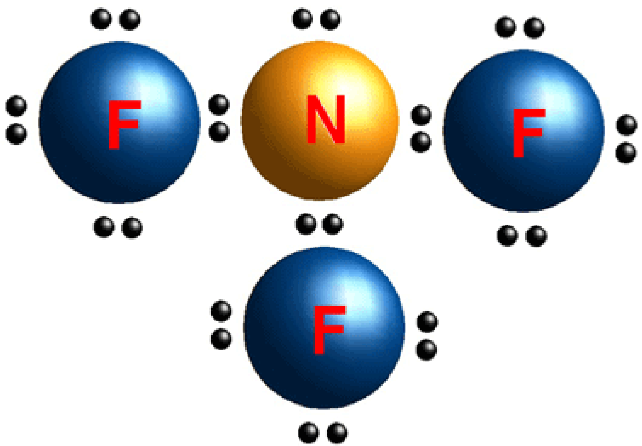
Molecule Polarity and Bigger Lewis Structures

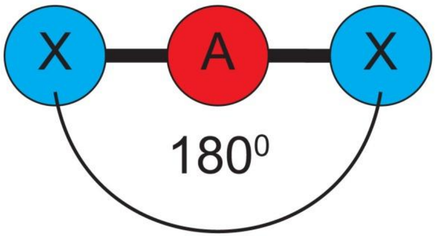


VSEPR

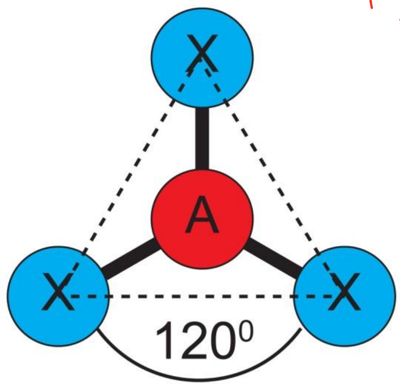
Valence **S**hell **E**lectron **P**air **R**epulsion

- Each region of electrons (bond or lone pair) counts as a balloon
- Balloons want to spread out as much as possible

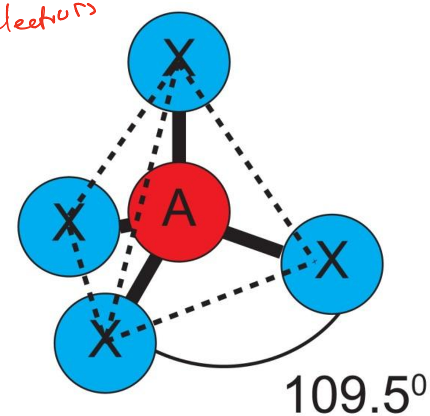
Maximize space for electrons and bonds



AX_2
Linear
sp



AX_3
Trigonal Planar
sp^2



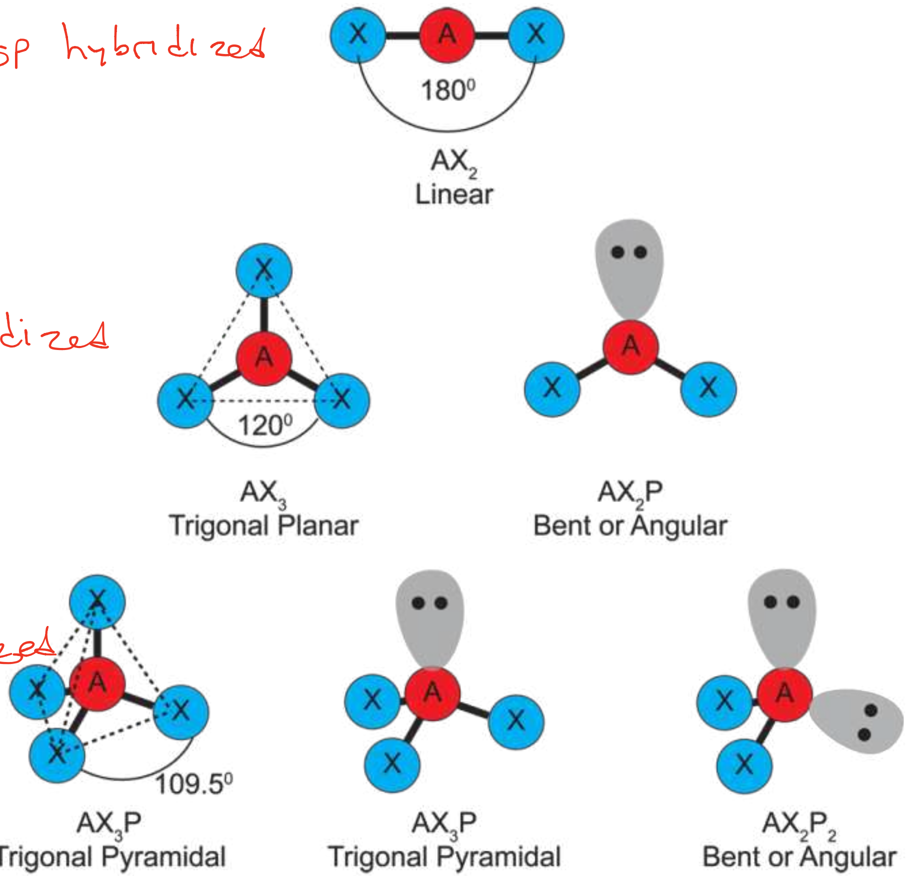
AX_4
Tetrahedral
sp^3

Molecular Shapes

sp hybridized

sp^2 hybridized

sp^3 hybridized



Polarity

Covalent Bonds can be Polar or Nonpolar

Polar molecules have different chemical properties than nonpolar

H 2.1																	He –
Li 1.0	Be 1.5											B 2.0	C 2.5	N 3.0	O 3.5	F 4.0	Ne –
Na 0.9	Mg 1.2											Al 1.5	Si 1.8	P 2.1	S 2.5	Cl 3.0	Ar –
K 0.8	Ca 1.0	Sc 1.3	Ti 1.5	V 1.6	Cr 1.6	Mn 1.5	Fe 1.8	Co 1.8	Ni 1.8	Cu 1.8	Zn 1.6	Ga 1.6	Ge 1.8	As 2.0	Se 2.4	Br 2.8	Kr –
Rb 0.8	Sr 1.0	Y 1.2	Zr 1.4	Nb 1.6	Mo 1.8	Tc 1.9	Ru 2.2	Rh 2.2	Pd 2.2	Ag 1.9	Cd 1.7	In 1.7	Sn 1.8	Sb 1.9	Te 2.1	I 2.5	Xe –
Cs 0.7	Ba 0.9	57–71 1.1–1.2	Hf 1.3	Ta 1.5	W 1.7	Re 1.9	Os 2.2	Ir 2.2	Pt 2.2	Au 2.4	Hg 1.9	Tl 1.8	Pb 1.8	Bi 1.9	Po 2.0	At 2.2	Rn –
Fr 0.7	Ra 0.9																

X-Y

Electronegativity difference

≥ 2	Ionic Bond
$0.4 \rightarrow 2$	Polar Covalent
≤ 0.4	Nonpolar Covalent

H-Cl

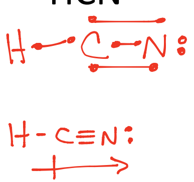
$\delta+$ $\delta-$

Molecule Polarity

Will each of these molecules be polar?

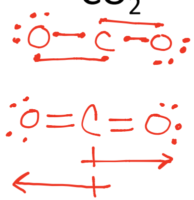
Try drawing these Lewis Structures:

HCN

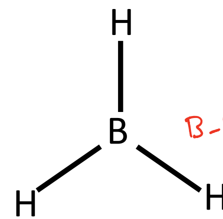


CO_2

NOT polar

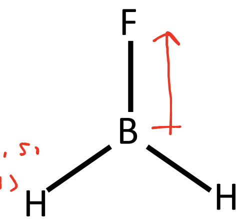


Cancel out



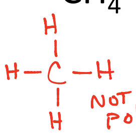
B-H bonds are not polar, so the molecule is NOT polar

POLAR



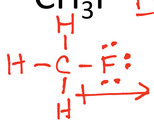
Remember bond angles are NOT 90°, so NO way to cancel out C-F bonds

CH_4

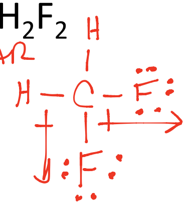


NOT polar

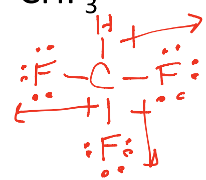
CH_3F POLAR



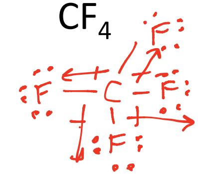
CH_2F_2 POLAR



CHF_3 POLAR



CF_4



Perfectly symmetrical, so polarity cancels out

NOT POLAR

Lewis Structures

Try with HSCN

Count Electrons

16

Draw Skeleton Structure

H S C N

Form bonds with 2 electrons

H-S-C-N

Fill Octet of TERMINAL atoms (only one bond)

H-S-C-N̤:

H and N are terminal

Are all electrons used?

Yes → Do all atoms have a full octet?

No → Place remaining electrons on CENTRAL atoms

put e- on most electronegative central atom 1st

H-S̤̈-C-N̤̈:

Do all atoms have a full octet?

Yes → GREAT SUCCESS!

No → Form Double or Triple bonds to satisfy octet rule

H-S̤̈-C≡N̤̈ ← not octet

$\boxed{\text{H-S̤̈-C≡N:}}$ ✓

this is one method you can use ... I like the other approach

Lewis Structures

Ethanol
CH_3CH_2OH

Acetaldehyde
CH_3CHO

Group (example)	Likely Position in Molecule	Number of bonds
1 (H)	Terminal	1
4 (C)	Central	4
5 (N)	usually Central	3
6 (O)	Central or Terminal	2
7 (F)	~~Central~~ Terminal	1

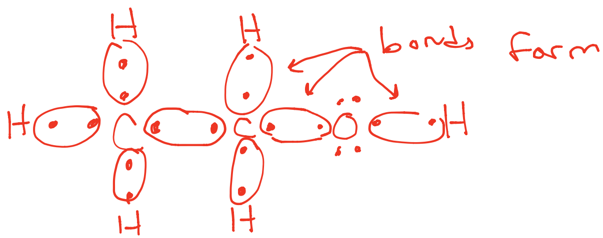
when terminal N has a triple bond (needs to share 3 electrons to fill octet)

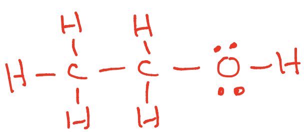
when terminal, double bond to fill octet

*****Note that these bond number correspond with how many electrons are needed to gain an octet!*****

Lewis Structures

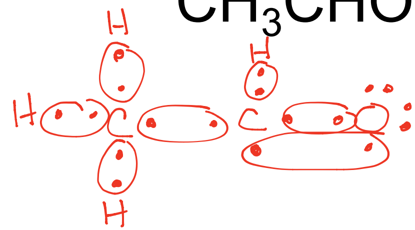
Ethanol
CH_3CH_2OH

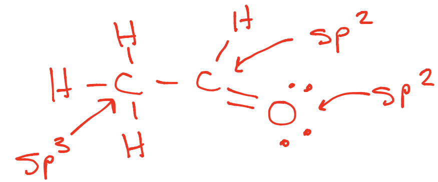




All central atoms are sp^3

Acetaldehyde
CH_3CHO





Alternate approach – start with sp^3 hybridized Lewis Symbols (except H) and connect the dots.

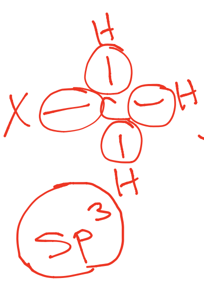
Ethanol
CH_3CH_2OH

Acetaldehyde
CH_3CHO

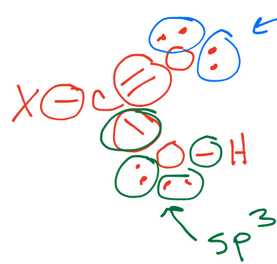
Did this above

To determine hybridization

Count the regions the e^- are found ... you need one orbital (or lobe) per region



4 circles
so need 4
lobes
1s + 3p

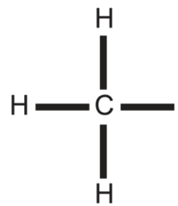


around carbon
- 3 lobes
s + 2p $\rightarrow$ sp^2

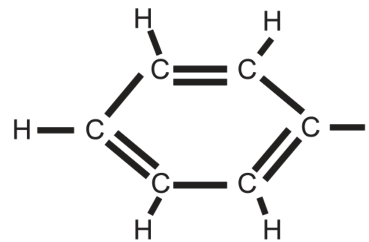
Oxygen
3 lobes
sp^2

Lewis Structures – common groups

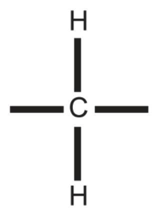
CH_3



C_6H_5

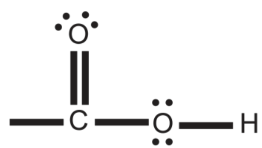


CH_2

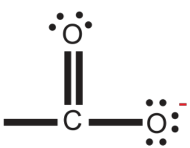


OH

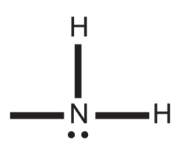
COOH
CO_2H



COO-
CO_2-



NH_2

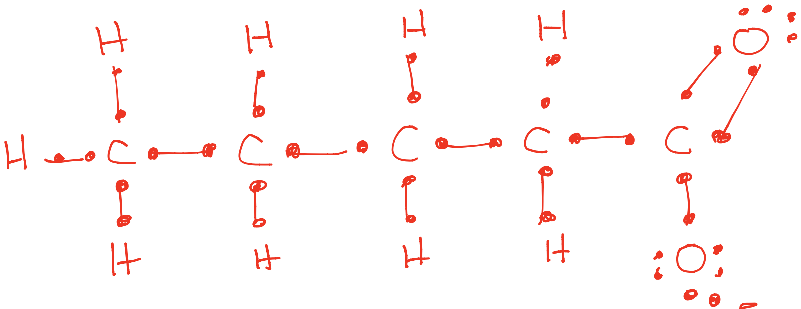


SH

Lewis Structures

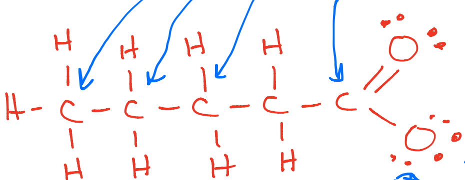
$CH_3CH_2CH_2CH_2CO_2^-$

one extra electron



extra electron

F.C. = 4 - 4 = 0



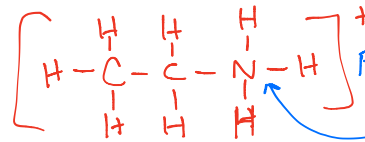
F.C. = 6 - 6 = 0

extra e⁻ is here so this O has formal charge of -1

F.C. = # VE − # EO = 6 − 7 = -1
(see next slide)

Formal charge is the charge on an atom

$CH_3CH_2NH_3^+$



F.C. = 5 − 4 = +1

Everything has a full octet, but where is (+) at?

since the Nitrogen has a F.C. of +1, the cation is on the Nitrogen!

Formal Charge

$CH_3CH_2CH_2CH_2CO_2^-$

$CH_3CH_2NH_3^+$

We can determine what atom is hosting the charge

E.O.

V.E.

$$\boxed{\text{Electrons owned by atom (1 electron per covalent bond and 2 electrons per lone pair)}} - \boxed{\text{Number of valence electrons for the neutral atom}} = \boxed{\textbf{\textit{Formal Charge}}}$$

crap, these should be switched

SO_2

Formal charge should <u>ALWAYS</u> be minimized on a molecule

If you drew the structure correctly, only one (maybe two) atoms will have a F.C. ≠ 0