Pearson

5.9: VSEPR Theory: Predicting Molecular Geometries

To determine the geometry of a molecule, we follow the procedure presented in Examples 5.10 and 5.11. The steps are in the left column, and two examples of applying the steps are in the center and right columns.

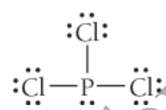
Example 5.10 Predicting Molecular Geometries

PROCEDURE FOR Predicting Molecular Geometries

Predict the geometry and bond angles of PCl_3.

1. ***Draw the Lewis structure for the molecule.***

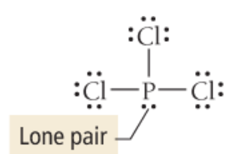
PCl_3 has 26 valence electrons.



2. ***Determine the total number of electron groups around the central atom.*** Lone pairs, single bonds, double bonds, triple bonds, and single electrons each count as one group.

The central atom (P) has four electron groups.

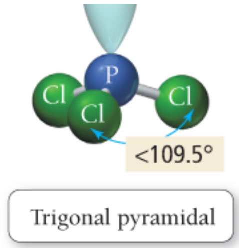
3. ***Determine the number of bonding groups and the number of lone pairs around the central atom.*** These should sum to your result from Step 2. Bonding groups include single bonds, double bonds, and triple bonds.



Three of the four electron groups around P are bonding groups, and one is a lone pair.

4. ***Refer to Table 5.5 to determine the electron geometry and molecular geometry.*** If no lone pairs are present around the central atom, the bond angles will be those of the ideal geometry. If lone pairs are present, the bond angles may be smaller than the ideal geometry.

The electron geometry is tetrahedral (four electron groups), and the molecular geometry—the shape of the molecule—is *trigonal pyramidal* (three bonding groups and one lone pair). Because of the presence of a lone pair, the bond angles are less than 109.5°.



FOR PRACTICE 5.10

Predict the molecular geometry and bond angle of ClNO.

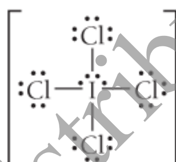
Example 5.11 Predicting Molecular Geometries

PROCEDURE FOR Predicting Molecular Geometries

Predict the geometry and bond angles of ICl_4^-.

1. ***Draw the Lewis structure for the molecule.***

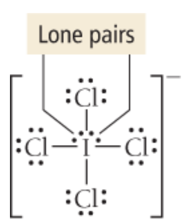
ICl_4^- has 36 valence electrons.



2. ***Determine the total number of electron groups around the central atom.*** Lone pairs, single bonds, double bonds, triple bonds, and single electrons each count as one group.

The central atom (I) has six electron groups.

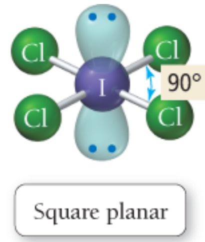
3. ***Determine the number of bonding groups and the number of lone pairs around the central atom.*** These should sum to your result from Step 2. Bonding groups include single bonds, double bonds, and triple bonds.



Four of the six electron groups around I are bonding groups, and two are lone pairs.

4. ***Refer to*** Table 5.5 ***to determine the electron geometry and molecular geometry.*** If no lone pairs are present around the central atom, the bond angles will be those of the ideal geometry. If lone pairs are present, the bond angles may be smaller than the ideal geometry.

The electron geometry is octahedral (six electron groups), and the molecular geometry—the shape of the molecule—is *square planar* (four bonding groups and two lone pairs). Even though lone pairs are present, the bond angles are 90° because the lone pairs are symmetrically arranged and do not compress the I—Cl bond angles.



FOR PRACTICE 5.11

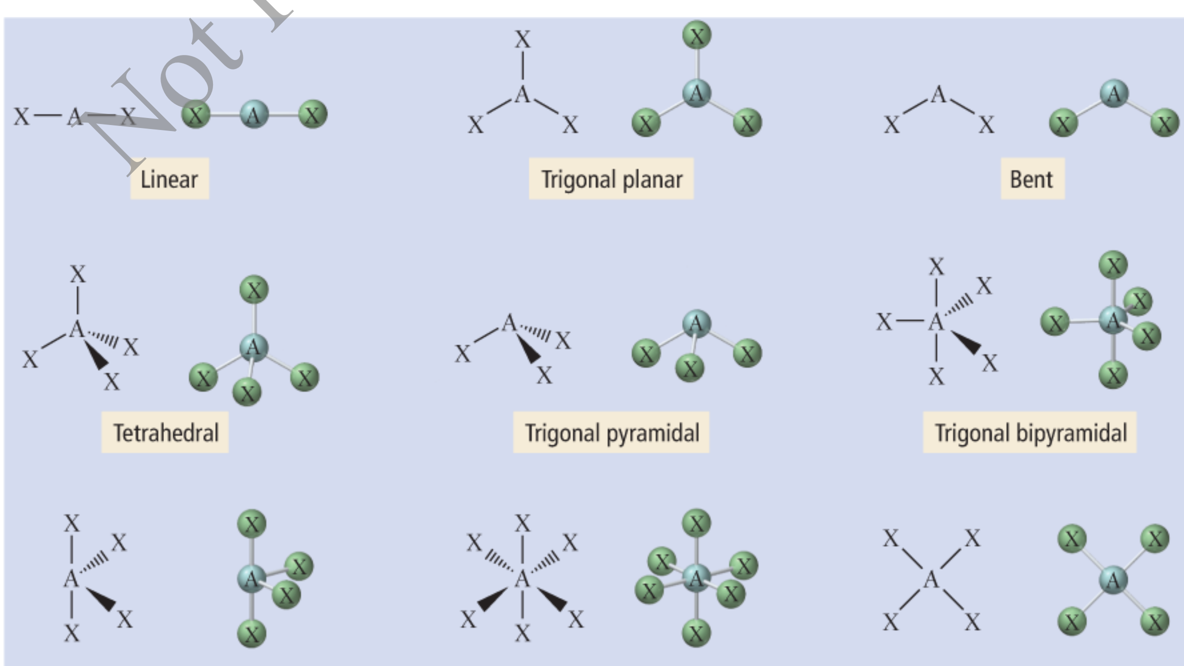
Predict the molecular geometry of I_3^-.

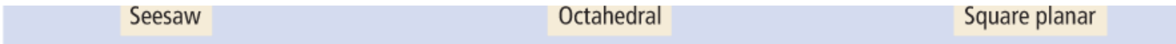
Interactive Worked Example 5.10 **Predicting Molecular Geometries**

Representing Molecular Geometries on Paper

Since molecular geometries are three-dimensional, they are often difficult to represent on two-dimensional paper. Many chemists use the notation shown here for bonds to indicate three-dimensional structures on two-dimensional paper.

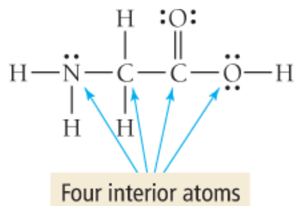
Some examples of the molecular geometries used in this book are shown here using this notation.



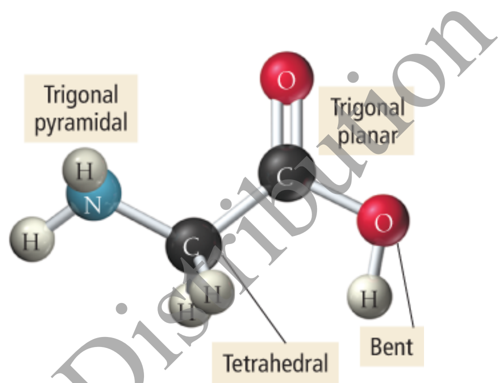


Predicting the Shapes of Larger Molecules

Larger molecules may have two or more *interior* atoms. When predicting the shapes of these molecules, we apply the principles we just covered to each interior atom. Consider glycine, an amino acid found in many proteins (such as those involved in opioid receptors discussed in Section 5.1). Glycine, contains four interior atoms: one nitrogen atom, two carbon atoms, and an oxygen atom. To determine the shape of glycine, we determine the geometry about each interior atom as shown in the following table and accompanying ball-and-stick model.



Glycine



Ball-and-Stick Model of Glycine

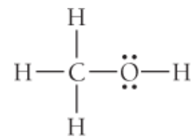
Atom (in Glycine)	Number of Electron Groups	Number of Lone Pairs	Molecular Geometry
Nitrogen	4	1	Trigonal pyramidal
Leftmost carbon	4	0	Tetrahedral
Rightmost carbon	3	0	Trigonal planar
Oxygen	4	2	Bent

Example 5.12 Predicting the Shape of Larger Molecules

Predict the geometry about each interior atom in methanol (CH_3OH) and sketch the molecule.

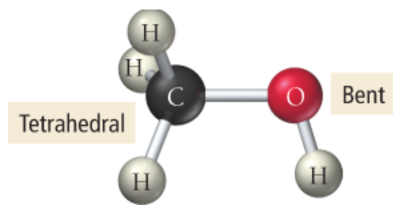
SOLUTION

Begin by drawing the Lewis structure of CH_3OH. CH_3OH contains two interior atoms: one carbon atom and one oxygen atom. To determine the shape of methanol, determine the geometry about each interior atom.



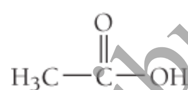
Atom	Number of Electron Groups	Number of Lone Pairs	Molecular Geometry
Carbon	4	0	Tetrahedral
Oxygen	4	2	Bent

Using the geometries of each of these, draw a three-dimensional sketch of the molecule as shown here.



FOR PRACTICE 5.12

Predict the geometry about each interior atom in acetic acid:



and sketch the molecule.

Interactive Worked Example 5.12 **Predicting the Shape of Larger Molecules**