LEC (2) CHEM 30A Oct 3rd

(1) CHEMICAL BONDING
(2) LEWIS STRUCTURES
(3) FORMAL CHARGE
(4) SHAPES OF MOLECULES

HWK: READ 1.3–1.4
PROBLEMS 1.6–1.13, 1.23–1.47
+ MOLECULAR SHAPE PROB SETS ON WEB

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(1) CHEMICAL BONDING

Valence electrons (outer shell electrons)
⟹ BOND FORMATION

# VALENCE e^-	1	2		3	4	5	6	7	8
	H								He
	Li	Be	d	B	C	N	O	F	Ne
	Na	Mg	BLOCK	Al	Si	P	S	Cl	Ar

ELECTRONEGATIVITY (EN)
– AN ATOM'S ATTRACTION FOR ELECTRONS IT SHARES IN A CHEMICAL BOND WITH ANOTHER ATOM

F HAS HIGHEST VALUE ⟹ 4.0

decreases ← F
↓ decreases

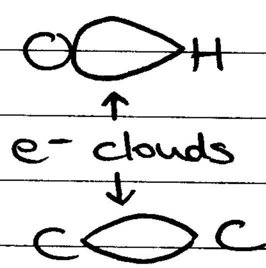
PAULING SCALE

(Linus Pauling 19∅1 – 1994) CHEM 1954 PEACE 1962

ORGANIC CHEMISTRY ⟹ COVALENT BONDS ⟹ EN DIFFERENCES < 2

So, consider:

Na 0.9	F 4.0	(3.1) ⟶	NaF	$(Na^+ F^-)$		IONIC SALT
O 3.5	H 2.1	(1.4) ⟶	δ- δ+ O—H			POLAR COVALENT
C 2.5	C 2.5	(∅) ⟶	C—C			NON POLAR COVALENT



EN difference < 0.5 ≃ NON POLAR

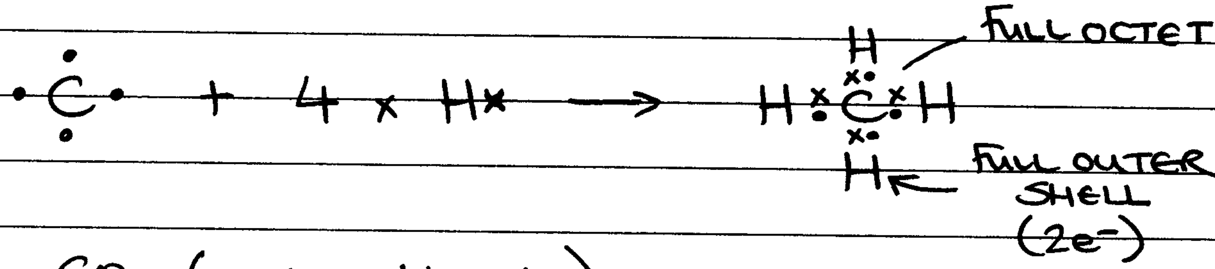
C — H Table 1.5 Page 7
2.5 2.1

Know values for common elements & Know TRENDS

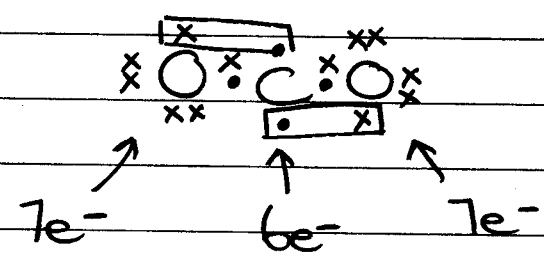
② LEWIS STRUCTURES

- # of Valence e^- on each atom
- least EN element in center (not H)
- form SINGLE BONDS
- fill octets (multiple bonds / charges)

a) CH_4 (methane)

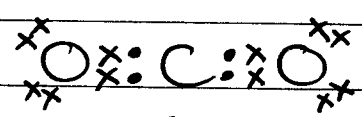


b) CO_2 (carbon dioxide)

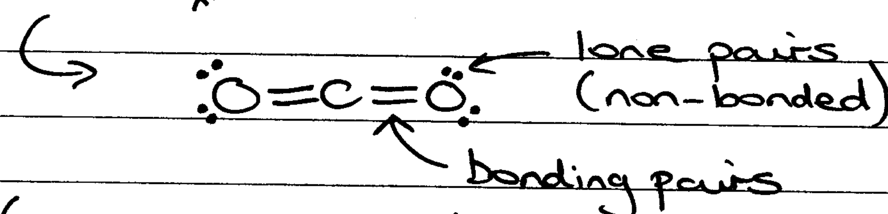


single bonds, but OCTETS not full

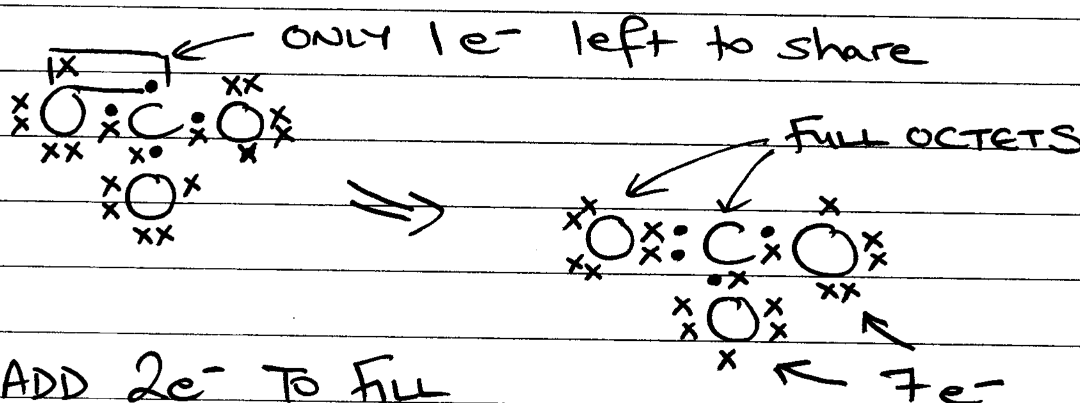
- share more electrons (MULTIPLE BONDS)
⟹ REDRAW



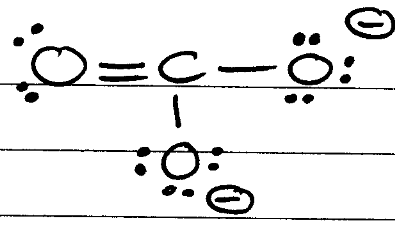
ALL ATOMS HAVE FULL OCTETS



c) CO_3^{2-} (CARBONATE ANION)

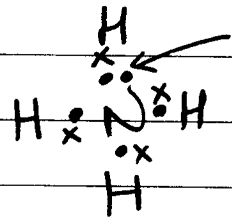


So, ADD $2e^-$ TO FILL OCTETS (DRAW THEM IN) ↗



CO_3^{2-}

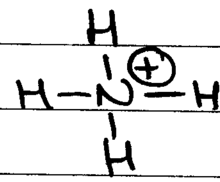
d) $NH_4^{\oplus}$ – AMMONIUM CATION



9e⁻ in VALENCE shell

VIOLATES OCTET RULE

so, get rid of it ⟹

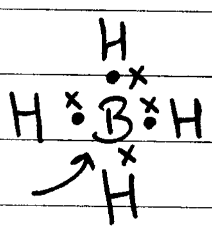


③ FORMAL CHARGE

– Draw LEWIS structure
for each atom:

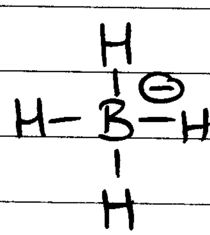
$$\text{FORMAL CHARGE} = \begin{array}{l}\text{\# VALENCE } e^- \\ \text{IN ISOLATED} \\ \text{NEUTRAL ATOM}\end{array} - \left(\begin{array}{l}\text{\# of NONBONDING } e^- \\ + \tfrac{1}{2}\text{\# BONDING } e^-\end{array}\right)$$

a) $BH_4^{\ominus}$



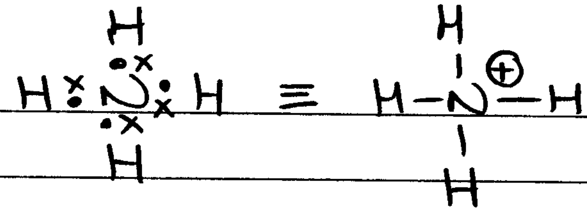
add in e⁻

≡



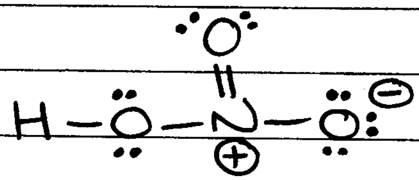
$\left(3 - \frac{8}{2}\right) = -1$

b) $NH_4^{\oplus}$



$(5 - 8/4) = +1$

c) HNO_3 (nitric acid)



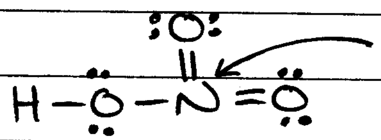
show how we get this.

N $(5 - 8/2) = +1$

O $(6 - (6 + 2/2)) = -1$

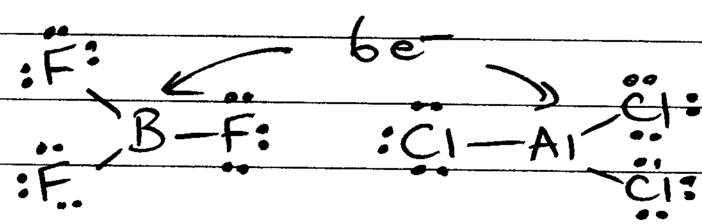
other Os $(6 - (4 + 4/2)) = \phi$

note: not



Note: there are exceptions to the OCTET rule

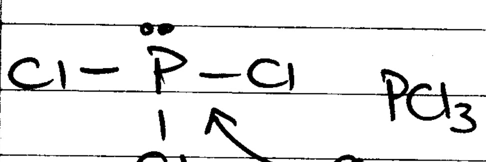
GROUP 3

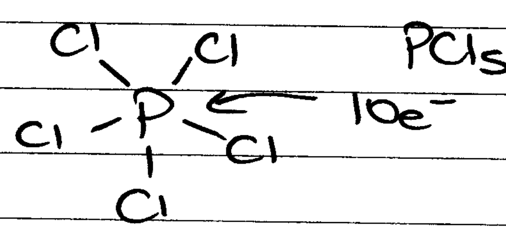


usually quite reactive species

3RD ROW ELEMENTS (P & S)

d orbitals ⇒ EXPAND octet



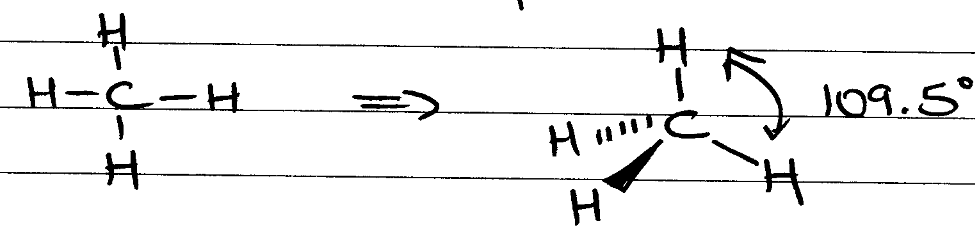


(4) SHAPES OF MOLECULES

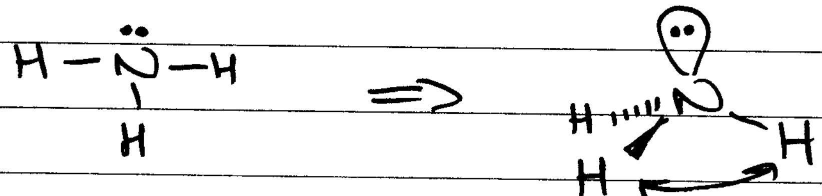
Valence Shell Electron Pair Repulsion Theory (VSEPR)
– simplified model

Geometry determined by valence shell e^- PAIRS both BONDED & NON BONDED arranging to minimize electrostatic repulsion

e.g.

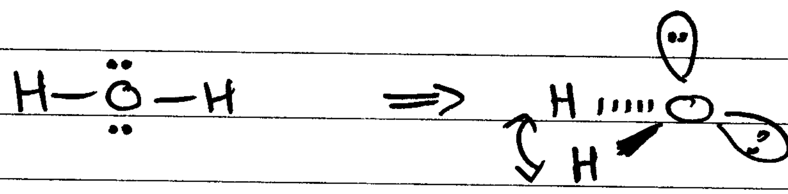


tetrahedral



PYRAMIDAL

107.3° compressed



BENT

104.5° more compressed

WHY? lone pair/lone pair > lone pair/bond pair > bond pair/bond pair REPULSION

Also: A≡B > A=B > A–B

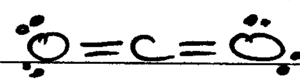
DISTINGUISH BETWEEN "SHAPE OF MOLECULE" VERSUS GEOMETRY AROUND AN ATOM.

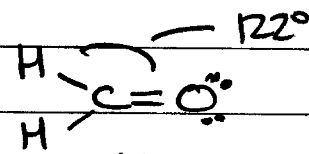
BASIC GEOMETRIES

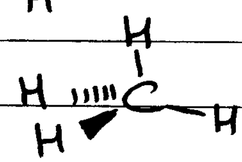
\# for the sake of geometry, treat MULTIPLE BONDS as SINGLE BONDS

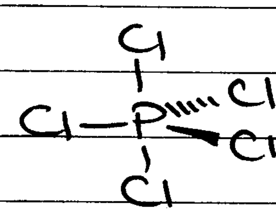
When considering geometry around a given atom, add # of ATOMS bonded to it to the # of LONE PAIRS.

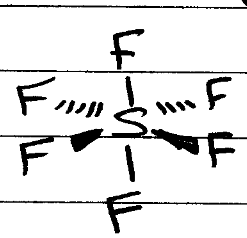
2 => LINEAR
3 => TRIGONAL PLANAR
4 => TETRAHEDRAL
5 => TRIGONAL BIPYRAMIDAL
6 => OCTAHEDRAL

2 → LINEAR 

3 → TRIGONAL PLANAR 

4 → TETRAHEDRAL  , NH_3, H_2O

5 → TRIGONAL PLANAR  PCl_5

6 → OCTAHEDRAL  SF_6