Molecular Modeling I - Three-dimensional Geometry
VSEPR & Dash-Wedge Notation

Basic Principles of VSEPR Theory

The basic ideas of VSEPR Theory are as follows:

1. Electrons in a Lewis structure are viewed as *groups*:

- Lone pair of electrons
- Single bond
- Double bond
- Triple bond

Each of these constitute one *group* of electrons.

TABLE 2-1 Various Types of Electron Groups in VSEPR Theory

Type of Group	Total Number of e^-	Number of Groups
1 Lone pair	2	1
1 Single bond	2	1
1 Double bond	4	1
1 Triple bond	6	1

2. Because the negatively charged electron groups strongly repel one another, they tend to arrange themselves as far away from each other as possible and generally demonstrate the following bond angles:

- Two electron groups surrounding the central atom tend to be 180° apart (a linear configuration).
- Three electron groups tend to be 120° apart (a triangular, planar configuration).
- Four electron groups tend to be 109.5° apart (a tetrahedral configuration).

3. *Electron geometry* describes the electron groups about a particular atom.

4. *Molecular geometry* describes the arrangement of atoms about a particular atom. Because atoms must be attached by bonding pairs of electrons, an atom's molecular geometry is governed by its electron geometry.

TABLE 2-2 Correlations between Electron Geometry and Bond Angle in VSEPR Theory

Number of Electron Groups	Electron Geometry	Approximate Bond Angle
2	Linear 	180°
3	Trigonal planar 	120°
4	Tetrahedral 	109.5°

Dash-Wedge Notation

Although molecules are three-dimensional, representing them on paper is confined to the two dimensions of the page. To work around this problem, chemists use *dash-wedge notation*, which provides a means to represent atoms both in front of, and behind the plane of the paper, in three dimensions.

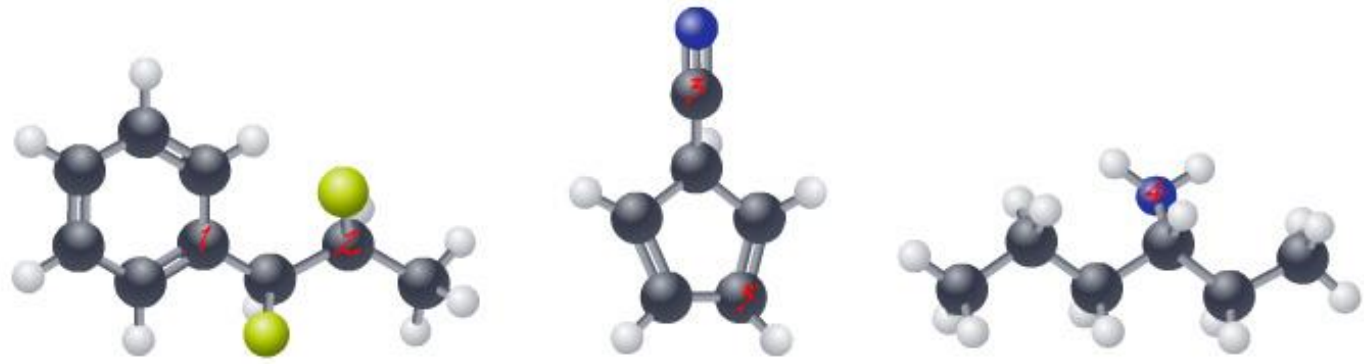
There are three components:

1. A straight line represents a bond that is in the plane of the paper. Atoms at either end of the bond are also in the plane of the paper.

2. A wedge represents a bond that comes out of the plane of the paper and toward the viewer. Generally, the atom at the thick end of the wedge is in front of the page, and the atom at the thin end of the wedge is in the plane of the paper.

3. A dash represents a bond that is pointed away from the viewer. You may assume that the atom at the thicker end of the dash is behind the plane of the paper.

Problem 1a. Construct models of the below molecules, then identify the molecular geometry, and bond angles around the atoms as numbered.



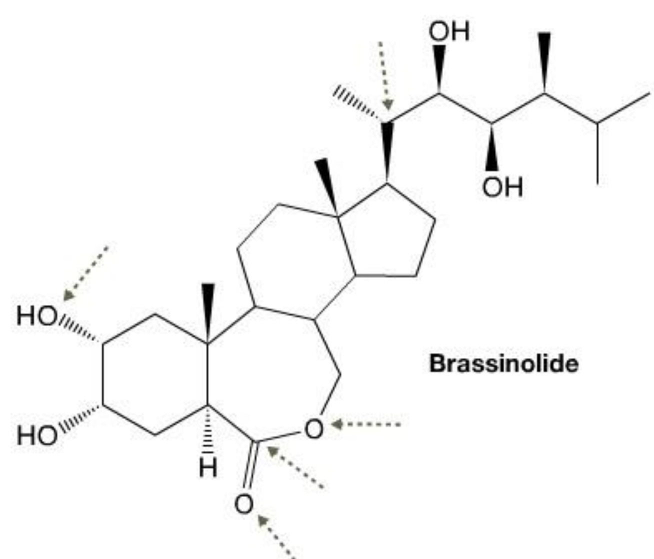
(a) (b) (c)

	1	2	3	4	5
Molecular Geometry					
Bond Angle					

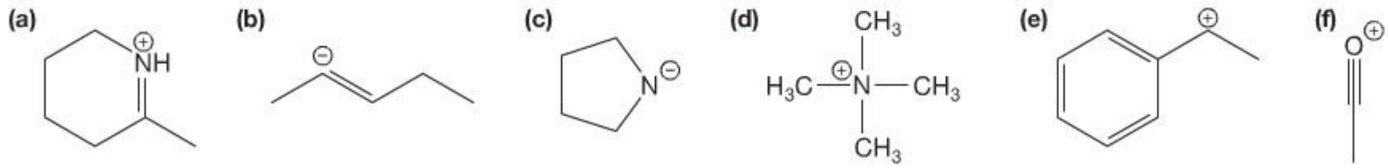
Problem 1b. Draw line structures of the molecules above in the space below using dash-wedge notation. Assume no atoms have any formal charges.

(a)	(b)	(c)

Problem 2. Brassinolide, a naturally occurring steroid derivative found in a wide variety of plants, is thought to promote plant growth. Identify the electron geometry for each atom indicated. Where applicable, describe the atoms molecular geometry and estimate the bond angle.

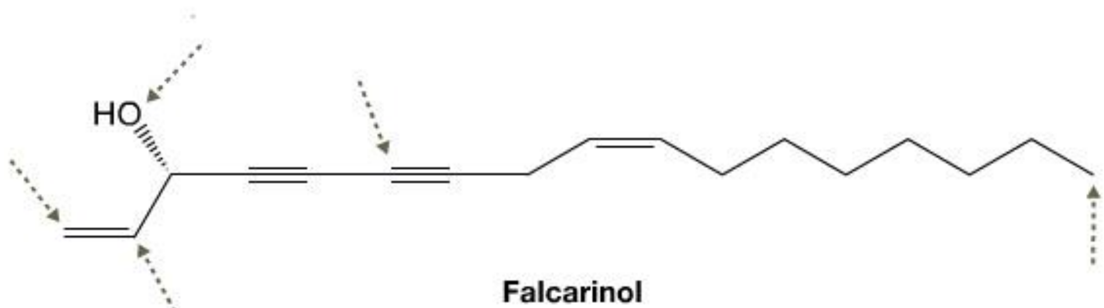


Problem 3. Identify the electron geometry about each charged atom. Where appropriate, indicate the molecular geometry and approximate bond angle as well.



	(a)	(b)	(c)	(d)	(e)	(f)
Electron Geometry						
Molecular Geometry						
Bond Angle						

Problem 4. Falcarinol, a naturally occurring pesticide found in carrots, is being studied as an anticancer agent. Identify the electron geometry for each atom indicated. Where applicable, describe the atom's molecular geometry and estimate the bond angle.



Falcarinol

Problem 5. Add dash-wedge notation to each line structure provided to accurately depict the ball-and-stick model appearing above it.