[4.3] Molecular Shapes

TEXTBOOK: 183 - 188

Drawing Molecules

1. central atom has least electronegativity, **H** is **never** the central atom

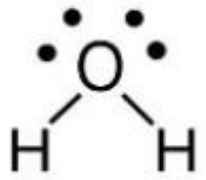
2. molecules tend to be s**ymmetrical,** like water molecule

3. **covalent bonds** are represented by **pairs of dots** between two atoms

4. **pairs of electrons** forming covalent bonds can be represented by a **line O=C=O**

Drawing Molecules

5. number of **dots/lines** you draw must equal the **sum of the valence electrons** of all atoms in the molecule



6. octet rule refers to how elements generally prefer to form bonds so as to attain an octet (8) configuration, i.e. have **8** electrons in their valence shell (H and He have **2**)

7. Try to **satisfy octet rule** for all atom, if impossible - at least for outer **atoms**.

Molecular Shapes

2.1 VSEPR

Use **VSEPR**

(VALENCE **S**HELL **E**LECTRON **P**AIR **R**EPULSION) theory to predict the **shape of molecules**.

2. Molecular Shape

2.1 VSEPR

Remember, molecules are **3D structures**. Their geometric shape is determined by:

- electron repulsion – **electron pairs in bonds** will orient **as far away** from each other **as possible**
- **valence** electrons – these occupy space too so these will **spread out evenly around the central atom**

"AXE" Notation of 3D Molecular Shape

A - this is the **central atom** of the molecule (or portion of a large molecule being focused on).

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No distinction is made between atoms of different elements. For example, $\mathbf{AX_4}$ can refer to $\mathbf{CH_4}$ or to $\mathbf{CCl_4}$.

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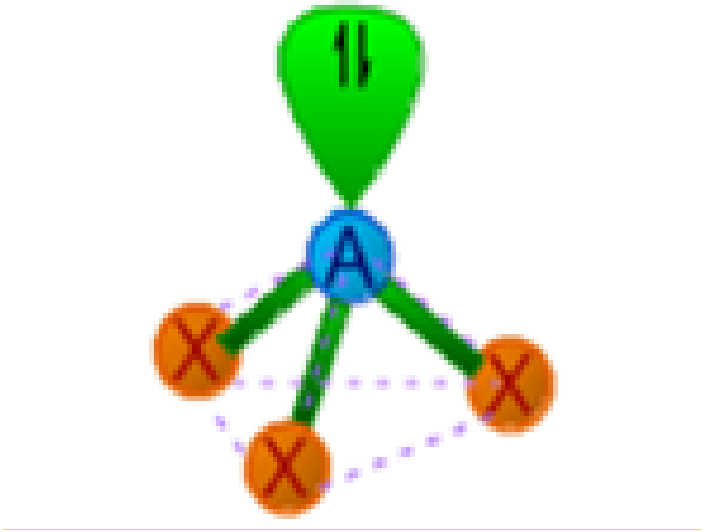
E - this stands for **nonbonding** electron **pairs**. For example, $\mathbf{AX_2E_2}$ can refer to $\mathbf{H_2O}$

"AXE" Notation of 3D Molecular Shape

Examples:



AX_3E - NH_3

AX_2E_2 - H_2O

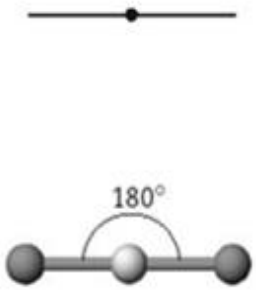
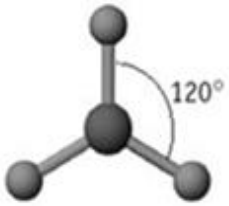
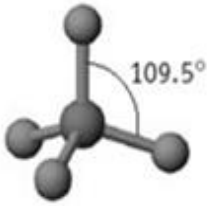
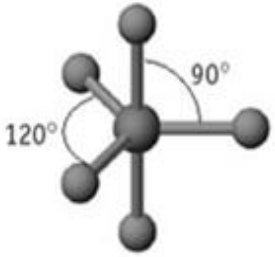
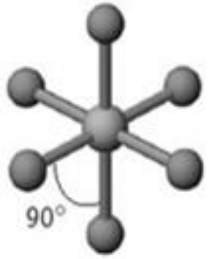
2.3 The Steric Number

(the # of lone pairs + bonded atoms) relates the **shape** of the **electron pairs** around a central atom

Steric number (GEOMETRY): 2=linear, 3=trigonal planar, 4=tetrahedral.

For water= $\mathbf{AX_2E_2}$ steric number is 2+2=**4 electron domains** (2 in bonds and 2 in **lone pairs**).

- If each shape is **symmetrical**, the bond dipoles will cancel resulting in a **nonpolar** molecule.
- If a shape has **lone pairs** of electrons on the central atom, the shape is often **unsymmetrical**, the molecule is **polar**.

Linear	Trigonal-planar	Tetrahedral	Trigonal-bipyramidal	Octahedral
				
AX_2 Example: BeF_2	AX_3 Example: BF_3	AX_4 Example: CF_4	AX_5 Example: PF_5	AX_6 Example: SF_6
Steric number: 2	3	4	5	6

Lewis Structures in 3D

Molecular Structure Movie Time!

Lewis Structures in 3D

These **normal lines** are used to represent bonds that lies **in the plane** of the drawing surface (i.e the computer screen, the paper, the chalkboard, etc.)

In order to represent bonds **projecting out** of this plane, we use "**dashed**" and "**wedged**" bonds.

2.4 Lewis Structures in 3D

- **Dashed**  bonds are used to represent bonds that project **backward** (*behind* the drawing plane

- **Wedged**  bonds are used to represent bonds that project **outward** (*in front* of the drawing plane).

Example: Draw the Lewis structure for the following molecules

a) CCl_4

C in the middle
total # of valence electrons = 4 + 4(7) = 32

b) NH_3

N in the middle
total # of valence electrons = 5 + 3(1) = 8

c) C_2H_6

two C's in the middle
total # of valence electrons = 2(4) + 6(1) = 14

d) CO_2

C in the middle
total # of valence electrons = 4 + 2(6) = 16

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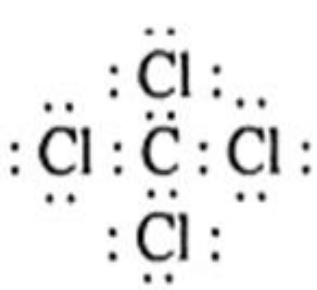

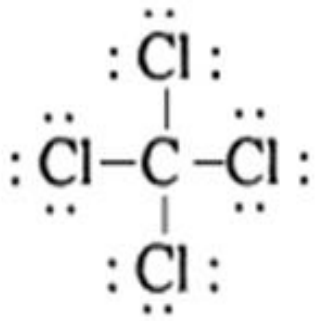

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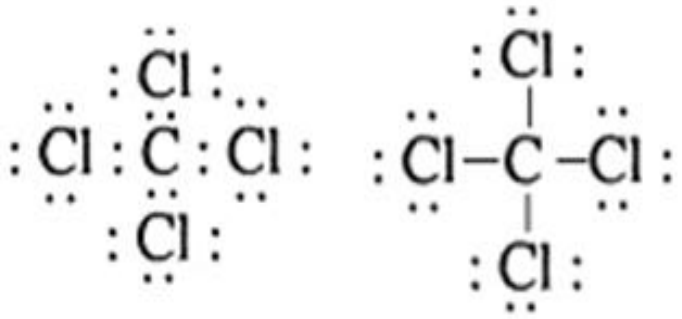

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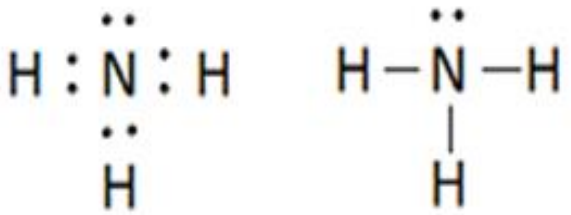

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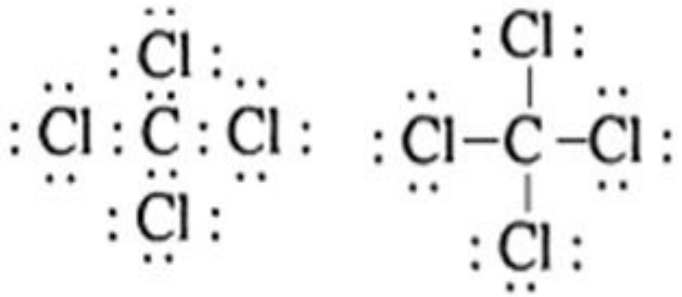

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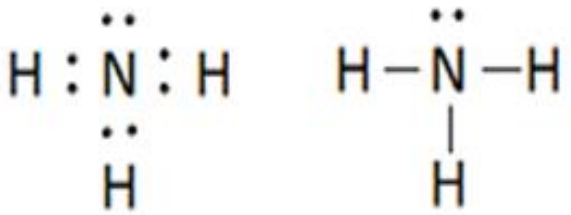

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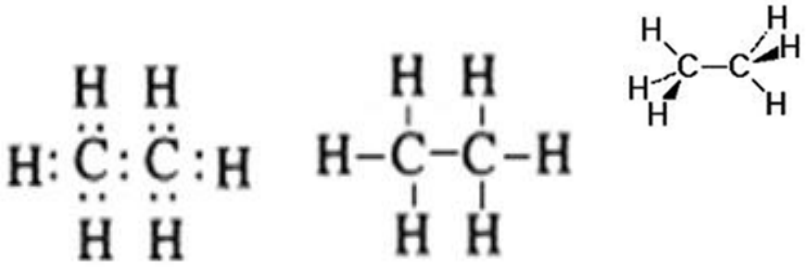

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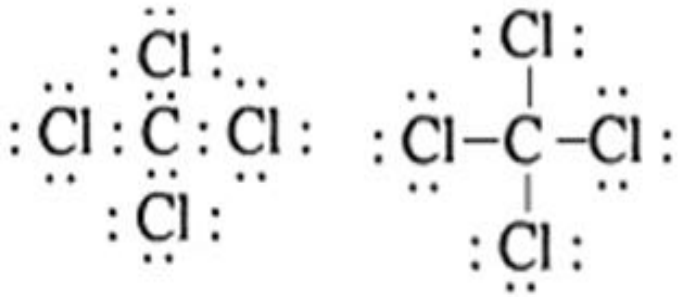

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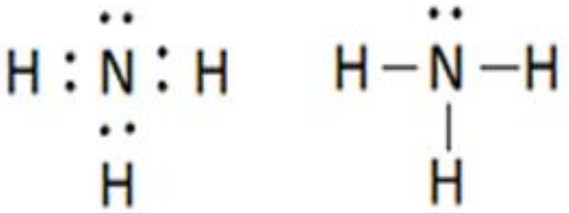

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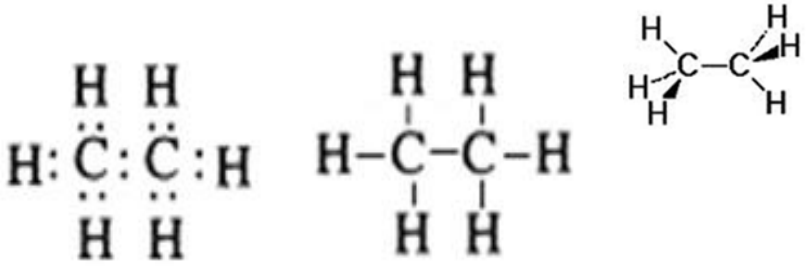

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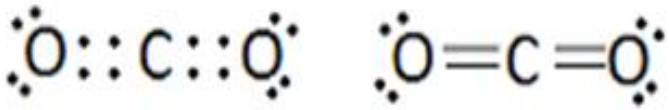
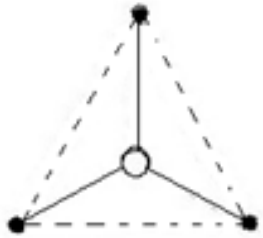
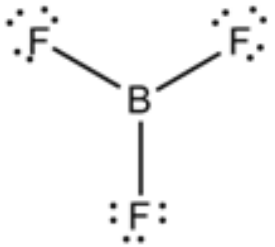
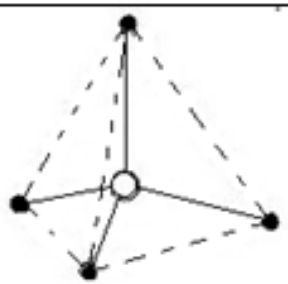
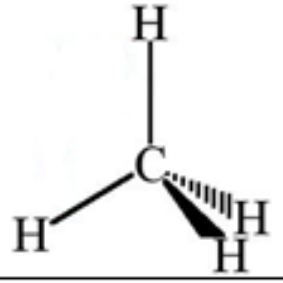
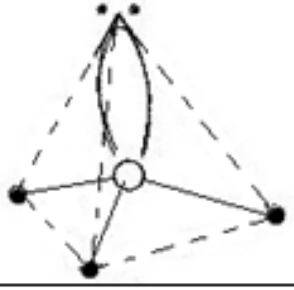
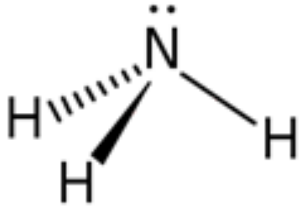
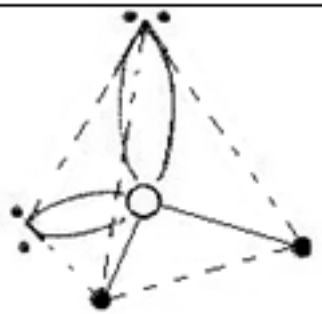
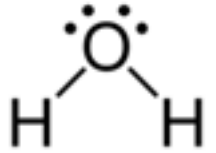
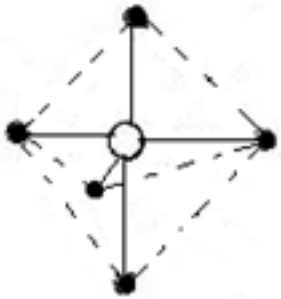
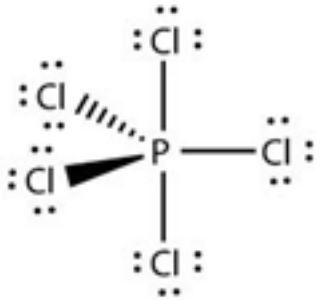
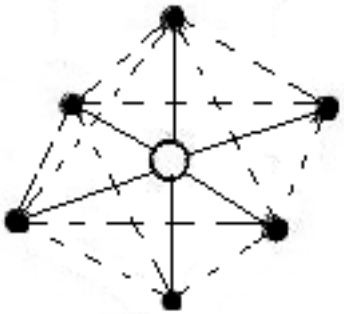
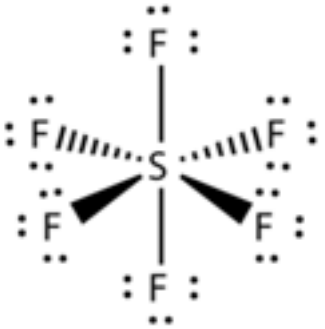
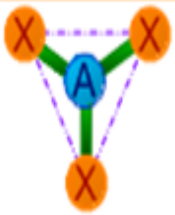
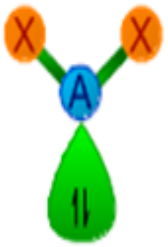
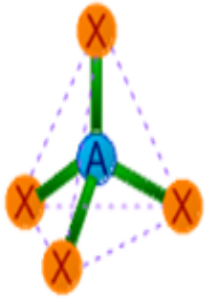
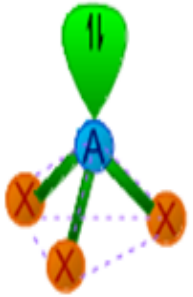
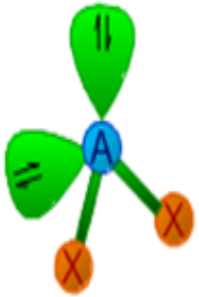


Name	Shape	Atoms Bonded to Central Atom	Lone Pairs of Electrons Bonded to Central Atom	Bond Angle	Example	
					Formula	Lewis Structure Represented in 3D
Linear		2	0	180°	BeH_2	
Trigonal planar		3	0	120°	BF_3	
Tetrahedral		4	0	109.5°	CH_4	
Trigonal pyramidal		3	1	107°	NH_3	

Angular		2	2	104.5°	H_2O	
Trigonal bipyramidal		5	0	90° 120° 180°	PCl_5	
Octahedral		6	0	90° 180°	SF_6	

Steric number	Number of Bond pairs	Number of Lone pairs	Formula	Shape of molecule		Approximate Bond angles	Examples
1	1	0	AX	Linear		-	ClF, BrF, BrCl, HF, O_2
2	2	0	AX_2	Linear		180°	$BeCl_2$, $HgCl_2$, CO_2
3	3	0	AX_3	Trigonal planar		120°	BF_3, CO_3^{2-}, NO_3^-, SO_3
	2	1	AX_2E	Angular		120°	SO_2, $SnCl_2$, O_3, NSF, NO_2^-

4	4	0	AX_4	Tetrahedral		109°28'	CH_4, $SiCl_4$, NH_4^+, PO_4^{3-}, SO_4^{2-}, ClO_4^-
	3	1	AX_3E	Trigonal pyramidal		around 109°28'	NH_3, PCl_3, XeO_3
	2	2	AX_2E_2	Angular		around 109°28'	H_2O, SCl_2, Cl_2O, OF_2

Homework