

What is Computational Chemistry?

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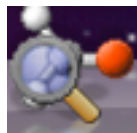
Objective: Students will be able to explain the overall methods and practical uses for computational Chemistry and the Computer software used

Gaussian View

- Gaussian View is a molecular building interface.
- Gaussian view allows its users to build molecules simply and interact with them in 3 dimensions by simply manipulating the mouse.
- We will use this software to practice building representations of ionic and covalent molecules

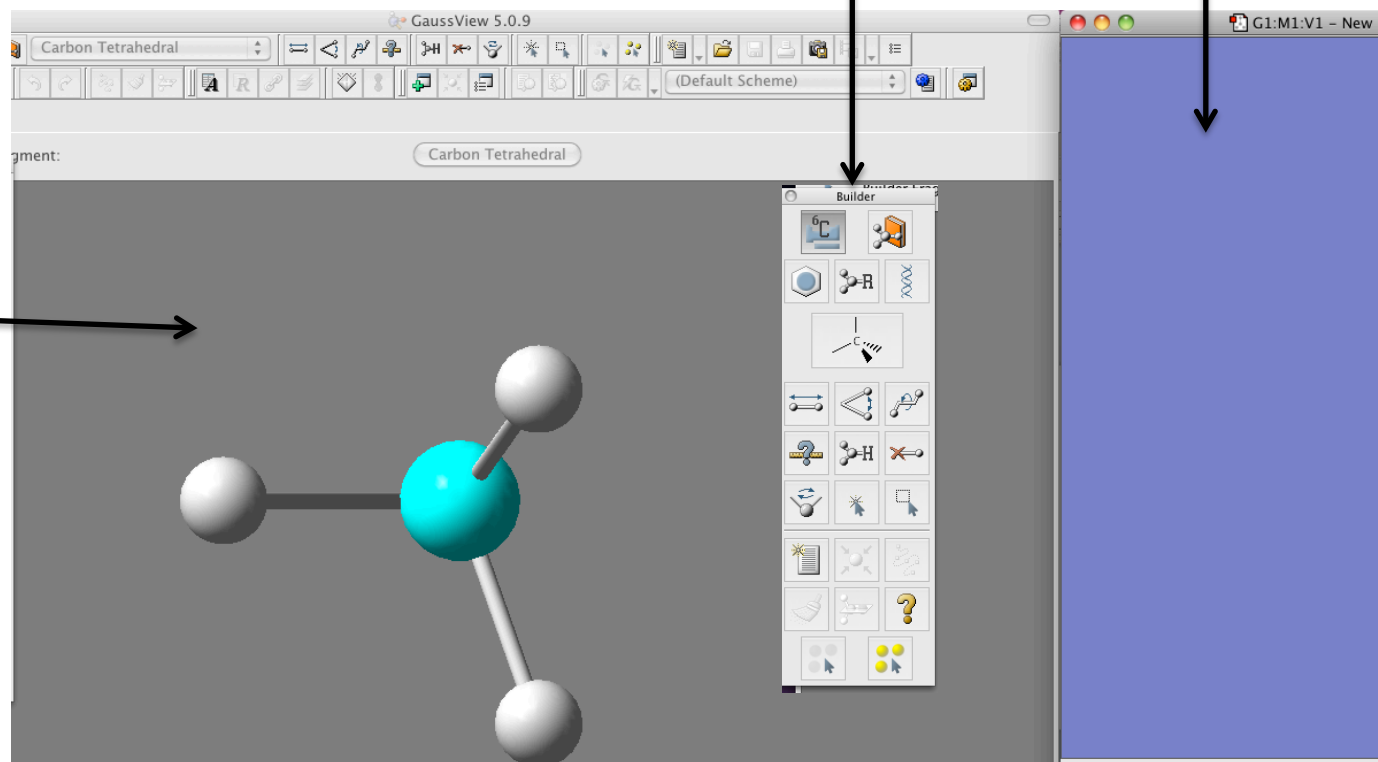
How to log into G View?

Click the icon on your computer screen to access software



These screens will appear

Menu screen



Click on this icon to pull up the periodic table



1. Use your mouse to hover over an element on the table. Click the element of choice.

2. Then Click atom.

3. Now click in the center of the purple

The periodic table below will appear.

Element Fragments

H	X Bq																He				
Li	Be															B	C	N	O	F	Ne
Na	Mg															Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr				
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe				
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn				
Fr	Ra	Ac	Rf	Db	Sg	Bh	Hs	Mt													
		Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu						
		Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr						

Select Carbon Fragment:

⁶ C Atom	<chem>C#C</chem>	<chem>C=C</chem>	<chem>C=C</chem>	<chem>C=C</chem>	<chem>C=C</chem>	<chem>C=C</chem>
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★ If you make a mistake click on the



and then click the mistake

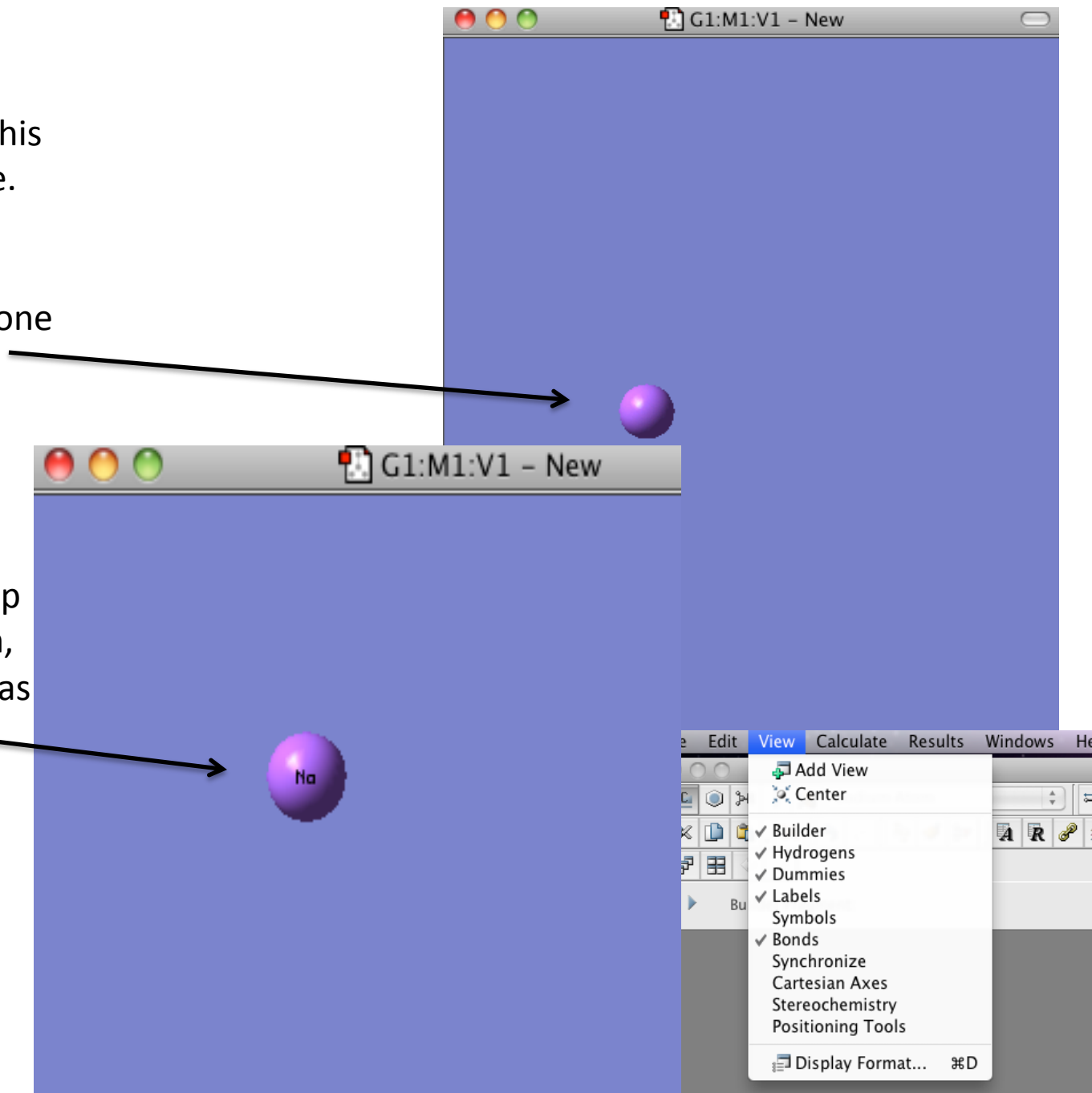
★ Let's try Sodium!

If you did it correctly this is what you should see.

- The sphere in the middle represents one atom of Nitrogen.

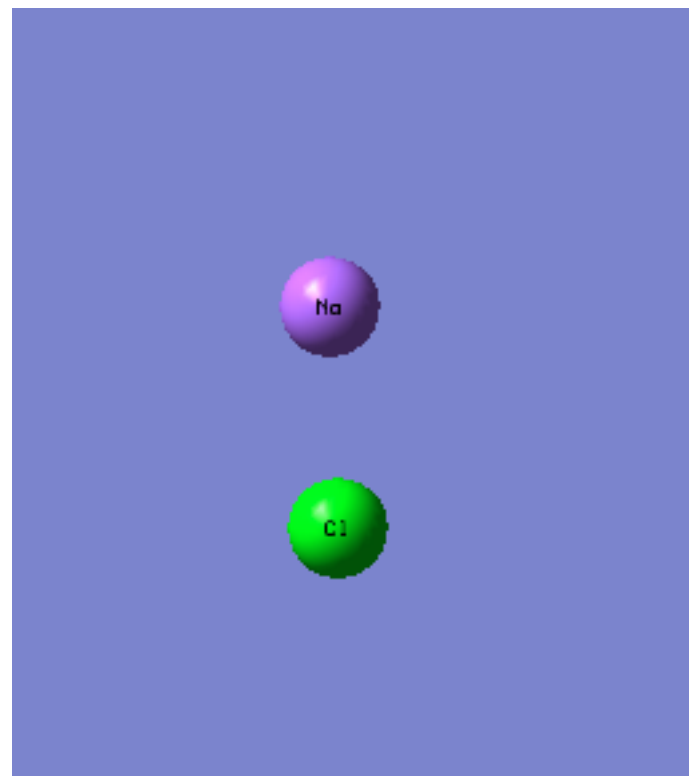
- You can label each atom.

★ Click **view** at the top of the menu screen, then click **symbols** as seen below



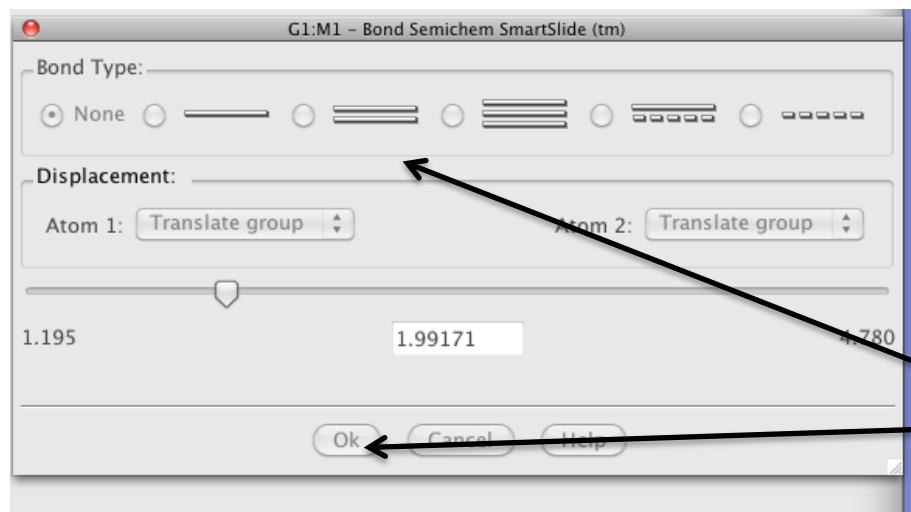
Now Let's add some another and work on some simple bonds!!

1. Look at your periodic table, think about what we have learned about ionic and covalent bonds.
2. How many valence electrons does Sodium have?
3. Is sodium a metal or a non metal?
4. What group on the periodic table would most likely form bonds with sodium?
5. Click the element of your choice
6. Now click atom
7. Next, click in the purple next to sodium





1. Click this icon in the builder menu



2. Now click both atoms, the should turn the same color

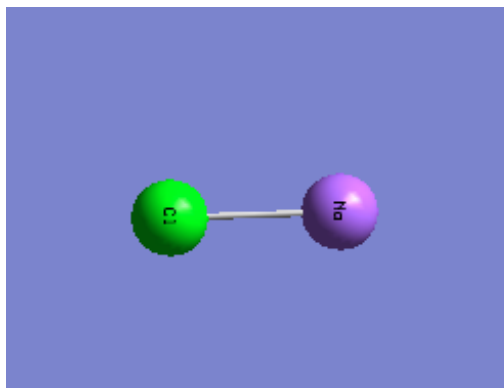
This screen will pop up.

3. Choose the number of bonds then click ok

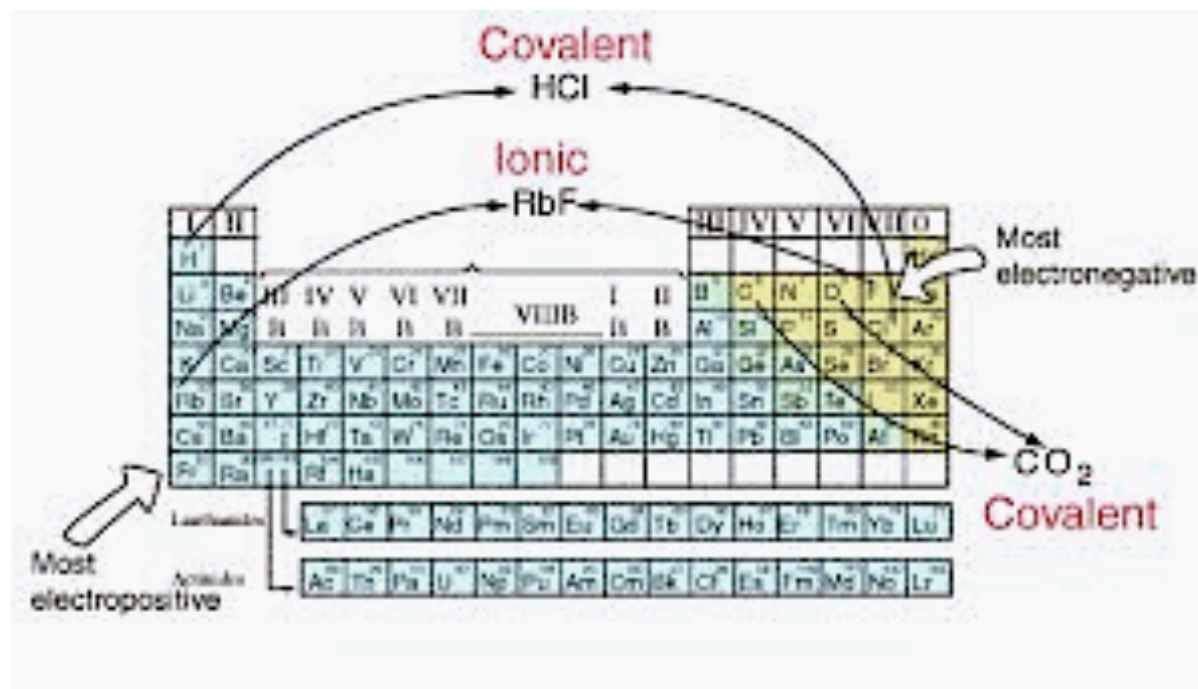
4. Now click the



This will give you the optimum shape



- ★ Try a few more molecules and draw them in your observation notebooks.
Label them ionic or covalent

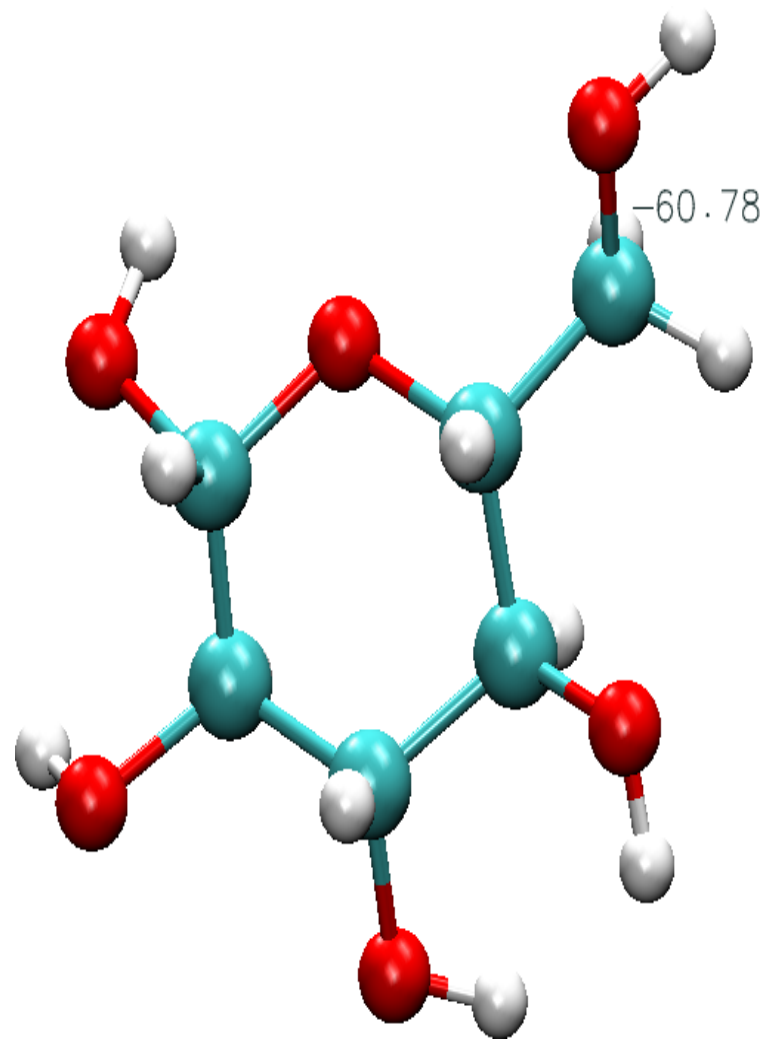


What is VMD?

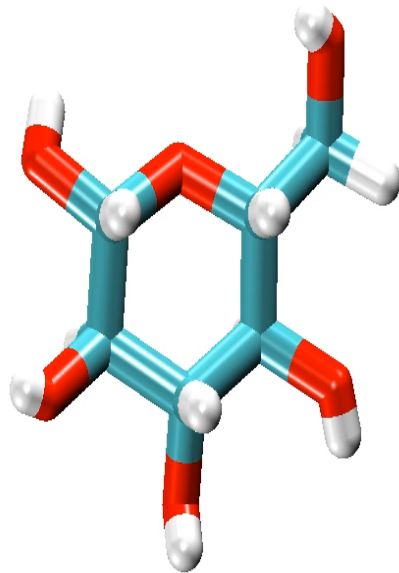
VMD stands for Visual Molecular Dynamics

- ◆ Visualize molecules in 3 dimensions
- ◆ Visualize how structures move in solutions

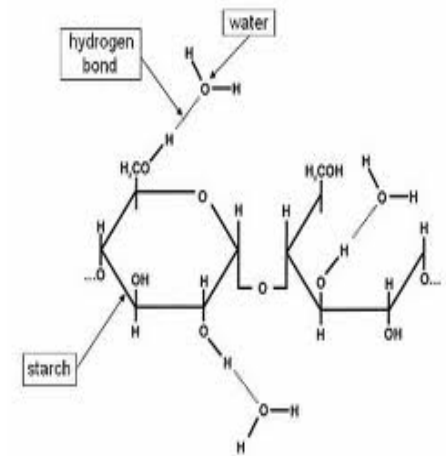
VMD is a molecular visualization program for displaying, animating, and analyzing large biomolecular systems using 3-D graphics and built in scripting



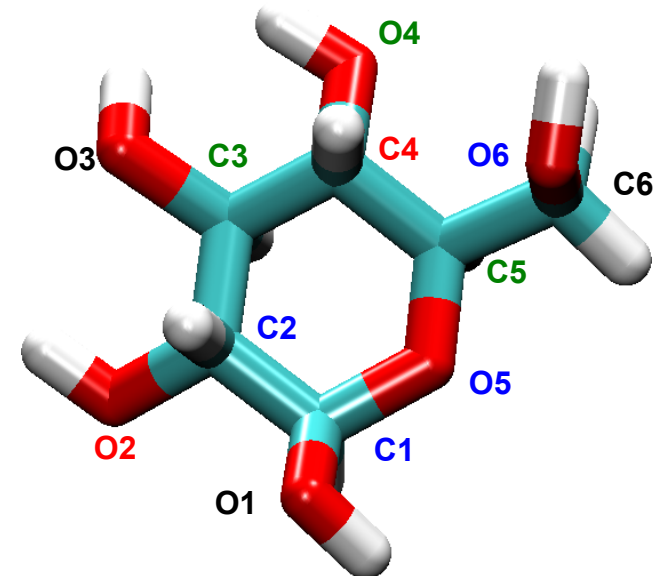
VMD Movie of Glucose Molecule in Water



Which carbons and oxygens have a better chance of interacting with the solvent? Why?

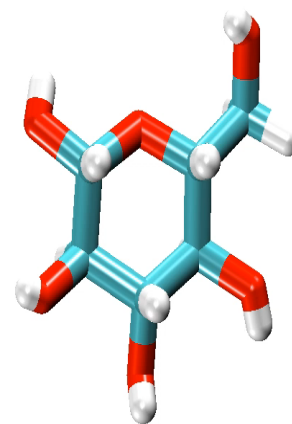
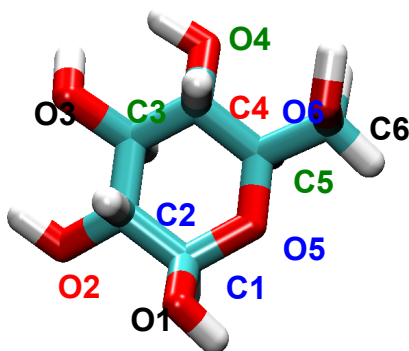
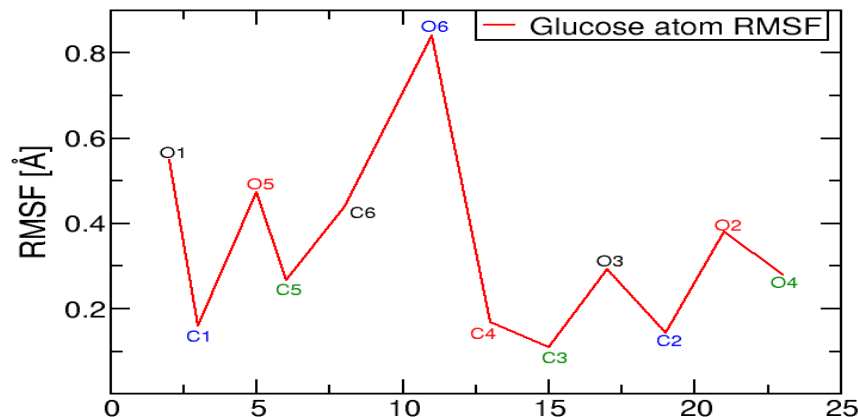


What type of bonds does glucose have the possibility of forming with water?



How do we get the data to analyze computationally?

- Simulations using Amber tools, VMD and Xmgrace-
- ♦ visualize changes due to differences in solution and molecule
 - ♦ Focusing on RDF and h-bonding as a indicator of dissolution
- ♦ Amber tools gather data based on angles, dihedrals, distance, and hydrogen bond count
- ♦ Xmgrace will produce the graphs



Sample Lab Report: Comparison: Comp vs. Experimental

Timekeeper _____

Manager/ Recorder _____/_____

Question: _____

This image shows a single sheet of white paper with horizontal blue or grey ruling lines. The lines are evenly spaced and run across the width of the page. There are approximately 20 lines visible. On the left side, there is a vertical margin line, creating a narrow left margin. The paper appears to be from a notebook or a standard ruled sheet of paper.

If _____ then _____

Independent _____

Independent _____

Procedure:

Title_____

Title_____

You will now write a lab report comparing what you have learned computationally to what you have learned in the science lab.