038e+02  5.5379e+02
    25    33    36     1  1.1038e+02  5.5379e+02
    26    25    33     1  1.1090e+02  5.3564e+02

[ dihedrals ]
;i  j   k  l      func    C0  ...  C5
    1    3    5    6     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    1    9   10   11     3     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000  ;
    1    9   10   12     3     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000  ;
    1    9   10   13     3     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000  ;
    2    1    3    4     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    2    1    3    5     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    2    1    9    8     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    2    1    9   10     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    9    1    3    4     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    4    3    5    6     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    4    3    5    7     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    5    7   14   15     3     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000  ;
    5    7   14   16     3     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000  ;
    5    7   14   17     3     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000  ;
    6    5    7    8     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    6    5    7   14     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    7    8   18   19     3     3.76560     0.00000    -3.76560     0.00000     0.00000     0.00000  ;
    8    7   14   15     3     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000  ;
    8    7   14   16     3     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000  ;
    8    7   14   17     3     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000  ;
    8    9   10   11     3     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000  ;
    8    9   10   12     3     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000  ;
    8    9   10   13     3     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000  ;
```

```
    9    8   18   19     3     3.76560     0.00000    -3.76560     0.00000     0.00000     0.00000  ;
   18   20   22   23     3     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000  ;
   18   20   22   24     3     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000  ;
   19   18   20   21     3    29.28800    -8.36800   -20.92000     0.00000     0.00000     0.00000  ;
   19   18   20   22     3    20.92000     0.00000   -20.92000     0.00000     0.00000     0.00000  ;
   21   20   22   23     3     3.68192    -4.35136     0.00000     1.33888     0.00000     0.00000  ;
   21   20   22   24     3     3.68192    -4.35136     0.00000     1.33888     0.00000     0.00000  ;
   22   25   26   27     3     1.25520     3.76560     0.00000    -5.02080     0.00000     0.00000  ;
   22   25   26   28     3     1.25520     3.76560     0.00000    -5.02080     0.00000     0.00000  ;
   22   25   33   34     3     1.25520     3.76560     0.00000    -5.02080     0.00000     0.00000  ;
   22   25   33   35     3     1.25520     3.76560     0.00000    -5.02080     0.00000     0.00000  ;
   23   22   25   26     3     1.25520     3.76560     0.00000    -5.02080     0.00000     0.00000  ;
   23   22   25   33     3     1.25520     3.76560     0.00000    -5.02080     0.00000     0.00000  ;
   24   22   25   26     3     1.25520     3.76560     0.00000    -5.02080     0.00000     0.00000  ;
   24   22   25   33     3     1.25520     3.76560     0.00000    -5.02080     0.00000     0.00000  ;
   25   26   29   30     3     0.65270     1.95811     0.00000    -2.61082     0.00000     0.00000  ;
   25   26   29   31     3     0.65270     1.95811     0.00000    -2.61082     0.00000     0.00000  ;
   25   26   29   32     3     0.65270     1.95811     0.00000    -2.61082     0.00000     0.00000  ;
   25   33   36   37     3     0.65270     1.95811     0.00000    -2.61082     0.00000     0.00000  ;
   25   33   36   38     3     0.65270     1.95811     0.00000    -2.61082     0.00000     0.00000  ;
   25   33   36   39     3     0.65270     1.95811     0.00000    -2.61082     0.00000     0.00000  ;
   26   25   33   34     3     1.25520     3.76560     0.00000    -5.02080     0.00000     0.00000  ;
   26   25   33   35     3     1.25520     3.76560     0.00000    -5.02080     0.00000     0.00000  ;
   27   26   25   33     3     1.25520     3.76560     0.00000    -5.02080     0.00000     0.00000  ;
   27   26   29   30     3     0.65270     1.95811     0.00000    -2.61082     0.00000     0.00000  ;
   27   26   29   31     3     0.65270     1.95811     0.00000    -2.61082     0.00000     0.00000  ;
   27   26   29   32     3     0.65270     1.95811     0.00000    -2.61082     0.00000     0.00000  ;
   28   26   25   33     3     1.25520     3.76560     0.00000    -5.02080     0.00000     0.00000  ;
   28   26   29   30     3     0.65270     1.95811     0.00000    -2.61082     0.00000     0.00000  ;
   28   26   29   31     3     0.65270     1.95811     0.00000    -2.61082     0.00000     0.00000  ;
   28   26   29   32     3     0.65270     1.95811     0.00000    -2.61082     0.00000     0.00000  ;
   34   33   36   37     3     0.65270     1.95811     0.00000    -2.61082     0.00000     0.00000  ;
   34   33   36   38     3     0.65270     1.95811     0.00000    -2.61082     0.00000     0.00000  ;
   34   33   36   39     3     0.65270     1.95811     0.00000    -2.61082     0.00000     0.00000  ;
   35   33   36   37     3     0.65270     1.95811     0.00000    -2.61082     0.00000     0.00000  ;
   35   33   36   38     3     0.65270     1.95811     0.00000    -2.61082     0.00000     0.00000  ;
   35   33   36   39     3     0.65270     1.95811     0.00000    -2.61082     0.00000     0.00000  ;
    2    1    9    3     3     9.20480     0.00000    -9.20480     0.00000     0.00000     0.00000  ;
    1    5    3    4     3     9.20480     0.00000    -9.20480     0.00000     0.00000     0.00000  ;
    3    7    5    6     3     9.20480     0.00000    -9.20480     0.00000     0.00000     0.00000  ;
   20    8   18   19     3     9.20480     0.00000    -9.20480     0.00000     0.00000     0.00000  ;
    1    3    5    7     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    1    9    8    7     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    1    9    8   18     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    3    1    9    8     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    3    1    9   10     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    3    5    7    8     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    3    5    7   14     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    9    1    3    5     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    5    7    8    9     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    5    7    8   18     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    7    8    9   10     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    7    8   18   20     3     3.76560     0.00000    -3.76560     0.00000     0.00000     0.00000  ;
    8   18   20   21     3    20.92000     0.00000   -20.92000     0.00000     0.00000     0.00000  ;
    8   18   20   22     3    20.92000     0.00000   -20.92000     0.00000     0.00000     0.00000  ;
    9    8    7   14     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    9    8   18   20     3     3.76560     0.00000    -3.76560     0.00000     0.00000     0.00000  ;
   10    9    8   18     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
   14    7    8   18     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
   18   20   22   25     3     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000  ;
   20   22   25   26     3     1.25520     3.76560     0.00000    -5.02080     0.00000     0.00000  ;
   20   22   25   33     3     1.25520     3.76560     0.00000    -5.02080     0.00000     0.00000  ;
   21   20   22   25     3     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000  ;
   22   25   26   29     3     5.27184     3.76560    -4.01664    -5.02080     0.00000     0.00000  ;
   22   25   33   36     3     5.27184     3.76560    -4.01664    -5.02080     0.00000     0.00000  ;
   26   25   33   36     3     5.27184     3.76560    -4.01664    -5.02080     0.00000     0.00000  ;
   29   26   25   33     3     5.27184     3.76560    -4.01664    -5.02080     0.00000     0.00000  ;
    5    8    7   14     3     9.20480     0.00000    -9.20480     0.00000     0.00000     0.00000  ;
    7    9    8   18     3     9.20480     0.00000    -9.20480     0.00000     0.00000     0.00000  ;
   10    1    9    8     3     9.20480     0.00000    -9.20480     0.00000     0.00000     0.00000  ;
   22   18   20   21     3    87.86400     0.00000   -87.86400     0.00000     0.00000     0.00000  ;

end--------------------------------------------------------------------------------------------------------------------------
```

Lidocaine (polarized charges, water)

```
[ moleculetype ]
; Name            nrexcl
Lidocaine             3

[ atoms ]
;   nr       type  resnr residue  atom   cgnr     charge       mass  typeB    chargeB
     1         ca      1    LIG      C      1   -0.38580  12.000000
     2         ha      1    LIG      H      2    0.20260   1.000000
     3         ca      1    LIG     C1      3   -0.10160  12.000000
     4         ha      1    LIG     H1      4    0.17180   1.000000
     5         ca      1    LIG     C2      5   -0.38580  12.000000
     6         ha      1    LIG     H2      6    0.20260   1.000000
     7         ca      1    LIG     C3      7    0.23220  12.000000
     8         ca      1    LIG     C4      8   -0.01690  12.000000
     9         ca      1    LIG     C5      9    0.25190  12.000000
```

```
    10         c3      1    LIG     C6     10   -0.29650  12.000000
    11         hc      1    LIG     H3     11    0.08960   1.000000
    12         hc      1    LIG     H4     12    0.08960   1.000000
    13         hc      1    LIG     H5     13    0.08960   1.000000
    14         c3      1    LIG     C7     14   -0.29650  12.000000
    15         hc      1    LIG     H6     15    0.08960   1.000000
    16         hc      1    LIG     H7     16    0.08960   1.000000
    17         hc      1    LIG     H8     17    0.08960   1.000000
    18          n      1    LIG      N     18   -0.46470  14.000000
    19         hn      1    LIG     H9     19    0.33750   1.000000
    20          c      1    LIG     C8     20    0.64440  12.000000
    21          o      1    LIG      O     21   -0.71880  16.000000
    22         c3      1    LIG     C9     22    0.01110  12.000000
    23         h1      1    LIG    H10     23    0.04750   1.000000
    24         h1      1    LIG    H11     24    0.04750   1.000000
    25         n3      1    LIG     N1     25   -0.15830  14.000000
    26         c3      1    LIG    C10     26   -0.04180  12.000000
    27         h1      1    LIG    H12     27    0.05780   1.000000
    28         h1      1    LIG    H13     28    0.05780   1.000000
    29         c3      1    LIG    C11     29   -0.14630  12.000000
    30         hc      1    LIG    H14     30    0.04720   1.000000
    31         hc      1    LIG    H15     31    0.04720   1.000000
    32         hc      1    LIG    H16     32    0.04720   1.000000
    33         c3      1    LIG    C12     33   -0.04180  12.000000
    34         h1      1    LIG    H17     34    0.05780   1.000000
    35         h1      1    LIG    H18     35    0.05780   1.000000
    36         c3      1    LIG    C13     36   -0.14630  12.000000
    37         hc      1    LIG    H19     37    0.04720   1.000000
    38         hc      1    LIG    H20     38    0.04720   1.000000
    39         hc      1    LIG    H21     39    0.04720   1.000000

[ bonds ]
;  ai    aj funct  r  k
    1     2     1  1.0870e-01  2.8811e+05
    3     4     1  1.0870e-01  2.8811e+05
    5     6     1  1.0870e-01  2.8811e+05
   10    11     1  1.0920e-01  2.8225e+05
   10    12     1  1.0920e-01  2.8225e+05
   10    13     1  1.0920e-01  2.8225e+05
   14    15     1  1.0920e-01  2.8225e+05
   14    16     1  1.0920e-01  2.8225e+05
   14    17     1  1.0920e-01  2.8225e+05
   18    19     1  1.0090e-01  3.4326e+05
   22    23     1  1.0930e-01  2.8108e+05
   22    24     1  1.0930e-01  2.8108e+05
   26    27     1  1.0930e-01  2.8108e+05
   26    28     1  1.0930e-01  2.8108e+05
   29    30     1  1.0920e-01  2.8225e+05
   29    31     1  1.0920e-01  2.8225e+05
   29    32     1  1.0920e-01  2.8225e+05
   33    34     1  1.0930e-01  2.8108e+05
   33    35     1  1.0930e-01  2.8108e+05
   36    37     1  1.0920e-01  2.8225e+05
   36    38     1  1.0920e-01  2.8225e+05
   36    39     1  1.0920e-01  2.8225e+05
    1     3     1  1.3870e-01  4.0033e+05
    1     9     1  1.3870e-01  4.0033e+05
    3     5     1  1.3870e-01  4.0033e+05
    5     7     1  1.3870e-01  4.0033e+05
    7     8     1  1.3870e-01  4.0033e+05
    7    14     1  1.5130e-01  2.7070e+05
    8     9     1  1.3870e-01  4.0033e+05
    8    18     1  1.4220e-01  3.1154e+05
    9    10     1  1.5130e-01  2.7070e+05
   18    20     1  1.3450e-01  4.0016e+05
   20    21     1  1.2140e-01  5.4225e+05
   20    22     1  1.5080e-01  2.7472e+05
   22    25     1  1.4700e-01  2.6828e+05
   25    26     1  1.4700e-01  2.6828e+05
   25    33     1  1.4700e-01  2.6828e+05
   26    29     1  1.5350e-01  2.5363e+05
   33    36     1  1.5350e-01  2.5363e+05

[ pairs ]
;  ai    aj funct
    1     6     1
    1    11     1
    1    12     1
    1    13     1
    2     4     1
    2     5     1
    2     8     1
    2    10     1
    9     4     1
    4     6     1
    4     7     1
    5    15     1
    5    16     1
    5    17     1
    6     8     1
    6    14     1
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     7     19      1
     8     15      1
     8     16      1
     8     17      1
     8     11      1
     8     12      1
     8     13      1
     9     19      1
    18     23      1
    18     24      1
    19     21      1
    19     22      1
    21     23      1
    21     24      1
    22     27      1
    22     28      1
    22     34      1
    22     35      1
    23     26      1
    23     33      1
    24     26      1
    24     33      1
    25     30      1
    25     31      1
    25     32      1
    25     37      1
    25     38      1
    25     39      1
    26     34      1
    26     35      1
    27     33      1
    27     30      1
    27     31      1
    27     32      1
    28     33      1
    28     30      1
    28     31      1
    28     32      1
    34     37      1
    34     38      1
    34     39      1
    35     37      1
    35     38      1
    35     39      1
     1      7      1
     1     18      1
     3      8      1
     3     10      1
     3     14      1
     9      5      1
     5     18      1
     7     10      1
     7     20      1
     8     21      1
     8     22      1
     9     14      1
     9     20      1
    10     18      1
    14     18      1
    18     25      1
    20     26      1
    20     33      1
    21     25      1
    22     29      1
    22     36      1
    26     36      1
    29     33      1

[ angles ]
;  ai    aj    ak funct  theta   cth
    1     3     4     1  1.2001e+02  4.0551e+02
    2     1     3     1  1.2001e+02  4.0551e+02
    2     1     9     1  1.2001e+02  4.0551e+02
    3     5     6     1  1.2001e+02  4.0551e+02
    4     3     5     1  1.2001e+02  4.0551e+02
    6     5     7     1  1.2001e+02  4.0551e+02
    7    14    15     1  1.1015e+02  3.9296e+02
    7    14    16     1  1.1015e+02  3.9296e+02
    7    14    17     1  1.1015e+02  3.9296e+02
    8    18    19     1  1.1594e+02  3.9631e+02
    9    10    11     1  1.1015e+02  3.9296e+02
    9    10    12     1  1.1015e+02  3.9296e+02
    9    10    13     1  1.1015e+02  3.9296e+02
   11    10    12     1  1.0835e+02  3.2995e+02
   11    10    13     1  1.0835e+02  3.2995e+02
   12    10    13     1  1.0835e+02  3.2995e+02
   15    14    16     1  1.0835e+02  3.2995e+02
   15    14    17     1  1.0835e+02  3.2995e+02
   16    14    17     1  1.0835e+02  3.2995e+02
   19    18    20     1  1.1846e+02  4.1179e+02
   20    22    23     1  1.0766e+02  3.9857e+02
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    20    22    24     1  1.0766e+02  3.9857e+02
    23    22    24     1  1.0955e+02  3.2786e+02
    23    22    25     1  1.0992e+02  4.1330e+02
    24    22    25     1  1.0992e+02  4.1330e+02
    25    26    27     1  1.0992e+02  4.1330e+02
    25    26    28     1  1.0992e+02  4.1330e+02
    25    33    34     1  1.0992e+02  4.1330e+02
    25    33    35     1  1.0992e+02  4.1330e+02
    26    29    30     1  1.1005e+02  3.8802e+02
    26    29    31     1  1.1005e+02  3.8802e+02
    26    29    32     1  1.1005e+02  3.8802e+02
    27    26    28     1  1.0955e+02  3.2786e+02
    27    26    29     1  1.1007e+02  3.8794e+02
    28    26    29     1  1.1007e+02  3.8794e+02
    30    29    31     1  1.0835e+02  3.2995e+02
    30    29    32     1  1.0835e+02  3.2995e+02
    31    29    32     1  1.0835e+02  3.2995e+02
    33    36    37     1  1.1005e+02  3.8802e+02
    33    36    38     1  1.1005e+02  3.8802e+02
    33    36    39     1  1.1005e+02  3.8802e+02
    34    33    35     1  1.0955e+02  3.2786e+02
    34    33    36     1  1.1007e+02  3.8794e+02
    35    33    36     1  1.1007e+02  3.8794e+02
    37    36    38     1  1.0835e+02  3.2995e+02
    37    36    39     1  1.0835e+02  3.2995e+02
    38    36    39     1  1.0835e+02  3.2995e+02
     1     3     5     1  1.1997e+02  5.6216e+02
     1     9     8     1  1.1997e+02  5.6216e+02
     1     9    10     1  1.2063e+02  5.3421e+02
     3     1     9     1  1.1997e+02  5.6216e+02
     3     5     7     1  1.1997e+02  5.6216e+02
     5     7     8     1  1.1997e+02  5.6216e+02
     5     7    14     1  1.2063e+02  5.3421e+02
     7     8     9     1  1.1997e+02  5.6216e+02
     7     8    18     1  1.1989e+02  5.6877e+02
     8     7    14     1  1.2063e+02  5.3421e+02
     8     9    10     1  1.2063e+02  5.3421e+02
     8    18    20     1  1.2371e+02  5.3798e+02
     9     8    18     1  1.1989e+02  5.6877e+02
    18    20    21     1  1.2203e+02  6.3455e+02
    18    20    22     1  1.1515e+02  5.6785e+02
    20    22    25     1  1.1114e+02  5.5723e+02
    21    20    22     1  1.2311e+02  5.6928e+02
    22    25    26     1  1.1090e+02  5.3564e+02
    22    25    33     1  1.1090e+02  5.3564e+02
    25    26    29     1  1.1038e+02  5.5379e+02
    25    33    36     1  1.1038e+02  5.5379e+02
    26    25    33     1  1.1090e+02  5.3564e+02

[ dihedrals ]
;i   j    k   l      func    C0   ...   C5
     1    3    5    6      3     30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
     1    9   10   11      3      0.00000     0.00000     0.00000     0.00000     0.00000     0.00000  ;
     1    9   10   12      3      0.00000     0.00000     0.00000     0.00000     0.00000     0.00000  ;
     1    9   10   13      3      0.00000     0.00000     0.00000     0.00000     0.00000     0.00000  ;
     2    1    3    4      3     30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
     2    1    3    5      3     30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
     2    1    9    8      3     30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
     2    1    9   10      3     30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
     9    1    3    4      3     30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
     4    3    5    6      3     30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
     4    3    5    7      3     30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
     5    7   14   15      3      0.00000     0.00000     0.00000     0.00000     0.00000     0.00000  ;
     5    7   14   16      3      0.00000     0.00000     0.00000     0.00000     0.00000     0.00000  ;
     5    7   14   17      3      0.00000     0.00000     0.00000     0.00000     0.00000     0.00000  ;
     6    5    7    8      3     30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
     6    5    7   14      3     30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
     7    8   18   19      3      3.76560     0.00000    -3.76560     0.00000     0.00000     0.00000  ;
     8    7   14   15      3      0.00000     0.00000     0.00000     0.00000     0.00000     0.00000  ;
     8    7   14   16      3      0.00000     0.00000     0.00000     0.00000     0.00000     0.00000  ;
     8    7   14   17      3      0.00000     0.00000     0.00000     0.00000     0.00000     0.00000  ;
     8    9   10   11      3      0.00000     0.00000     0.00000     0.00000     0.00000     0.00000  ;
     8    9   10   12      3      0.00000     0.00000     0.00000     0.00000     0.00000     0.00000  ;
     8    9   10   13      3      0.00000     0.00000     0.00000     0.00000     0.00000     0.00000  ;
     9    8   18   19      3      3.76560     0.00000    -3.76560     0.00000     0.00000     0.00000  ;
    18   20   22   23      3      0.00000     0.00000     0.00000     0.00000     0.00000     0.00000  ;
    18   20   22   24      3      0.00000     0.00000     0.00000     0.00000     0.00000     0.00000  ;
    19   18   20   21      3     29.28800    -8.36800   -20.92000     0.00000     0.00000     0.00000  ;
    19   18   20   22      3     20.92000     0.00000   -20.92000     0.00000     0.00000     0.00000  ;
    21   20   22   23      3      3.68192    -4.35136     0.00000     1.33888     0.00000     0.00000  ;
    21   20   22   24      3      3.68192    -4.35136     0.00000     1.33888     0.00000     0.00000  ;
    22   25   26   27      3      1.25520     3.76560     0.00000    -5.02080     0.00000     0.00000  ;
    22   25   26   28      3      1.25520     3.76560     0.00000    -5.02080     0.00000     0.00000  ;
    22   25   33   34      3      1.25520     3.76560     0.00000    -5.02080     0.00000     0.00000  ;
    22   25   33   35      3      1.25520     3.76560     0.00000    -5.02080     0.00000     0.00000  ;
    23   22   25   26      3      1.25520     3.76560     0.00000    -5.02080     0.00000     0.00000  ;
    23   22   25   33      3      1.25520     3.76560     0.00000    -5.02080     0.00000     0.00000  ;
    24   22   25   26      3      1.25520     3.76560     0.00000    -5.02080     0.00000     0.00000  ;
    24   22   25   33      3      1.25520     3.76560     0.00000    -5.02080     0.00000     0.00000  ;
    25   26   29   30      3      0.65270     1.95811     0.00000    -2.61082     0.00000     0.00000  ;
    25   26   29   31      3      0.65270     1.95811     0.00000    -2.61082     0.00000     0.00000  ;
```

```
    25   26   29   32     3     0.65270     1.95811     0.00000    -2.61082     0.00000     0.00000  ;
    25   33   36   37     3     0.65270     1.95811     0.00000    -2.61082     0.00000     0.00000  ;
    25   33   36   38     3     0.65270     1.95811     0.00000    -2.61082     0.00000     0.00000  ;
    25   33   36   39     3     0.65270     1.95811     0.00000    -2.61082     0.00000     0.00000  ;
    26   25   33   34     3     1.25520     3.76560     0.00000    -5.02080     0.00000     0.00000  ;
    26   25   33   35     3     1.25520     3.76560     0.00000    -5.02080     0.00000     0.00000  ;
    27   26   25   33     3     1.25520     3.76560     0.00000    -5.02080     0.00000     0.00000  ;
    27   26   29   30     3     0.65270     1.95811     0.00000    -2.61082     0.00000     0.00000  ;
    27   26   29   31     3     0.65270     1.95811     0.00000    -2.61082     0.00000     0.00000  ;
    27   26   29   32     3     0.65270     1.95811     0.00000    -2.61082     0.00000     0.00000  ;
    28   26   25   33     3     1.25520     3.76560     0.00000    -5.02080     0.00000     0.00000  ;
    28   26   29   30     3     0.65270     1.95811     0.00000    -2.61082     0.00000     0.00000  ;
    28   26   29   31     3     0.65270     1.95811     0.00000    -2.61082     0.00000     0.00000  ;
    28   26   29   32     3     0.65270     1.95811     0.00000    -2.61082     0.00000     0.00000  ;
    34   33   36   37     3     0.65270     1.95811     0.00000    -2.61082     0.00000     0.00000  ;
    34   33   36   38     3     0.65270     1.95811     0.00000    -2.61082     0.00000     0.00000  ;
    34   33   36   39     3     0.65270     1.95811     0.00000    -2.61082     0.00000     0.00000  ;
    35   33   36   37     3     0.65270     1.95811     0.00000    -2.61082     0.00000     0.00000  ;
    35   33   36   38     3     0.65270     1.95811     0.00000    -2.61082     0.00000     0.00000  ;
    35   33   36   39     3     0.65270     1.95811     0.00000    -2.61082     0.00000     0.00000  ;
     2    1    9    3     3     9.20480     0.00000    -9.20480     0.00000     0.00000     0.00000  ;
     1    5    3    4     3     9.20480     0.00000    -9.20480     0.00000     0.00000     0.00000  ;
     3    7    5    6     3     9.20480     0.00000    -9.20480     0.00000     0.00000     0.00000  ;
    20    8   18   19     3     9.20480     0.00000    -9.20480     0.00000     0.00000     0.00000  ;
     1    3    5    7     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
     1    9    8    7     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
     1    9    8   18     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
     3    1    9    8     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
     3    1    9   10     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
     3    5    7    8     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
     3    5    7   14     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
     9    1    3    5     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
     5    7    8    9     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
     5    7    8   18     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
     7    8    9   10     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
     7    8   18   20     3     3.76560     0.00000    -3.76560     0.00000     0.00000     0.00000  ;
     8   18   20   21     3    20.92000     0.00000   -20.92000     0.00000     0.00000     0.00000  ;
     8   18   20   22     3    20.92000     0.00000   -20.92000     0.00000     0.00000     0.00000  ;
     9    8    7   14     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
     9    8   18   20     3     3.76560     0.00000    -3.76560     0.00000     0.00000     0.00000  ;
    10    9    8   18     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    14    7    8   18     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    18   20   22   25     3     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000  ;
    20   22   25   26     3     1.25520     3.76560     0.00000    -5.02080     0.00000     0.00000  ;
    20   22   25   33     3     1.25520     3.76560     0.00000    -5.02080     0.00000     0.00000  ;
    21   20   22   25     3     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000  ;
    22   25   26   29     3     5.27184     3.76560    -4.01664    -5.02080     0.00000     0.00000  ;
    22   25   33   36     3     5.27184     3.76560    -4.01664    -5.02080     0.00000     0.00000  ;
    26   25   33   36     3     5.27184     3.76560    -4.01664    -5.02080     0.00000     0.00000  ;
    29   26   25   33     3     5.27184     3.76560    -4.01664    -5.02080     0.00000     0.00000  ;
     5    8    7   14     3     9.20480     0.00000    -9.20480     0.00000     0.00000     0.00000  ;
     7    9    8   18     3     9.20480     0.00000    -9.20480     0.00000     0.00000     0.00000  ;
    10    1    9    8     3     9.20480     0.00000    -9.20480     0.00000     0.00000     0.00000  ;
    22   18   20   21     3    87.86400     0.00000   -87.86400     0.00000     0.00000     0.00000  ;

end--------------------------------------------------------------------------------------------------------------------
```

Lidocaine (polarized charges, hexadecane)

```
[ moleculetype ]
; Name            nrexcl
Lidocaine             3

[ atoms ]
;   nr       type  resnr residue  atom   cgnr     charge       mass  typeB    chargeB
     1         ca      1    LIG      C      1   -0.3681  12.000000
     2         ha      1    LIG      H      2    0.1902   1.000000
     3         ca      1    LIG     C1      3   -0.0927  12.000000
     4         ha      1    LIG     H1      4    0.1608   1.000000
     5         ca      1    LIG     C2      5   -0.3681  12.000000
     6         ha      1    LIG     H2      6    0.1902   1.000000
     7         ca      1    LIG     C3      7    0.2372  12.000000
     8         ca      1    LIG     C4      8   -0.0200  12.000000
     9         ca      1    LIG     C5      9    0.2451  12.000000
    10         c3      1    LIG     C6     10   -0.3072  12.000000
    11         hc      1    LIG     H3     11    0.0902   1.000000
    12         hc      1    LIG     H4     12    0.0902   1.000000
    13         hc      1    LIG     H5     13    0.0902   1.000000
    14         c3      1    LIG     C7     14   -0.3072  12.000000
    15         hc      1    LIG     H6     15    0.0902   1.000000
    16         hc      1    LIG     H7     16    0.0902   1.000000
    17         hc      1    LIG     H8     17    0.0902   1.000000
    18          n      1    LIG      N     18   -0.4665  14.000000
    19         hn      1    LIG     H9     19    0.3287   1.000000
    20          c      1    LIG     C8     20    0.6213  12.000000
    21          o      1    LIG      O     21   -0.6684  16.000000
    22         c3      1    LIG     C9     22    0.1071  12.000000
    23         h1      1    LIG    H10     23    0.0073   1.000000
    24         h1      1    LIG    H11     24    0.0073   1.000000
    25         n3      1    LIG     N1     25   -0.1512  14.000000
    26         c3      1    LIG    C10     26   -0.0300  12.000000
```

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    27         h1      1    LIG    H12     27    0.0506   1.000000
    28         h1      1    LIG    H13     28    0.0506   1.000000
    29         c3      1    LIG    C11     29   -0.1755  12.000000
    30         hc      1    LIG    H14     30    0.0536   1.000000
    31         hc      1    LIG    H15     31    0.0536   1.000000
    32         hc      1    LIG    H16     32    0.0536   1.000000
    33         c3      1    LIG    C12     33   -0.0300  12.000000
    34         h1      1    LIG    H17     34    0.0506   1.000000
    35         h1      1    LIG    H18     35    0.0506   1.000000
    36         c3      1    LIG    C13     36   -0.1755  12.000000
    37         hc      1    LIG    H19     37    0.0536   1.000000
    38         hc      1    LIG    H20     38    0.0536   1.000000
    39         hc      1    LIG    H21     39    0.0536   1.000000

[ bonds ]
;  ai    aj funct  r  k
    1     2     1  1.0870e-01  2.8811e+05
    3     4     1  1.0870e-01  2.8811e+05
    5     6     1  1.0870e-01  2.8811e+05
   10    11     1  1.0920e-01  2.8225e+05
   10    12     1  1.0920e-01  2.8225e+05
   10    13     1  1.0920e-01  2.8225e+05
   14    15     1  1.0920e-01  2.8225e+05
   14    16     1  1.0920e-01  2.8225e+05
   14    17     1  1.0920e-01  2.8225e+05
   18    19     1  1.0090e-01  3.4326e+05
   22    23     1  1.0930e-01  2.8108e+05
   22    24     1  1.0930e-01  2.8108e+05
   26    27     1  1.0930e-01  2.8108e+05
   26    28     1  1.0930e-01  2.8108e+05
   29    30     1  1.0920e-01  2.8225e+05
   29    31     1  1.0920e-01  2.8225e+05
   29    32     1  1.0920e-01  2.8225e+05
   33    34     1  1.0930e-01  2.8108e+05
   33    35     1  1.0930e-01  2.8108e+05
   36    37     1  1.0920e-01  2.8225e+05
   36    38     1  1.0920e-01  2.8225e+05
   36    39     1  1.0920e-01  2.8225e+05
    1     3     1  1.3870e-01  4.0033e+05
    1     9     1  1.3870e-01  4.0033e+05
    3     5     1  1.3870e-01  4.0033e+05
    5     7     1  1.3870e-01  4.0033e+05
    7     8     1  1.3870e-01  4.0033e+05
    7    14     1  1.5130e-01  2.7070e+05
    8     9     1  1.3870e-01  4.0033e+05
    8    18     1  1.4220e-01  3.1154e+05
    9    10     1  1.5130e-01  2.7070e+05
   18    20     1  1.3450e-01  4.0016e+05
   20    21     1  1.2140e-01  5.4225e+05
   20    22     1  1.5080e-01  2.7472e+05
   22    25     1  1.4700e-01  2.6828e+05
   25    26     1  1.4700e-01  2.6828e+05
   25    33     1  1.4700e-01  2.6828e+05
   26    29     1  1.5350e-01  2.5363e+05
   33    36     1  1.5350e-01  2.5363e+05

[ pairs ]
;  ai    aj funct
    1     6     1
    1    11     1
    1    12     1
    1    13     1
    2     4     1
    2     5     1
    2     8     1
    2    10     1
    9     4     1
    4     6     1
    4     7     1
    5    15     1
    5    16     1
    5    17     1
    6     8     1
    6    14     1
    7    19     1
    8    15     1
    8    16     1
    8    17     1
    8    11     1
    8    12     1
    8    13     1
    9    19     1
   18    23     1
   18    24     1
   19    21     1
   19    22     1
   21    23     1
   21    24     1
   22    27     1
   22    28     1
   22    34     1
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    22     35      1
    23     26      1
    23     33      1
    24     26      1
    24     33      1
    25     30      1
    25     31      1
    25     32      1
    25     37      1
    25     38      1
    25     39      1
    26     34      1
    26     35      1
    27     33      1
    27     30      1
    27     31      1
    27     32      1
    28     33      1
    28     30      1
    28     31      1
    28     32      1
    34     37      1
    34     38      1
    34     39      1
    35     37      1
    35     38      1
    35     39      1
     1      7      1
     1     18      1
     3      8      1
     3     10      1
     3     14      1
     9      5      1
     5     18      1
     7     10      1
     7     20      1
     8     21      1
     8     22      1
     9     14      1
     9     20      1
    10     18      1
    14     18      1
    18     25      1
    20     26      1
    20     33      1
    21     25      1
    22     29      1
    22     36      1
    26     36      1
    29     33      1

[ angles ]
;  ai    aj    ak funct  theta   cth
    1     3     4     1  1.2001e+02  4.0551e+02
    2     1     3     1  1.2001e+02  4.0551e+02
    2     1     9     1  1.2001e+02  4.0551e+02
    3     5     6     1  1.2001e+02  4.0551e+02
    4     3     5     1  1.2001e+02  4.0551e+02
    6     5     7     1  1.2001e+02  4.0551e+02
    7    14    15     1  1.1015e+02  3.9296e+02
    7    14    16     1  1.1015e+02  3.9296e+02
    7    14    17     1  1.1015e+02  3.9296e+02
    8    18    19     1  1.1594e+02  3.9631e+02
    9    10    11     1  1.1015e+02  3.9296e+02
    9    10    12     1  1.1015e+02  3.9296e+02
    9    10    13     1  1.1015e+02  3.9296e+02
   11    10    12     1  1.0835e+02  3.2995e+02
   11    10    13     1  1.0835e+02  3.2995e+02
   12    10    13     1  1.0835e+02  3.2995e+02
   15    14    16     1  1.0835e+02  3.2995e+02
   15    14    17     1  1.0835e+02  3.2995e+02
   16    14    17     1  1.0835e+02  3.2995e+02
   19    18    20     1  1.1846e+02  4.1179e+02
   20    22    23     1  1.0766e+02  3.9857e+02
   20    22    24     1  1.0766e+02  3.9857e+02
   23    22    24     1  1.0955e+02  3.2786e+02
   23    22    25     1  1.0992e+02  4.1330e+02
   24    22    25     1  1.0992e+02  4.1330e+02
   25    26    27     1  1.0992e+02  4.1330e+02
   25    26    28     1  1.0992e+02  4.1330e+02
   25    33    34     1  1.0992e+02  4.1330e+02
   25    33    35     1  1.0992e+02  4.1330e+02
   26    29    30     1  1.1005e+02  3.8802e+02
   26    29    31     1  1.1005e+02  3.8802e+02
   26    29    32     1  1.1005e+02  3.8802e+02
   27    26    28     1  1.0955e+02  3.2786e+02
   27    26    29     1  1.1007e+02  3.8794e+02
   28    26    29     1  1.1007e+02  3.8794e+02
   30    29    31     1  1.0835e+02  3.2995e+02
   30    29    32     1  1.0835e+02  3.2995e+02
   31    29    32     1  1.0835e+02  3.2995e+02
```

```
    33    36    37     1  1.1005e+02  3.8802e+02
    33    36    38     1  1.1005e+02  3.8802e+02
    33    36    39     1  1.1005e+02  3.8802e+02
    34    33    35     1  1.0955e+02  3.2786e+02
    34    33    36     1  1.1007e+02  3.8794e+02
    35    33    36     1  1.1007e+02  3.8794e+02
    37    36    38     1  1.0835e+02  3.2995e+02
    37    36    39     1  1.0835e+02  3.2995e+02
    38    36    39     1  1.0835e+02  3.2995e+02
     1     3     5     1  1.1997e+02  5.6216e+02
     1     9     8     1  1.1997e+02  5.6216e+02
     1     9    10     1  1.2063e+02  5.3421e+02
     3     1     9     1  1.1997e+02  5.6216e+02
     3     5     7     1  1.1997e+02  5.6216e+02
     5     7     8     1  1.1997e+02  5.6216e+02
     5     7    14     1  1.2063e+02  5.3421e+02
     7     8     9     1  1.1997e+02  5.6216e+02
     7     8    18     1  1.1989e+02  5.6877e+02
     8     7    14     1  1.2063e+02  5.3421e+02
     8     9    10     1  1.2063e+02  5.3421e+02
     8    18    20     1  1.2371e+02  5.3798e+02
     9     8    18     1  1.1989e+02  5.6877e+02
    18    20    21     1  1.2203e+02  6.3455e+02
    18    20    22     1  1.1515e+02  5.6785e+02
    20    22    25     1  1.1114e+02  5.5723e+02
    21    20    22     1  1.2311e+02  5.6928e+02
    22    25    26     1  1.1090e+02  5.3564e+02
    22    25    33     1  1.1090e+02  5.3564e+02
    25    26    29     1  1.1038e+02  5.5379e+02
    25    33    36     1  1.1038e+02  5.5379e+02
    26    25    33     1  1.1090e+02  5.3564e+02

[ dihedrals ]
;i   j    k   l      func    C0   ...   C5
     1    3    5    6      3     30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
     1    9   10   11      3      0.00000     0.00000     0.00000     0.00000     0.00000     0.00000  ;
     1    9   10   12      3      0.00000     0.00000     0.00000     0.00000     0.00000     0.00000  ;
     1    9   10   13      3      0.00000     0.00000     0.00000     0.00000     0.00000     0.00000  ;
     2    1    3    4      3     30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
     2    1    3    5      3     30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
     2    1    9    8      3     30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
     2    1    9   10      3     30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
     9    1    3    4      3     30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
     4    3    5    6      3     30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
     4    3    5    7      3     30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
     5    7   14   15      3      0.00000     0.00000     0.00000     0.00000     0.00000     0.00000  ;
     5    7   14   16      3      0.00000     0.00000     0.00000     0.00000     0.00000     0.00000  ;
     5    7   14   17      3      0.00000     0.00000     0.00000     0.00000     0.00000     0.00000  ;
     6    5    7    8      3     30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
     6    5    7   14      3     30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
     7    8   18   19      3      3.76560     0.00000    -3.76560     0.00000     0.00000     0.00000  ;
     8    7   14   15      3      0.00000     0.00000     0.00000     0.00000     0.00000     0.00000  ;
     8    7   14   16      3      0.00000     0.00000     0.00000     0.00000     0.00000     0.00000  ;
     8    7   14   17      3      0.00000     0.00000     0.00000     0.00000     0.00000     0.00000  ;
     8    9   10   11      3      0.00000     0.00000     0.00000     0.00000     0.00000     0.00000  ;
     8    9   10   12      3      0.00000     0.00000     0.00000     0.00000     0.00000     0.00000  ;
     8    9   10   13      3      0.00000     0.00000     0.00000     0.00000     0.00000     0.00000  ;
     9    8   18   19      3      3.76560     0.00000    -3.76560     0.00000     0.00000     0.00000  ;
    18   20   22   23      3      0.00000     0.00000     0.00000     0.00000     0.00000     0.00000  ;
    18   20   22   24      3      0.00000     0.00000     0.00000     0.00000     0.00000     0.00000  ;
    19   18   20   21      3     29.28800    -8.36800   -20.92000     0.00000     0.00000     0.00000  ;
    19   18   20   22      3     20.92000     0.00000   -20.92000     0.00000     0.00000     0.00000  ;
    21   20   22   23      3      3.68192    -4.35136     0.00000     1.33888     0.00000     0.00000  ;
    21   20   22   24      3      3.68192    -4.35136     0.00000     1.33888     0.00000     0.00000  ;
    22   25   26   27      3      1.25520     3.76560     0.00000    -5.02080     0.00000     0.00000  ;
    22   25   26   28      3      1.25520     3.76560     0.00000    -5.02080     0.00000     0.00000  ;
    22   25   33   34      3      1.25520     3.76560     0.00000    -5.02080     0.00000     0.00000  ;
    22   25   33   35      3      1.25520     3.76560     0.00000    -5.02080     0.00000     0.00000  ;
    23   22   25   26      3      1.25520     3.76560     0.00000    -5.02080     0.00000     0.00000  ;
    23   22   25   33      3      1.25520     3.76560     0.00000    -5.02080     0.00000     0.00000  ;
    24   22   25   26      3      1.25520     3.76560     0.00000    -5.02080     0.00000     0.00000  ;
    24   22   25   33      3      1.25520     3.76560     0.00000    -5.02080     0.00000     0.00000  ;
    25   26   29   30      3      0.65270     1.95811     0.00000    -2.61082     0.00000     0.00000  ;
    25   26   29   31      3      0.65270     1.95811     0.00000    -2.61082     0.00000     0.00000  ;
    25   26   29   32      3      0.65270     1.95811     0.00000    -2.61082     0.00000     0.00000  ;
    25   33   36   37      3      0.65270     1.95811     0.00000    -2.61082     0.00000     0.00000  ;
    25   33   36   38      3      0.65270     1.95811     0.00000    -2.61082     0.00000     0.00000  ;
    25   33   36   39      3      0.65270     1.95811     0.00000    -2.61082     0.00000     0.00000  ;
    26   25   33   34      3      1.25520     3.76560     0.00000    -5.02080     0.00000     0.00000  ;
    26   25   33   35      3      1.25520     3.76560     0.00000    -5.02080     0.00000     0.00000  ;
    27   26   25   33      3      1.25520     3.76560     0.00000    -5.02080     0.00000     0.00000  ;
    27   26   29   30      3      0.65270     1.95811     0.00000    -2.61082     0.00000     0.00000  ;
    27   26   29   31      3      0.65270     1.95811     0.00000    -2.61082     0.00000     0.00000  ;
    27   26   29   32      3      0.65270     1.95811     0.00000    -2.61082     0.00000     0.00000  ;
    28   26   25   33      3      1.25520     3.76560     0.00000    -5.02080     0.00000     0.00000  ;
    28   26   29   30      3      0.65270     1.95811     0.00000    -2.61082     0.00000     0.00000  ;
    28   26   29   31      3      0.65270     1.95811     0.00000    -2.61082     0.00000     0.00000  ;
    28   26   29   32      3      0.65270     1.95811     0.00000    -2.61082     0.00000     0.00000  ;
    34   33   36   37      3      0.65270     1.95811     0.00000    -2.61082     0.00000     0.00000  ;
    34   33   36   38      3      0.65270     1.95811     0.00000    -2.61082     0.00000     0.00000  ;
    34   33   36   39      3      0.65270     1.95811     0.00000    -2.61082     0.00000     0.00000  ;
```

```
    35   33   36   37    3     0.65270     1.95811     0.00000    -2.61082     0.00000     0.00000  ;
    35   33   36   38    3     0.65270     1.95811     0.00000    -2.61082     0.00000     0.00000  ;
    35   33   36   39    3     0.65270     1.95811     0.00000    -2.61082     0.00000     0.00000  ;
    2    1    9    3     3     9.20480     0.00000    -9.20480     0.00000     0.00000     0.00000  ;
    1    5    3    4     3     9.20480     0.00000    -9.20480     0.00000     0.00000     0.00000  ;
    3    7    5    6     3     9.20480     0.00000    -9.20480     0.00000     0.00000     0.00000  ;
    20   8    18   19    3     9.20480     0.00000    -9.20480     0.00000     0.00000     0.00000  ;
    1    3    5    7     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    1    9    8    7     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    1    9    8    18    3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    3    1    9    8     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    3    1    9    10    3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    3    5    7    8     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    3    5    7    14    3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    9    1    3    5     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    5    7    8    9     3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    5    7    8    18    3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    7    8    9    10    3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    7    8    18   20    3     3.76560     0.00000    -3.76560     0.00000     0.00000     0.00000  ;
    8    18   20   21    3    20.92000     0.00000   -20.92000     0.00000     0.00000     0.00000  ;
    8    18   20   22    3    20.92000     0.00000   -20.92000     0.00000     0.00000     0.00000  ;
    9    8    7    14    3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    9    8    18   20    3     3.76560     0.00000    -3.76560     0.00000     0.00000     0.00000  ;
    10   9    8    18    3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    14   7    8    18    3    30.33400     0.00000   -30.33400     0.00000     0.00000     0.00000  ;
    18   20   22   25    3     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000  ;
    20   22   25   26    3     1.25520     3.76560     0.00000    -5.02080     0.00000     0.00000  ;
    20   22   25   33    3     1.25520     3.76560     0.00000    -5.02080     0.00000     0.00000  ;
    21   20   22   25    3     0.00000     0.00000     0.00000     0.00000     0.00000     0.00000  ;
    22   25   26   29    3     5.27184     3.76560    -4.01664    -5.02080     0.00000     0.00000  ;
    22   25   33   36    3     5.27184     3.76560    -4.01664    -5.02080     0.00000     0.00000  ;
    26   25   33   36    3     5.27184     3.76560    -4.01664    -5.02080     0.00000     0.00000  ;
    29   26   25   33    3     5.27184     3.76560    -4.01664    -5.02080     0.00000     0.00000  ;
    5    8    7    14    3     9.20480     0.00000    -9.20480     0.00000     0.00000     0.00000  ;
    7    9    8    18    3     9.20480     0.00000    -9.20480     0.00000     0.00000     0.00000  ;
    10   1    9    8     3     9.20480     0.00000    -9.20480     0.00000     0.00000     0.00000  ;
    22   18   20   21    3    87.86400     0.00000   -87.86400     0.00000     0.00000     0.00000  ;

end-------------------------------------------------------------------------------------------------------------------
```

Methanol (gas phase charges)

```
[ moleculetype ]
; Name            nrexcl
Methanol             3

[ atoms ]
;   nr       type  resnr residue  atom   cgnr     charge       mass  typeB    chargeB
     1         c3      1    LIG      C      1    0.1615  12.000000
     2         h1      1    LIG      H      2    0.0194   1.000000
     3         h1      1    LIG     H1      3    0.0194   1.000000
     4         h1      1    LIG     H2      4    0.0194   1.000000
     5         oh      1    LIG      O      5   -0.6019  16.000000
     6         ho      1    LIG     H3      6    0.3822   1.000000

[ bonds ]
;  ai    aj funct  r  k
    1     2     1  1.0930e-01  2.8108e+05
    1     3     1  1.0930e-01  2.8108e+05
    1     4     1  1.0930e-01  2.8108e+05
    5     6     1  9.7400e-02  3.0928e+05
    1     5     1  1.4260e-01  2.6284e+05

[ pairs ]
;  ai    aj funct
     2      6      1
     3      6      1
     4      6      1

[ angles ]
;  ai    aj    ak funct  theta   cth
    1     5     6     1  1.0816e+02  3.9405e+02
    2     1     3     1  1.0955e+02  3.2786e+02
    2     1     4     1  1.0955e+02  3.2786e+02
    2     1     5     1  1.0988e+02  4.2652e+02
    3     1     4     1  1.0955e+02  3.2786e+02
    3     1     5     1  1.0988e+02  4.2652e+02
    4     1     5     1  1.0988e+02  4.2652e+02

[ dihedrals ]
;i  j   k  l      func    C0  ...  C5
    2    1    5    6      3     0.69873     2.09618     0.00000    -2.79491     0.00000     0.00000  ;
    3    1    5    6      3     0.69873     2.09618     0.00000    -2.79491     0.00000     0.00000  ;
    4    1    5    6      3     0.69873     2.09618     0.00000    -2.79491     0.00000     0.00000  ;

end----------------------------------------------------------------------------------------------------------------------------
```

Methanol (polarized charges, water)

```
[ moleculetype ]
; Name            nrexcl
Methanol             3

[ atoms ]
;   nr       type  resnr residue  atom   cgnr     charge       mass  typeB    chargeB
     1         c3      1    LIG      C      1    0.2049  12.000000
     2         h1      1    LIG      H      2    0.0189   1.000000
     3         h1      1    LIG     H1      3    0.0189   1.000000
     4         h1      1    LIG     H2      4    0.0189   1.000000
     5         oh      1    LIG      O      5   -0.6903  16.000000
     6         ho      1    LIG     H3      6    0.4287   1.000000

[ bonds ]
;  ai    aj funct  r  k
    1     2     1  1.0930e-01  2.8108e+05
    1     3     1  1.0930e-01  2.8108e+05
    1     4     1  1.0930e-01  2.8108e+05
    5     6     1  9.7400e-02  3.0928e+05
    1     5     1  1.4260e-01  2.6284e+05

[ pairs ]
;  ai    aj funct
     2      6      1
     3      6      1
     4      6      1

[ angles ]
;  ai    aj    ak funct  theta   cth
    1     5     6     1  1.0816e+02  3.9405e+02
    2     1     3     1  1.0955e+02  3.2786e+02
    2     1     4     1  1.0955e+02  3.2786e+02
    2     1     5     1  1.0988e+02  4.2652e+02
    3     1     4     1  1.0955e+02  3.2786e+02
    3     1     5     1  1.0988e+02  4.2652e+02
    4     1     5     1  1.0988e+02  4.2652e+02

[ dihedrals ]
;i  j   k  l      func    C0  ...  C5
    2    1    5    6      3     0.69873     2.09618     0.00000    -2.79491     0.00000     0.00000  ;
    3    1    5    6      3     0.69873     2.09618     0.00000    -2.79491     0.00000     0.00000  ;
    4    1    5    6      3     0.69873     2.09618     0.00000    -2.79491     0.00000     0.00000  ;
```

```
end--------------------------------------------------------------------------------------------------------------------
```

Methanol (polarized charges, hexadecane)

```
[ moleculetype ]
; Name            nrexcl
Methanol             3

[ atoms ]
;   nr       type  resnr residue  atom   cgnr     charge       mass  typeB    chargeB
     1         c3      1    LIG      C      1    0.1780  12.000000
     2         h1      1    LIG      H      2    0.0193   1.000000
     3         h1      1    LIG     H1      3    0.0193   1.000000
     4         h1      1    LIG     H2      4    0.0193   1.000000
     5         oh      1    LIG      O      5   -0.6357  16.000000
     6         ho      1    LIG     H3      6    0.3998   1.000000

[ bonds ]
;  ai    aj funct  r  k
    1     2     1  1.0930e-01  2.8108e+05
    1     3     1  1.0930e-01  2.8108e+05
    1     4     1  1.0930e-01  2.8108e+05
    5     6     1  9.7400e-02  3.0928e+05
    1     5     1  1.4260e-01  2.6284e+05

[ pairs ]
;  ai    aj funct
     2     6     1
     3     6     1
     4     6     1

[ angles ]
;  ai    aj    ak funct  theta   cth
    1     5     6     1  1.0816e+02  3.9405e+02
    2     1     3     1  1.0955e+02  3.2786e+02
    2     1     4     1  1.0955e+02  3.2786e+02
    2     1     5     1  1.0988e+02  4.2652e+02
    3     1     4     1  1.0955e+02  3.2786e+02
    3     1     5     1  1.0988e+02  4.2652e+02
    4     1     5     1  1.0988e+02  4.2652e+02

[ dihedrals ]
;i  j   k  l      func    C0  ...  C5
    2    1    5    6      3     0.69873     2.09618     0.00000    -2.79491     0.00000     0.00000  ;
    3    1    5    6      3     0.69873     2.09618     0.00000    -2.79491     0.00000     0.00000  ;
    4    1    5    6      3     0.69873     2.09618     0.00000    -2.79491     0.00000     0.00000  ;

end--------------------------------------------------------------------------------------------------------------------
```

1. Gromacs topologies

1,3,5 trichlorobenzene

```
135trichlorobenzene
 12
    10       C1    1  -0.109   0.088   0.000
    10       H2    2  -0.193   0.156   0.000
    10       C3    3  -0.128  -0.049   0.000
    10       C4    4  -0.022  -0.138   0.000
    10       H5    5  -0.039  -0.245  -0.000
    10       C6    6   0.107  -0.087  -0.000
    10       C7    7   0.131   0.050   0.000
    10       H8    8   0.232   0.089   0.000
    10       C9    9   0.022   0.136  -0.000
    10      X10   10   0.049   0.308  -0.000
    10      X11   11   0.242  -0.197  -0.000
    10      X12   12  -0.292  -0.112  -0.000
    0.24230   -0.19670   -0.00000

end--------------------------------------------------------------------------------------------------------------------------
```

Chlorobenzene

```
Chlorobenzene
   12
    1LIG      C    1   0.018  -0.120  -0.000
    1LIG      H    2  -0.037  -0.214   0.000
    1LIG     C1    3   0.157  -0.120  -0.000
    1LIG     H1    4   0.211  -0.214   0.000
    1LIG     C2    5   0.226   0.000   0.000
    1LIG     H2    6   0.335  -0.000  -0.000
    1LIG     C3    7   0.157   0.120   0.000
    1LIG     H3    8   0.211   0.214  -0.000
    1LIG     C4    9   0.018   0.120   0.000
    1LIG     H4   10  -0.037   0.214  -0.000
    1LIG     C5   11  -0.051  -0.000  -0.000
    1LIG     CL   12  -0.224   0.000   0.000
  10.05020  10.00000  10.00000

end--------------------------------------------------------------------------------------------------------------------------
```

Chloroform

```
Chloroform
    5
    1LIG      C    1   0.000   0.000   0.046
    1LIG      H    2  -0.000  -0.000   0.155
    1LIG     CL    3   0.079   0.151  -0.009
    1LIG    Cl1    4   0.091  -0.144  -0.009
    1LIG    Cl2    5  -0.170  -0.007  -0.009
   1.00000   1.00000   1.00000

end--------------------------------------------------------------------------------------------------------------------------
```

2,4,5 trichloroaniline

```
245trichloroaniline
 14
    1LIG      C    1   0.088  -0.071   0.000
    1LIG     C1    2  -0.042  -0.119   0.000
    1LIG      H    3  -0.060  -0.226   0.000
    1LIG     C2    4  -0.150  -0.032   0.000
    1LIG     C3    5  -0.132   0.108  -0.000
    1LIG     C4    6   0.001   0.155   0.000
    1LIG     H1    7   0.020   0.261  -0.000
    1LIG     C5    8   0.109   0.067   0.000
    1LIG     CL    9   0.221  -0.185  -0.000
    1LIG    Cl1   10   0.270   0.135   0.000
    1LIG    Cl2   11  -0.313  -0.097   0.000
    1LIG      N   12  -0.238   0.195  -0.000
    1LIG     H2   13  -0.332   0.160   0.000
    1LIG     H3   14  -0.223   0.294   0.000
   -0.33190    0.16040    0.00000

end--------------------------------------------------------------------------------------------------------------------------
```

Lidocaine

```
Lidocaine
   39
    1LIG      C    1   0.308  -0.055  -0.069  0.0012 -0.0007 -0.0009
    1LIG      H    2   0.382  -0.052  -0.149  0.0013  0.0001 -0.0014
    1LIG     C1    3   0.296  -0.170   0.008  0.0006 -0.0008 -0.0002
    1LIG     H1    4   0.361  -0.255  -0.011  0.0008 -0.0011 -0.0002
    1LIG     C2    5   0.202  -0.174   0.110  0.0005 -0.0016  0.0004
    1LIG     H2    6   0.194  -0.263   0.171 -0.0001 -0.0016  0.0011
    1LIG     C3    7   0.120  -0.065   0.133 -0.0003 -0.0011  0.0009
    1LIG     C4    8   0.131   0.049   0.055 -0.0001  0.0002  0.0000
    1LIG     C5    9   0.227   0.054  -0.046  0.0009  0.0003 -0.0011
    1LIG     C6   10   0.246   0.178  -0.131  0.0002  0.0015 -0.0010
    1LIG     H3   11   0.241   0.269  -0.071 -0.0000  0.0007  0.0005
    1LIG     H4   12   0.169   0.183  -0.208 -0.0006  0.0000 -0.0006
    1LIG     H5   13   0.343   0.176  -0.181  0.0008 -0.0000 -0.0004
    1LIG     C7   14   0.020  -0.073   0.247 -0.0012 -0.0001  0.0013
    1LIG     H6   15   0.048  -0.002   0.326  0.0002  0.0005  0.0006
    1LIG     H7   16   0.017  -0.173   0.290 -0.0000 -0.0008  0.0003
    1LIG     H8   17  -0.080  -0.048   0.212 -0.0008  0.0002 -0.0003
    1LIG      N   18   0.045   0.160   0.078 -0.0002  0.0017  0.0012
    1LIG     H9   19   0.069   0.223   0.153  0.0006  0.0015  0.0018
    1LIG     C8   20  -0.070   0.190   0.015 -0.0008  0.0002 -0.0004
    1LIG      O   21  -0.129   0.290   0.052 -0.0005  0.0008  0.0003
    1LIG     C9   22  -0.118   0.101  -0.097 -0.0002 -0.0004 -0.0010
    1LIG    H10   23  -0.031   0.078  -0.158  0.0006 -0.0001 -0.0004
    1LIG    H11   24  -0.187   0.159  -0.159 -0.0005  0.0004 -0.0004
    1LIG     N1   25  -0.184  -0.022  -0.051 -0.0001 -0.0003  0.0002
    1LIG    C10   26  -0.194  -0.124  -0.157 -0.0000 -0.0001 -0.0001
    1LIG    H12   27  -0.245  -0.082  -0.244 -0.0000  0.0000 -0.0001
    1LIG    H13   28  -0.254  -0.208  -0.121 -0.0001 -0.0001  0.0000
    1LIG    C11   29  -0.058  -0.181  -0.198  0.0000 -0.0000 -0.0000
    1LIG    H14   30  -0.003  -0.215  -0.110  0.0000 -0.0000  0.0000
    1LIG    H15   31   0.003  -0.108  -0.252  0.0000  0.0000 -0.0000
    1LIG    H16   32  -0.072  -0.267  -0.264 -0.0000 -0.0000 -0.0000
    1LIG    C12   33  -0.313   0.008   0.013 -0.0001  0.0001  0.0000
    1LIG    H17   34  -0.385   0.043  -0.062 -0.0001  0.0000 -0.0001
    1LIG    H18   35  -0.299   0.089   0.086  0.0000  0.0001  0.0001
    1LIG    C13   36  -0.372  -0.111   0.090 -0.0000 -0.0000  0.0000
    1LIG    H19   37  -0.298  -0.155   0.157  0.0000 -0.0000  0.0000
    1LIG    H20   38  -0.410  -0.188   0.023 -0.0000 -0.0000 -0.0000
    1LIG    H21   39  -0.456  -0.077   0.151 -0.0000  0.0000  0.0000
   2.50890   2.02520   2.10950

end----------------------------------------------------------------------------------------------------------------------
```

Methanol

```
Methanol
    6
    1LIG      C    1   0.070  -0.003  -0.000
    1LIG      H    2   0.104  -0.058  -0.088
    1LIG     H1    3   0.101  -0.055   0.090
    1LIG     H2    4   0.115   0.097  -0.001
    1LIG      O    5  -0.072   0.009  -0.003
    1LIG     H3    6  -0.110  -0.081  -0.002
   0.57520   0.51230   0.50000

end----------------------------------------------------------------------------------------------------------------------
```