

LEC (4)

CHEM 30A

Oct 7th

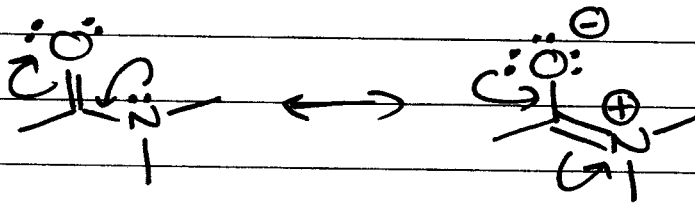
- ① RESONANCE
- ② ATOMIC ORBITALS
- ③ MOLECULAR ORBITALS
- ④ HYBRIDISATION

HWK 1.18, 1.55-1.71 + RESONANCE PROBLEMS ON WEB

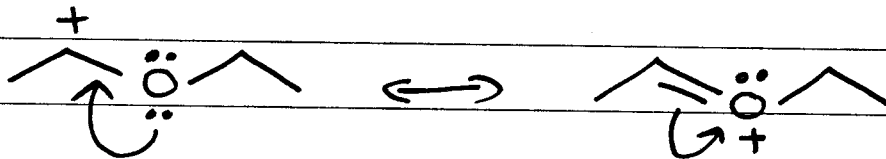
① RESONANCE

- Patterns

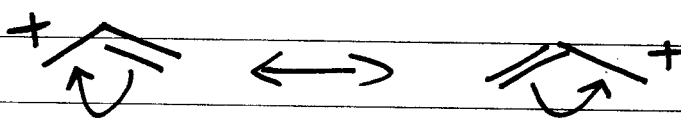
a) LONE PAIR / π BOND



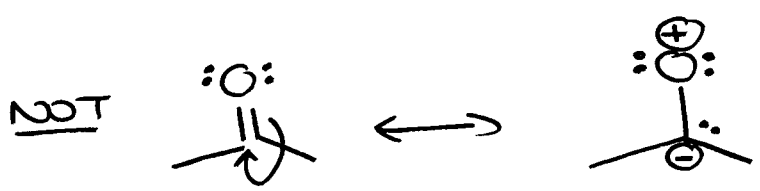
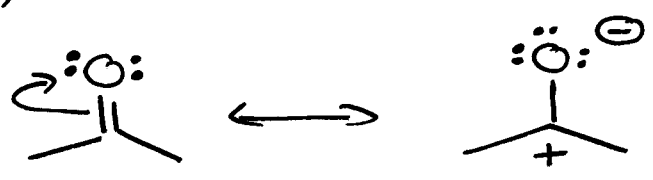
b) LONE PAIR / +ve CHARGE



c) π BOND / +ve CHARGE

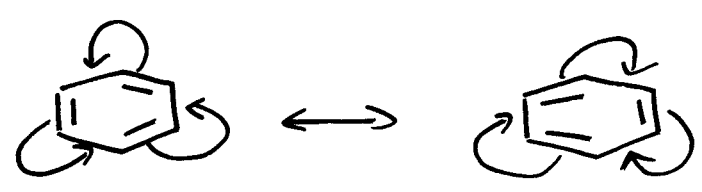


d) π BOND / TWO EN ATOMS



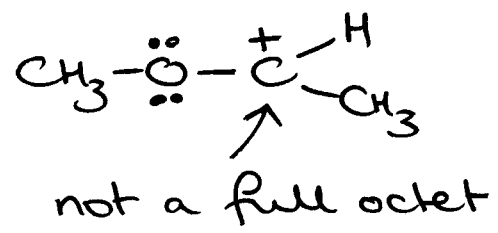
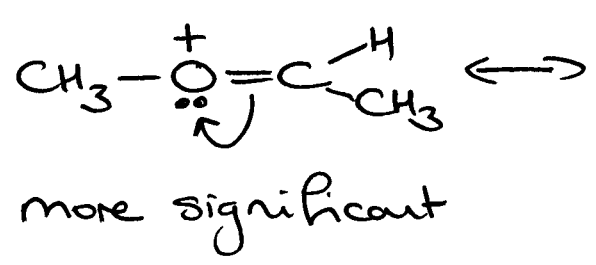
O is more EN than C

e) π BONDS in a RING

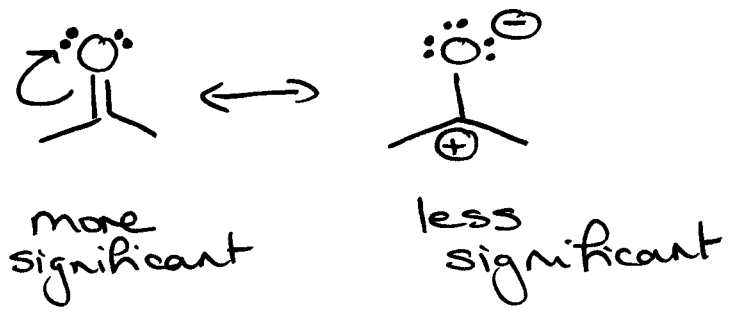


RELATIVE IMPORTANCE OF CONTRIBUTING STRUCTURES

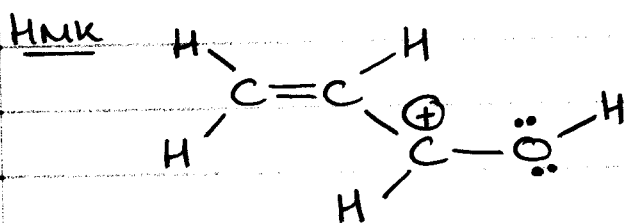
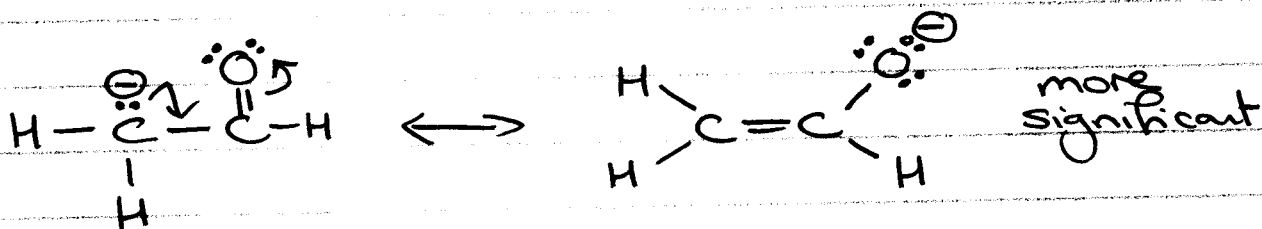
a) MAXIMISE OCTETS



b) MINIMISE CHARGES



c) Put -ve charge on more EN element



DRAW OTHER TWO RESONANCE FORMS

- which is most significant?
- structure of hybrid?

② ATOMIC ORBITALS

Schrödinger equation

Probability distributions of electron density

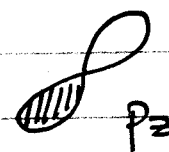
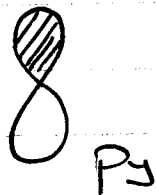
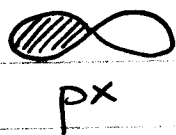
Orbitals (shapes)
this class

s, p, d, f

sharp
principal
diffuse
fundamental



2p ORBITALS



/// = phase

③ MOLECULAR ORBITALS

molecules \Rightarrow many atoms \Rightarrow many atomic orbitals

(LCAO - linear combination of atomic orbitals)

$$n \text{ AOs} \rightarrow n \text{ MOs}$$

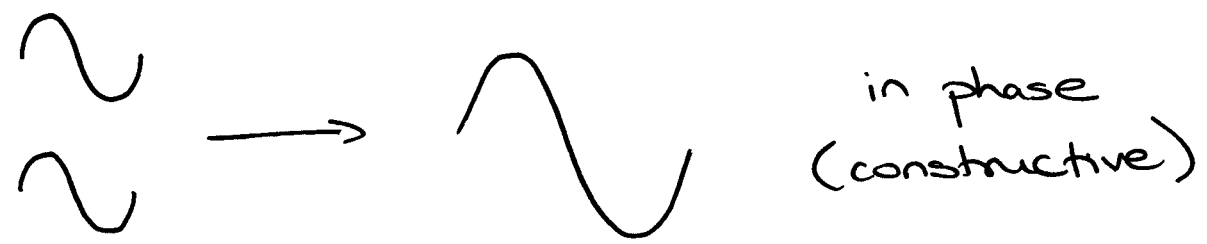
- same filling rules

AUFBAU PRINCIPLE (lowest energy first)

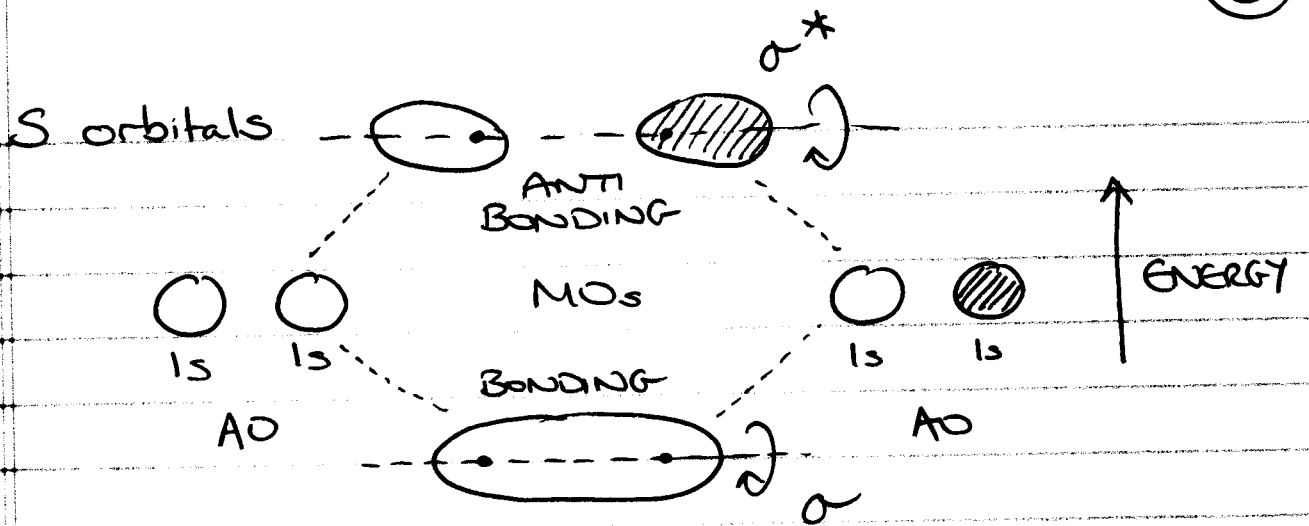
PAULI EXCLUSION PRINCIPLE (two e^- , opp spin)

HUND'S RULE (don't pair until you have to)

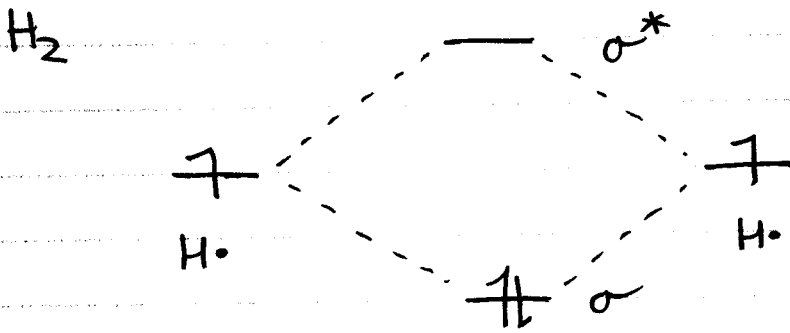
Orbitals \rightarrow wave functions - combine like waves



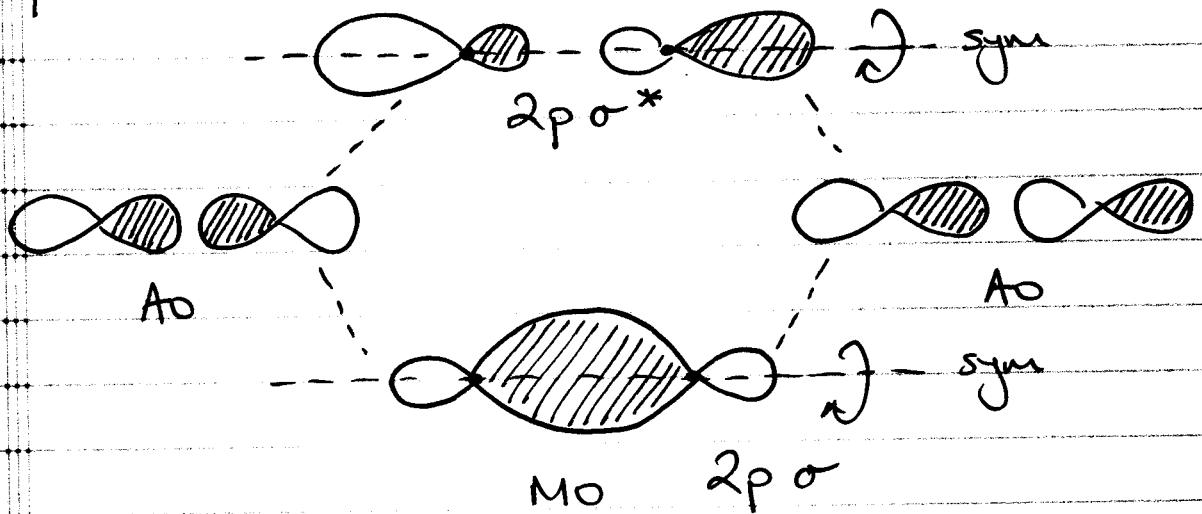
5



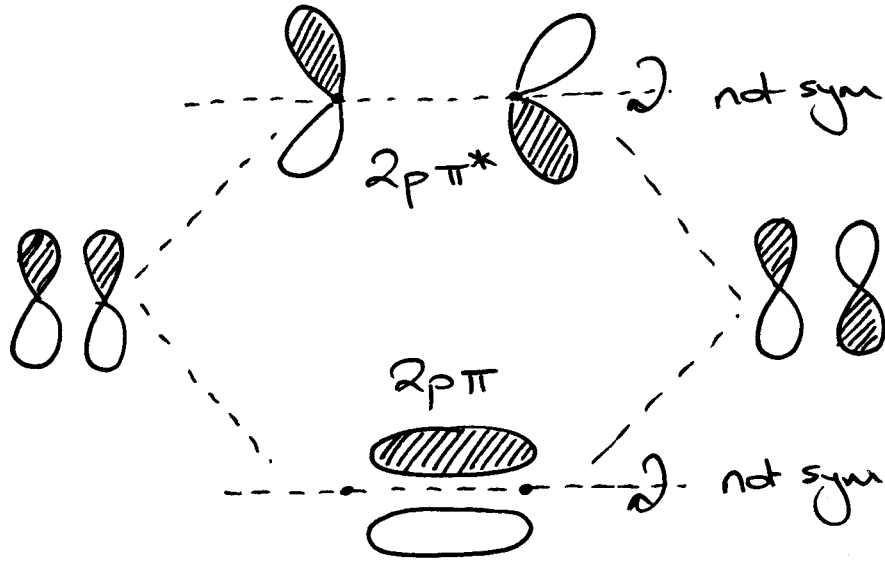
Symmetrical about axis $\Rightarrow \sigma$



p orbitals

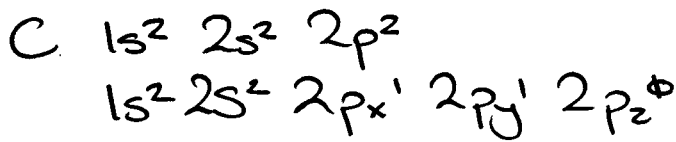


p ORBITALS can also overlap side on...



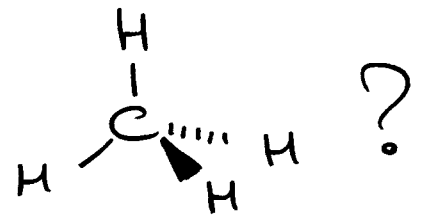
σ BONDS stronger than π BONDS \Rightarrow more overlap

④ HYBRIDISATION



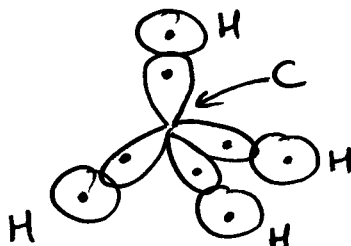
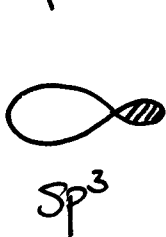
ONLY 2 UNPAIRED e^- AND
 p ORBITALS are 90° apart

So, how do we explain



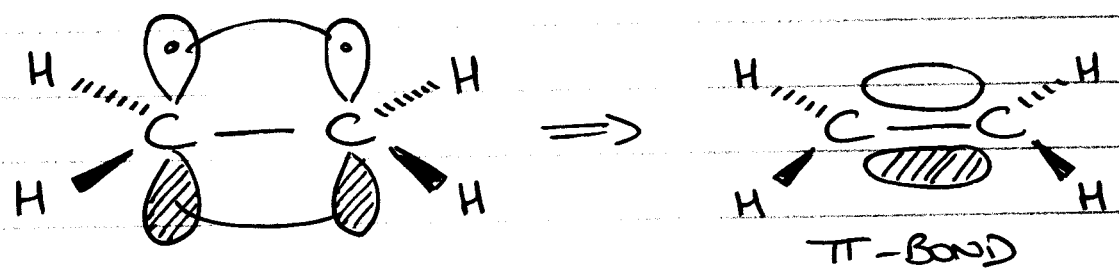
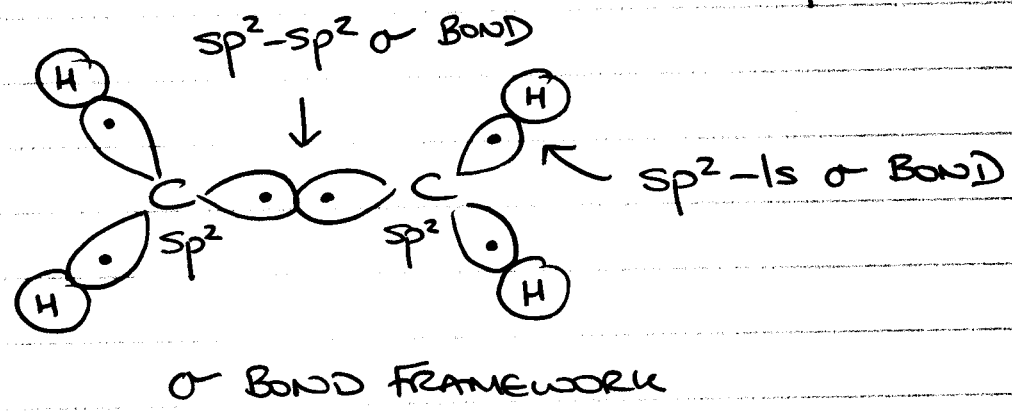
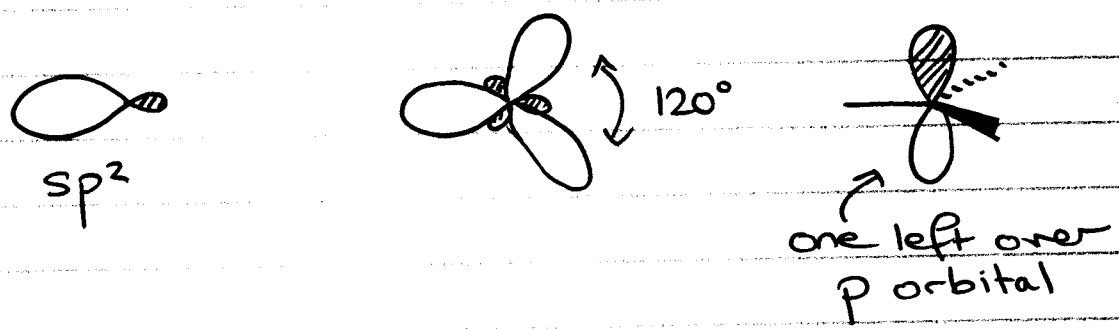
HYBRID ORBITALS (PAULING)

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

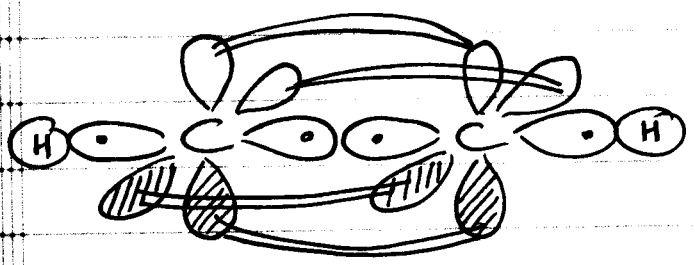
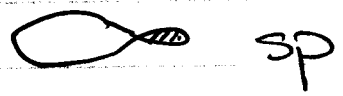


1s - $2sp^3$
 σ BONDS

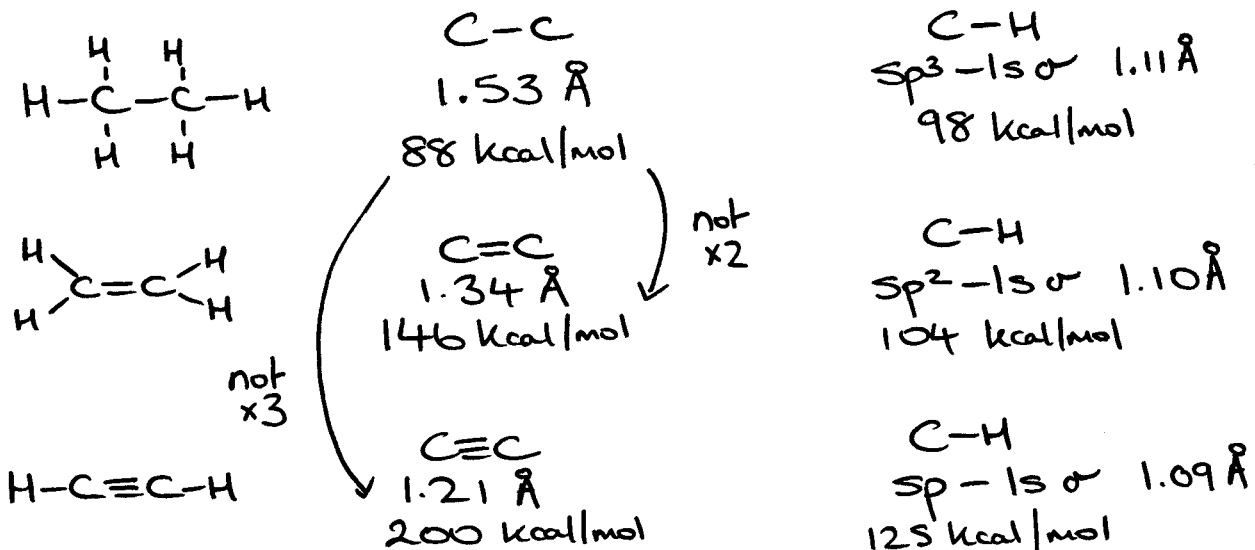
sp^2 (1 x 2s, 2 x 2p) \Rightarrow 3 sp^2 orbitals



sp (1 x 2s, 1 x 2p) \Rightarrow 2 sp orbitals



$H-C \equiv C-H$
 1 x $sp-sp$ σ
 2 x $2p-2p$ π

CONSIDER

$$\text{\AA} = 10^{-10} \text{ m}$$

more s character

- electrons closer to nucleus
- stronger/shorter bonds

To determine HYBRIDIZATION of an ATOM

ADD # BONDED ATOMS to # LONE PAIRS

$$4 \rightarrow \text{sp}^3$$

$$3 \rightarrow 3 \times \text{sp}^2 + 1 \times \text{p}$$

$$2 \rightarrow 2 \times \text{sp} + 2 \times \text{p}$$