Chemistry 121

Exercise 4: Using VSEPR to predict molecular shapes, polarity and solubility

Objective:

a. Use molecular model kits to apply VSEPR rules to determine the shapes of various molecules

b. Using the shape of a molecule and the electronegativities of the atoms in the molecule, predict the overall polarity of a molecule

c. Determining which substances will dissolve in a given solvent, given their polarities

VSEPR stands for "valence shell electron pair repulsion" and is the principal theory that predicts the **shapes** of molecules. At its most basic level, it uses the interactions of **lone** and **bonded pairs of electrons** around each atom in a molecule to determine the overall arrangement of atoms in a molecule (the molecular shape). Combined with electronegativities of atoms, it will provide the basis for determining the **polarity** (the electrical charge distribution) of a molecule.

Reading: Section 4.8 in the textbook.

Materials needed:

- Molecular model kit
- Distilled water bottle
- Test tube rack
- Three small test tubes
- Small dropper bottle of hexane
- Small dropper bottle of ethanol

Safety issues: Hexane and ethanol are volatile solvents so avoid inhaling too much of them (toxic and explosion hazards). **Close the containers** after use! **Solvents should be disposed of properly in the container provided**.

Procedure:

A. Draw the Lewis (electron) dot structures of the molecules on the data sheet.

B. Determine the number of bonded and lone pairs around each molecule's central atom. Describe the arrangement of electron pairs around the central atom. Predict the shape of the molecules on the data sheet, based on the rules of VSEPR.

C. Build the model of the molecule using the kit and confirm or deny the validity of your shape prediction. Sketch your model as accurately as you can on the data sheet.

The **rules**:

- White represents **hydrogen**
- Red represents **oxygen**
- Black represents **carbon**
- Blue represents **nitrogen** (some of these blue balls have five holes but use only **three adjacent holes**)

• For other atoms, use family relationships to determine which color you should use
• Short sticks and long sticks represent chemical bonds (which are merely a pair of shared electrons between atoms); length doesn't matter
• For a molecule to be "happy" (i.e., have all of its bonding requirements satisfied), all holes must be filled with bonds. Note this is simply a way of stating the **octet** or duet **rule**

D. Using the rules developed in class about the central atom **bond angles** (that is, the angle between bonds coming out of the central atom), predict whether the bond angles will be the ideal angle for the electronic arrangement of that molecule, less than ideal or greater than ideal.

E. Using the individual bond polarities in the molecule, combine them to get an overall **dipole moment** for the molecule, and determine whether each molecule is thus polar or nonpolar.

Further rules:
• Two liquids are said to be **miscible** (and therefore form a solution) if, after mixing, there is no line separating the two liquids.
• Two liquids are said to be **immiscible** if, after mixing, they separate and a clear line divides both liquids.

1. What do the **holes** represent in each atom? Hint: consider why there are different numbers of holes in the different color spheres. Therefore, what type of bonding (ionic or covalent) is represented by these model kits?

2. Can a molecule **change** shape simply by being ionized? If so, give an example and show how the bond angles changed.

3. Why was it **difficult** to get the shape of the last two molecules on the data sheet?

4. Given the polarities of each of the following molecules **you predicted** on the data sheet:

a. Should water and hexane be **miscible**? Explain your reasoning for this answer only.

b. Should water and ethanol be miscible?

c. Should ethanol and hexane be miscible?

F. I will perform the following demonstration: in separate test tubes, I will mix equal portions of a) water/hexane, b) water/ethanol and c) ethanol/hexane.

G. Sketch each test tube's contents on the data sheet. Clearly indicate any immiscibility lines.

H. Clean up all materials and dispose of the solvent waste properly.

5. Given **your observations** of the behavior of these solvents in the test tubes:

a. Are water and hexane miscible? Explain your reasoning for this answer only.

b. Are water and ethanol miscible?

c. Are ethanol and hexane miscible?

6. Were there any **discrepancies** (inconsistencies) between your predictions and your observations? If so, give a reason that might help explain the discrepancy.