

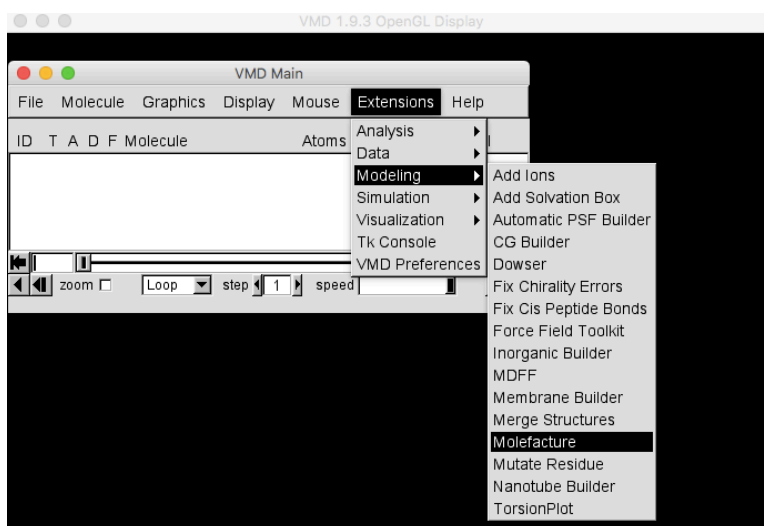
VMD: Molefacture

The molefacture plugin provides VMD users with an interface to edit molecules. This includes the ability to add, delete, or manipulate their structure at an atomic level, and to build new components from a library of common fragments.

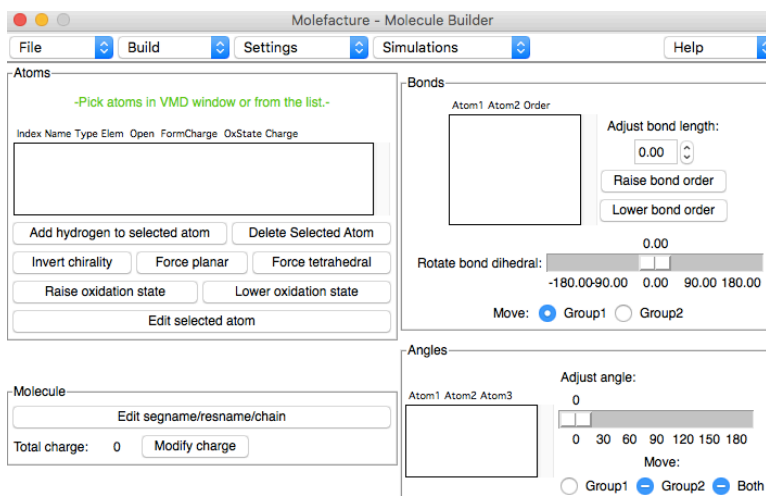
In this tutorial, we will learn how to build a united atom n-butane and generate topology file and pdb file for single n-butane.

1. Molefacture

Open the VMD by typing “vmd” in your terminal. Under the “Extensions” tab, “Modeling”, select “Molefacture”.

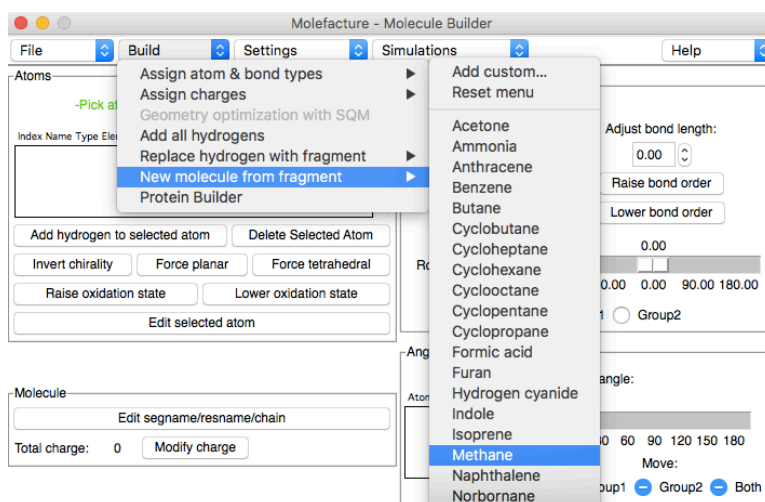


Click on “Start Molefacture” to open the “Molefacture” window.

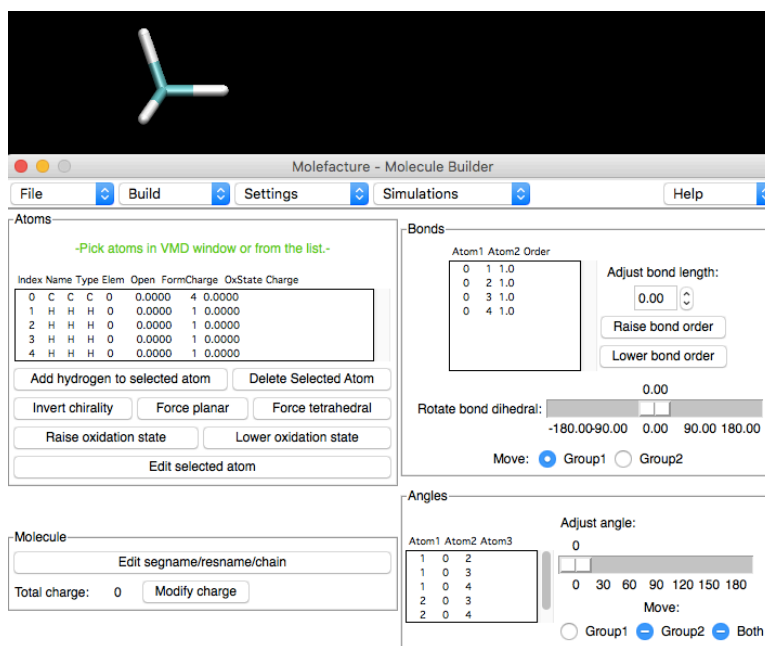


2. Building n-butane

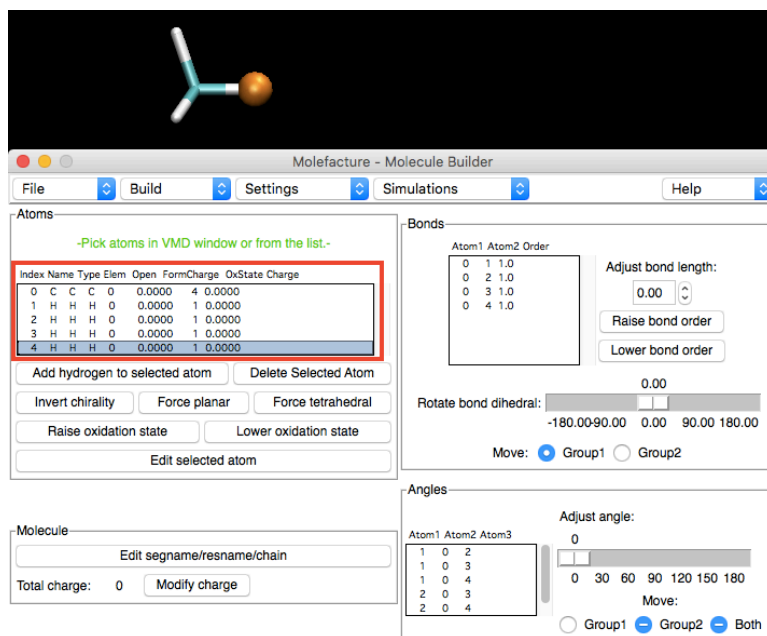
We will start building n-butane, from methane molecule. Under the “Build” tab, select “New Molecule from fragment”, and click on “Methane”.



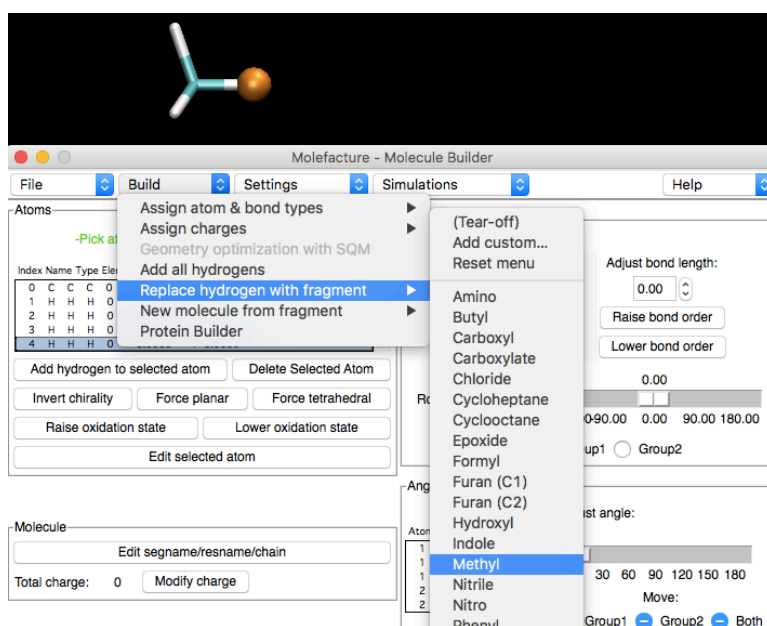
You will receive an error regarding “abandon all editing on the current molecule”, click yes button. You will see an all atom methane.



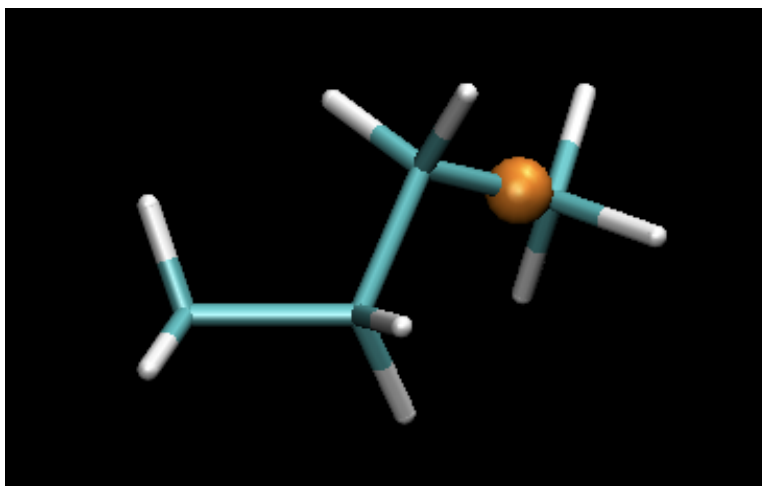
Now we start building the rest of the n-butane molecule by replacing a hydrogen atom with a methyl group. Select one hydrogen from atoms listed in the “Atoms” section.



Under the “Build” tab, select “Replace hydrogen with fragment”, and then select “Methyl”.



Continue this process until you build all atom of n-butane. Note that, you should choose the hydrogen atom to be replaced, in a way to accurately demonstrate the n-butane structure. The final molecule structure will be like this:



3. United Atom n-butane

In united atom force field, hydrogen are incorporated in the carbon atom. To remove the hydrogen atom, under the “Atoms” section, select all the hydrogen and click on “Delete Selected Atoms”.

Atoms

-Pick atoms in VMD window or from the list.-

Index	Name	Type	Elem	Open	FormCharge	OxState	Charge
9	C	C	C	0	0.0000	4	0.0000
10	H	H	H	0	0.0000	1	0.0000
11	H	H	H	0	0.0000	1	0.0000
12	H	H	H	0	0.0000	1	0.0000
13	H	H	H	0	0.0000	1	0.0000

Buttons: Add hydrogen to selected atom, **Delete Selected Atom**, Invert chirality, Force planar, Force tetrahedral, Raise oxidation state, Lower oxidation state, Edit selected atom

Bonds

Atom1	Atom2	Order
0	1	1.0
0	2	1.0
0	3	1.0
0	4	1.0
4	5	1.0
4	6	1.0
4	7	1.0
7	8	1.0

Adjust bond length: 0.00
Buttons: Raise bond order, Lower bond order

Rotate bond dihedral: -180.00 90.00 0.00 90.00 180.00
Move: ☒ Group1 ☐ Group2

Angles

Atom1	Atom2	Atom3
1	0	2
1	0	3
1	0	4
2	0	3
2	0	4

Adjust angle: 0
Buttons: Group1, Group2, Both

Molecule

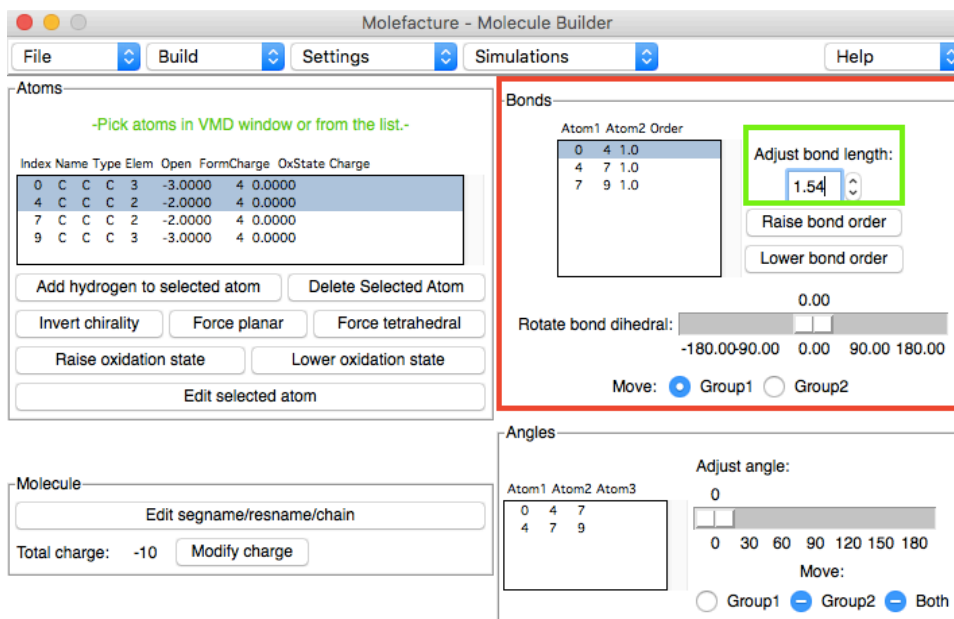
Edit segname/resname/chain

Total charge: 0

Under the “Settings” tab, you can disable “Display valences” and “Display electrons”.

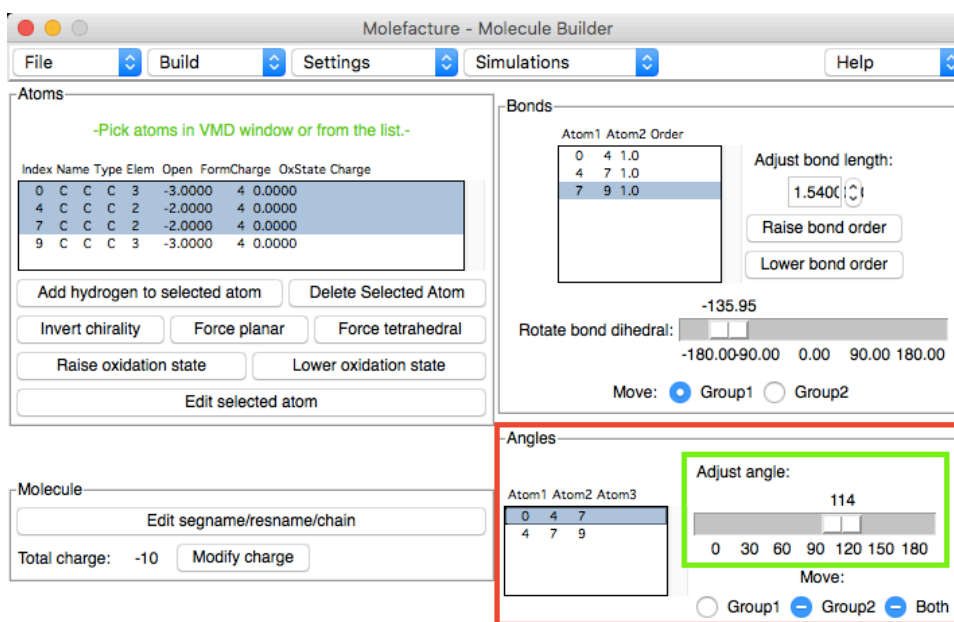
4. Adjust Bonds

Mie potential for n-alkanes uses fix bond length of 1.54 Å. To adjust the bond value, under the “Bonds” section, select the first bond, and adjust the bond length to 1.54 Å and press enter. Repeat this process for remaining bonds.



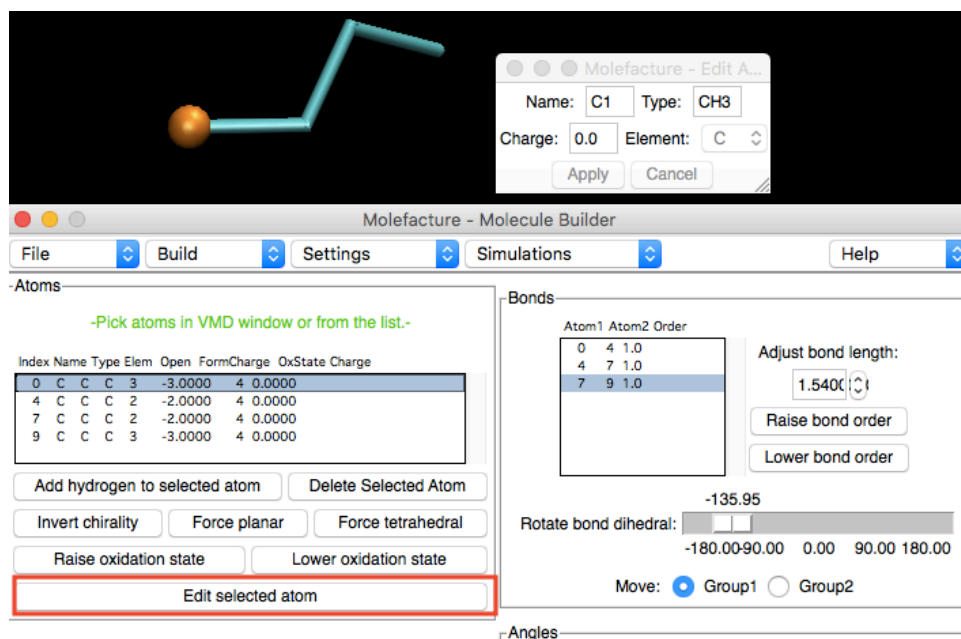
5. Adjust Angles

In Mie potential for n-alkanes, all the equilibrium bend angles are 114°. To adjust the angle value, under the “Angles” section, select the first angle, and adjust the angle to 114° and press enter. Repeat this process for remaining angles.



6. Assign Atom Name and Type

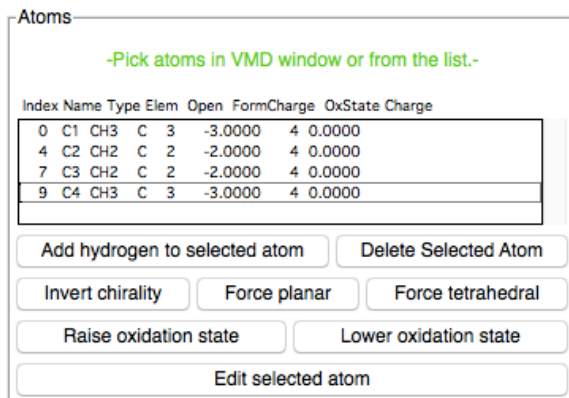
To assign atom name and type, under “Atoms” section, select the first atom (index 0), and click on “Edit selected atom”. In the opened window, change the atom name to “C1”, and atom type to “CH3” since the first atom incorporated three hydrogen, and click “Apply”. Note that in the potential for alkane, there are no charges.



Repeat the same process for other atoms as follow:

- Second atom “Index 4”, change the atom name to “C2”, and atom type to “CH2”.
- Second atom “Index 7”, change the atom name to “C3”, and atom type to “CH2”.
- Second atom “Index 9”, change the atom name to “C4”, and atom type to “CH3”.

The atom parameter in “Atoms” section should be similar to this:



7. Assign Resname and Chain

To assign the residue name (resname), under “Molecule” section, click on “Edit segname/resname/chain” and change the resname to “C4A”. You can also change the chain value to “A”. Then press “Apply” and “Done”.

The screenshot displays the Molecule Builder software interface. At the top, a 3D ball-and-stick model of a molecule is shown. Below it, a dialog box titled 'Molefacture - Edit Re...' is open, showing fields for 'resname: C4A', 'segname: 1', 'chain: A', and 'resid: 1'. The main window has a menu bar with 'File', 'Build', 'Settings', 'Simulations', and 'Help'. The 'Atoms' panel on the left contains a table of atom properties and buttons for editing. The 'Bonds' panel on the right shows a table of bond properties and sliders for adjusting bond length and dihedral angle. The 'Angles' panel at the bottom right shows a table of angle properties and a slider for adjusting the angle. The 'Molecule' section at the bottom left is highlighted with a red box, showing the 'Edit segname/resname/chain' button and the 'Total charge: -10' field.

Index	Name	Type	Elem	Open	FormCharge	OxState	Charge
0	C1	CH3	C	3	-3.0000	4	0.0000
4	C2	CH2	C	2	-2.0000	4	0.0000
7	C3	CH2	C	2	-2.0000	4	0.0000
9	C4	CH3	C	3	-3.0000	4	0.0000

Atom1	Atom2	Order
0	4	1.0
4	7	1.0
7	9	1.0

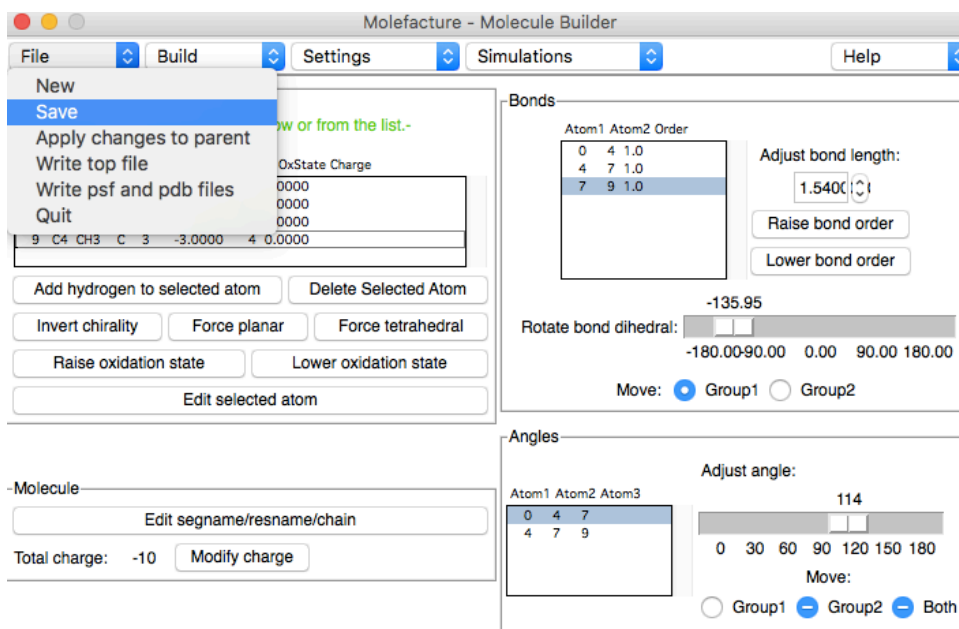
Atom1	Atom2	Atom3
0	4	7
4	7	9

8. Assign Molecule Charge

Since atoms of n-butane have no charge, we need to adjust the total charges to zero. Under “Molecule” section, click on “Modify charge” and in the opened window, set the value of total charge to zero, press “Apply” and “Done”.

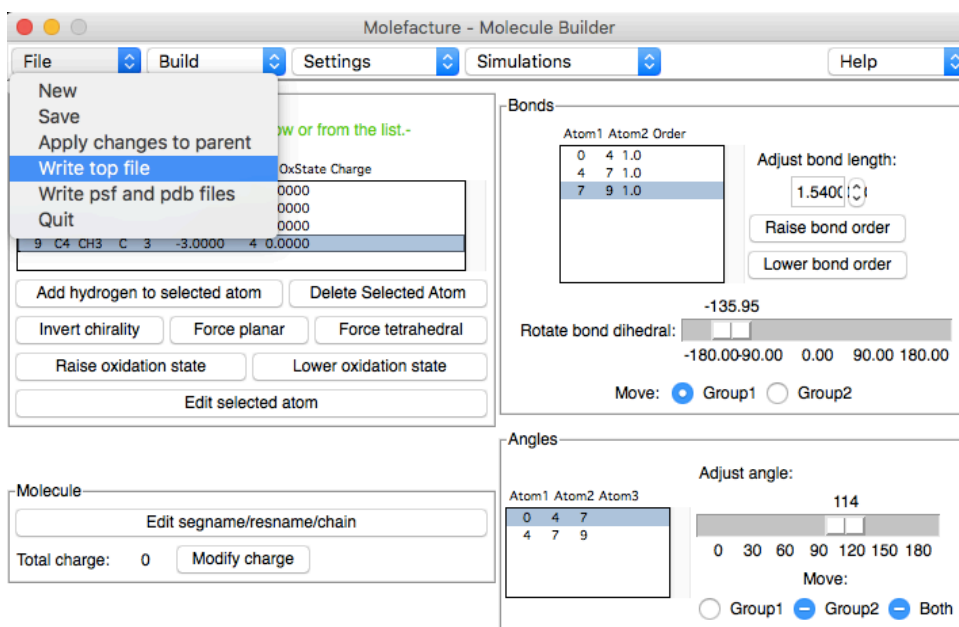
9. Save PDB File

To save the PDB file for n-butane, under the “File” tab, select “Save”. In the opened window, change the “Files of type” to “PDB Files (*.pdb)”, and save the it as “butane_ua.pdb”.



10. Save Topology file

To save the topology file for n-butane, under the “File” tab, select “Write top file”. In the opened window, save the topology file as “top_butane_ua.top”.



11. Adjust Atom Mass

Since we are using united atom force field, the mass of the carbon atom is not 12.011 u. Open the “top_butane_ua.top” and adjust the mass of CH3 to 15.035 u, and mass of CH2 to 14.027 u. Here is the n-butane topology file after the adjustment:

```
*>>>>> CHARMM topology file generated by Molefacture <<<<<<

27 1

MASS      1 CH3    15.03500  C
MASS      1 CH2    14.02700  C

AUTO ANGLES DIHE

RESI  C4A      0.00

GROUP

ATOM  C1  CH3  0.00000
ATOM  C2  CH2  0.00000
ATOM  C3  CH2  0.00000
ATOM  C4  CH3  0.00000
BOND C1 C2  C2 C3  C3 C4

END
```