MOLECULAR SHAPES

When bonds form between atoms molecules are created. Depending on how many bonds exist a molecule will take on different shapes. The bonds between atoms generally contain two electrons. These electron pairs will repulse each other, therefore the bonds will be equally spread around the surface of the atom.

The **Valence-Shell Electron Pair Repulsion theory (VSEPR)** states that in a small molecule, the pairs of electrons are arranged as far apart from each other as possible. (*of course there are always exceptions) The VSEPR effect helps determine the **bond angle**, the geometric angle between two bonds. This arrangement of bonds creates the shape of a molecule. Although bonds appear flat when drawn on paper we have to remember that a molecule is actually 3-dimensional.

There are seven basic shapes – linear, trigonal planar, tetrahedral, pyramidal, bent, trigonal bipyramidal, and octahedral. When determining the shape of a molecule you must first draw the Lewis Dot Diagram for the molecule or ion. Next, count the total number of regions of high electron density (bonding and unshared electron pairs) around the central atom.

Rules for determining high electron density:

1. Double and triple bonds count as ONE REGION OF HIGH ELECTRON DENSITY.
2. An unpaired electron counts as ONE REGION OF HIGH ELECTRON DENSITY.
3. For molecules or ions that have resonance structures, you may use any one of the resonance structures.

Third, identify the most stable arrangement of the regions of high electron density as ONE of the following:

1. **linear** - molecules have bonds that form a straight line, the atoms are 180° apart. A molecule may be linear if it contains double or triple bonds that create a symmetry.

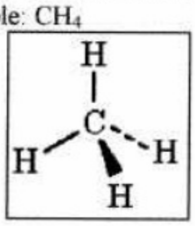
- For example: O_2 O=O (diatomic)

CO_2 O=C=O

2. **trigonal planar** - molecules form a flat triangle with the bond angle at 120°. Because the bond angle is greater than 90° the bonds may remain on the same plane.

3. **Tetrahedral** - molecules have four equal bonds. All bond angles are 109.5°.

- For example: CH_4



1/8/16

1. B
2. C
3. A
4. D
5. B
6. D
7. D
8. B
9. - no answer Tetrahedral
10. C

11. H-Ö: water has a bent shape because the natural pair of e^- push the bonds away - VSPER

12. Polarity

13. sp — sp^2 — sp^3

linear 180° — trigonal planar 120° — tetrahedral 109.5°

Seven diatomic molecules

H_2 $^7N_2$ O_2 F_2 Cl_2 Br_2 I_2

14. Dipoles — +/-

15. they are diatomic molecules

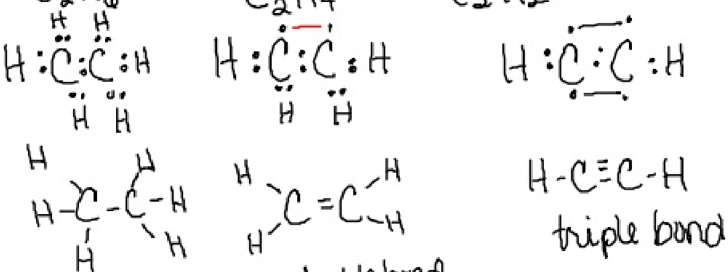
16. generally acquire additional e^-

17. VSEPR

Valence
Shell
Electron
Pair
Repulsion

natural pairs of electrons have greater repulsion than bonded pairs.

18. C_2H_6 — C_2H_4 — C_2H_2



Single C-C — double bond — triple bond

alkane — alkene — alkyne

$C_1-C_2-C_3-C_4-C_5$ pentane

$C_1-C_2=C_3-C_4$ 2-butene

$C_1-C_2\equiv C_3-C_4-C_5-C_6-C_7$ 2-heptyne

C-C-C propane

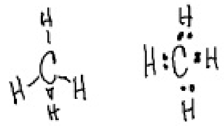
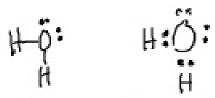
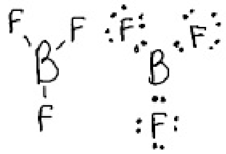
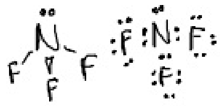
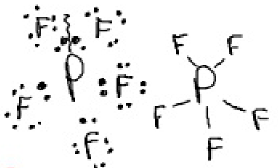
1C = meth
2C = eth
3C = prop
4C = but

$C_1-C_2-C_3\equiv C_4-C_5-C_6-C_7-C_8$

3-octyne

Octane C_8H_{18}

C
H
O
N
P
S
halogens

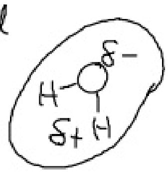
CH_4		C 2.5 H 2.1 0.4 NPC	tetrahedral	non-polar molecule
H_2O		O 3.5 H 2.1 1.4 PC	bent	Polar molecule
BF_3		F 4.0 B 2.0 2.0 I	trigonal planar	non-polar molecule
NF_3		F 4.0 N 3.0 1.0 PC	pyramidal	Polar molecule
PF_5		F 4.0 P 2.1 1.9 PC	~	non-polar

Type of bond
Subtract electronegativity for the 2 elements in a bond – look # up on chart
- 0.49 or less nonpolar covalent (NPC)
- 0.5 to 1.9 polar covalent (PC)
- 2.0 or greater ionic (I)

Molecule Polarity

Determine Type of Bonds are Present
- all bonds NPC → $\boxed{\text{Non-Polar Molecule}}$
- PC or I → apply arrows toward element w/ higher electronegativity
  - Equal + opposite → $\boxed{\text{Non-polar molecules}}$ trigonal planar + tetrahedral
  - unbalanced movement → $\boxed{\text{Polar Molecules}}$ bent + pyramidal

O 3.5
H 2.1
1.4 PC



Oxidation

* (ions +/- go behind #, for oxidation # the +/- go infront)

The sum of the oxidation # must equal zero.

There can only be <u>one</u> negative element in a molecule. O_2 $O=0$

Pure, unreacted elements + diatomic molecules = zero Mg $Mg=0$

any ion w/a given charge charge = oxidation

Ca^{2+} $Ca = +2$

Oxygen is generally -2, except when H_2O_2 $\boxed{\text{peroxide } O_2^{2-} \quad O=-1}$

Hydrogen can be +1 if attached to a non-metal

-1 if attached to a metal (hydride)

Practice: Determine the oxidation number for each of the elements in the following molecules and ions.

1.	Ag	Ag= 0	11.	Ag_2S	Ag= S=
2.	CdS (-2)	Cd= +2 S= -2	12.	HgCl	Hg= Cl=
3.	$CdCl_2$ (-2)	Cd= +2 Cl= -1	13.	$HgCl_2$	Hg= Cl=
4.	I_2	I= 0	14.	$H(NO_3)$ (+1 {+5 -6 (-1))	H= +1 N= +5 O= -2
5.	$SnCl_2$ (+2 -2)	Sn= +2 Cl= -1	15.	NaOH	Na= O= H=
6.	$SnCl_4$ (+4 -4)	Sn= +4 Cl= -1	→ 16.	H_2O_2	H= O=
7.	$FeCl_2$	Fe= +2 Cl= -1	17.	LiH	Li= H=
8.	$FeCl_3$	Fe= +3 Cl= -1	18.	$K(ClO_3)$	K= Cl= O=
9.	NO_2^{-1} (+3 -4)	N= +3 O= -2	19.	$H_2(SO_4)$	H= S= O=
10.	N_2O (+2 -2)	N= +1 O= -2	20.	$Fe(NO_3)_3$	Fe= N= O=

Practice: Determine the oxidation number for each of the elements in the following molecules and ions.

1.	Ag	Ag= 0	11.	Ag_2S	Ag= S=
2.	CdS	Cd= +2 S= -2	12.	HgCl	Hg= Cl=
3.	$CdCl_2$	Cd= +2 Cl= -1	13.	$HgCl_2$	Hg= Cl=
4.	I_2	I= 0	14.	$H(NO_3)$	H= +1 N= +5 O= -2
5.	$SnCl_2$	Tin (II) chloride Sn= +2 Cl= -1	15.	NaOH	Na= +1 O= -2 H= +1
6.	$SnCl_4$	Tin (IV) chloride Sn= +4 Cl= -1	16.	H_2O_2	H= +1 O= -1
7.	$FeCl_2$	Fe= +2 Cl= -1	17.	LiH	lithium hydride Li= +1 H= -1
8.	$FeCl_3$	Fe= +3 Cl= -1	18.	$K(ClO_3)$	K= +1 Cl= +5 O= -2
9.	NO_2^{-1}	N= +3 O= -2	19.	$H_2(SO_4)$	H= +1 S= +6 O= -2
10.	N_2O	N= +1 O= -2	20.	$Fe(NO_3)_3$	Fe= +3 N= +5 O= -2

+1 H { -1 NO_3 : + -6 = -1

+1 Na { -1 OH : -2 + = -1

+3 Fe { -3 $(NO_3)_3$: + -6 = -1

* Start w/ element that has highest electronegativity.
It will keep the normal neg. charge.

NH_4^{1+} ammonium

CN^{1-} cyanide

SO_4^{2-} sulfate

ClO_3^{1-} Chlorate

PO_4^{3-} Phosphate

OH^{1-} hydroxide

$C_2H_3O_2^{1-}$ acetate

O_2^{2-} peroxide

CO_3^{2-} carbonate

NO_3^{1-} nitrate

Practice: Determine the oxidation number for each of the elements in the following molecules and ions.

1.	Ag	Ag= 0	11.	Ag_2S	Ag= S=
2.	CdS ($-2=0$)	Cd= +2 S= -2	12.	HgCl	Hg= Cl=
3.	$CdCl_2$ ($-2=0$)	Cd= +2 Cl= -1	13.	$HgCl_2$	Hg= Cl=
4.	I_2	I= 0	14.	$H(NO_3)$ ($+1$ -1 $=0$; -6)	H= +1 N= +5 O= -2. ($+\ -6=-1$)
5.	$SnCl_2$ ($-2=0$) tin (II) chloride	Sn= +2 Cl= -1	15.	NaOH	Na= +1 O= -2 H= +1
6.	$SnCl_4$ (-4) tin (IV) chloride	Sn= +4 Cl= -1	*16.	H_2O_2 ($+2$ -2 $=0$)	H= +1 O= -1 O_2^{2-}
7.	$FeCl_2$ (-2)	Fe= +2 Cl= -1	17.	LiH	Li= +1 H= -1 lithium hydride
8.	$FeCl_3$ (-3)	Fe= +3 Cl= -1	18.	$K(ClO_3)$	K= +1 Cl= +5 O= -2
9.	NO_2^{-1} ($-4=-1$)	N= +3 O= -2	19.	$H_2(SO_4)$	H= +1 S= +6 O= -2
10.	N_2O ($+2$ -2 $=0$)	N= +1 O= -2	20.	$Fe(NO_3)_3$ ($+3$ -3; -6 $=-1$)	Fe= +3 N= +5 O= -2

IA	IIA	B	IIIA	IVA	VA	VIA	VIIA	VIIIA
1+	2+		3+	4+ 4−	3−	2−	1−	0

$+2 \mid -2.$

$+6 + -8 = -2$

$H_2(SO_4)$

H= +1 S= +6 O= -2