Miranda House
University of Delhi

INSPIRE INTERNSHIP PROGRAMME 2024

Innovation in Science Pursuits for Inspired Research
An Initiative of DST, Govt of India

8-12 JULY 2024

The World of Molecules: Playing with structures

Offered by:
Chemistry Department

The World of Molecules: Playing with structures

Aims: To learn and apply the Valence Shell Electron Pair Repulsion theory using computational modeling.

Objectives:

a) To build 3-D models of simple molecules using open source software Argus Lab.
b) To visualize the three dimensional arrangement of the atoms in the molecule and see the correct orientation of the atoms and bonds with respect to each other.
c) To optimize the structures.
d) To apply Valence Shell Electron Pair Repulsion theory using computational modeling to simple structures.
e) To compare to the results obtained by Argus with results obtained from VSEPR theory.

Procedure:

1. Use ArgusLab to build the water molecule: **H_2O**

Start out with a chain of three atoms. Then click on the yellow arrow  in the tool bar to select the atoms individually. Select the middle atom and right click it. Then select the change atom option. Then select the O[sp3] tab and then click the O_3 tetrahedral option. Your central atom should now be a "red" oxygen atom. Now select the other two atoms (select one, then hold down ctrl then select the 2nd). Right click and then change these 2 to hydrogen atoms.

The number of valence electrons in water is _____

The number of electron domains in water is _____

What is the shape of the molecules you have originally drawn? (circle one): *Linear Bent*

2. Go up to the calculations tab on the top. Click it and then select the energy option. In the upper right hand corner choose the PM3 option and then OK. Now you can click on the optimizegeometry button  , which is on the right side of the tool bar. Save the file as h2o

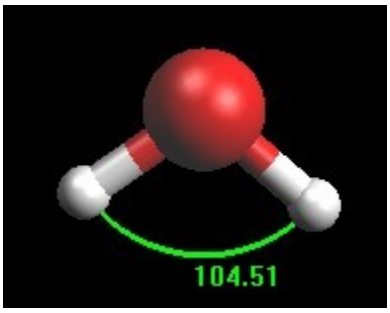
What did you see? Did the molecule arrange in a straight line or is it bent?

---

3. In order to display the H-O-H angle, click on the button. This allows you to select atoms. Select the three atoms by clicking on each while holding down the CRTL key. The selected atoms should appear yellow. Now go to the Monitor tab on top, and select Angle.

Record the angle value here: _____

Does the result given by the computer match your prediction based on VSEPR? Explain.



4. Build and optimize the following molecules and ions:

NO_3^-, CH_4, SF_6, SO_2, PCl_5

Building Hints: For **NO_3^-:** start with four atoms in a pattern. There should be a total of 3 bonds and the three outer atoms should be connected to the central atom. The central atom should be changed into a nitrogen (tetrahedral). The three surrounding atoms should be changed to oxygens. Before optimizing (i.e clicking on the) click on the calculations tab on top then energy and make sure to adjust the charge to -1.

For **CH_4**: Start with an atom in the middle. Then make a shape similar to NO_3^-. Now you

will have to rotate your atom so all the atoms are in a horizontal plane. Left click and hold on the central atom then drag your mouse slowly towards the top of the screen. Stop when you can only see 3 atoms. Now add a fourth atom straight down to form a "T". The central atom will stay a carbon. The other four atoms should be changed to hydrogen.

For **SF_6**: Sulfur is the central atom.

For **SO_2**: Sulfur is the central atom.

For **PCl_5**: Phosphorus is the central atom.

5. Use VSEPR to predict the molecular geometries for these molecules/ions. Compare to the results obtained by Argus. Use the following table to summarize your results

Molecule/Ion	**VSEPR Molecular geometry**	**Geometry obtained by Argus**	**Bond Angles Predicted by VSPER**	**Bond Angles Predicted by Argus**
NO_3^-				
CH_4				
SF_6				
SO_2				
PCl_5				

Did most of the geometries obtained by Argus match the molecular geometries predicted by VSEPR? To what extent? If any did not agree at all, provide a reasonable explanation.

Exercise

Molecules with more than one central atom:

Start with an empty window (File then New). Click on the add fragment button  . Select fragment library. Then select the folder labeled amino acids, then scroll down and select tryptophan and then ok. Right click in the middle of your screen and a molecule of tryptophan will appear. Rotate it so that you can see the two carbon rings. Now look at the carbon and two oxygen atoms on the end.

Is this structure correctly displaying the rules of VSEPR? Explain your answer.

Now go back to the fragment library  and select the pharmaceuticals folder. Then select aspirin and then ok. Right click on the screen and an aspirin molecule will appear. Look at the carbon atom double bonded to the oxygen atom.

Does this portion of the molecule display correct VSEPR? Explain your answer.

Arrange these molecules in order of increasing bong angle (smallest bond angle to largest):

H_2O, ICl_2^-, NH_2^-, NO_2^- = _____<_____<_____<
<_____