LEC (4) CHEM 30A Jan 14th

1. RESONANCE
2. ATOMIC ORBITALS
3. MOLECULAR ORBITALS
4. HYBRIDIZATION

HMK 1.18, 1.55 – 1.70
UCLA CLOSED ON MONDAY
QUIZ IN CLASS NEXT WEDS
OFFICE HOURS TUES 4pm

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1. RESONANCE

- drawing resonance structures

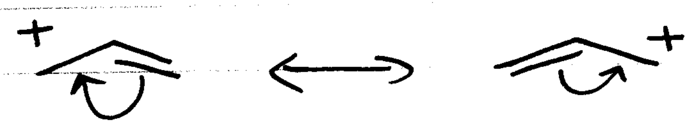
CANNOT BREAK SINGLE BONDS, SO WE can only move electrons from double (or triple) bonds and lone pairs

- PATTERNS

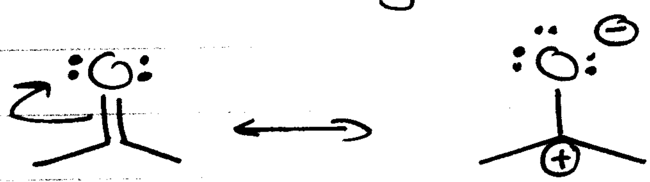
a) LONE PAIR NEXT TO π BOND (DOUBLE/TRIPLE)
('next to' means one single bond away)

b) LONE PAIR next to +ve CHARGE

c) π BOND next to +ve CHARGE



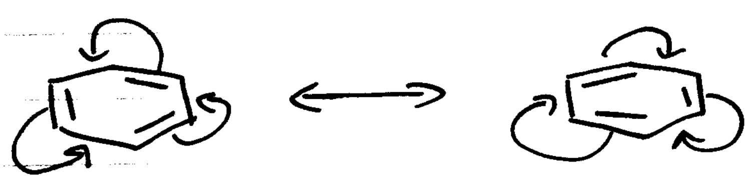
d) π BOND between two ATOMS where one is very EN



NOT

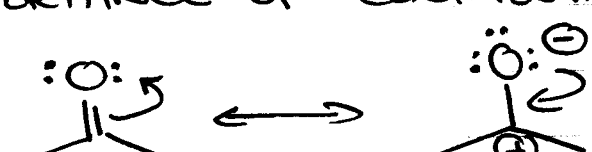
O is more EN than C

e) ALTERNATING π BONDS in a RING



– RELATIVE IMPORTANCE OF CONTRIBUTING STRUCTURES

① MINIMIZE CHARGES



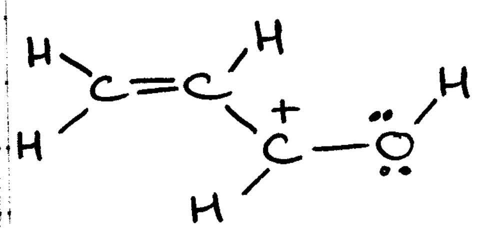
more significant

(2) MAXIMISE OCTETS

more significant

not a full octet

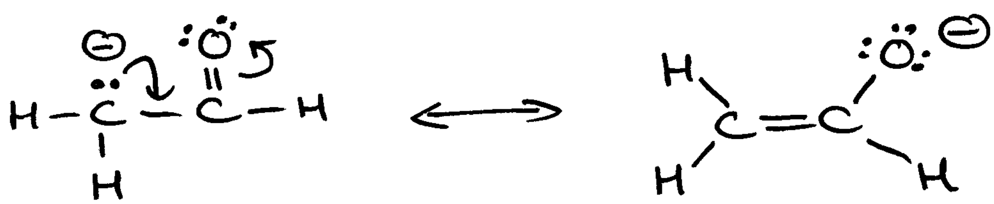
e.g.



DRAW OTHER TWO RESONANCE FORMS

- WHICH IS THE MOST SIGNIFICANT?
- WHAT IS THE STRUCTURE OF THE RESONANCE HYBRID

(3) NEGATIVE CHARGE ON MORE EN ELEMENT



more significant

(2) ATOMIC ORBITALS

Schrödinger equation

⇓

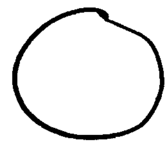
Probability distributions of electron density

⇓

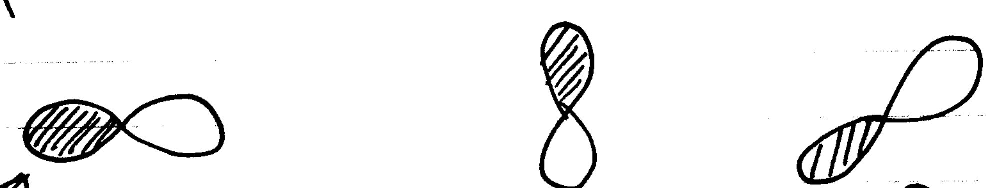
Orbitals (shapes)

this class

$\underline{\underline{s, p}}$, d, f — sharp, principal, diffuse, fundamental

1s  2s 

2p orbitals



p_x p_y p_z

different phases

(3) MOLECULAR ORBITALS

molecules ⟹ many atoms ⟹ many atomic orbitals

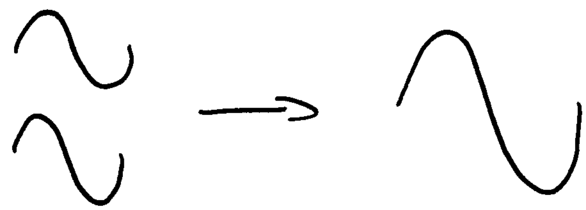
(LCAO – linear combination of atomic orbitals)

n AOs ⟶ n MOs

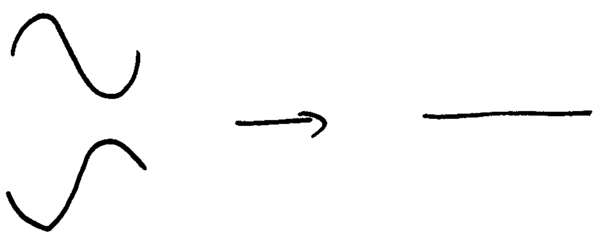
- same filling rules

AUFBAU PRINCIPLE (lowest energy first)
PAULI EXCLUSION PRINCIPLE (two e^-, opp spin)
HUND'S RULE (don't pair until you have to)

Orbitals → wavefunctions
- combine like waves

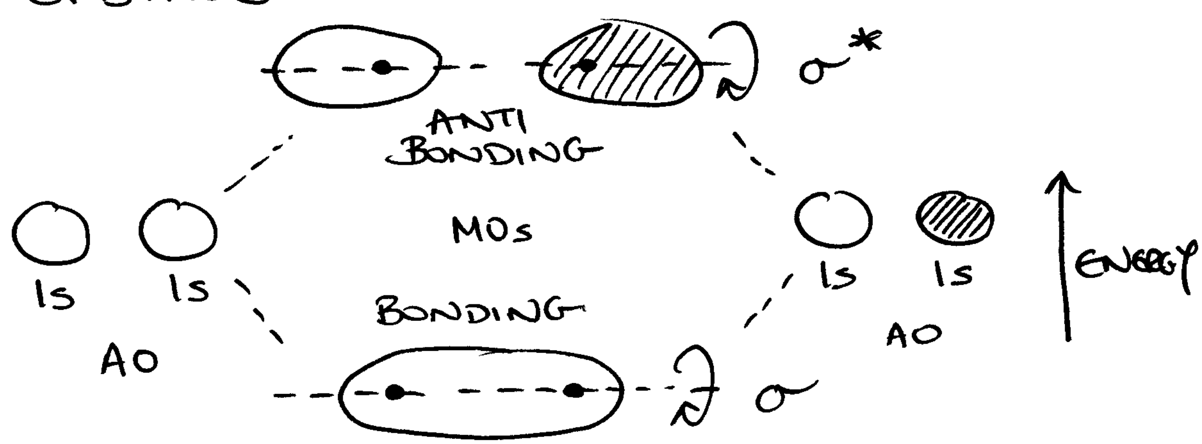


in phase
(constructive)



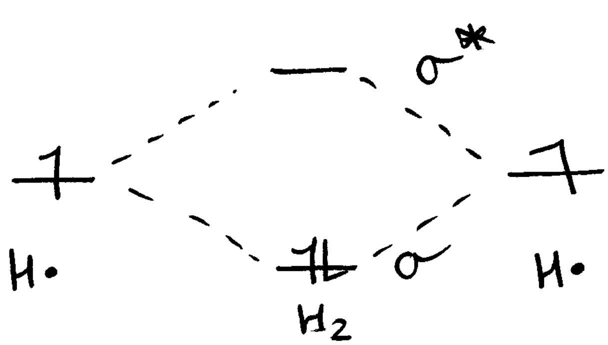
out of phase
(destructive)

- s orbitals

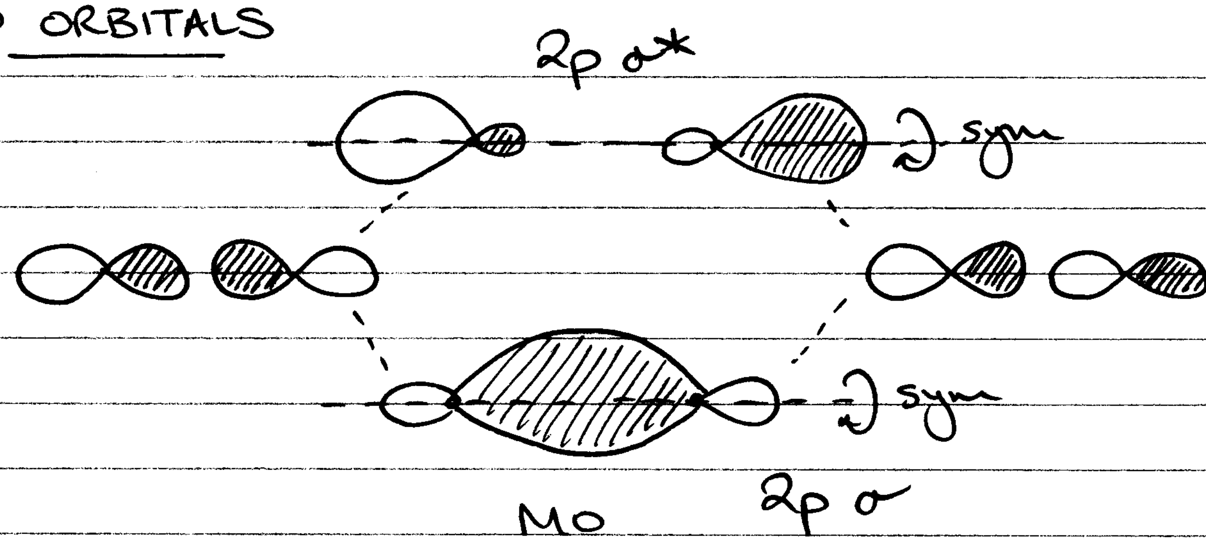


SYMMETRICAL ABOUT AXIS ⇒ σ

H_2



p ORBITALS



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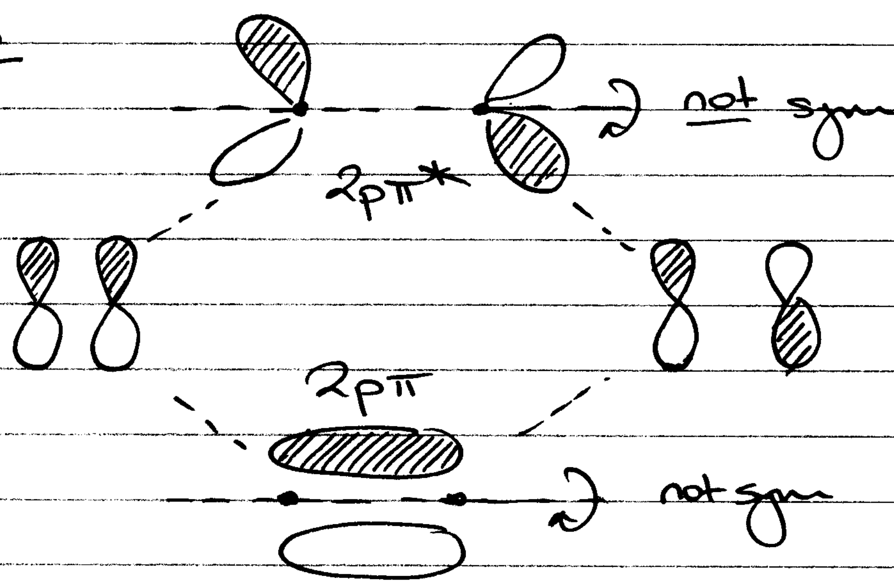


σ BONDS stronger than π BONDS – MORE OVERLAP

④ HYBRIDISATION

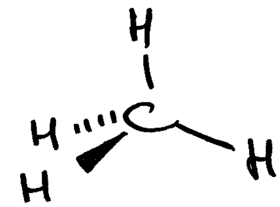
C $1s^2\ 2s^2\ 2p^2$

$1s^2\ 2s^2\ 2p_x^1\ 2p_y^1\ 2p_z^0$

ONLY 2 UNPAIRED ELECTRONS

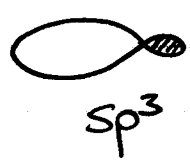
and p ORBITALS 90° apart

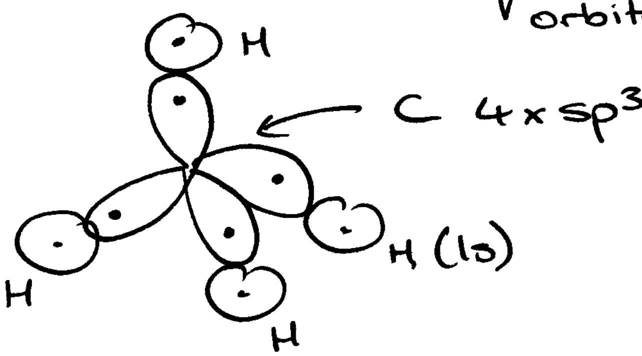
So, how do we explain



HYBRID ORBITALS (PAULING)

$\underline{sp^3}$ $1 \times 2s$ $3 \times 2p$ $\Rightarrow$ $4 sp^3$ equivalent orbitals

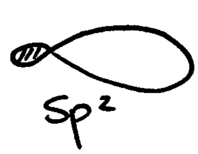


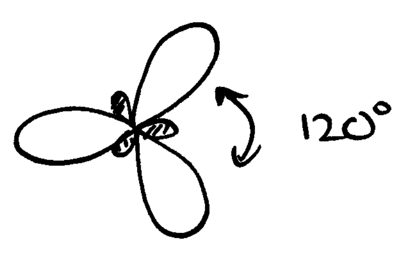


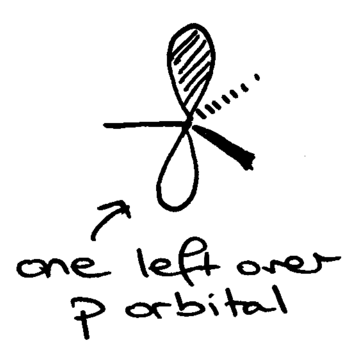
$4 \times$ $1s - 2sp^3$ σ BONDS

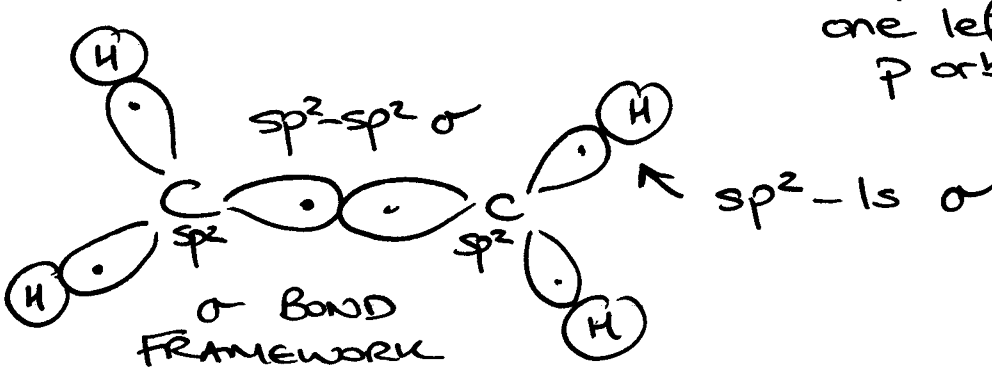
$\underline{sp^2}$ $1 \times 2s$ and $2 \times 2p$

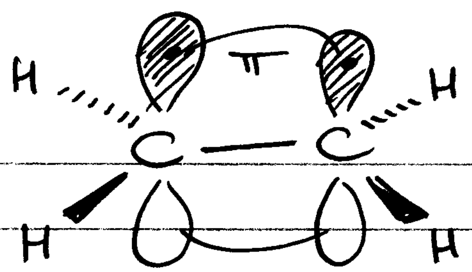
$\Rightarrow$ $3 \times sp^2$ orbitals



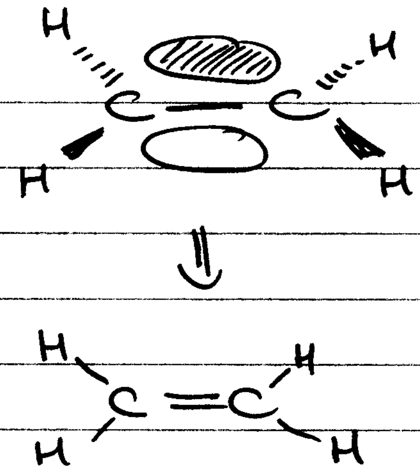




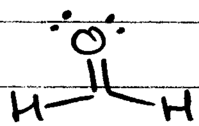


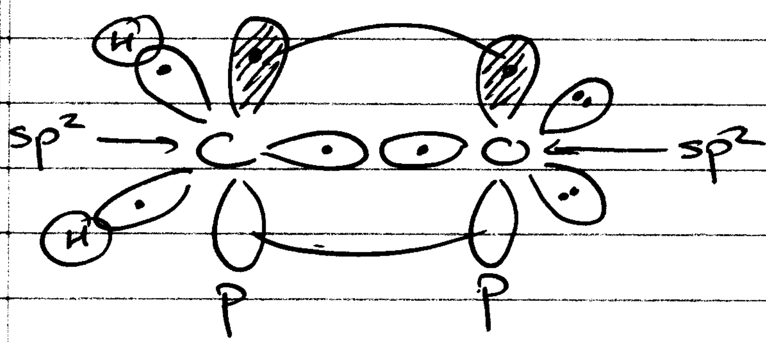


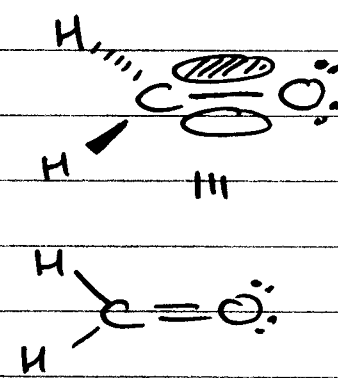
π BOND



FLAT



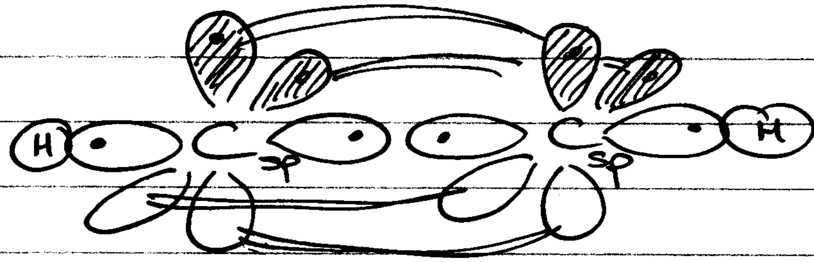




FLAT

sp 1 x 2s and 1 x 2p

 sp



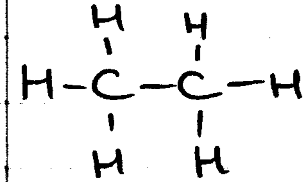
H−C≡C−H

↑

1 x sp−sp σ

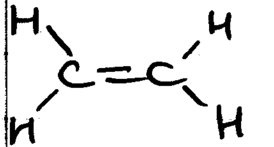
2 x 2p−2p π

CONSIDER



C—C
1.53 Å
88 Kcal/mol

C—H
$sp^3 - 1s$ σ
1.11 Å
98 Kcal/mol



C=C
1.34 Å
146 Kcal/mol

(not ×2)

C—H
$sp^2 - 1s$ σ
1.10 Å
104 Kcal/mol

(not ×3)

H—C≡C—H

C≡C
1.21 Å
200 Kcal/mol

C—H
$sp - 1s$ σ
1.09 Å
125 Kcal/mol

$Å = 10^{-10}$ m

more s character
→ electrons closer to nucleus
→ stronger/shorter bonds

So, to determine HYBRIDIZATION of an atom

ADD # BONDED ATOMS TO # LONE PAIRS

4 → sp^3
3 → $3 \times sp^2 + 1 \times p$
2 → $2 \times sp + 2 \times p$