VR Instruction
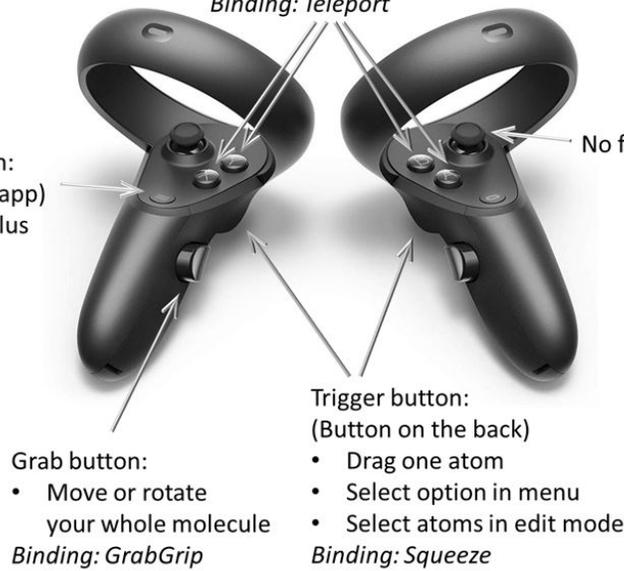

Adjust the size.

Menu button:
(All the same)
- Pause & enter menu
- Resume & leave menu

Binding: Teleport

No function for now.

Oculus Menu button:
(No function in this app)
- Enter or exit oculus menu

Trigger button:
(Button on the back)
- Drag one atom
- Select option in menu
- Select atoms in edit mode

Binding: Squeeze

Grab button:
- Move or rotate your whole molecule

Binding: GrabGrip

Hardware requirements:

GPU: NVIDIA GTX 960 / 1050Ti or greater
CPU: Intel i3-6100 or greater
Memory: 8GB+ RAM
VR: Oculus Rift S (or other VR devices)
Ports: DisplayPort 1.2 / Mini DisplayPort + 1 x USB 3.0 (for Oculus Rift S)

Software requirements:

System: Windows 10
Driver: NVIDIA driver released after 2019
            Oculus App (for Oculus Rift S)
SteamVR: Steam + SteamVR

Note: Oculus Rift S is the recommended VR device, because it's used in development, and a binding is provided. For other VR devices, you need to make your own customized binding. The names of the actions for binding is provided in the controller instruction figure.

Instruction:

1. General:
   Press the menu button, hit the "Molecule" using the trigger button, in the "Molecule" dropdown list select the one you are interested. Exit the menu by hit the menu button again.
   Reach your controller INTO one atom, and drag it using the trigger button. You can use two controllers to drag two atoms simultaneously.
   Move the whole system using the grab button. Rotate the whole system by holding both grab buttons.
   Discover other functions yourself!

2. Add a new molecule:
   Generate an xyz file of your molecule or system. It is recommended that your system contains less than 20 atoms.
   Open "VROption.txt", under the line "#ifdef Molecule", add the complete absolute path of you xyz file. It will occur in the "Molecule" dropdown list.
   If your molecule or system has a net charge (-1 for example), in the second line of your xyz file, which is intended for a description, write "charge=-1.0".

Note: Current backend is xtb 6.3 (semiempirical, https://github.com/grimme-lab/xtb). The TeraChem backend (HF) wil come soon.

Structure and Steric Effects

Chemists like to use Lewis structures to show a simple picture of how atoms are bonded to one another in a molecule. Below are Lewis structures for methane, the simplest hydrocarbon, and ammonia, the simplest amine.
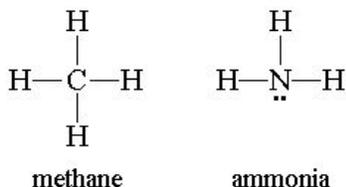
Using your molecular modeling kit, build a methane and ammonia molecule and use them to answer the following questions.

1. What is the name of each shape (or how would you describe them)?

2. Using other atom pieces instead of the 4-hole black carbon, can you make any other geometrical shapes with four hydrogen atoms? Compared to the usual structure of methane, what makes your structure better or worse?

VR Challenge 1: Planar Methane
- Open the menu using the A, B, X, or Y buttons. Point the controller to hover over buttons and click the index trigger to select them.
  - Go to Molecule and select **ch4** to open methane.
  - Go to Dynamics > Force and select **4x** to increase the force.
  - Go to Edit > Freeze and select 2 hydrogen atoms and the carbon atom.
- Exit out of the menu by pressing the A, B, X, or Y buttons again.
- Get the molecule in front of you by pressing and holding the middle finger grip trigger to move the entire scene - one hand pans, two hands rotate.
- Place your controllers over the non-frozen hydrogen atoms. Press and hold the index triggers to grab the atoms, and try to pull the atoms so that the molecule is flat. How easy is this to do? Is this structure stable?
- Pay attention to the potential energy diagram in the bottom left corner. Just like a ball rolling down a hill, the molecule is "more stable" when it has low potential energy. Does the graph support your previous answer or not?

3. Looking just at the hydrogen atoms, one may have expected ammonia to be planar (i.e. all atoms in a single plane). Why do you think this is not the case?

4. Comparing the bond angles in methane with those in ammonia, which are wider? Why would this be the case?

VR Challenge 2: Ammonia "Umbrella Flip"
Consider the following two structures for ammonia, which are related by a 180 degree rotation. Convert your ammonia from hydrogen atoms down to hydrogen atoms up WITHOUT any rotation.
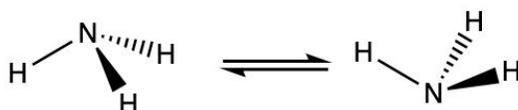

- Open the menu, make the following changes, and exit as above.
  - Go to Molecule and select **nh3** to open ammonia.
- WITHOUT rotating the entire system, flip the hydrogen atoms from one side of the nitrogen to the other. How easy is this "umbrella flip" motion?
- For an extra challenge, see if you can do the flip while only touching the nitrogen atom.
  - If needed, go to Dynamics > Force and select **4x** to increase the force.

Single vs Double Bonds
Use your molecular modeling kits to make ethane and ethene, shown below with a 3D representation of a Lewis diagram.
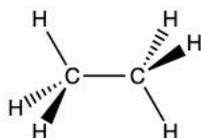

Ethane
(C_2H_6)
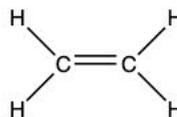
Ethene
(C_2H_4)

5. List at least two geometric differences between ethane and ethene.

6. Is the C-C bond in ethane or the C=C bond in ethene easier to twist? Why do you think this is the case?

VR Challenge 3: C-C Bond Torsions
- Open the Molecule menu and select **ethane**.
- Spin the two methyl (CH_3) groups in opposite directions by pulling on the hydrogens.
- Now, open the Molecule menu and select **ethene**.
- Try to spin the two methylene (CH_2) groups in opposite directions as you did in ethane. Is this bond easier or harder to twist around? Approximately how much less or more force did you have to use?
    - If more force is needed, open the menu and change Dynamics > Force to **4x**.

Cyclic Molecules
Molecules can also form cycles, such as cyclohexane (below left) and benzene (below right). Analogous to ethane and ethene above, cyclohexane is not flat while benzene is.
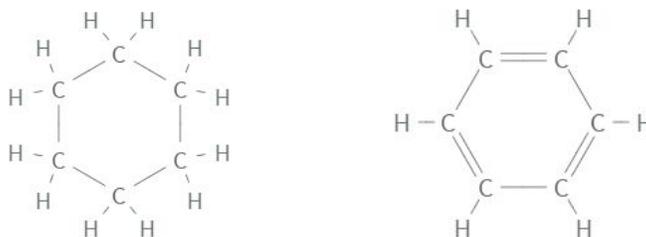
7. Cyclohexane has two main conformations: "chair" and "boat". Based on your molecular modeling kit, which conformer do you think is more stable and why?

flip this end
of the chair up

chair   boat
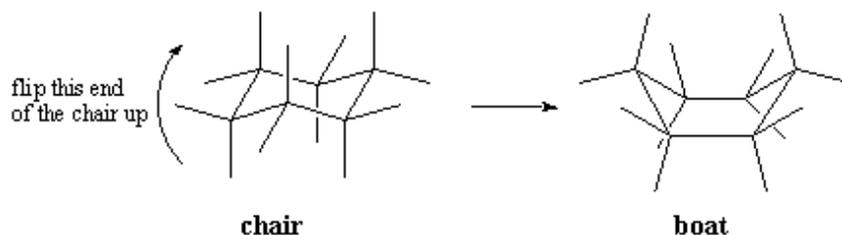
VR Challenge 4: Cyclohexane Conformer Flip
- Open the Molecule menu and select **cyclohexane**.
- Pull on atoms to switch between the "chair" and "boat". Do you notice any differences between what you expect to happen from the modeling kits and what actually happens?

8. Benzene is planar and only has one conformer for the nuclei. However, some of the electrons in benzene can change between configurations, an effect often called "resonance". Draw the two Lewis structures for benzene (often called "resonance structures").

VR Challenge 5: Through the Benzene
- Open the Molecule menu and select **benzene+h**.
- Try to pull the hydrogen atom through the benzene ring. Do you notice any differences between what is expected based on the modeling kits and the simulation?
    - If more force is needed, open the menu and change Dynamics > Force to **4x**.

Hypervalency and Pseudorotations

Molecules involving heavier atoms can take on interesting geometries as atoms can become *hypervalent* - that is, they can accept more than four bonds. This can lead to cool conformer rearrangements; for example, PF_5 can perform a *pseudorotation* where the fluorine atoms can take a different configuration around the central phosphorus atom.

trigonal bipyramidal   square pyramidal   trigonal bipyramidal
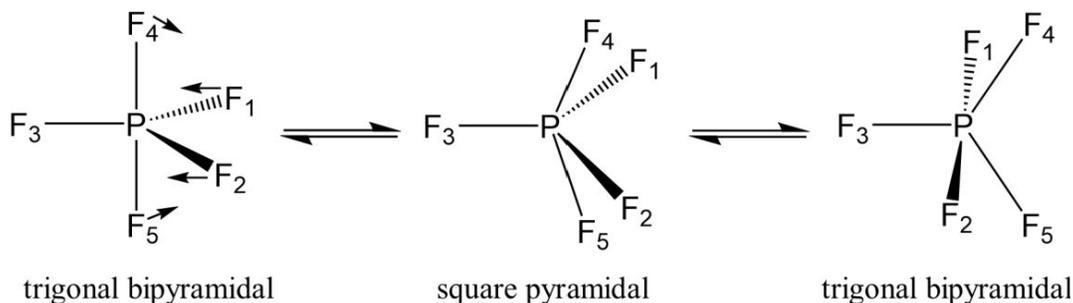
9. Consider the complex PH_3F_2. Draw out all the different trigonal bipyramidal geometries can be formed with these atoms.

VR Challenge 6: Pseudorotations
- Open the Molecule menu and select **ph3f2**.
- Try to convert between the conformers of PH_3F_2 without breaking any bonds. Did you find all the conformers and rotations between them with the modeling kit?

Acid-Base Reactions
Chemistry is most interesting when molecules react! You may have already heard of acid-base reactions, where an H^+ is transferred between two molecules.

10. Given carbonic acid (H_2CO_3) and water (H_2O), draw Lewis structures for the reactants and the most likely products. Using your molecular modeling kit, propose a mechanism for this reaction.

VR Challenge 7: Not So Basic After All
- Open the Molecule menu and select **H2CO3_H2O**.
- Try to carry out the acid-base reaction you proposed in Question 10. Is the system more stable (i.e. lower in energy) before or after the reactions? Why do you think this might be the case?
    - If more force is needed, open the menu and change Dynamics > Force to **4x**.
- As an added challenge, see if you can create a proton shuttle by making one H^+ transfer to water, transfer another H^+ between water molecules, and finally a third H^+ back to a different oxygen atom on the carbonic acid.

Simple Organic Reactions

Chemical reactions that involve bond formation between heavier atoms (carbon, nitrogen, or oxygen) are very useful, as they can be used to build large molecules, such as pharmaceuticals for medicine, amino acids for proteins, or polymers for materials.

11. Consider the following substitution reaction between methyl fluoride and hydroxide:

$$CH_3F + OH^- \Leftrightarrow CH_3OH + F^-$$
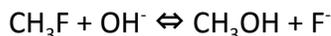
Using your molecular modeling kit, propose a mechanism for this reaction.

VR Challenge 8: Substitution Reaction Part I
- Open the Molecule menu and select **MeF_OH**.
- Try to carry out the substitution reaction you proposed in Question 11. Are there any other mechanisms that seem to work? Are there any competing reactions that lead to other products?
    - Open the Molecule menu, switch to any molecule, and switch back to **MeF_OH** to reset the system as needed.

12. Now consider a related substitution reaction with tert-butyl fluoride instead:

$$C(CH_3)_3F + OH^- \Leftrightarrow C(CH_3)_3OH + F^-$$
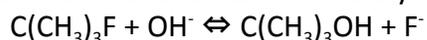
Do you expect the most likely mechanism to change in any way?

VR Challenge 9: Substitution Reaction Part II
- Open the Molecule menu and select **tBuF_OH**.
- Try to carry out the substitution reaction with the new system. Does the system behave as you expect?
    - Open the Molecule menu, switch to any molecule, and switch back to **tBuF_OH** to reset the system as needed.