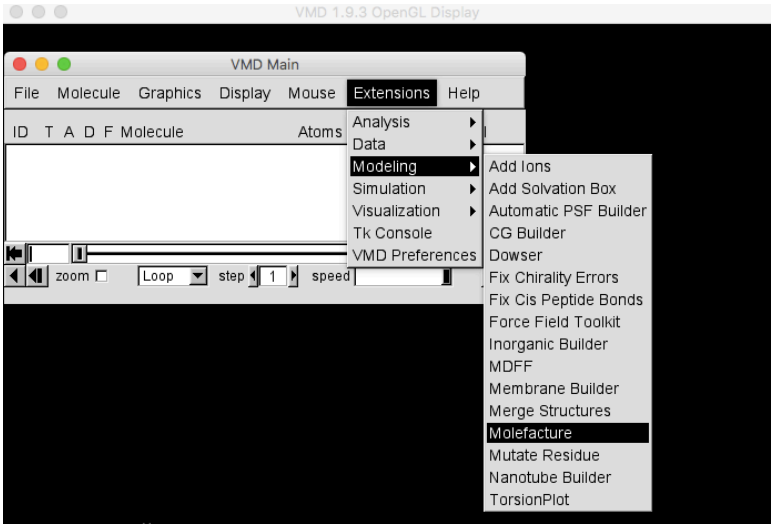
VMD: Molefacture

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.

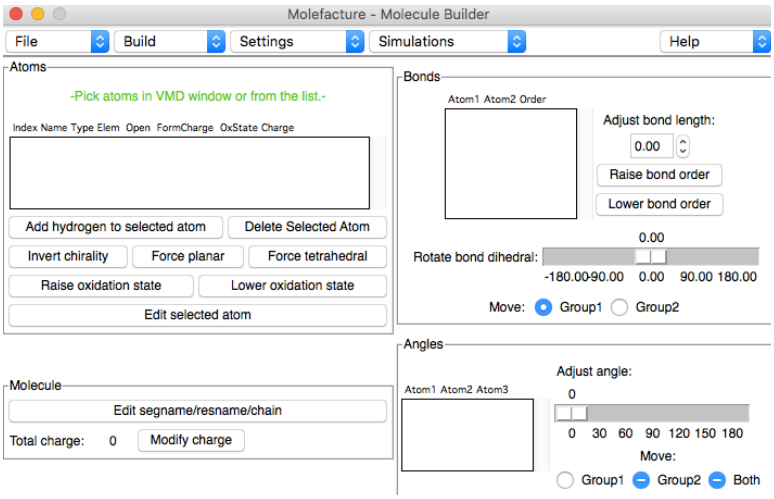
In this tutorial, we will learn how to build a united atom n-butane and generate topology file and pdb file for single n-butane.

1. Molefacture

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

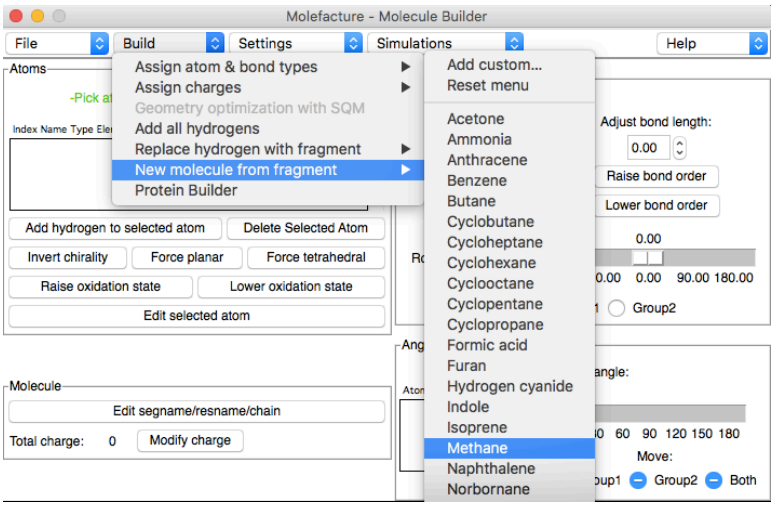


Click on “Start Molefacture” to open the “Molefacture” window.

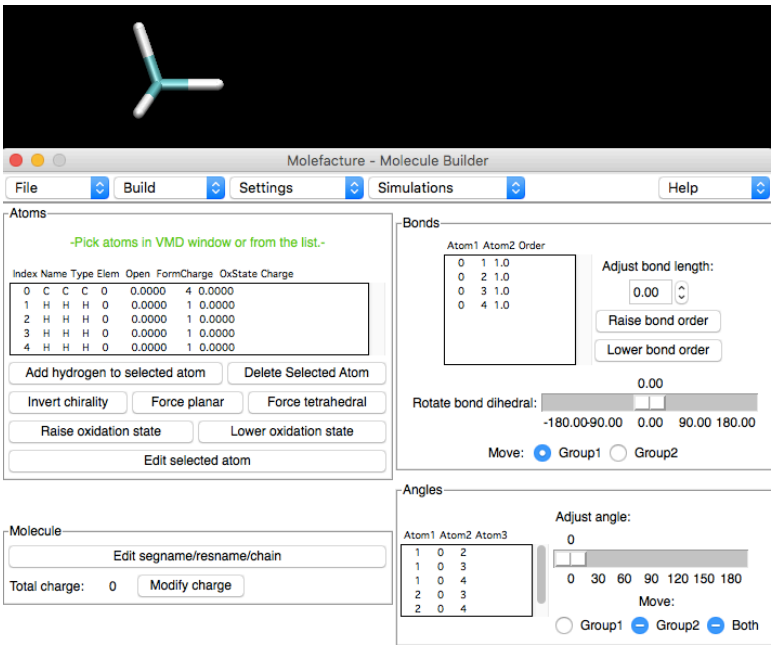


2. Building n-butane

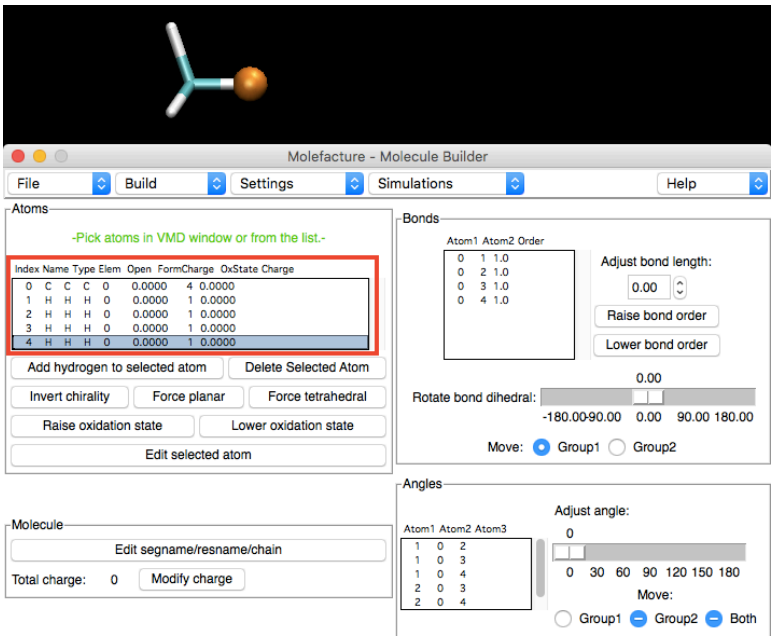
We will start building n-butane, from methane molecule. Under the “Build” tab, select “New Molecule from fragment”, and click on “Methane”.



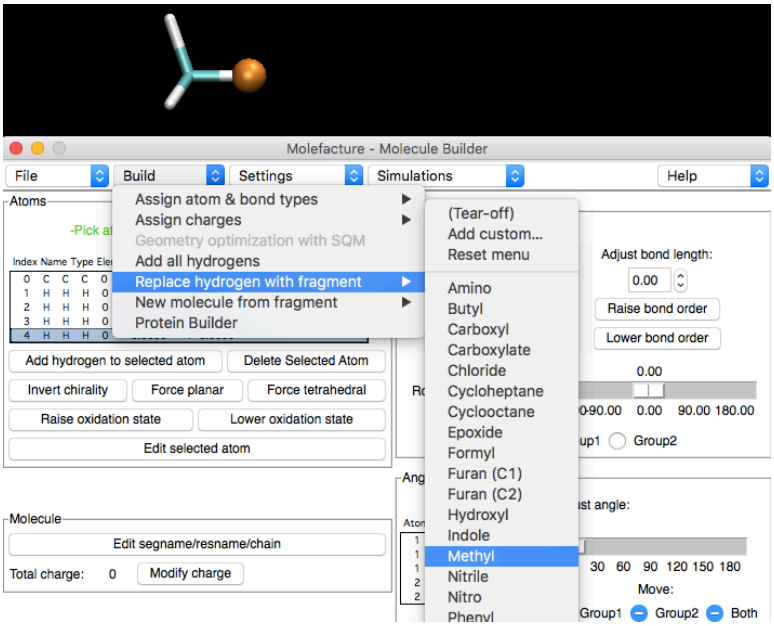
You will receive and error regarding “abandon all editing on the current molecule”, click yes button. You will see an all atom methane.



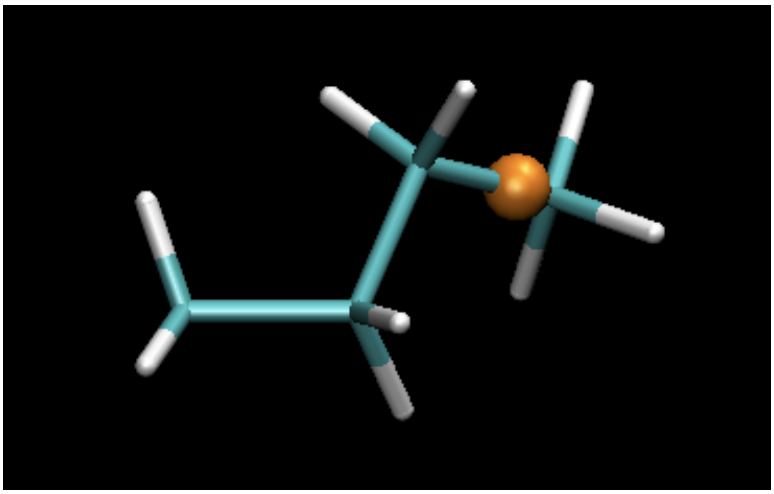
Now we start building the rest of the n-butane molecule by replacing a hydrogen atom with a methyl group. Select one hydrogen from atoms listed in the “Atoms” section.



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

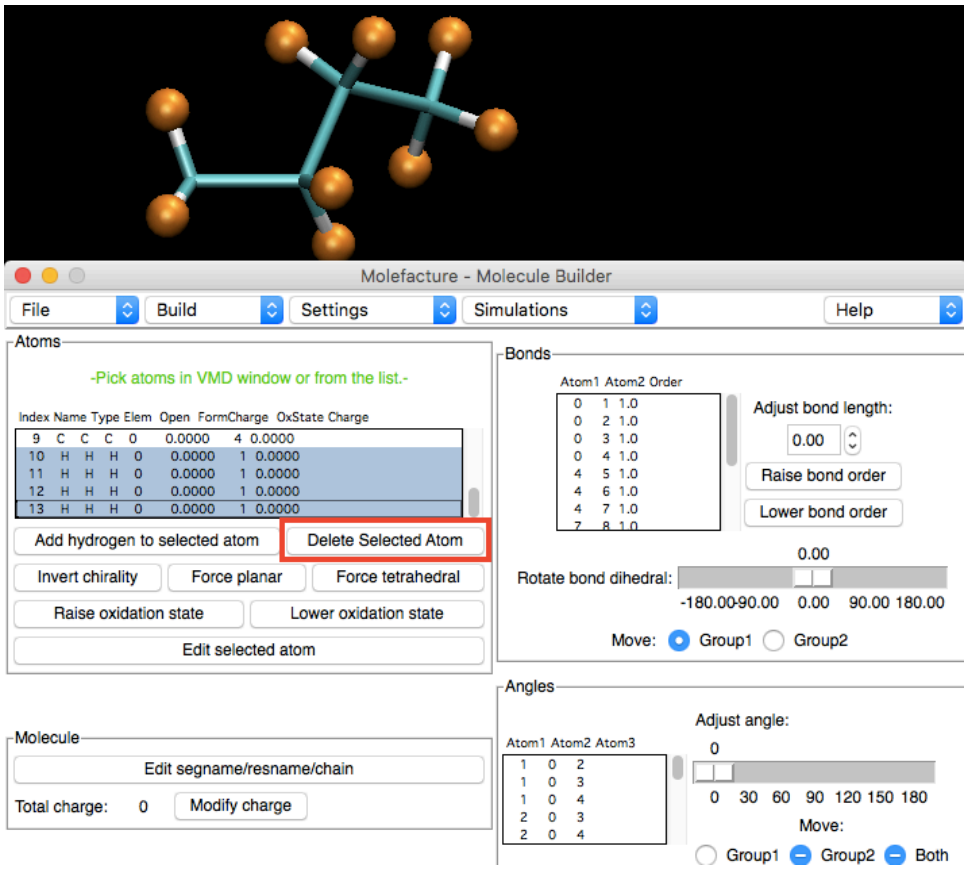


Continue this process until you build all atom of n-butane. Note that, you should choose the hydrogen atom to be replaced, in a way to accurately demonstrate the n-butane structure. The final molecule structure will be like this:



3. United Atom n-butane

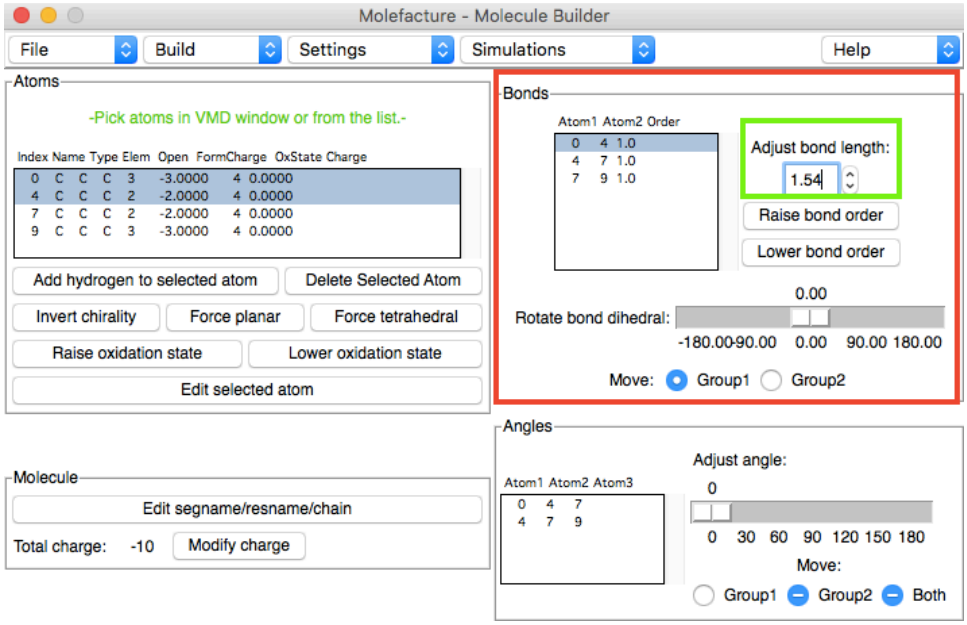
In united atom force field, hydrogen are incorporated in the carbon atom. To remove the hydrogen atom, under the “Atoms” section, select all the hydrogen and click on “Delete Selected Atoms”.



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

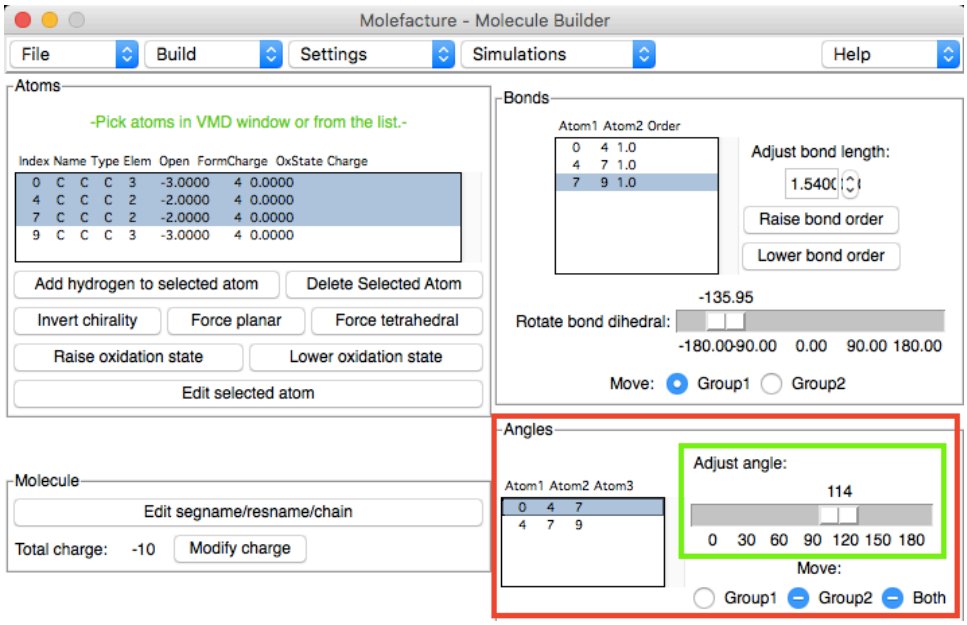
4. Adjust Bonds

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.



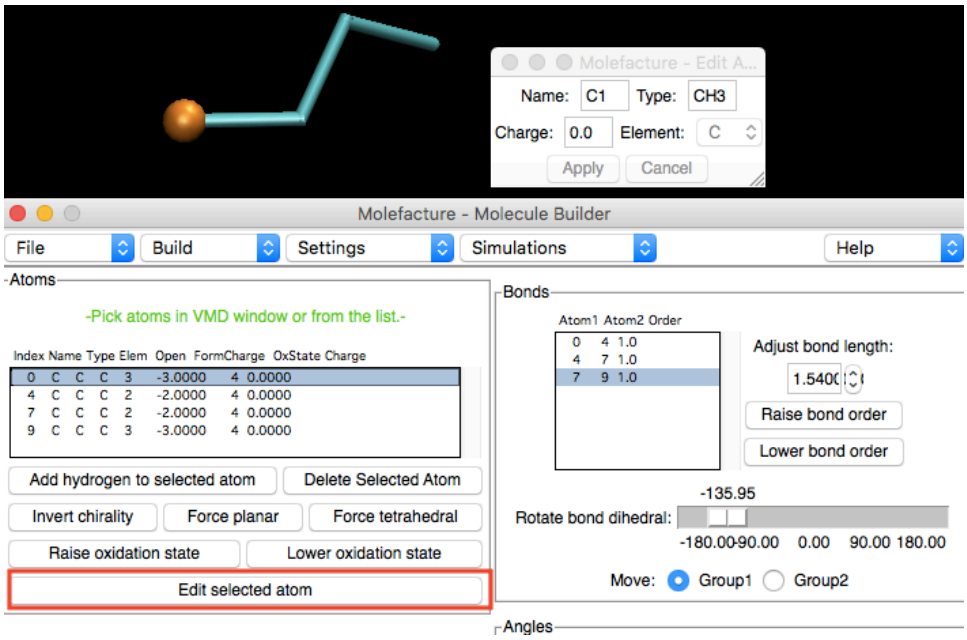
5. Adjust Angles

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

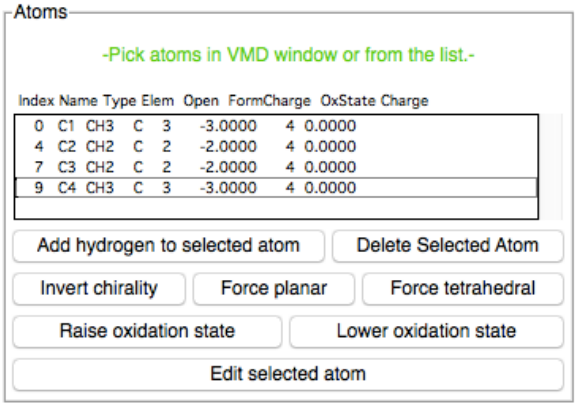
To assign atom name and type, under “Atoms” section, select the first atom (index 0), and click on “Edit selected atom”. In the opened window, change the atom name to “C1”, and atom type to “CH3” since the first atom incorporated three hydrogen, and click “Apply”. Note that In Mie potential for alkane,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



Repeat the same process for other atoms as follow:

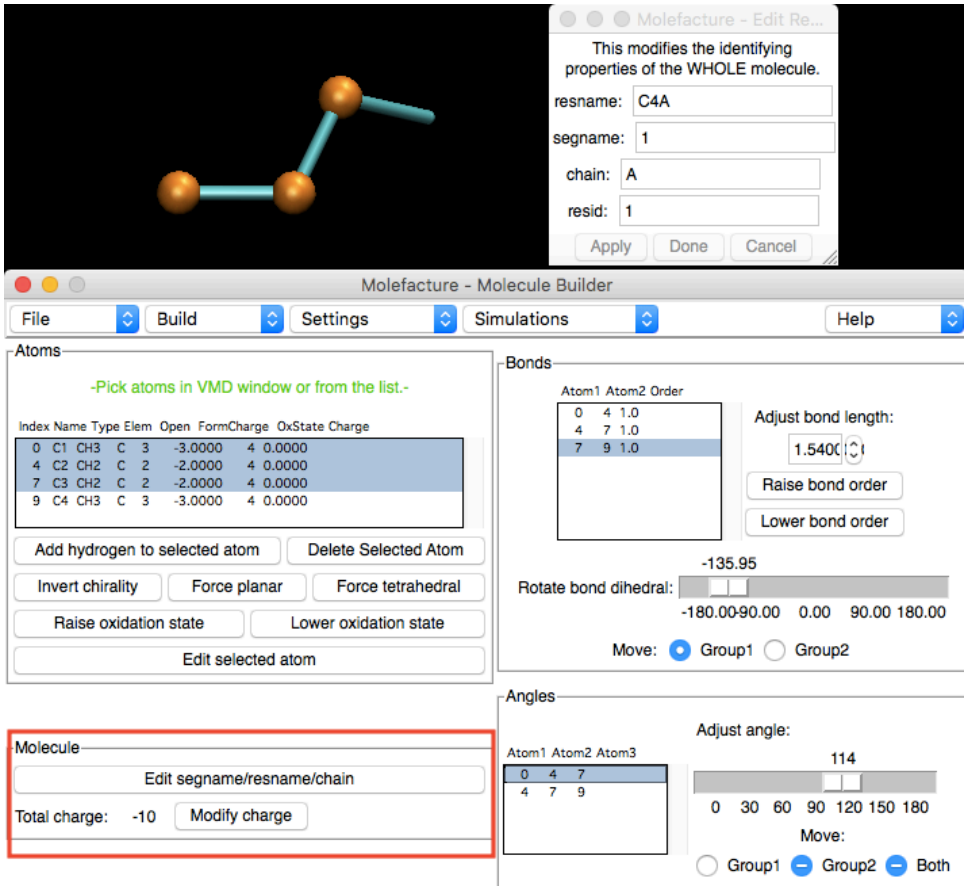
- Second atom “Index 4”, change the atom name to “C2”, and atom type to “CH2”.
- Second atom “Index 7”, change the atom name to “C3”, and atom type to “CH2”.
- Second atom “Index 9”, change the atom name to “C4”, and atom type to “CH3”.

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".

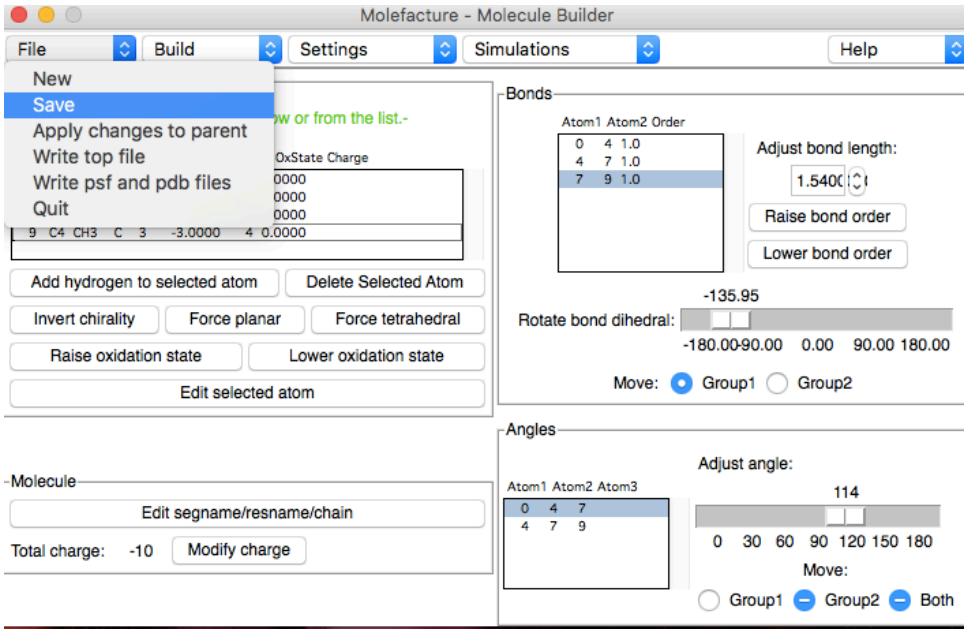


8. Assign Molecule Charge

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".

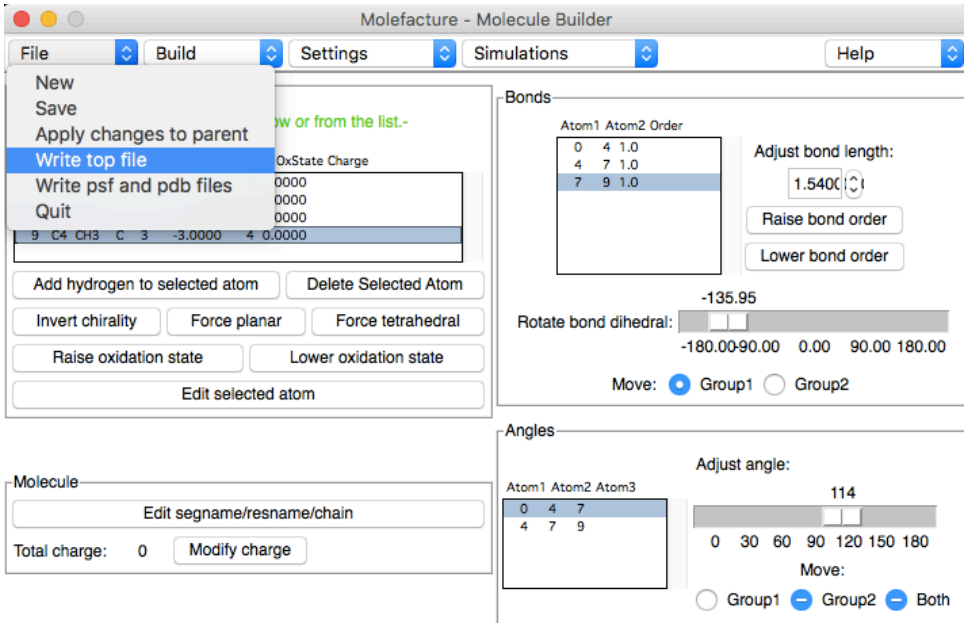
9. Save PDB File

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 filed, 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
```