GENERAL CHEMISTRY LABORATORY

CH101

Post-lab assignment on exp. #6

Molecular Structure

Name:____

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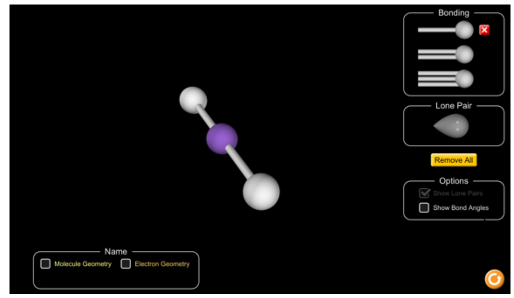
TF:____

Lab section:

BOSTON UNIVERSITY

Exp.#6: Molecular Structures

Part A – Lewis and VSPER— Practice and Theory



In the first part of the lab, we will use molecular visualization tools to look at molecules in three dimensions. To start, log on to the PheT Molecular Shapes simulation located at: https://phet.colorado.edu/en/simulation/molecule-shapes

Click on the play arrow and then select the "**Model**" option to enter the simulation area. You will see a screen like the one on the right. Take a moment to see the options:

- You can add (or remove) bonds to the structure using the *Bonding* palette in the top right. You can add (or remove) lone pairs as well. "Remove All" gets rid of everything but the central atom.
- Notice that there is also an option to see the bond angle, molecule geometry (shape), and electron geometry (this is not really interesting).

1. Let's investigate the molecule BF_3.

   a. Draw the Lewis structure for the molecule in the space provided.

   b. What is the steric number (SN) of central atom?

   c. What is the class of molecule ($AX_{\#}E_{\#}$)?

   d. Use the PheT simulation to model the molecule. Add another single-bonded atom to make a total of three grey atoms bonded to the purple central atom. Based on the simulation, what is the molecular geometry (i.e., shape) of the molecule?

   e. Redraw your Lewis structure, this time as a 3D representation (if necessary, use dashes and wedges to illustrate 3D structure). You can rotate the simulated molecule to get a better view.

   f. Use the simulation to measure the bond angles. What is (are) the bond angle(s) between the terminal atoms (grey) and the central atom?

   g. Draw bond dipoles on your 3D sketch for any polar bonds. Based on your sketch, is the molecule polar? Explain briefly.

Lewis:

SN =

Class =

Shape =

3D sketch:

Bond angles =

2. Let's repeat our investigation for NH_3.

   a. Draw the Lewis structure for the molecule in the space provided.

   b. What is the steric number (SN) of central atom?

   c. What is the class of molecule ($AX_{\#}E_{\#}$)?

   d. Use the PheT simulation to model the molecule. Add another single-bonded atom to make a total of three grey atoms bonded to the purple central atom. Based on the simulation, what is the molecular geometry (i.e., shape) of the molecule?

   e. Redraw your Lewis structure, this time as a 3D representation (if necessary, use dashes and wedges to illustrate 3D structure). You can rotate the simulated molecule to get a better view.

   f. Use the simulation to measure the bond angles. What is (are) the bond angle(s) between the terminal atoms (grey) and the central atom?

Lewis:

SN =

Class =

Shape =

3D sketch:

Bond angles =

   g. Draw bond dipoles on your 3D sketch for any polar bonds. Based on your sketch, is the molecule polar? Explain briefly.

3. Why is it important to know the molecular shape before making determinations about molecular polarity?

4. Do you agree with the bond angle that the simulation reported for ammonia in question 2? Let's investigate! At the bottom of the simulation screen it should say "Real Molecules". Select NH_3 from the drop-down list of molecules. What is the bond angle that is reported for the actual ammonia molecule? Explain the difference that you observed between these bond angles.

5. Methane (CH_4) and water (H_2O) both have steric number 4, but they have different bond angles. Which bond angle do you expect to be larger? Your explanation should include a discussion of the molecular shape of the molecules. You can check your work in the "Real molecules" part of the PheT simulation.

6. We're going to do a few more examples. For each molecule below, follow the guidance in questions (1) and (2) to help you with your work. Report <u>real</u> bond angles (<120º, <90º), where applicable (but you don't need exact values).

XeF_2

Lewis:	3D sketch:
SN = / Class =	Bond angles =
Shape =	Is the molecule polar?

$TeCl_4$

Lewis:	3D sketch:
SN = / Class =	Bond angles =
Shape =	Is the molecule polar?

I_3^-

Lewis:	3D sketch:
SN = / Class =	Bond angles =
Shape =	Is the molecule polar?

H_2CO

Lewis:	3D sketch:
SN = / Class =	Bond angles =
Shape =	Is the molecule polar?

$BFCl_2$

Lewis:

3D sketch:

SN =

Class =

Bond angles =

Shape =

Is the molecule polar?

AsF_5

Lewis:

3D sketch:

SN =

Class =

Bond angles =

Shape =

Is the molecule polar?

SCl_4

Lewis:

3D sketch:

SN =

Class =

Bond angles =

Shape =

Is the molecule polar?

7. In the trigonal bipyramidal structure we place lone pairs in the equatorial plane first. Use the concepts of lone-pair–lone-pair repulsion and lone-pair–bonding-pair repulsion to show why a T-shaped molecular geometry is preferred over other possibilities for molecules with an AX_3E_2 configuration.

Part B – Resonance-practice and theory

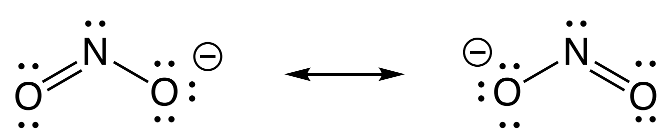
Two videos on resonance are posted on Blackboard. Watch the two videos and answer the questions on resonance below. To access the videos:

- Go to blackboard (learn.bu.edu)
- Click on "Lab content" and then "Lab 6 Videos"
- There will be two video links in that folder.

Start with the video 2.3 called "Introduction to Resonance" and then work through "Drawing Resonance Structures."

1. Consider the two resonance forms to the right for the nitrite ion, NO_2^-. Answer the following questions based on your understanding from the videos about what resonance forms indicate.

a. True or false: nitrite behaves like the form on the left 50% of the time and the form on the right 50% of the time. If the statement is false, explain why.



b. What are the O–N bond orders in the nitrite molecule? Explain briefly.

c. What can you say about the formal charge of the oxygen atoms in the nitrite ion?

2. Write resonance forms that describe the distribution of electrons in each of these molecules or ions. Make sure to include non-zero formal charges where relevant.

a. Selenium dioxide, OSeO

b. Nitrate ion, NO_3^-

c. Benzene, C_6H_6:

d. Carbonate ion, CO_3^{2-}

Part C – Bonding and antibonding 1s molecular orbitals

For this part of the experiment you will need to install the (free) Wolfram Player on your computer or look on with another student who has it installed. The link to install the player is: https://www.wolfram.com/player/

After you've installed the wolfram player, download or open the CDF simulation that is posted at:

http://quantum.bu.edu/CDF/101/1sMolecularOrbitals.cdf

Click on the little "+" sign in a box next to the Separation slider. Start by tuning the separation all the way to the right so that separation is maximized (the value will read 0).

a. Focusing on the green orbitals on the bottom: what orbitals are these representing?

b. What do the black dots in the simulation area represent?

c. Slowly move the slider to the left to decrease the separation. Stop when the value of Separation is equal to 1. Notice that the bottom orbitals/waves have the same phase (the loop of the wave on the left and right are both up). Notice that the top orbitals/waves have *opposite phases* (the wave on the left has its loop pointed up, and the wave on the right has its loop pointed down). What do you expect to happen when the two bottom (in-phase) waves start to overlap with each other?

d. What do you expect to happen when the two top waves (out-of-phase) start to overlap with each other?

e. Keep moving the slider until the separation value reads 1.75. At this point the waves have overlapped with each other by about half. If you wanted, you could keep moving the slider and force the waves to overlap completely. While that is mathematically fine, it will not happen in atoms. Why not?

f. Sketch the cartoon of the new orbital that is made by the in-phase overlap of the atoms' electrons (this is the bottom image). Does this agree with your prediction that you made in (c)?

g. Sketch the cartoon of the new orbital that is made by the out-of-phase overlap of the atoms' electrons (this is the top image). Does this agree with your prediction that you made in (d)?

h. What happened to the original atomic orbitals when they overlapped with each other? Where did they go? What are the names of the new orbitals that were made?