**Tutorial: Generating an OPLS-AA topology file from a pdb/xyz file**

This tutorial focuses on the protocols for generating an OPLS topology file, including a gromacs structure file (.gro file) from a plain coordinate data.

Files that you need: Oplsatom2, OPLS-top.f90, pdb-gro.f90, the pdb file that you want to convert

**Put these files in the same directory**

Also, please prepare the ffbonded.itp and ffnonbond.itp by yourself. These two files are OPLS-AA force field files describing bonded interactions and non-bonded interactions.

**Step 1: Using the topotools version 1.8 plugin in vmd to create an incomplete topology file (CANNOT use version 1.7, it will not work)**

1. Start vmd and load your pdb structure (make sure the structure does not show any weird bond connectivities)
2. Start the Tcl/Tk console (Extensions -> Tk console)
3. In the Tk console, type the following (hit return after each line):

* pbc set {x y z } (eg. {100.0 100.0 100.0 90.0 90.0 90.0}) to set simulation cell with dimensions (Å) x, y, z and angles . (this line can be omitted if the structure (pdb) already has a pbc cell.)
* topo guessbonds (this will detect the bonds in the structure)
* topo guessangles (this will detect the angles in the structure
* topo guessdihedrals (this will detect the dihedrals in the structure)
* topo guessimpropers (this will detect the impropers in the structure)
* topo writegmxtop filename.top (this will write out the structure as a half-baked gromacs topology file)
* topo writelammpsdata data.filename (this will give the number of bonds, angles, dihedrals, impropers. You will need it later)

When using xyz file to generate the topology, make sure all carbon, oxygen and hydrogen atoms are labelled as C, O and H, respectively, to prevent weird bond connectivities.

**Step 2: Editing the incomplete topology file**

1. Delete the first 37 and last 9 lines in the filename.top file, as highlighted in the figures below.

Text

Description automatically generated

Shape

Description automatically generated with medium confidence

Run OPLS-top.f90 to complete step2 ii, iii, and iv. Before running OPLS-top.f90, carefully check the masses of the atoms to make sure **C, H** and **O** has a mass of **12.0110**, **1.0080** and **15.9994**, respectively.

In the file OPLS-top.f90, change the following lines:

Line 30, replace the number of natoms to the number you have, see the file generated early on 🡪 data.filename

Line 31, replace the number of nbonds to the number you have, see the file generated early on 🡪 data.filename

Line 32, replace the number of nangles to the number you have, see the file generated early on 🡪 data.filename

Line 33, replace the number of ndihedrals to the number you have, see the file generated early on 🡪 data.filename

Line 34, replace the number of nimpropers to the number you have, see the file generated early on 🡪 data.filename

Line 47, change the GO\_sheet\_stitch.itp to the filename that you want

Command to run this code (OPLS-top.f90):

gfortran -o half\_product OPLS-top.f90

./half\_product

This calculation will also sum the charge of the system, and it should be zero. (If the number is -0.0000xx, it is also fine)

1. Under the [ atoms ] section in the .top file, replace the atom types and charges with the appropriate OPLS atom types and charges. Change the residues for easy identification.



1. The bond connectivity and angle connectivity entries should be fine. However, in the case of the dihedral and improper connectivity entries, change the functions (func) from 1 to 3. This is because Ryckaert-Bellemans potentials are used inthe OPLS force field in combination with 1-4 interactions for dihedral interactions.



1. Finally, add a section for the 1-4 pair interactions which can be obtained from the dihedral connectivity entities, i.e., *i* and *l* and save the file with the extension **.itp**

A picture containing text

Description automatically generated

**Step 3: Generating a gromacs structural file from pdb/xyz file**

1. To convert pdb to gro file, type gmx editconf -f input.pdb -o output.gro

Run code pdb-gro.f90 to conduct step 3 ii

In the file pdb-gro.f90: line 19 output.gro is the file generated in step 3 i

Line 25 is the result file generated in this step, you can change the result.gro the name that you want.

1. Edit the residue names in the output.gro file to match that of the filename.top

Text

Description automatically generated with low confidence

A picture containing text

Description automatically generated

Alternatively,

1. Start vmd and load your xyz file
2. Save the coordinates as a gro file in vmd
3. Add the column containing the residue names

A picture containing text

Description automatically generatedA picture containing text

Description automatically generated

Test the generated topology file via energy minimisation.

The following error you may not encounter.

Look out for missing default angle types and dihedral types when you perform gmx grompp. These could be fixed by carefully selecting similar angle types and dihedral types from the ffbonded.itp file and renaming the atoms to match the atoms with the missing parameters.

Graphical user interface, text

Description automatically generated

For example, to fix the above errors,

1. open the new-GO.itp file (the itp file that you generated in step 2) and look for the dihedral entries at line 5652 and 5678.

Table

Description automatically generated

1. Check for the OPLS atom types corresponding to these numbers from the [ atoms ] section in the .itp file

5652 35 61 62 90 -> opls\_147 opls\_184 opls\_147 opls\_159

5678 63 64 65 66 -> opls\_147 opls\_159 opls\_147 opls\_159

1. Open the ffnonbonded.itp file and check for the default names for these atom types

opls\_147 opls\_184 opls\_147 opls\_159 -> CA CT CA CT

opls\_147 opls\_159 opls\_147 opls\_159 -> CA CT CA CT

1. Check the ffbonded.itp file for similar dihedral types

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Description automatically generated

1. Copy the highlighted line and edit the dihedral arrangement to match iii.

CA CT CA CT 3 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

Do not make these changes in the original ffbonded.itp file.