LEC (2) CHEM 30A Oct 4th

1. CHEMICAL BONDING
2. LEWIS STRUCTURES
3. FORMAL CHARGE
4. SHAPES OF MOLECULES
5. DRAWING ORGANIC STRUCTURES
6. DIPOLE MOMENTS
7. RESONANCE

HMK Read FUNCTIONAL GROUPS Sect 1.3
1.6-1.14, 1.23-1.49

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(1) Chemical Bonding

Valence electrons (outer shell electrons)
⇒ these are what form bonds

1	2		3	4	5	6	7	8	# valence e⁻
H								He	
Li	Be	d-BLOCK	B	C	N	O	F	Ne	
Na	Mg		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 AT 4.0

decreases ← F

↓

decreases

PAULING SCALE
(Linus Pauling 1901–1994)
CHEM 1954
PEACE 1962

WEDNESDAY

~$1M DEC 10TH (NOBEL DEATH)

Organic chemistry – mainly concerned w/ COVALENT BONDS

EN differences < 2

Na F → NaF or $Na^+ F^-$
0.9 4 ionic salt
(3.1)

O H → δ^- δ^+ polar
3.5 2.1 O–H covalent
(1.4)

C C → C–C nonpolar covalent
2.5 2.5
(0)

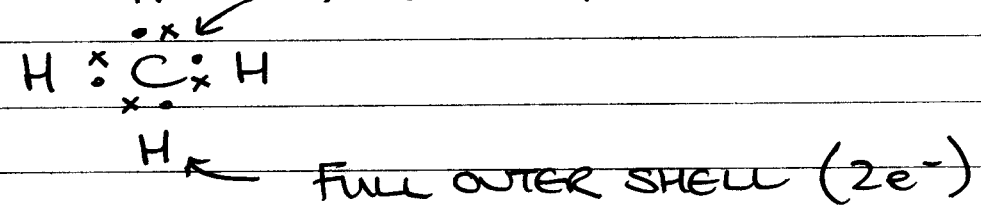
EN difference < 0.5 ⇒ NON POLAR

C–H (TABLE 1.5 pg 7)
2.5 2.1
↳ know values for common elements

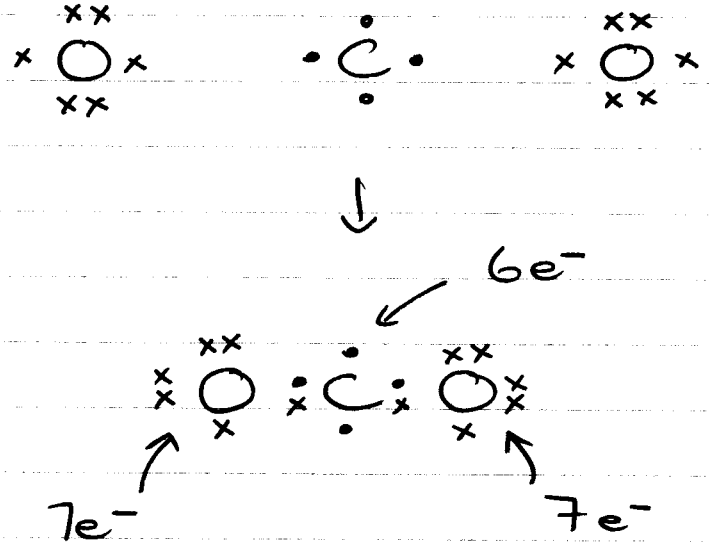
② LEWIS STRUCTURES

- # of VALENCE ELECTRONS ON EACH ATOM
- IN GENERAL, PUT LEAST EN ELEMENT IN THE MIDDLE (ignore H)
- FORM SINGLE BONDS - FILL OCTETS

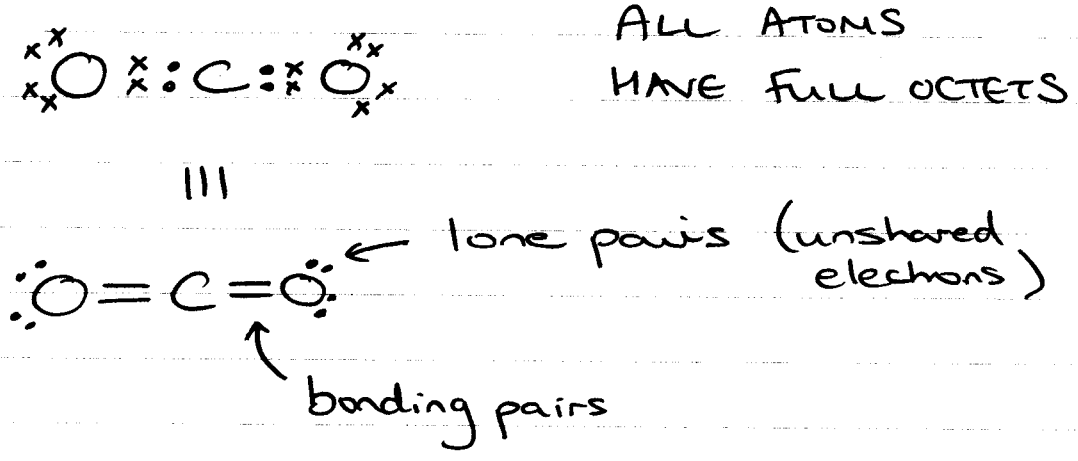
a) CH_4



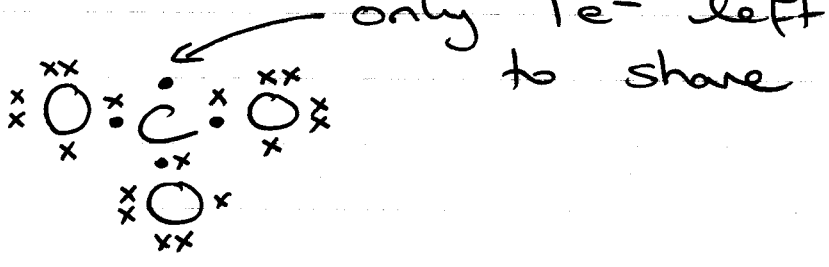
b) CO_2

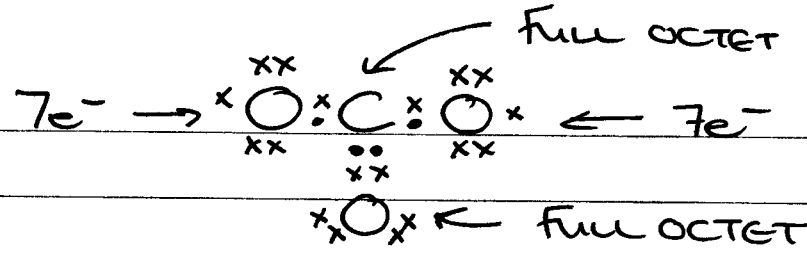


SO, SHARE MORE ELECTRONS

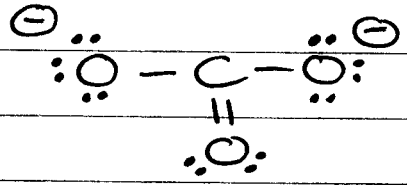


c) CO_3^{2-} (ANION)

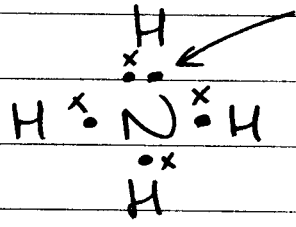




BUT 2^- SO ADD TWO ELECTRONS (DRAW THEM IN ABOVE)

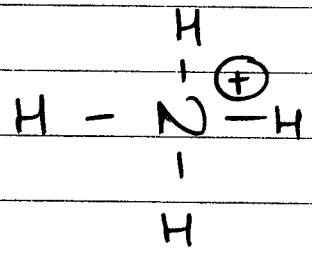


d) NH_4^+ (CATION)



VIOLATES OCTET RULE

So, get rid of it. (ERASE IT)



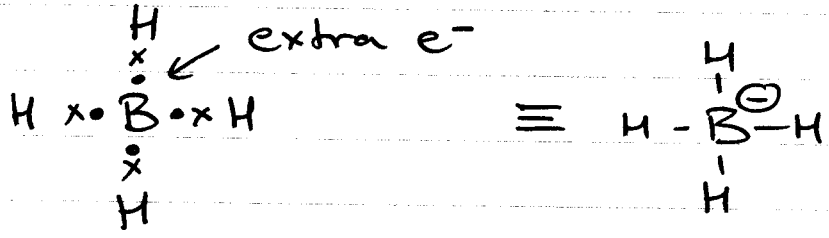
③ FORMAL CHARGE

- DRAW LEWIS STRUCTURE

For each atom's valence shell,
ADD # of NON-BONDING electrons
$\frac{1}{2}$ # of BONDING electrons

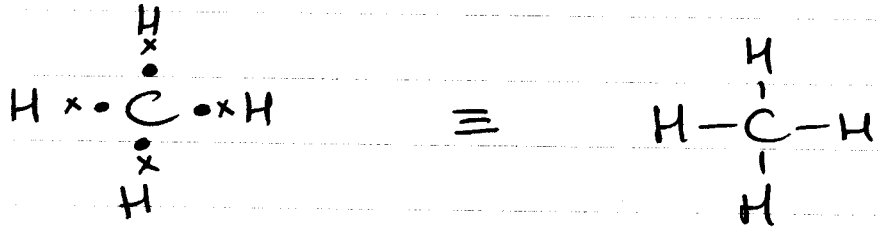
FORMAL CHARGE = # VALENCE ELECTRONS IN ISOLATED NEUTRAL ATOM − THIS NUMBER

a) $BH_4^{\ominus}$



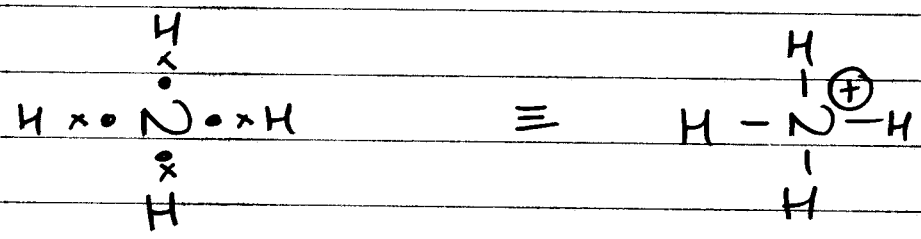
$(3 - 8/2) = -1$

b)



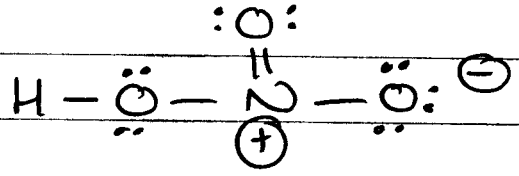
$(4 - 8/2) = 0$

c) NH_4^+
(already seen)



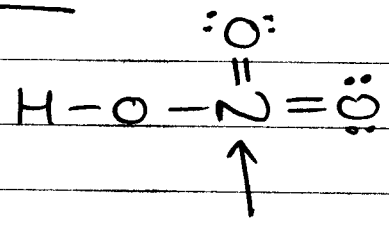
$(5 - {}^8/_4) = +1$

d) HNO_3 (nitric acid)



$N\,(5 - {}^8/_2) = +1$
$O\,(6 - ({}^2/_2 + 6)) = -1$

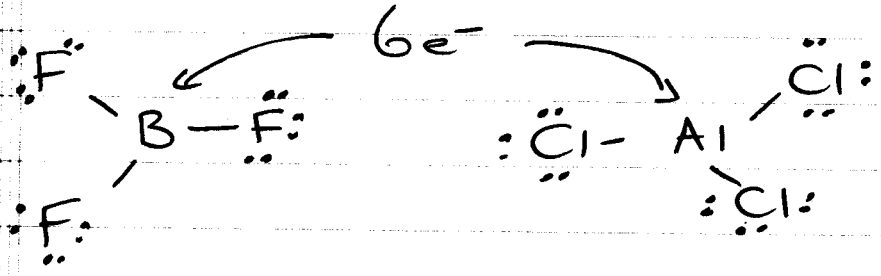
NOT



$10e^-$ VIOLATES
OCTET RULE

Note: EXCEPTIONS TO OCTET RULE

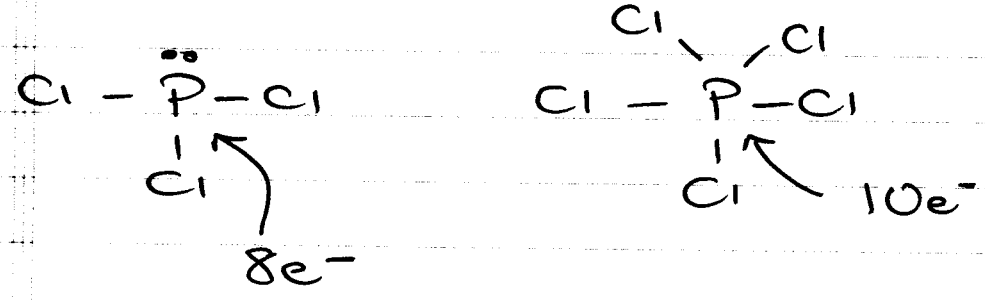
GROUP 3



3rd Row ELEMENTS (P & S)

– d orbitals ⇒ EXPAND OCTET

PCl_3 and PCl_5



④ SHAPES OF MOLECULES

Valence Shell Electron Pair Repulsion THEORY (VSEPR)

Simplified model

Geometry determined by valence shell ELECTRON PAIRS (σ and lp not π) arranging to minimize electrostatic repulsions.

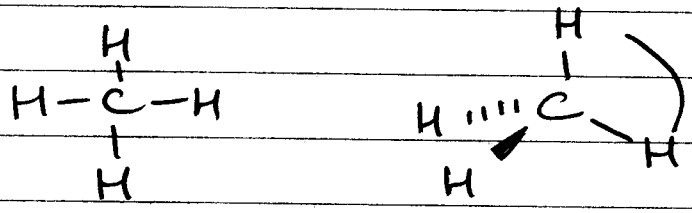
other considerations

lp − lp > lp − bp > bp − bp

and

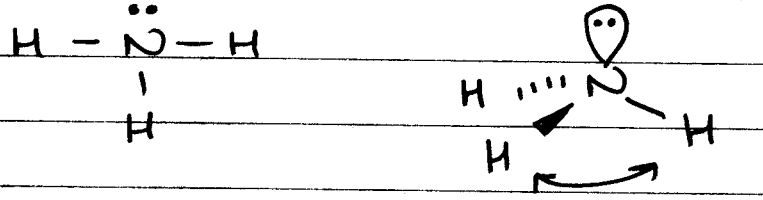
A ≡ B > A = B > A − B

So



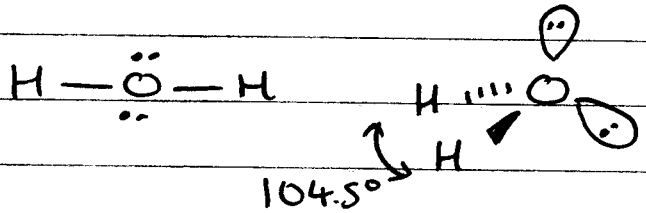
REGULAR TETRAHEDRON

tetrahedral



PYRAMIDAL

Compressed

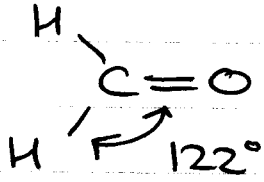


BENT

more compressed

linear

linear

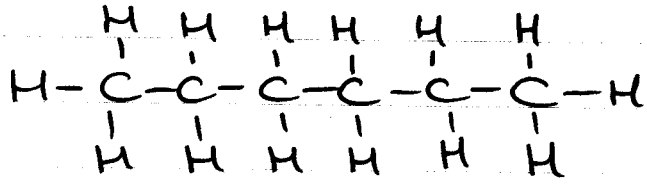


trigonal planar

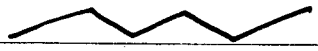
2 LINEAR
3 TRIGONAL PLANAR
4 TETRAHEDRAL
5 TRIGONAL BIPYRAMIDAL
6 OCTAHEDRAL

(5) DRAWING ORGANIC STRUCTURES

- Draw chains of atoms as a zigzag
- Miss out H atoms from C atoms (not from heteroatoms)
- Miss out Cs of C atoms
- Draw all lone pairs



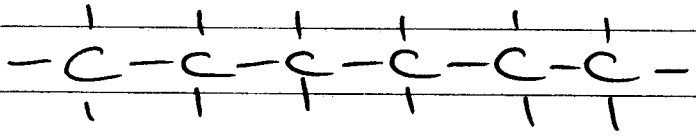
HEXANE (naming later)



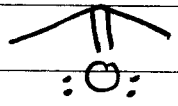
DO NOT WRITE

C–C–C–C–C–C WRONG

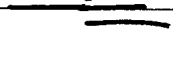
or

 WRONG

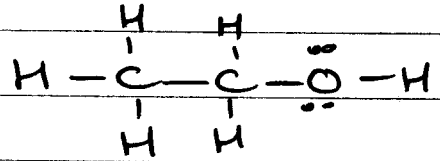
Try to be as true to molecular shape as possible

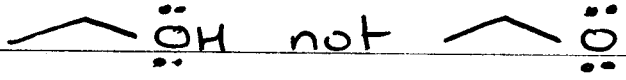
 BAD  GOOD

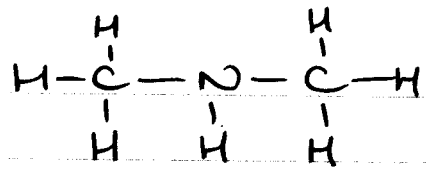
 BAD  GOOD

 BAD  GOOD

HETEROATOMS







not

C_5H_{12}

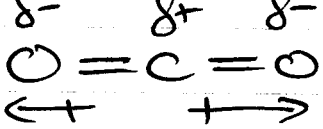
all C_5H_{12}

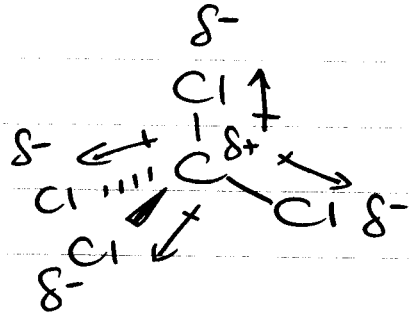
CONSTITUTIONAL ISOMERS
- same molecular formula, different arrangements of atoms

QUICKER TO DRAW

⑥ DIPOLE MOMENTS

Vector Sum of BOND dipoles

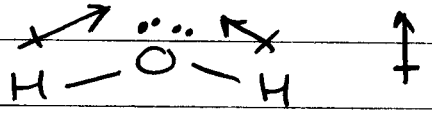




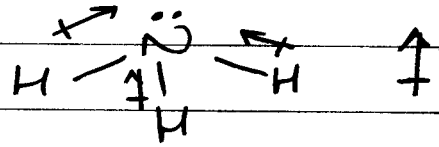
μ = 0D

μ = 0D

D = debye



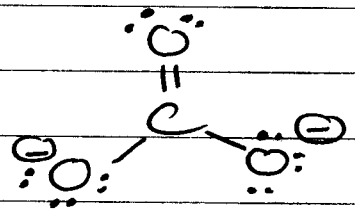
$\mu = 1.85$ D



$\mu = 1.47$ D

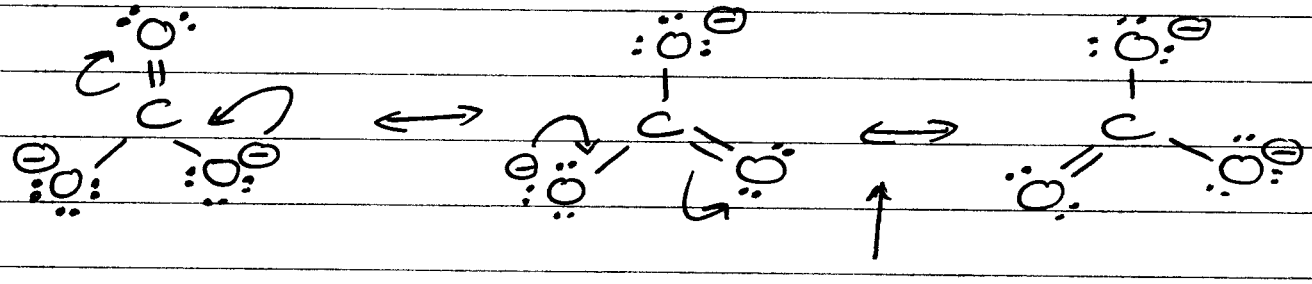
(7) RESONANCE

consider CO_3^{2-}



one C=O bond
two C–O bonds

However all carbon–oxygen bonds are the same

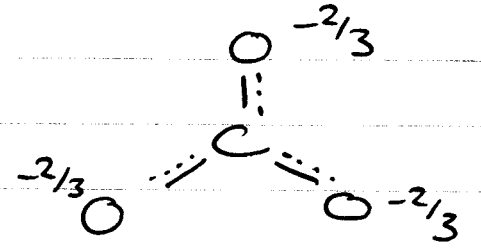


means RESONANCE

↷ movement of pair of electrons

THREE RESONANCE CONTRIBUTORS
(ALL EQUIVALENT)

NONE OF THEM ARE REAL



RESONANCE HYBRID

- NON EQUIVALENT CONTRIBUTORS

DIFFERENT ENERGIES

- RULES FOR DRAWING RESONANCE STRUCTURES

- RULES FOR DETERMINING IMPORTANCE OF CONTRIBUTING STRUCTURES