LEC 4 CHEM 30A Apr 11th

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

HMK 1.18, 1.55 – 1.71 (1.70 3rd ed) + RESONANCE PROBLEMS ON WEB

QUIZ IN CLASS ON WEDNESDAY

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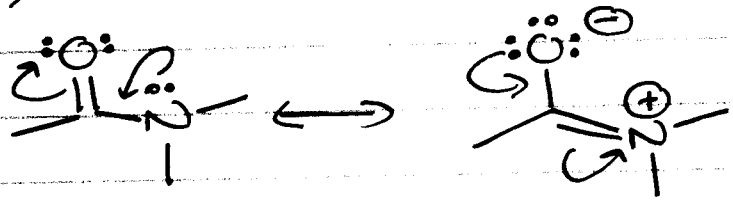
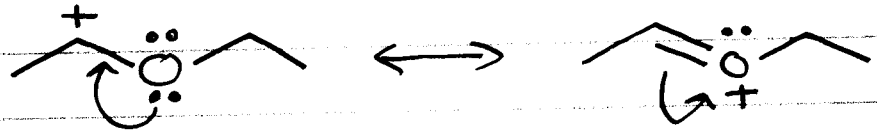
1. RESONANCE

– Patterns

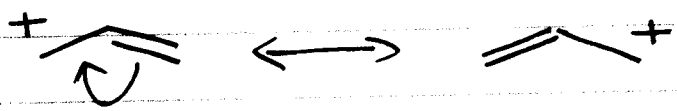
a) LONE PAIR / π-BOND



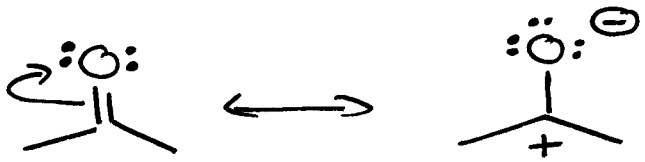
b) LONE PAIR / +ve CHARGE



c) π BOND / +ve CHARGE



d) π BOND / TWO EN ATOMS



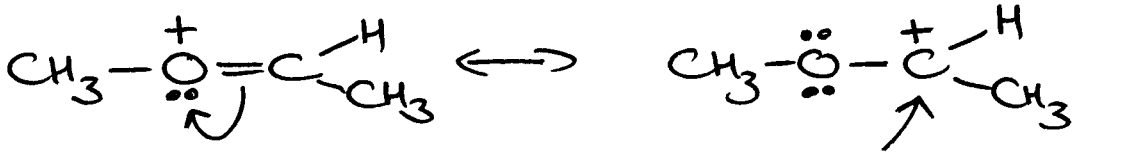
NOT

O is more EN than C

e) π BONDS in a RING

— RELATIVE IMPORTANCE OF CONTRIBUTING STRUCTURES

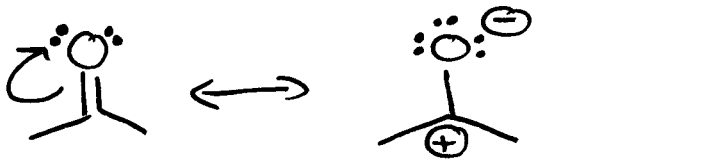
a) MAXIMISE OCTETS



more significant

not a full octet

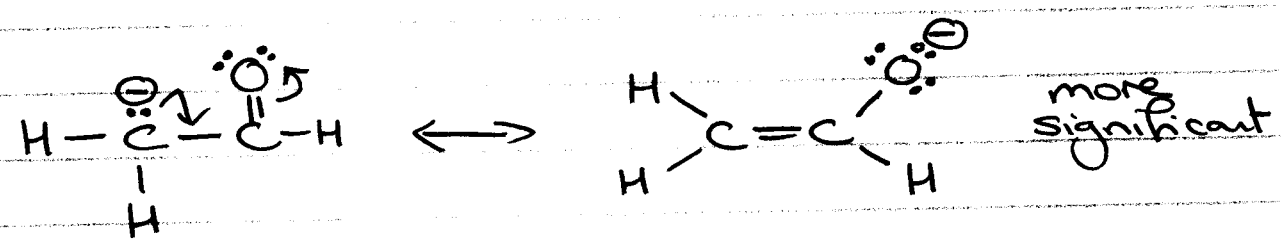
b) MINIMISE CHARGES



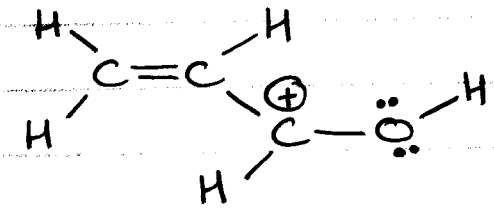
more significant

less significant

c) PUT -ve CHARGE ON MORE EN ELEMENT



HMK



DRAW OTHER TWO RESONANCE FORMS

- which is most significant?
- structure of hybrid?

(2) ATOMIC ORBITALS

Schrödinger equation

⇓

Probability distributions of electron density

⇓

Orbitals (shapes) s, p, d, f

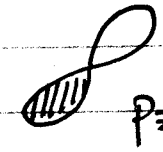
this class

sharp
principal
diffuse
fundamental

1s 

2s 

2p ORBITALS



(3) MOLECULAR ORBITALS

molecules => many atoms => many atomic orbitals

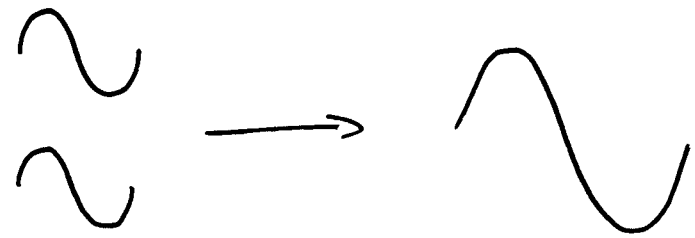
(LCAO - linear combination of atomic orbitals)

nAOs $\longrightarrow$ nMOs

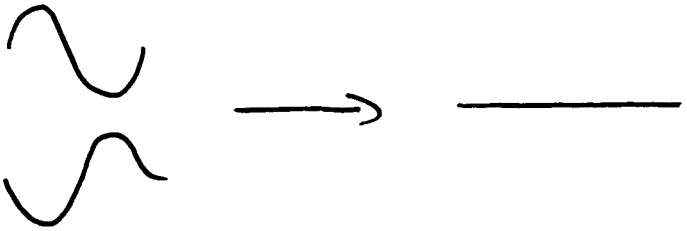
- same filling rules

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

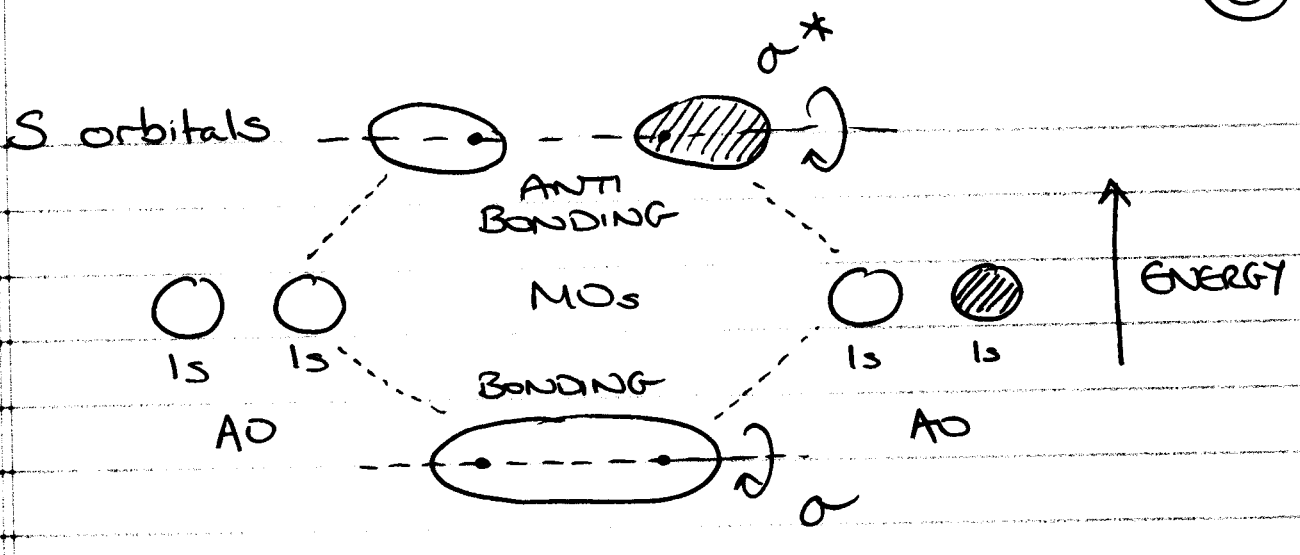
Orbitals → wavefunctions - combine like waves



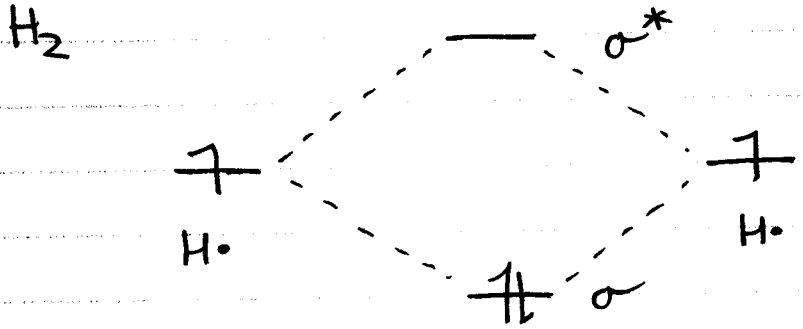
in phase
(constructive)



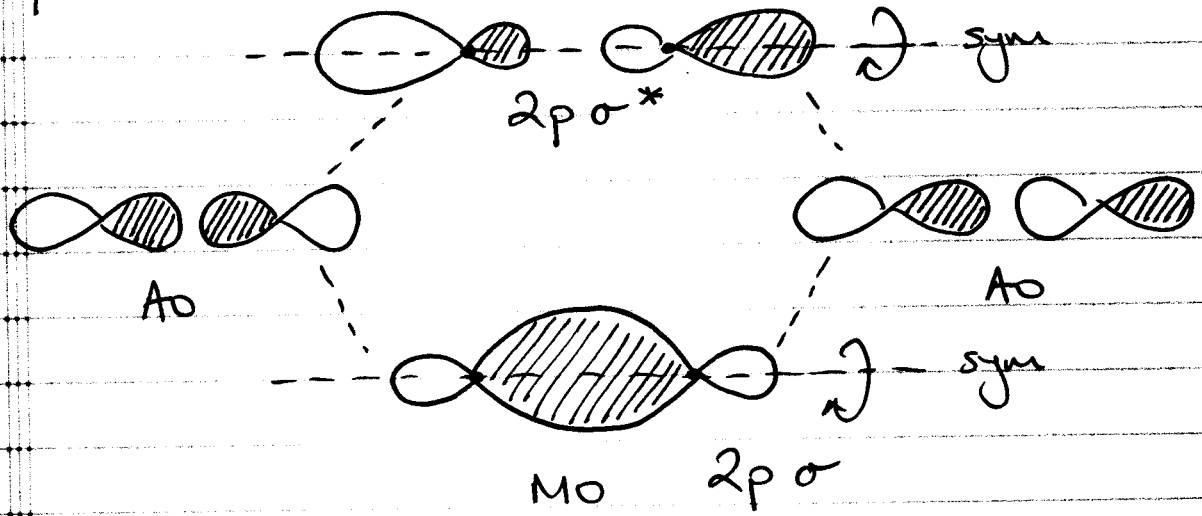
out of phase
(destructive)



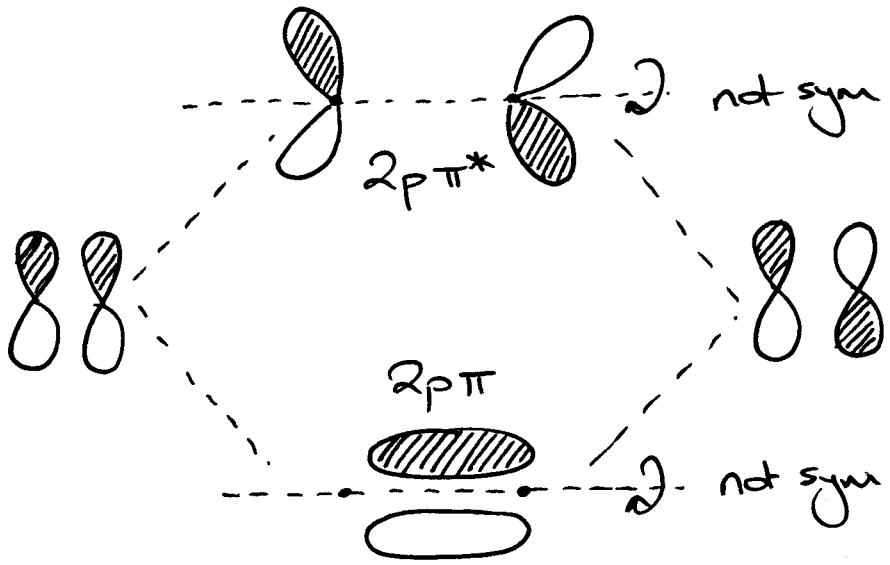
Symmetrical about axis ⇒ σ



p orbitals



p ORBITALS can also overlap side on...

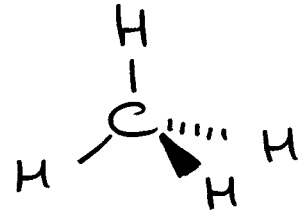


σ BONDS stronger than π BONDS ⇒ More overlap

④ HYBRIDISATION

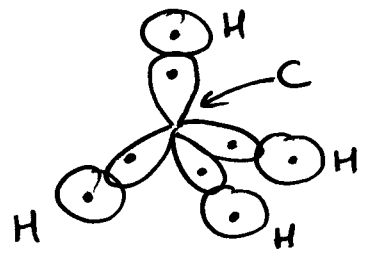
C $1s^2\ 2s^2\ 2p^2$
$1s^2\ 2s^2\ 2p_x^1\ 2p_y^1\ 2p_z^0$

ONLY 2 UNPAIRED e^- AND
p ORBITALS are 90° apart

So, how do we explain  ?

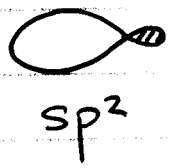
HYBRID ORBITALS (PAULING)

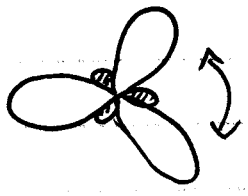
sp^3 (1 x 2s, 3 x 2p) ⇒ 4 sp^3 orbitals

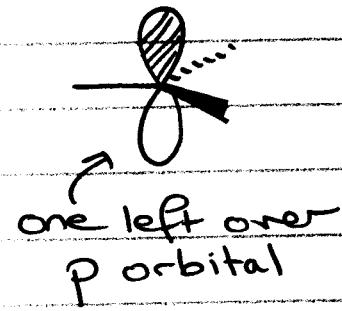


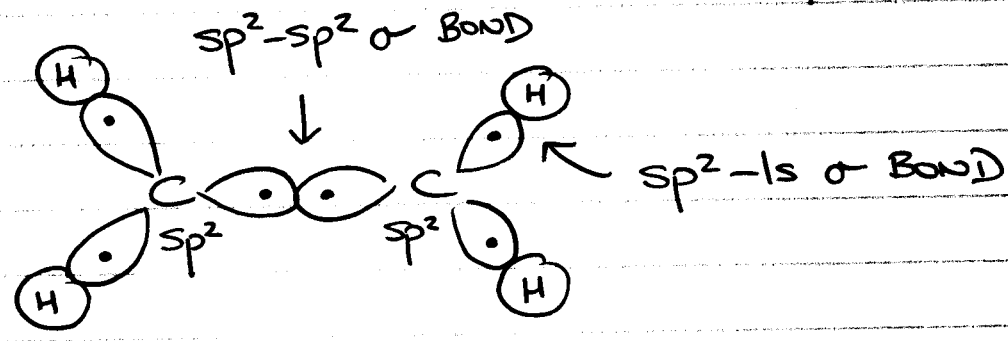
1s - $2sp^3$ σ BONDS

sp^2 $(1 \times 2s, 2 \times 2p) \Rightarrow 3\,sp^2$ orbitals

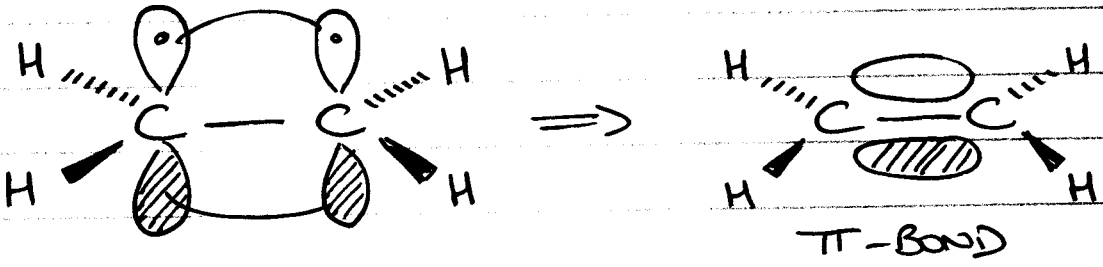




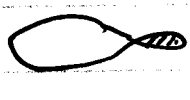


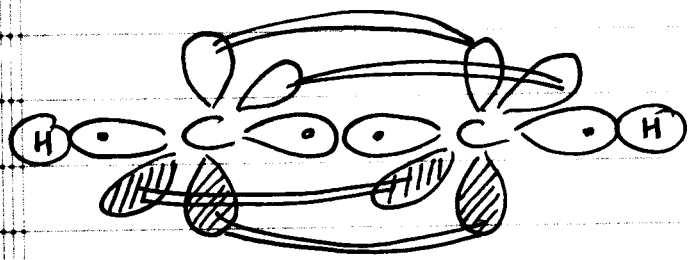


σ BOND FRAMEWORK



sp $(1 \times 2s, 1 \times 2p) \Rightarrow 2\,sp$ orbitals



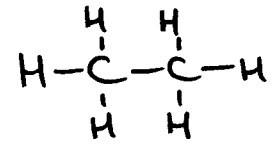


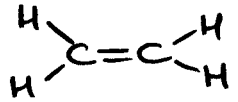
$H-C \equiv C-H$

$1 \times sp\text{-}sp\ \sigma$

$2 \times 2p\text{-}2p\ \pi$

CONSIDER





H–C≡C–H

C–C	C=C	C≡C
1.53 Å	1.34 Å	1.21 Å
88 kcal/mol	146 kcal/mol	200 kcal/mol

not ×2

not ×3

C–H	C–H	C–H
sp^3–1s σ 1.11 Å	sp^2–1s σ 1.10 Å	sp–1s σ 1.09 Å
98 kcal/mol	104 kcal/mol	125 kcal/mol

$\text{Å} = 10^{-10}\ m$

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

To determine HYBRIDIZATION of an ATOM

ADD # BONDED ATOMS to # LONE PAIRS

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