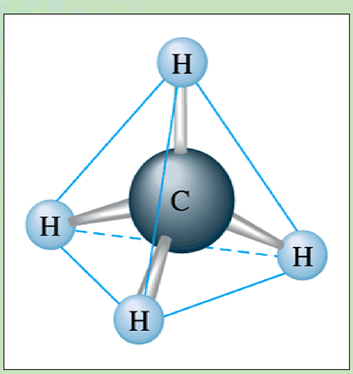
VSEPR Model

- The structure around a given atom is determined *principally* by minimizing electron pair repulsions.

The Valence-Shell Electron Pair Repulsion Model

- The **valence-shell electron pair repulsion (VSEPR) model** predicts the shapes of molecules and ions by assuming that the valence shell electron pairs are arranged as far from one another as possible.
  - To predict the relative positions of atoms around a given atom using the VSEPR model, you first note the **arrangement of the electron pairs around that central atom**.

Figure 8.14: The molecular structure of methane. The tetrahedral arrangement of electron pairs produces a tetrahedral arrangement of hydrogen atoms.



Predicting Molecular Geometry

- The following rules and figures will help discern electron pair arrangements.

1. Draw the Lewis structure
2. Determine how many electrons pairs are around the central atom. Count a multiple bond as one pair.
3. Arrange the electrons pairs are shown in Table 8.8.

The direction in space of the bonding electron pairs gives the molecular geometry

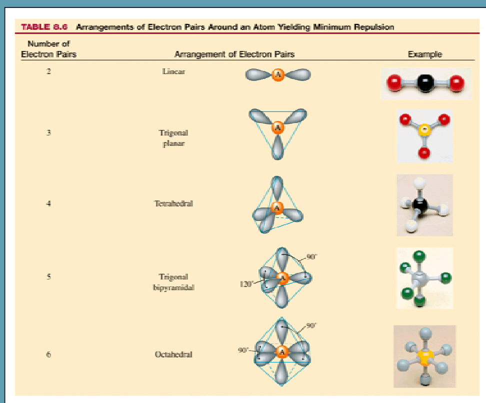


TABLE 8.6 Arrangements of Electron Pairs Around an Atom Yielding Minimum Repulsion

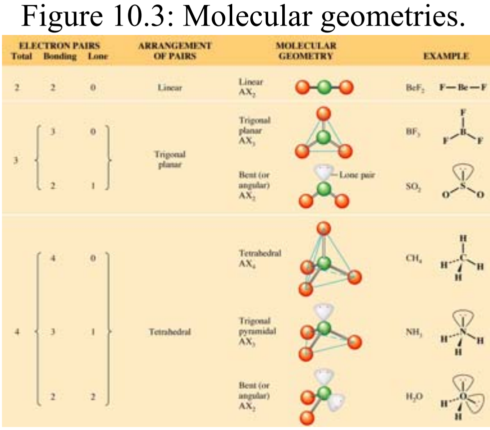
Number of Electron Pairs	Arrangement of Electron Pairs	Example
2	Linear	
3	Trigonal planar	
4	Tetrahedral	
5	Trigonal bipyramidal	
6	Octahedral	

Predicting Molecular Geometry

- The following rules and figures will help discern electron pair arrangements.

4. Obtain the molecular geometry from the directions of bonding pairs, as shown in Figures 10.3 and 10.8.

Figure 10.3: Molecular geometries.



ELECTRON PAIRS Total	Bonding	Lone	ARRANGEMENT OF PAIRS	MOLECULAR GEOMETRY	EXAMPLE
2	2	0	Linear	Linear AX_2	BeF_2 F—Be—F
3	3	0	Trigonal planar	Trigonal planar AX_3	BF_3
	2	1		Bent (or angular) AX_2	SO_2
4	4	0	Tetrahedral	Tetrahedral AX_4	CH_4
	3	1		Trigonal pyramidal AX_3	NH_3
	2	2		Bent (or angular) AX_2	H_2O

Figure 8.18: (a) In a bonding pair of electrons, the electrons are shared by two nuclei. (b) In a lone pair, both electrons must be close to a single nucleus and tend to take up more of the space around that atom.

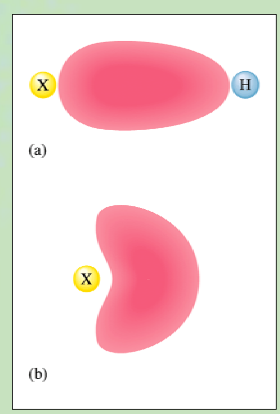


Figure 8.17: The bond angles in the CH_4, NH_3, and H_2O molecules.

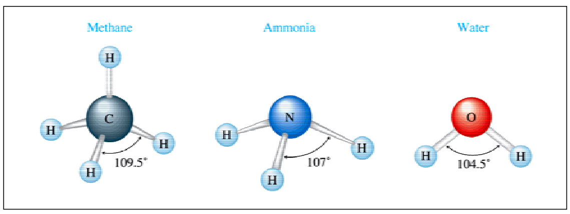


Figure 10.1: Molecular models of BF_3 and PF_3.

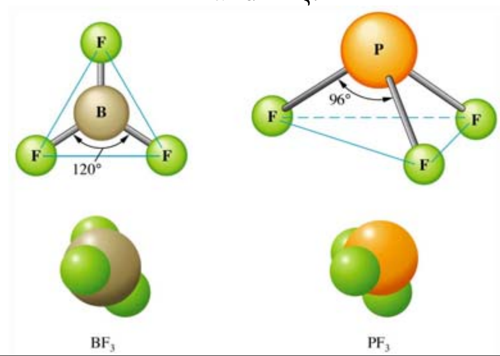


Figure 10.6: H—A—H bond angles in some molecules.

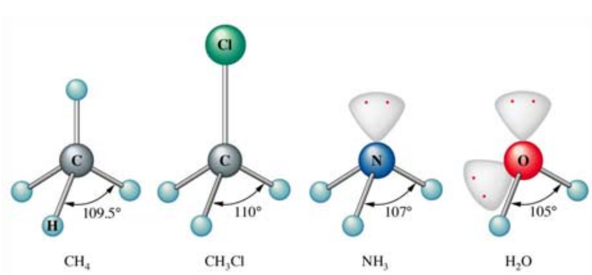
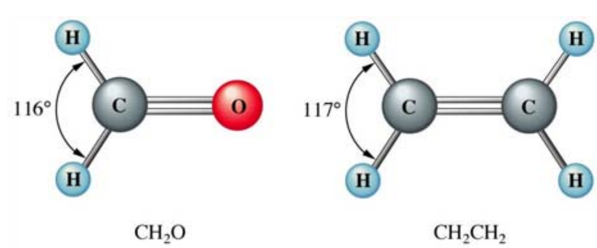
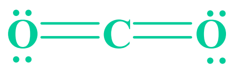


Figure 10.7: H—C—H bond angles in molecules with carbon double bond.



Predicting Molecular Geometry

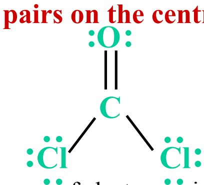
- Two electron pairs (linear arrangement).



- You have two double bonds, or two electron groups about the carbon atom.
- Thus, according to the VSEPR model, the bonds are arranged linearly, and the molecular shape of carbon dioxide is **linear**. This molecule has an AX_2 general formula with “2 bonding pairs” & no lone pairs. The bond angle is 180°.

Predicting Molecular Geometry

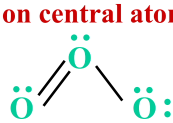
- Three electron pairs - **(trigonal planar arrangement - AX_3 with “3 bonding pairs” & no lone pairs on the central atom).**



- The three groups of electron pairs are arranged in a trigonal plane. Thus, the molecular shape of $COCl_2$ is **trigonal planar.** Bond angle is 120°.

Predicting Molecular Geometry

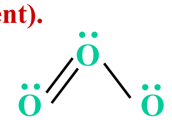
- Three electron pairs - **(trigonal planar arrangement - AX_2 with “2 bonding pairs” & 1 lone pair on central atom).**



- Ozone has three electron groups about the central oxygen. One group is a lone pair.
- These groups have a **trigonal planar arrangement**.

Predicting Molecular Geometry

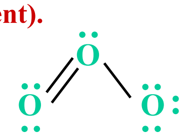
- Three electron pairs **(trigonal planar arrangement).**



- Since one of the groups is a lone pair, the molecular geometry is described as **bent** or **v-shaped**. When lone pairs are present in a bent molecule with bond angle ≥ **120°** very little distortion occurs.

Predicting Molecular Geometry

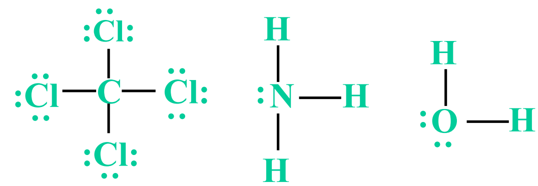
- Three electron pairs **(trigonal planar arrangement).**



- Note that the **electron pair arrangement** includes the lone pairs, but the **molecular geometry** refers to the spatial arrangement of just the atoms.

Predicting Molecular Geometry

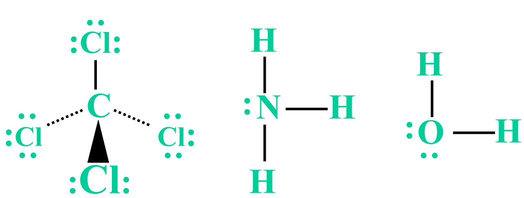
- Four electron pairs **(tetrahedral arrangement).**



- Four electron pairs about the central atom lead to three different molecular geometries.

Predicting Molecular Geometry

- Four electron pairs **(tetrahedral arrangement).**

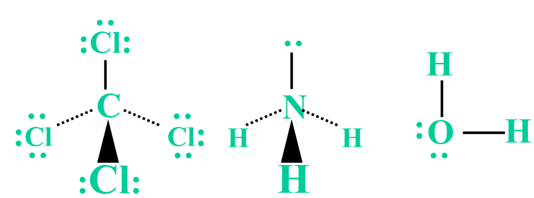


tetrahedral

Solid line - in plane of screen, dotted lines projecting back behind screen, dark wedge projecting toward you.

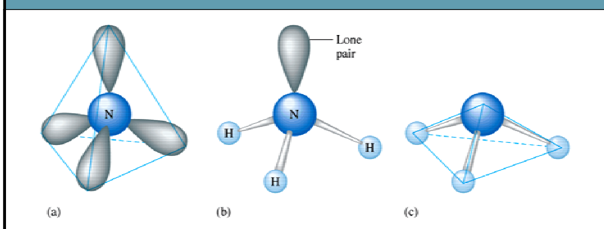
Predicting Molecular Geometry

- Four electron pairs **(tetrahedral arrangement).**



tetrahedral **trigonal pyramid**

Figure 8.15:(a) The tetrahedral arrangement of electron pairs around the nitrogen atom in the ammonia molecule.
(b) Three of the electron pairs around nitrogen are shared with hydrogen atoms as shown and one is a lone pair. Although the arrangement of electron pairs is tetrahedral, as in the methane molecule, the hydrogen atoms in the ammonia molecule occupy only three corners of the tetrahedron. A lone pair occupies the fourth corner.
(c) Note that molecular geometry is trigonal pyramidal, not tetrahedral.



Predicting Molecular Geometry

- Four electron pairs **(tetrahedral arrangement).**

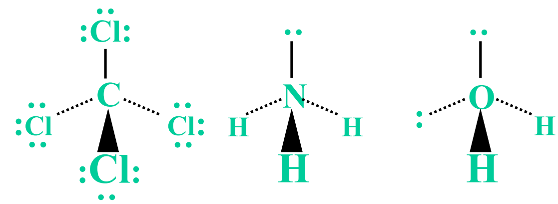
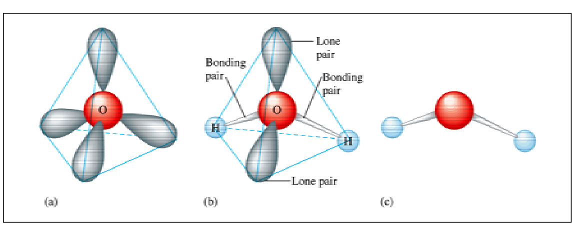


Figure 8.16: (a) The tetrahedral arrangement of the four electron pairs around oxygen in the water molecule. (b) Two of the electron pairs are shared between oxygen and the hydrogen atoms and two are lone pairs. (c) The V-shaped molecular structure of the water molecule.



CONCEPT CHECK 10.1

An atom in a molecule is surrounded by four pairs of electrons: one lone pair and three bonding pairs. Describe how the four electron pairs are arranged about the atom. How are any three of these pairs arranged in space? What is the geometry about this central atom, taking into account just the bonded atoms?

4 pairs = tetrahedral arrangement

Molecular geometry: AX_3 with a lone pair - trigonal pyramidal

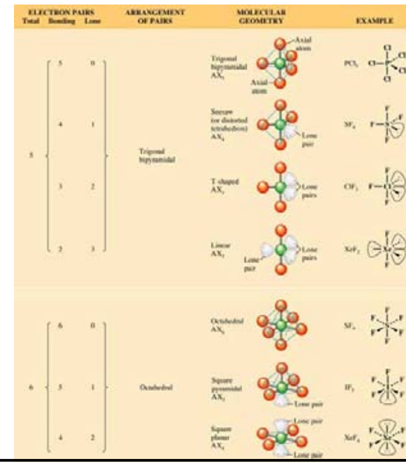
Models of CH_4, NH_3, H_2O.

tetrahedral

trigonal planar

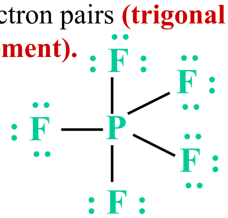
Bent or V-shaped

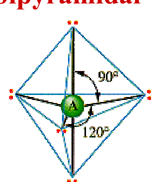
Figure 10.8: Molecular geometries



Predicting Molecular Geometry

- Five electron pairs **(trigonal bipyramidal arrangement).**

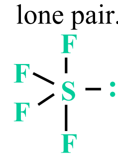




- This structure results in both 90° and 120° bond angles.

Predicting Molecular Geometry

- Other molecular geometries are possible when one or more of the electron pairs is a lone pair.



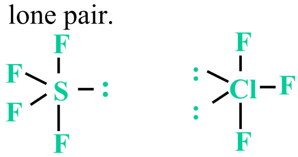
see-saw

ClF_3

XeF_2

Predicting Molecular Geometry

- Other molecular geometries are possible when one or more of the electron pairs is a lone pair.

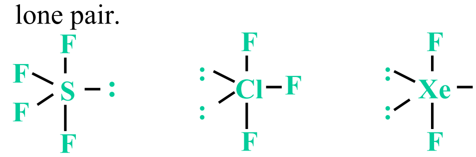


XeF_2

see-saw T-shape

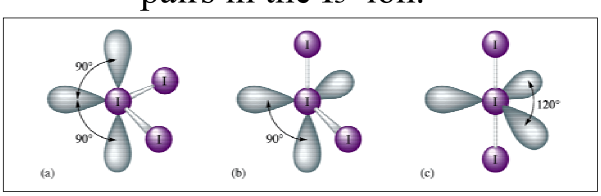
Predicting Molecular Geometry

- Other molecular geometries are possible when one or more of the electron pairs is a lone pair.



see-saw T-shape linear

Figure 8.20: Three possible arrangements of the electron pairs in the I_3^- ion.



I_3^- (3 x 7 e) + 1 e = 22 e or 11 pairs

I-I-I

Place 1 pair between each peripheral I and central I, 3 prs on each peripheral I, and 3 pairs on central I.

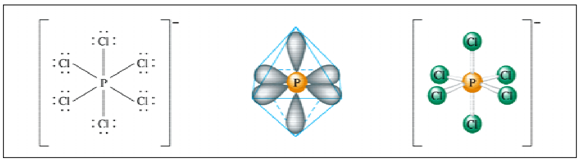
Predicting Molecular Geometry

- Other molecular geometries are possible when one or more of the electron pairs is a lone pair.

SF_4 ClF_3 XeF_2

- Let's try their Lewis structures.

Molecular structure of PCl_6^-



5 e (P) + 6 x 7 e (Cl) + 1 e = 48 e

Predicting Molecular Geometry

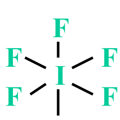
- Six electron pairs **(octahedral arrangement).**

IF_5 XeF_4

- Six electron pairs also lead to other molecular geometries.

Predicting Molecular Geometry

- Six electron pairs **(octahedral arrangement).**

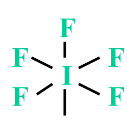


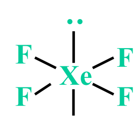
XeF_4

square pyramid

Predicting Molecular Geometry

- Six electron pairs **(octahedral arrangement).**





square pyramid **square planar**

- Figures 10.2, 10.3, and 10.8 summarize all the possible molecular geometries.

Octahedral electron arrangement for Xe

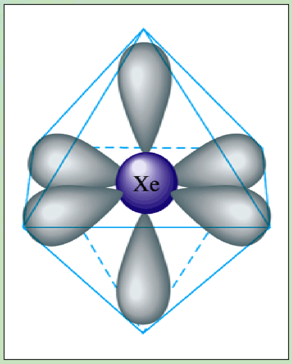


Figure 8.19: Possible electron-pair arrangements for XeF_4.

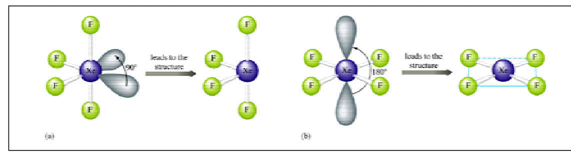
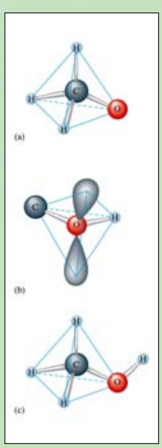


Figure 8.21: The molecular structure of methanol.
(a) The arrangement of electron pairs and atoms around the carbon atom.
(b) The arrangement of bonding and lone pairs around the oxygen atom.
(c) The molecular structure.



Dipole Moment and Molecular Geometry

- The **dipole moment** is a measure of the degree of charge separation in a molecule.
  - We can view the polarity of individual bonds within a molecule as vector quantities.
  - Thus, molecules that are perfectly symmetric have a zero dipole moment. These molecules are considered **nonpolar**. (see Table 10.1)

$$\delta^- \, O = C^{\delta^+} = O \, \delta^-$$

Table 10.1
Relationship Between Molecular Geometry and Dipole Moment

Formula	Molecular Geometry	Dipole Moment*
AX	Linear	Can be nonzero
AX_2	Linear	Zero
	Bent	Can be nonzero
AX_3	Trigonal planar	Zero
	Trigonal pyramidal	Can be nonzero
	T-shaped	Can be nonzero
AX_4	Tetrahedral	Zero
	Square planar	Zero
	Seesaw	Can be nonzero
AX_5	Trigonal bipyramidal	Zero
	Square pyramidal	Can be nonzero
AX_6	Octahedral	Zero

*All X atoms are assumed to be identical.

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Dipole Moment and Molecular Geometry

- However, molecules that exhibit **any asymmetry** in the arrangement of electron pairs would have a nonzero dipole moment. These molecules are considered **polar**.