VSEPR Theory and Molecular Shapes

Instructions: Work through the exercises below. If you have access to molecular model kits, use them to build three dimensional models of the molecules (or polyatomic ions) in the exercises and to help you answer the questions.

Learning Objectives:
By the end of these exercises, the student should be able to demonstrate the following proficiencies:

1. Draw Lewis electron-dot structures of polyatomic ions and molecules.
2. Given a Lewis electron-dot structure, distinguish between bonded pairs and non-bonded pairs of electrons.
3. Draw resonance forms (hybrids) for cases where more than one valid Lewis structure is possible
4. Use the Valence Shell Electron Pair Repulsion (VSEPR) theory to predict the geometries of molecules and polyatomic ions, including those with more than one central atom.
5. Given a Lewis electron-dot structure, assign hybridization to the atoms.
6. Explain how the combination of Valence Bond Theory (theory of hybrid atomic orbitals) and Molecular Orbital Theory can be used to explain the structure and bonding of delocalized π systems (such as ozone, carbonate ion, and benzene, for example).

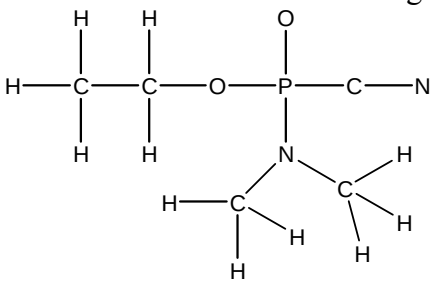
Part A: There is a table attached to the end of this document. For each molecule or ion in the table, provide entries for columns I through IX. You can check your answers at http://www.chemistry.usna.edu/plebeChem/vsepr/ (requires Internet Explorer and the Chime plugin)

Column I:	Draw a valid Lewis electron dot structure.
Column II:	Draw any appropriate resonance structures.
Column III:	Give the number of bonded atoms attached to the central atom.
Column IV:	Give the number of lone pairs attached to the central atom.
Column V:	Electron-Pair Geometry: Give the number of charge clouds, and their geometry, around the central atom (this is the number of bonded atoms plus the number of lone pairs on the central atom).
Column VI:	Molecular Geometry: Give the name of the arrangement of the atoms (for example: linear, trigonal planar, tetrahedral, trigonal bipyramidal, octahedral, bent, trigonal pyramidal, see-saw, T-shaped, square pyramidal, square planar).
Column VII:	Give values of the bond angles around the central atom. (for example, 109.5 °, less than 109.5°, 120°, less than 120°, etc.).
Column VIII:	Give the hybridization of the central atom.
Column IX:	State how many sigma bonds and pi bonds are present in the molecule (or polyatomic ion).

Part B: **More Complex Molecules**: The questions below make use of more interesting, and more complex, molecules. Many of these examples have more than one central atom. Also, many of these molecules have an important role in naval applications or other applied areas of chemistry.

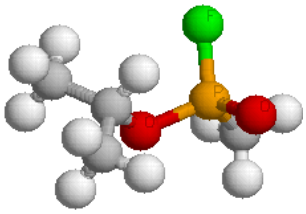
If you have access to molecular models, build 3-D models of the molecules to help you answer the questions. Or, you can work on these questions interactively, with online 3D molecular models, at: http://www.chemistry.usna.edu/plebeChem/vsepr/ (Requires Internet Explorer and the Chime plugin.)

1. The figure below shows how the atoms in the nerve agent Tabun are connected to each other. Draw the complete Lewis dot structure shown (include any multiple bonds or lone pairs). Assign the hybridization to each atom (except hydrogens). Give an estimate of the P-C-N angle.



2. A 3-D molecular model of the nerve agent Sarin is provided below. Based on this model, draw the Lewis structure of Sarin. Label the formal charges on the phosphorous and the atoms connected directly to the phosphorous. Can you draw more than one valid Lewis Structure? If so, what is the relationship between them?

Click here for a 3-D model of sarin.



3. The molecular formula for ethanol is CH_3CH_2OH. What is the C-O-H angle? What is the hybridization of the oxygen atom? Give an estimate of the C-O-H bond angle.

4. The molecular formula for octane is C_8H_{18}. Draw the Lewis structure and answer the questions below. Remember, carbon atoms can form 4 bonds but hydrogens can only form one!

   Pick one of the carbon atoms.
   a. What is its hybridization?

   b. Do all of the carbon atoms have the same hybridization?

   c. Give an estimate of the H-C-H bond angles on this carbon atom.

   d. Are all of the H-C-H bond angles the same?

5. The molecular formula for ozone is O_3. Draw the Lewis structure and any resonance structures. Label any atoms that bear formal charges and answer the questions below.
   a. What is the O-O-O bond angle?

   b. What is the hybridization of the central oxygen atom?

6. The molecular formula for acetic acid is CH_3COOH. Draw the Lewis structure. Hint: In determining how to put the atoms together follow the following rules: carbon forms a total of four bonds, oxygen forms 2 bonds, and hydrogen forms one bond.
   a. What is the hybridization of each of the atoms (except the hydrogens)?

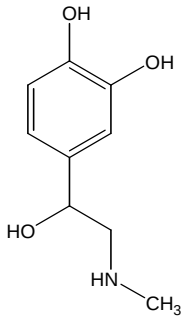
   b. Give an estimate of the H-C-H angles.

   c. Give an estimate of the O-C-O angle.

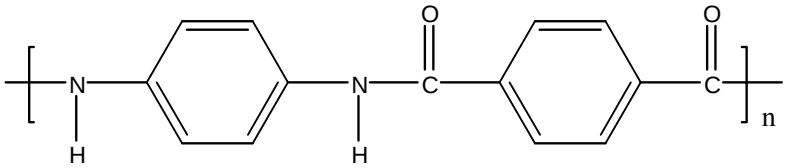
7. The molecular formula for the acetate ion is CH_3COO^-. Draw all possible valid Lewis structures. Calculate the formal charge on all of the atoms. Label all of the π bonds, including bonds which contain partial π-character that arises from resonance. Give an estimate of the O-C-O bond angle.

8. The structure below is the molecule adrenaline (also called epinephrine). The structure has been drawn using a shorthand notation commonly used by chemists where the bonds between carbon atoms are shown but the carbons (and their attached hydrogens) are omitted from the structure. Draw the complete Lewis structure of adrenaline showing all of the atoms (including hydrogens) and lone pairs. Remember: Carbon forms a total of four bonds.

   Give an estimate of the bond angles involving the carbon atoms in the ring



9. Kevlar is a very strong material that is used in bullet-proof vests and many other applications. It is an example of a class of compounds called polymers which are large molecules made up of small units (monomers) linked together to make a huge chain. The structural formula for the repeat unit of Kevlar® is shown below. The brackets indicate that the structure shown below is repeated over and over again.



   a. Complete the Lewis structure (i.e., add in the lone pairs).

   b. Provide the hybridization of the non-hydrogen atoms?

10. Methyl ethyl ketone (MEK) is a solvent that is sometimes used in the Fleet for cleaning and degreasing. The molecular formula is $CH_3C(O)CH_2CH_3$. The O atom is in parentheses to indicate that it is branched off of the second carbon atom.
    a. Draw the Lewis structure.

    b. Give an estimate of the C-C-O bond angles.

    c. What is the hybridization of the non-hydrogen atoms?

    d. How many π bonds are there?

Part A: SC111 VSEPR Molecular Shapes Assignment

Formula	I Lewis Structure	II Resonance	III Bonded Atoms	IV Lone Pairs	V Electron-Pair Geometry	VI Molecular Geometry	VII Bond Angles	VIII Hybridization	IX Sigma/ Pi Bonds
CN^-									
CO_2									
NO_2^-									
SO_2									
CO_3^{2-}									
BCl_3									

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SO_4^{2-}									
CH_3Cl									
NH_3									
PCl_5									
SF_6									