LEC 4 CHEM 30 A Oct 8th

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

HMK 1.18, 1.55-1.70

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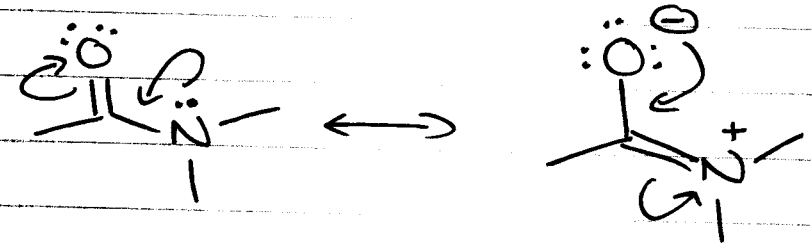
## 1 RESONANCE CONTINUED...

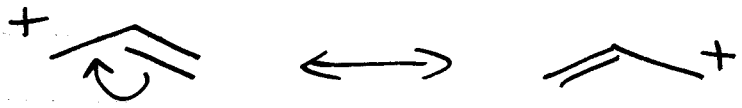
Patterns

### 1 LONE PAIR / π-BOND

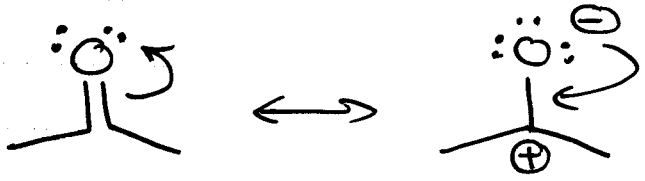


### 2 LONE PAIR / ⊕ve charge

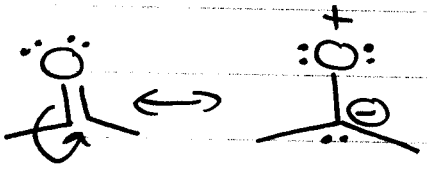
(3) π BOND / ⊕ve charge



(4) π BOND between two atoms where one is quite electronegative



NOT



$e^-$ go to more EN ATOM

(5) ALTERNATING π BONDS IN A RING

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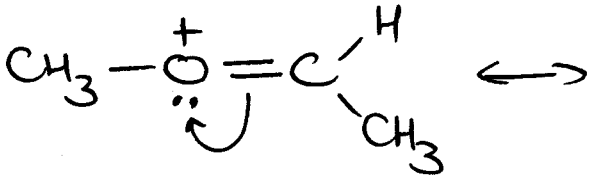
RELATIVE IMPORTANCE OF CONTRIBUTING STRUCTURES

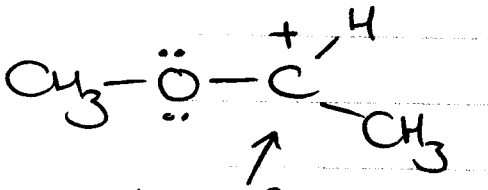
(1) MINIMIZE CHARGES

more significant

## ② MAXIMIZE OCTETS

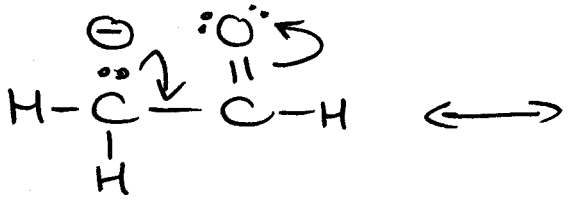


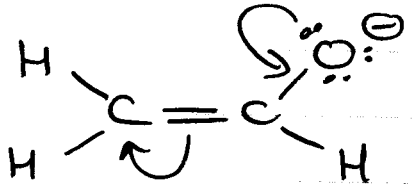
MORE SIGNIFICANT



not a full octet

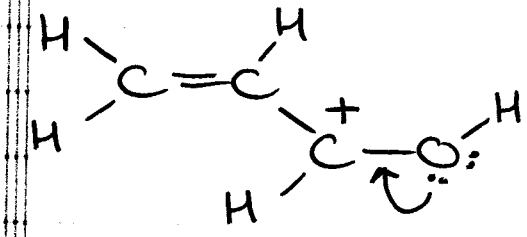
## ③ NEGATIVE CHARGE ON MORE EN ELEMENT

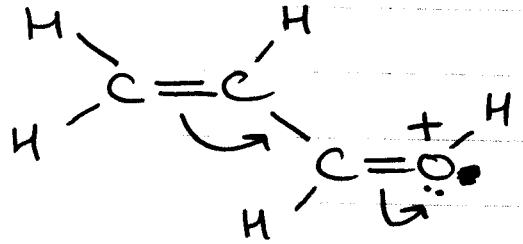




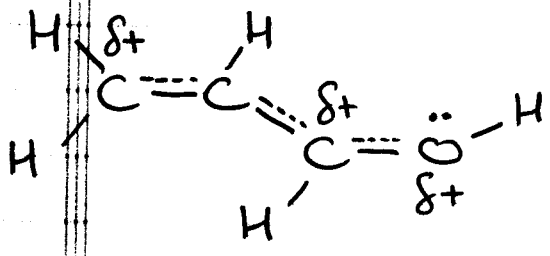
more significant

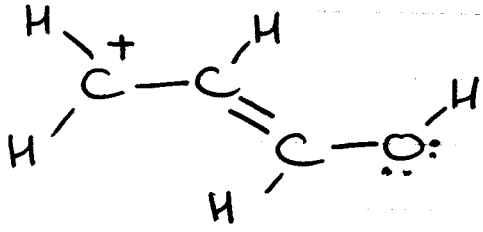
EXAMPLE





HYBRID





## (2) ATOMIC ORBITALS

SCHRÖDINGER EQUATION

⇓

PROBABILITY DISTRIBUTIONS OF ELECTRON DENSITY

⇓

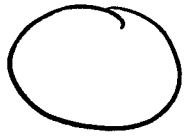
SHAPES OF ORBITALS

⇓

s, p, d, f

sharp, principal, diffuse, fundamental

1s 

2s 

### 2p ORBITALS

Px

Py

Pz

## (3) MOLECULAR ORBITALS

Molecules => many atoms => many atomic orbitals

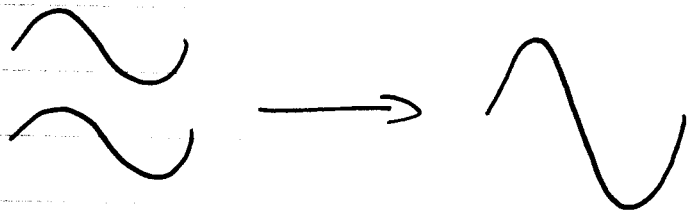
- LCAO (linear combination of atomic orbitals)

$n$ AOs $\longrightarrow$ $n$ MOs

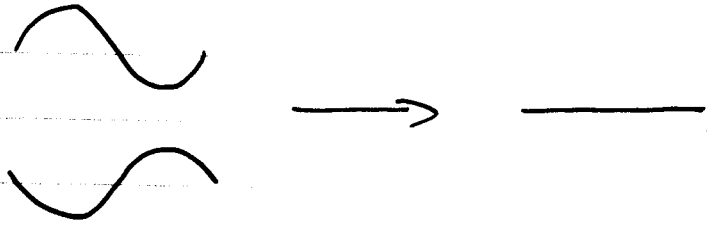
Same filling rules

- AUFBAU PRINCIPLE (lowest energy first)
- PAULI EXCLUSION PRINCIPLE (2 e⁻ OPP SPIN)
- HUND'S RULE (don't pair until you must)

Orbitals $\Rightarrow$ Wavefunctions
- combine like waves

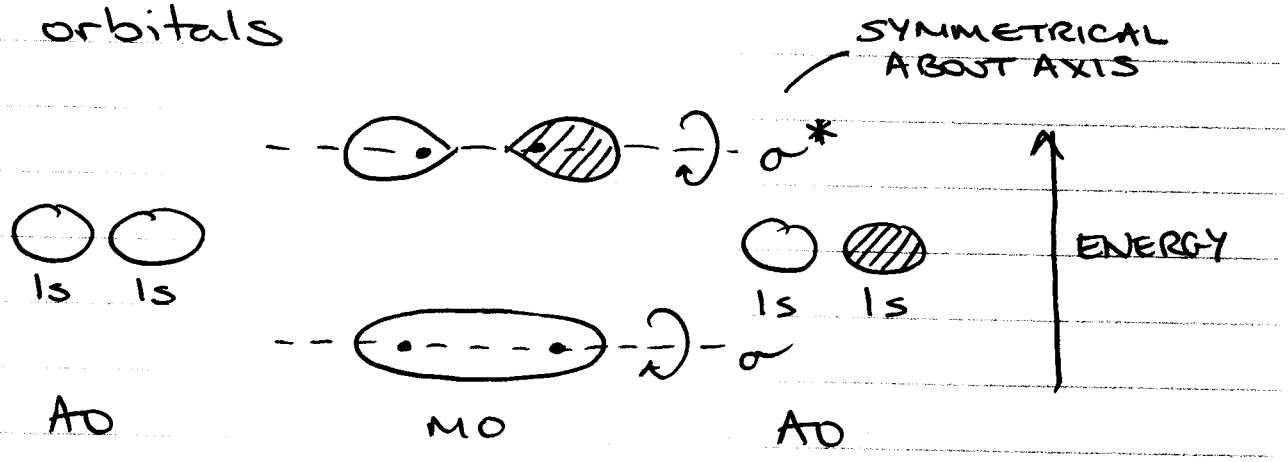


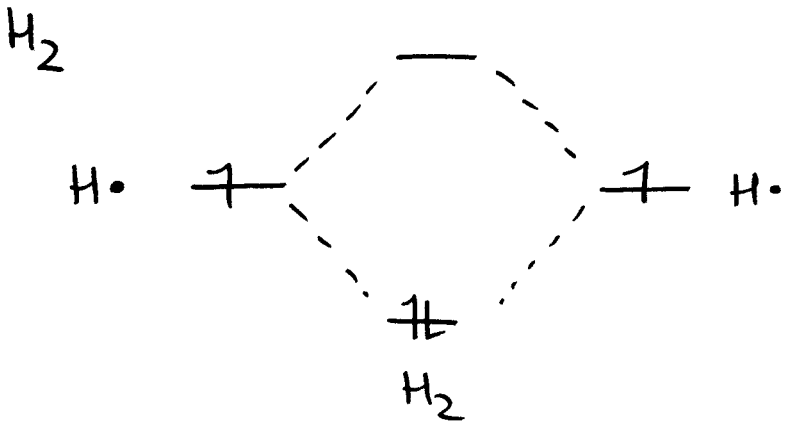
in phase (constructive)



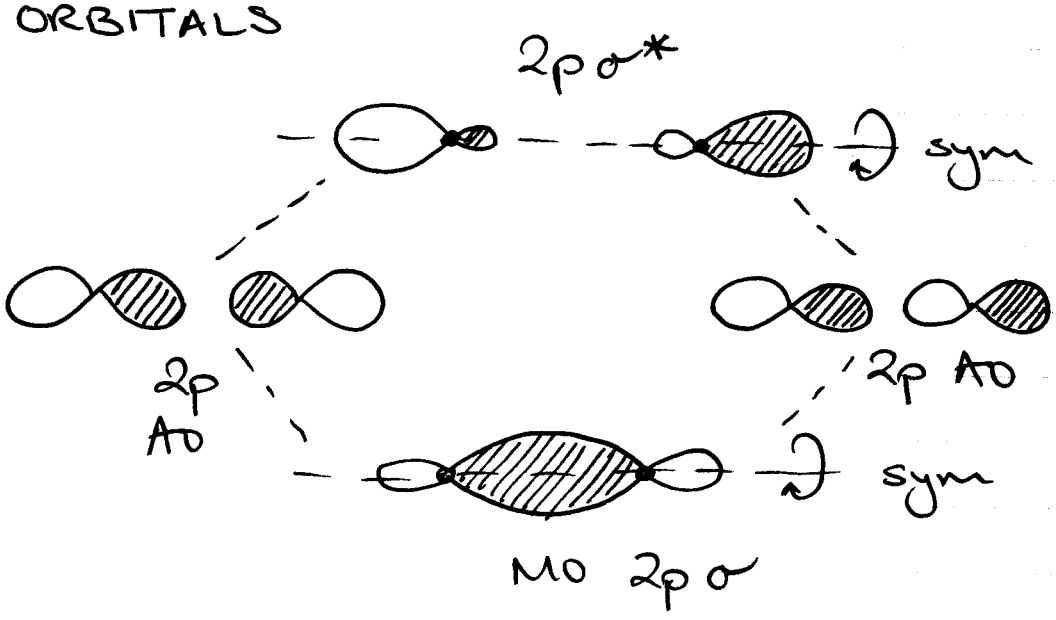
out of phase (destructive)

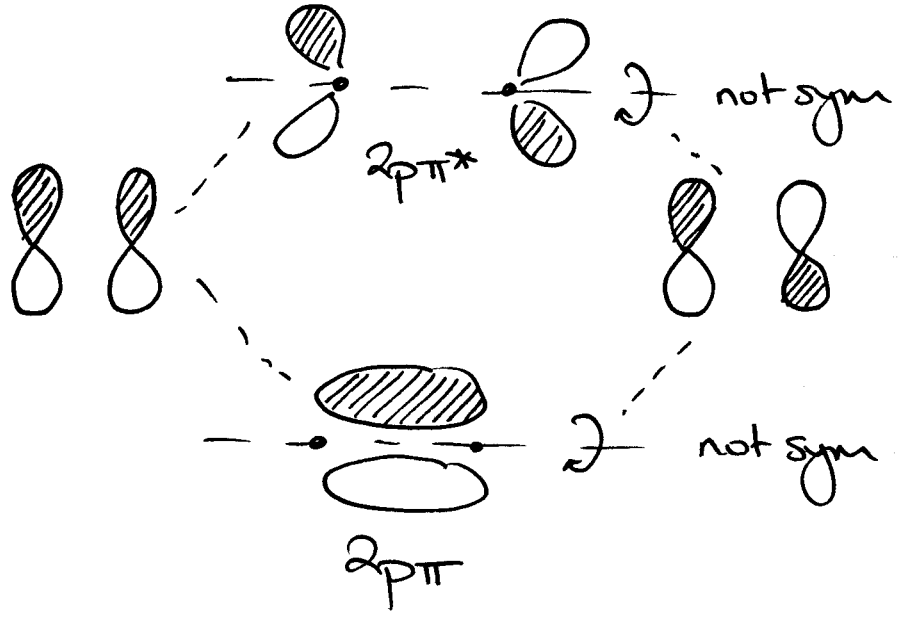
- S orbitals






p ORBITALS



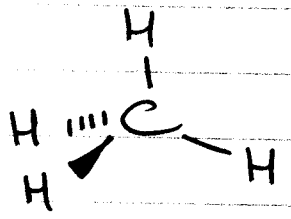

σ BONDS STRONGER THAN π BONDS — MORE OVERLAP

## ④ HYBRIDIZATION

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

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

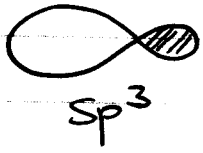
ONLY 2 unpaired electrons
and p orbitals are 90° apart

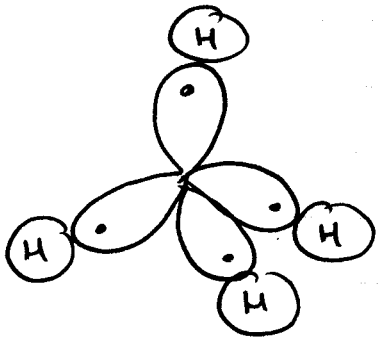
So, how do we explain 


HYBRID ORBITALS (PAULING)

$sp^3$ 1 x 2s 3 x 2p ⟹ 4 x $sp^3$

equiv hybrid orbitals



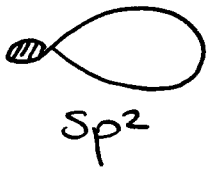



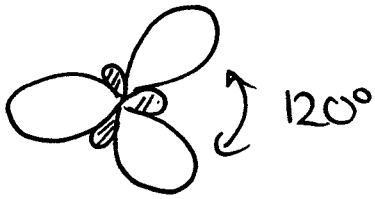

$CH_4$

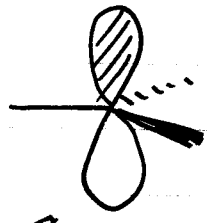
4 x 1s – $2sp^3$ σ BONDS

$sp^2$ 1 × 2s and 2 × 2p

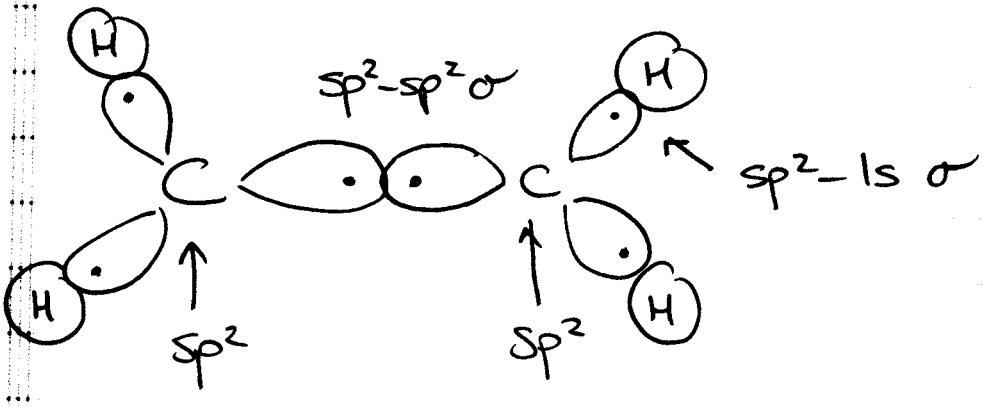
$\Rightarrow$ 3 × $sp^2$ orbitals



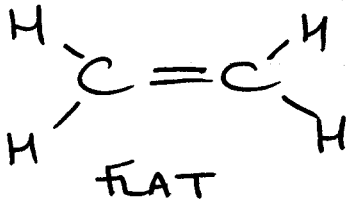
one left over p orbital



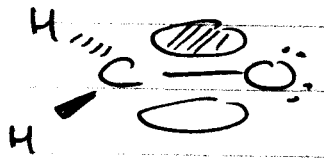

σ BOND FRAMEWORK

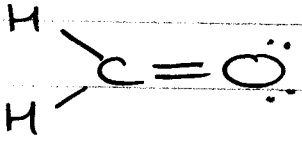

π BOND


≡

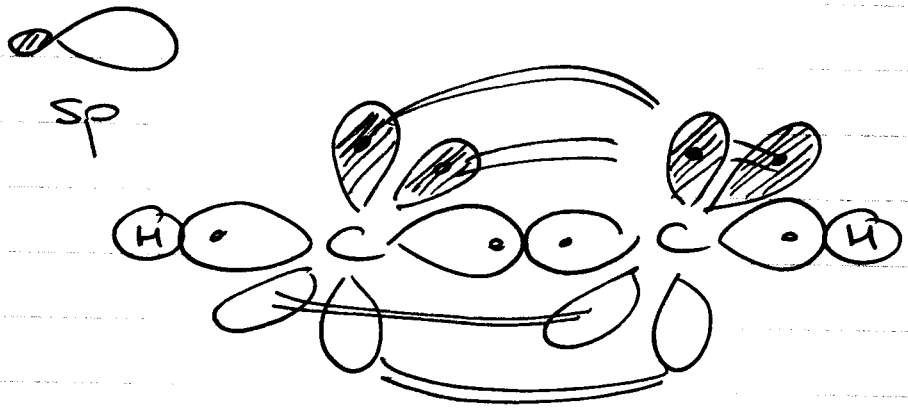


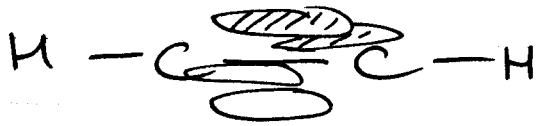

FLAT



sp 1 x 2s and 1 x 2p



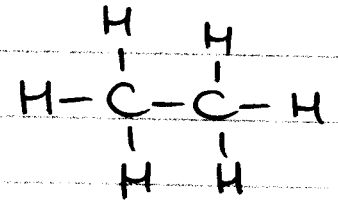
$H-C\equiv C-H$

↑

1 x sp–sp σ

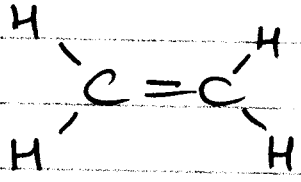
2 x $2p_{\pi}$

CONSIDER



C–C
1.53 Å
88 kcal mol$^{-1}$

C–H
$sp^3$–1s σ
1.11 Å
98 kcal/mol



not ×2

C=C
1.34 Å
146 kcal mol$^{-1}$

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$^{-1}$

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

ADD # of BONDED ATOMS TO # LONE PAIRS

4 → $sp^3$
3 → 3 × $sp^2$ + 1 × p
2 → 2 × sp + 2 × p