The formation of topology file of a molecule:

After studying this chapter, you will be able to

1) Generate the topology file of small molecule like EtOH, MeOH, DMSO, etc.
2) Generate the topology file of protein molecules like phenyl alanine etc.
3) Generate the topology file of Toluene from phenyl alanine.

Keywords: topology file

Introduction

Here we are going to discuss how you can make a topology file of a molecule that is defined in the **aminoacids.rtp**fileand this file is present in the force field directory that is present in gromacs. You can see this file in the following directory

cd home/user/gromacs-4.5.4/gro4.5.4/share/gromacs/top

<enter>

Then you will see following force field directories

****

amber03.ffatommass.dat co-shift.dat encadv.ff ffG53a5.itp flexspc.itp**gromos53a5.ffoplsaa.ff** spc216.gro table6-10.xvg tip4p.itp

amber94.ff atom_nom.tbl defselection.dat export.dlg ffG53a6.itp flexwat-ferguson.itp **gromos53a6.ff** phbres.dat spce.itp table6-11.xvg tip5p.gro

amber96.ff bonds.dlg dgsolv.dat ffencads.itp ffgmx2.itp**gmx2.ff** gurgle.dat ps.m2p spc.itp table6-12.xvg vdwradii.dat

amber99.ff bromacs.dat edissoc.dat ffencadv.itpffgmx.itp**gmx.ff** ha-shift.dat random.dat specbond.dat table6-8.xvg xlateat.dat

amber99sb.ff ca-shift.dat electroneg.dat ffG43a1.itp ffoplsaa.itp gromos43a1.ff highway.dat refi_aa.dat ss.map table6-9.xvg

amber99sb-ildn.ff cb-shift.dat elements.dat ffG43a2.itp ffoplsaa-n.tst gromos43a2.ff ions.itp residuetypes.dat surface.dat tip3p.itp

note: the directories are shown in bold and underlined.

amberGS.ffcharmm27.ffencads.ff ffG45a3.itp flexspce.itp gromos45a3.ff
links.dat sfactor.dat sw.itp tip4p.gro

****

cdoplsaa.ff

<enter>

ls

<enter>

ls

<enter>

Now you will see following files

1propanol.itp aminoacids.hdb aminoacids.r2b aminoacids.vsd atomtypes.atp ffbonded.itp forcefield.doc gbsa.itp methanol.itp spc.itp tip4p.itp watermodels.dat

aminoacids.c.tdbaminoacids.n.tdbaminoacids.rtp atomname2type.n2t ethanol.itp ffnonbonded.itp forcefield.itp ions.itp spce.itp tip3p.itp tip5p.itp

Now type

vi**aminoacids.rtp**

In the above file, you will see

****

; Ethanol - CA is the carbon bound to the OH group

[EtOH]

[atoms]

CB opls_135 -0.180 1

HB1 opls_140 0.060 1

HB2 opls_140 0.060 1

HB3 opls_140 0.060 1

CA opls_157 0.145 2

HA1 opls_140 0.060 2

HA2 opls_140 0.060 2

OH opls_154 -0.683 2

HO opls_155 0.418 2

[bonds]

CB HB1

CB HB2

CB HB3

CB CA

CA HA1

CA HA2

CA OH

OH HO

****

Now you have got the EtOH.gro file

****

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1LIG C 1 -0.415 0.410 -0.016

1LIG C 2 -0.263 0.410 -0.015

1LIG H 3 -0.453 0.513 -0.021

1LIG H 4 -0.454 0.365 0.075

1LIG H 5 -0.453 0.355 -0.102

1LIG O 6 -0.215 0.480 0.098

1LIG H 7 -0.223 0.457 -0.106

1LIG H 8 -0.226 0.307 -0.010

1LIG H 9 -0.249 0.571 0.092

4.00000 4.00000 4.00000

****

From column 5 to 6, residue names are there, the residue name of ethanol defined in the **aminoacids.rtp file** is **EtOH.** Therefore you have to replace **LIG** by **EtOH**. Now you have to replace atom name of EtOH.gro file with atom name defined in the **aminoacids.rtp file.**

C→ CB

C→ CA

H→ HB1

H→ HB2

H→ HB3

O→ OH

H→ HA1

H→ HA2

H→ HO

****

The modified **EtOHmodified.gro** file is given below

****

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1EtOH CB 1 -0.415 0.410 -0.016

1EtOH CA 2 -0.263 0.410 -0.015

1EtOH HB1 3 -0.453 0.513 -0.021

1EtOH HB2 4 -0.454 0.365 0.075

1EtOH HB3 5 -0.453 0.355 -0.102

1EtOH OH 6 -0.215 0.480 0.098

1EtOH HA1 7 -0.223 0.457 -0.106

1EtOH HA2 8 -0.226 0.307 -0.010

1EtOH HO 9 -0.249 0.571 0.092

4.00000 4.00000 4.00000

****

Generation of topology file of ethanol molecule:

Now we will generate the topology file for ethanol molecule by giving following command

pdb2gmx -f EtOHmodified.gro

<enter>

The system will ask you to select the force filed.

****

Select the Force Field:

From '/usr/local/gromacs/share/gromacs/top':

1: AMBER03 force field (Duan et al., J. Comp. Chem. 24, 1999-2012, 2003)

2: AMBER94 force field (Cornell et al., JACS 117, 5179-5197, 1995)

3: AMBER96 force field (Kollman et al., Acc. Chem. Res. 29, 461-469, 1996)

4: AMBER99 force field (Wang et al., J. Comp. Chem. 21, 1049-1074, 2000)

5: AMBER99SB force field (Hornak et al., Proteins 65, 712-725, 2006)

6: AMBER99SB-ILDN force field (Lindorff-Larsen et al., Proteins 78, 1950-58, 2010)

7: AMBERGS force field (Garcia &Sanbonmatsu, PNAS 99, 2782-2787, 2002)

8: CHARMM27 all-atom force field (with CMAP) - version 2.0

9: GROMOS96 43a1 force field

10: GROMOS96 43a2 force field (improved alkane dihedrals)

11: GROMOS96 45a3 force field (Schuler JCC 2001 22 1205)

12: GROMOS96 53a5 force field (JCC 2004 vol 25 pag 1656)

13: GROMOS96 53a6 force field (JCC 2004 vol 25 pag 1656)

14: OPLS-AA/L all-atom force field (2001 aminoacid dihedrals)

15: [DEPRECATED] Encad all-atom force field, using full solvent charges

16: [DEPRECATED] Encad all-atom force field, using scaled-down vacuum charges

17: [DEPRECATED] Gromacs force field (see manual)

18: [DEPRECATED] Gromacs force field with hydrogens for NMR

****

Type 14 (OPLS-AA/L all-atom force field)

<enter>

Then it will ask you to select a water model.

****

Select the Water Model:

1: TIP4P TIP 4-point, recommended

2: TIP3P TIP 3-point

3: TIP5P TIP 5-point

4: SPC simple point charge

5: SPC/E extended simple point charge

6: None

****

You can select any water model.

Here we are selecting SPC/E extended simple point charge model.

Type 4

<enter>

After that topol.top file for ethanol is generated. You can view the topology file of ethanol.

```
;
;       File 'topol.top' was generated
;       By user: onbekend (0)
;       On host: onbekend
;       At date: Tue Nov 20 14:35:39 2012
;
;       This is a standalone topology file
;
;       It was generated using program:
;       pdb2gmx - VERSION 4.5.4
;
;       Command line was:
;       pdb2gmx -f EtOH.gro
;
;       Force field was read from the standard Gromacs share directory.
;


; Include forcefield parameters
#include "oplsaa.ff/forcefield.itp"


[ moleculetype ]
; Name            nrexcl
Other             3
```

```
[ atoms ]
;   nr       type  resnr residue  atom   cgnr     charge       mass  typeBchargeBmassB
; residue   1 ETOH rtpEtOH q  0.0
     1   opls_135     1   ETOH    CB     1     -0.18     12.011   ; qtot -0.18
     2   opls_140     1   ETOH    HB1    1      0.06      1.008   ; qtot -0.12
     3   opls_140     1   ETOH    HB2    1      0.06      1.008   ; qtot -0.06
     4   opls_140     1   ETOH    HB3    1      0.06      1.008   ; qtot 0
     5   opls_157     1   ETOH    CA     2     0.145     12.011   ; qtot 0.145
     6   opls_140     1   ETOH    HA1    2      0.06      1.008   ; qtot 0.205
     7   opls_140     1   ETOH    HA2    2      0.06      1.008   ; qtot 0.265
     8   opls_154     1   ETOH    OH     2    -0.683    15.9994   ; qtot -0.418
     9   opls_155     1   ETOH    HO     2     0.418      1.008   ; qtot 0

[ bonds ]
;  aiajfunct          c0          c1          c2          c3
    1    2    1
    1    3    1
    1    4    1
    1    5    1
    5    6    1
    5    7    1
    5    8    1
    8    9    1

[ pairs ]
```

```
;  aiajfunct        c0        c1        c2        c3
    1    9    1
    2    6    1
    2    7    1
    2    8    1
    3    6    1
    3    7    1
    3    8    1
    4    6    1
    4    7    1
    4    8    1
    6    9    1
    7    9    1

[ angles ]
;  aiajakfunct        c0        c1        c2        c3
    2    1    3    1
    2    1    4    1
    2    1    5    1
    3    1    4    1
    3    1    5    1
    4    1    5    1
    1    5    6    1
    1    5    7    1
    1    5    8    1
```

```
    6    5    7    1
    6    5    8    1
    7    5    8    1
    5    8    9    1

[ dihedrals ]
;  aiajak    al funct         c0         c1         c2         c3         c4         c5
    2    1    5    6    3
    2    1    5    7    3
    2    1    5    8    3
    3    1    5    6    3
    3    1    5    7    3
    3    1    5    8    3
    4    1    5    6    3
    4    1    5    7    3
    4    1    5    8    3
    1    5    8    9    3
    6    5    8    9    3
    7    5    8    9    3

; Include Position restraint file
#ifdef POSRES
#include "posre.itp"
#endif
```

```
; Include water topology
#include "oplsaa.ff/spc.itp"

#ifdef POSRES_WATER
; Position restraint for each water oxygen
[ position_restraints ]
;  ifunctfcxfcyfcz
   1    1       1000       1000       1000
#endif

; Include topology for ions
#include "oplsaa.ff/ions.itp"

[ system ]
; Name
UNNAMED

[ molecules ]
; Compound        #mols
Other               1
```

****

In the same way, you can generate topology files of other molecules.

Generation of topology file of phenyl alanine:

We are going to discuss how to generate the topology file for phenyl alanine protein molecule

The pdb file (Phe_alanine.pdb) of phenyl alanine molecule is given below

****

```
ATOM      1  N   PHEA  1      -1.564   1.397   0.770  1.00  0.00           N
ATOM      2  CA  PHE A  1      -0.115   1.397   0.770  1.00  0.00           C
ATOM      3  C   PHE A  1       0.408   2.826   0.770  1.00  0.00           C
ATOM      4  O   PHE A  1       1.301   3.093   1.571  1.00  0.00           O
ATOM      5  OXT PHE A  1      -0.102   3.607  -0.030  1.00  0.00           O
ATOM      6  CB  PHE A  1       0.436   0.696  -0.462  1.00  0.00           C
ATOM      7  CG  PHE A  1       0.178  -0.791  -0.515  1.00  0.00           C
ATOM      8  CD1 PHE A  1      -0.896  -1.288  -1.263  1.00  0.00           C
ATOM      9  CD2 PHE A  1       1.014  -1.671   0.182  1.00  0.00           C
ATOM     10  CE2 PHE A  1       0.775  -3.050   0.133  1.00  0.00           C
ATOM     11  CZ  PHE A  1      -0.299  -3.548  -0.615  1.00  0.00           C
ATOM     12  CE1 PHE A  1      -1.135  -2.667  -1.312  1.00  0.00           C
CONECT    3    2    4    5
CONECT    2    1    3    6
CONECT    6    2    7
CONECT    8    7   12
CONECT    9    7   10
CONECT   12    8   11
CONECT   10    9   11
CONECT    7    6    8    9
CONECT   11   10   12
CONECT    1    2
CONECT    4    3
```

CONECT 5 3

END

****

First convert this file into .gro format by giving the following command.

editconf –f Phe_alanine.pdb –o Phe_alanine.gro

<enter>

The

****

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12

1PHE N 1 -0.156 0.140 0.077

1PHE CA 2 -0.012 0.140 0.077

1PHE C 3 0.041 0.283 0.077

1PHE O 4 0.130 0.309 0.157

1PHE OXT 5 -0.010 0.361 -0.003

1PHE CB 6 0.044 0.070 -0.046

1PHE CG 7 0.018 -0.079 -0.052

1PHE CD1 8 -0.090 -0.129 -0.126

1PHE CD2 9 0.101 -0.167 0.018

1PHE CE2 10 0.078 -0.305 0.013

1PHE CZ 11 -0.030 -0.355 -0.062

1PHE CE1 12 -0.113 -0.267 -0.131

4.00000 4.00000 4.00000

****

Now you can change the residue name and atom name as defined in the **aminoacid.rtp** file of **gromos53a6.ff force field**.

Now give the following command to generate the topology file

pdb2gmx -f Phe_alaninemodified.gro

<enter>

Now select the force field

****

Select the Force Field:

From '/usr/local/gromacs/share/gromacs/top':

1: AMBER03 force field (Duan et al., J. Comp. Chem. 24, 1999-2012, 2003)

2: AMBER94 force field (Cornell et al., JACS 117, 5179-5197, 1995)

3: AMBER96 force field (Kollman et al., Acc. Chem. Res. 29, 461-469, 1996)

4: AMBER99 force field (Wang et al., J. Comp. Chem. 21, 1049-1074, 2000)

5: AMBER99SB force field (Hornak et al., Proteins 65, 712-725, 2006)

6: AMBER99SB-ILDN force field (Lindorff-Larsen et al., Proteins 78, 1950-58, 2010)

7: AMBERGS force field (Garcia &Sanbonmatsu, PNAS 99, 2782-2787, 2002)

8: CHARMM27 all-atom force field (with CMAP) - version 2.0

9: GROMOS96 43a1 force field

10: GROMOS96 43a2 force field (improved alkane dihedrals)

11: GROMOS96 45a3 force field (Schuler JCC 2001 22 1205)

12: GROMOS96 53a5 force field (JCC 2004 vol 25 pag 1656)

13: GROMOS96 53a6 force field (JCC 2004 vol 25 pag 1656)

14: OPLS-AA/L all-atom force field (2001 aminoacid dihedrals)

15: [DEPRECATED] Encad all-atom force field, using full solvent charges

16: [DEPRECATED] Encad all-atom force field, using scaled-down vacuum charges

17: [DEPRECATED] Gromacs force field (see manual)

18: [DEPRECATED] Gromacs force field with hydrogens for NMR

****

Type 13 (GROMOS96 53a6 force field)

<enter>

Then it will ask to select water model

****

Select the Water Model:

1: SPC simple point charge, recommended

2: SPC/E extended simple point charge

3: None

Type***'2'***

<enter>

****

The topology file of phyenyl alanine is generated. It is given below

****

; File 'topol.top' was generated

; By user: onbekend (0)

; On host: onbekend

; At date: Tue Nov 20 15:23:09 2012

;

; This is a standalone topology file

;

; It was generated using program:

```
;       pdb2gmx - VERSION 4.5.4
;
;       Command line was:
;       pdb2gmx -f phe_top.top.gro
;
;       Force field was read from the standard Gromacs share directory.
;


; Include forcefield parameters
#include "gromos53a6.ff/forcefield.itp"

[ moleculetype ]
; Name            nrexcl
Protein             3

[ atoms ]
;   nr       type  resnr residue  atom   cgnr     charge       mass  typeBchargeBmassB
; residue   1 PHE rtpPHE  q  0.0
     1        NL     1    PHE     N      1      0.129    14.0067   ; qtot 0.129
     2         H     1    PHE     H1     1      0.248     1.008    ; qtot 0.377
     3         H     1    PHE     H2     1      0.248     1.008    ; qtot 0.625
     4         H     1    PHE     H3     1      0.248     1.008    ; qtot 0.873
     5       CH1     1    PHE     CA     2      0.127     13.019   ; qtot 1
     6       CH2     1    PHE     CB     2          0     14.027   ; qtot 1
     7         C     1    PHE     CG     2          0     12.011   ; qtot 1
```

```
     8       C     1    PHE    CD1     3     -0.14     12.011   ; qtot 0.86
     9       HC    1    PHE    HD1     3      0.14      1.008   ; qtot 1
    10       C     1    PHE    CD2     4     -0.14     12.011   ; qtot 0.86
    11       HC    1    PHE    HD2     4      0.14      1.008   ; qtot 1
    12       C     1    PHE    CE1     5     -0.14     12.011   ; qtot 0.86
    13       HC    1    PHE    HE1     5      0.14      1.008   ; qtot 1
    14       C     1    PHE    CE2     6     -0.14     12.011   ; qtot 0.86
    15       HC    1    PHE    HE2     6      0.14      1.008   ; qtot 1
    16       C     1    PHE    CZ      7     -0.14     12.011   ; qtot 0.86
    17       HC    1    PHE    HZ      7      0.14      1.008   ; qtot 1
    18       C     1    PHE    C       8      0.27     12.011   ; qtot 1.27
    19       OM    1    PHE    O1      8     -0.635    15.9994  ; qtot 0.635
    20       OM    1    PHE    O2      8     -0.635    15.9994  ; qtot 0

[ bonds ]
;  aiajfunct          c0          c1          c2          c3
    1    2    2    gb_2
    1    3    2    gb_2
    1    4    2    gb_2
    1    5    2    gb_21
    5    6    2    gb_27
    5   18    2    gb_27
    6    7    2    gb_27
    7    8    2    gb_16
    7   10    2    gb_16
```

```
   8    9    2   gb_3
   8   12    2   gb_16
  10   11    2   gb_3
  10   14    2   gb_16
  12   13    2   gb_3
  12   16    2   gb_16
  14   15    2   gb_3
  14   16    2   gb_16
  16   17    2   gb_3
  18   19    2   gb_6
  18   20    2   gb_6

[ pairs ]
;  aiajfunct      c0        c1        c2        c3
   1    7    1
   1   19    1
   1   20    1
   2    6    1
   2   18    1
   3    6    1
   3   18    1
   4    6    1
   4   18    1
   5    8    1
   5   10    1
```

```
    6   19    1
    6   20    1
    7   18    1


 [ angles ]
 ;  aiajakfunct       c0        c1        c2        c3
    2    1    3    2    ga_10
    2    1    4    2    ga_10
    2    1    5    2    ga_11
    3    1    4    2    ga_10
    3    1    5    2    ga_11
    4    1    5    2    ga_11
    1    5    6    2    ga_13
    1    5   18    2    ga_13
    6    5   18    2    ga_13
    5    6    7    2    ga_15
    6    7    8    2    ga_27
    6    7   10    2    ga_27
    8    7   10    2    ga_27
    7    8    9    2    ga_25
    7    8   12    2    ga_27
    9    8   12    2    ga_25
    7   10   11    2    ga_25
    7   10   14    2    ga_27
   11   10   14    2    ga_25
```

```
   8   12   13    2   ga_25
   8   12   16    2   ga_27
  13   12   16    2   ga_25
  10   14   15    2   ga_25
  10   14   16    2   ga_27
  15   14   16    2   ga_25
  12   16   14    2   ga_27
  12   16   17    2   ga_25
  14   16   17    2   ga_25
   5   18   19    2   ga_22
   5   18   20    2   ga_22
  19   18   20    2   ga_38

[ dihedrals ]
;  aiajak    al funct          c0          c1          c2          c3          c4          c5
   2    1    5   18    1   gd_29
   1    5    6    7    1   gd_34
   1    5   18   20    1   gd_40
   5    6    7    8    1   gd_40

[ dihedrals ]
;  aiajak    al funct          c0          c1          c2          c3
   5    1   18    6    2   gi_2
   6   10    8    7    2   gi_1
   7    8   12   16    2   gi_1
```

```
 7   10   14   16    2   gi_1
 8    7   12    9    2   gi_1
 8    7   10   14    2   gi_1
 8   12   16   14    2   gi_1
10    7   14   11    2   gi_1
10    7    8   12    2   gi_1
10   14   16   12    2   gi_1
12   16    8   13    2   gi_1
14   16   10   15    2   gi_1
16   12   14   17    2   gi_1
18    5   20   19    2   gi_1

; Include Position restraint file
#ifdef POSRES
#include "posre.itp"
#endif

; Include water topology
#include "gromos53a6.ff/spce.itp"

#ifdef POSRES_WATER
; Position restraint for each water oxygen
[ position_restraints ]
;  ifunctfcxfcyfcz
   1    1       1000       1000       1000
```

#endif

; Include topology for ions

#include "gromos53a6.ff/ions.itp"

[system]

; Name

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[molecules]

; Compound #mols

Protein 1

****

Formation of topology file of Toluene from phenyl alanine

With the help of **.gro** file of phenyl alanine, we can make .gro file of toluene.

The **.gro** file of phenyl alanine is

****

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20

1PHE N 1 -0.156 0.140 0.077

1PHE H1 2 -0.190 0.045 0.077

1PHE H2 3 -0.190 0.187 0.159

1PHE H3 4 -0.190 0.187 -0.005

1PHE CA 5 -0.012 0.140 0.077

1PHE CB 6 0.044 0.070 -0.046

1PHE CG 7 0.018 -0.079 -0.052

1PHE CD1 8 -0.090 -0.129 -0.126

1PHE HD1 9 -0.149 -0.066 -0.176

1PHE CD2 10 0.101 -0.167 0.018

1PHE HD2 11 0.178 -0.132 0.071

1PHE CE1 12 -0.113 -0.267 -0.131

1PHE HE1 13 -0.190 -0.302 -0.184

1PHE CE2 14 0.078 -0.305 0.013

1PHE HE2 15 0.137 -0.368 0.063

1PHE CZ 16 -0.030 -0.355 -0.062

1PHE HZ 17 -0.047 -0.453 -0.065

1PHE C 18 0.041 0.283 0.077

1PHE O1 19 0.130 0.309 0.157

1PHE O2 20 -0.010 0.361 -0.003

0.36846 0.81398 0.34314

****

Now from this **.gro** file you can make the **.gro** file of toluene

The tolune.gro file of Toluene is

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12

1PHE CA 5 -0.012 0.140 0.077

1PHE CB 6 0.044 0.070 -0.046

1PHE CG 7 0.018 -0.079 -0.052

1PHE CD1 8 -0.090 -0.129 -0.126

1PHE HD1 9 -0.149 -0.066 -0.176

1PHE CD2 10 0.101 -0.167 0.018

1PHE HD2 11 0.178 -0.132 0.071

1PHE CE1 12 -0.113 -0.267 -0.131

1PHE HE1 13 -0.190 -0.302 -0.184

1PHE CE2 14 0.078 -0.305 0.013

1PHE HE2 15 0.137 -0.368 0.063

1PHE CZ 16 -0.030 -0.355 -0.062

1PHE HZ 17 -0.047 -0.453 -0.065

4.0004.0004.000

****

Now give the following command to generate topology file

pdb2gmx -f tolune.gro –missing

<enter>

It will ask to select force field

****

Select the Force Field:

From '/usr/local/gromacs/share/gromacs/top':

1: AMBER03 force field (Duan et al., J. Comp. Chem. 24, 1999-2012, 2003)

2: AMBER94 force field (Cornell et al., JACS 117, 5179-5197, 1995)

3: AMBER96 force field (Kollman et al., Acc. Chem. Res. 29, 461-469, 1996)

4: AMBER99 force field (Wang et al., J. Comp. Chem. 21, 1049-1074, 2000)

5: AMBER99SB force field (Hornak et al., Proteins 65, 712-725, 2006)

6: AMBER99SB-ILDN force field (Lindorff-Larsen et al., Proteins 78, 1950-58, 2010)

7: AMBERGS force field (Garcia &Sanbonmatsu, PNAS 99, 2782-2787, 2002)

8: CHARMM27 all-atom force field (with CMAP) - version 2.0

9: GROMOS96 43a1 force field

10: GROMOS96 43a2 force field (improved alkane dihedrals)

11: GROMOS96 45a3 force field (Schuler JCC 2001 22 1205)

12: GROMOS96 53a5 force field (JCC 2004 vol 25 pag 1656)

13: GROMOS96 53a6 force field (JCC 2004 vol 25 pag 1656)

14: OPLS-AA/L all-atom force field (2001 aminoacid dihedrals)

15: [DEPRECATED] Encad all-atom force field, using full solvent charges

16: [DEPRECATED] Encad all-atom force field, using scaled-down vacuum charges

17: [DEPRECATED] Gromacs force field (see manual)

18: [DEPRECATED] Gromacs force field with hydrogens for NMR

****

Type ***13*** (GROMOS96 53a6 force field)

<enter>

Then it ask to select water model

****

Select the Water Model:

1: SPC simple point charge, recommended

2: SPC/E extended simple point charge

3: None

****

Type ***2***

<enter>

It will give the topology file of toluene. The file is given below

****

```
;       File 'topol.top' was generated
;       By user: onbekend (0)
;       On host: onbekend
;       At date: Tue Nov 20 17:14:54 2012
;
;       This is a standalone topology file
;
;       It was generated using program:
;       pdb2gmx - VERSION 4.5.4
;
;       Command line was:
;       pdb2gmx -f tolune.gro -missing
;
;       Force field was read from the standard Gromacs share directory.
;


; Include forcefield parameters
#include "gromos53a6.ff/forcefield.itp"


[ moleculetype ]
; Name            nrexcl
Protein             3


[ atoms ]
;   nr       type  resnr residue  atom   cgnr     charge       mass  typeBchargeBmassB
```

```
; residue   1 PHE rtp PHE  q  0.0
     1       CH2     1    PHE     CB     1         0     14.027   ; qtot 0
     2         C     1    PHE     CG     1         0     12.011   ; qtot 0
; replaceCH2 by CH3 then it will become toluene and change mass also
     3         C     1    PHE    CD1     2     -0.14     12.011   ; qtot -0.14
     4        HC     1    PHE    HD1     2      0.14      1.008   ; qtot 0
     5         C     1    PHE    CD2     3     -0.14     12.011   ; qtot -0.14
     6        HC     1    PHE    HD2     3      0.14      1.008   ; qtot 0
     7         C     1    PHE    CE1     4     -0.14     12.011   ; qtot -0.14
     8        HC     1    PHE    HE1     4      0.14      1.008   ; qtot 0
     9         C     1    PHE    CE2     5     -0.14     12.011   ; qtot -0.14
    10        HC     1    PHE    HE2     5      0.14      1.008   ; qtot 0
    11         C     1    PHE     CZ     6     -0.14     12.011   ; qtot -0.14
    12        HC     1    PHE     HZ     6      0.14      1.008   ; qtot 0

[ bonds ]
;  aiajfunct          c0          c1          c2          c3
    1    2    2    gb_27
    2    3    2    gb_16
    2    5    2    gb_16
    3    4    2    gb_3
    3    7    2    gb_16
    5    6    2    gb_3
    5    9    2    gb_16
    7    8    2    gb_3
```

```
   7   11    2   gb_16
   9   10    2   gb_3
   9   11    2   gb_16
  11   12    2   gb_3

[ angles ]
;  aiajakfunct        c0        c1        c2        c3
   1    2    3    2   ga_27
   1    2    5    2   ga_27
   3    2    5    2   ga_27
   2    3    4    2   ga_25
   2    3    7    2   ga_27
   4    3    7    2   ga_25
   2    5    6    2   ga_25
   2    5    9    2   ga_27
   6    5    9    2   ga_25
   3    7    8    2   ga_25
   3    7   11    2   ga_27
   8    7   11    2   ga_25
   5    9   10    2   ga_25
   5    9   11    2   ga_27
  10    9   11    2   ga_25
   7   11    9    2   ga_27
   7   11   12    2   ga_25
   9   11   12    2   ga_25
```

```
[ dihedrals ]
;  aiajak    al funct          c0          c1          c2          c3
    1     5     3     2     2    gi_1
    2     3     7    11     2    gi_1
    2     5     9    11     2    gi_1
    3     2     7     4     2    gi_1
    3     2     5     9     2    gi_1
    3     7    11     9     2    gi_1
    5     2     9     6     2    gi_1
    5     2     3     7     2    gi_1
    5     9    11     7     2    gi_1
    7    11     3     8     2    gi_1
    9    11     5    10     2    gi_1
   11     7     9    12     2    gi_1

; Include Position restraint file
#ifdef POSRES
#include "posre.itp"
#endif

; Include water topology
#include "gromos53a6.ff/spce.itp"

#ifdef POSRES_WATER
```

```
; Position restraint for each water oxygen
[ position_restraints ]
;  ifunctfcxfcyfcz
   1    1       1000       1000       1000
#endif

; Include topology for ions
#include "gromos53a6.ff/ions.itp"

[ system ]
; Name
Giving Russians Opium May Alter Current Situation

[ molecules ]
; Compound        #mols
Protein             1
SOL                 1000
```

****

Exercise:

Read the gromacs manual and generate the topology files of a few amino acids.