CHM 103

ORGANIC CHEMSTRY I

Department of Chemical Sciences
Faculty of Science and Technology
Bingham University, Karu

Course Lecturer: Joseph C. Oguegbulu
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COURSE CONTENT

PART A – Mr. Joseph

- Introduction. History, classifications — 0.5 week
- Carbon: Bonding in organic compounds, structure — 0.5 week
- Functional groups — 0.5 week
- IUPAC nomenclature — 1 week
- Isomerism – Structural & Stereo-isomerism — 2 weeks
- Hybridisation – Resonance effects & others — 2 weeks

PART B – Assoc. Prof. Okoli

- Alkanes, Alkenes, Alkynes
- Alkyl halides, Alkanols
- Carbonyl compounds: Alkanals and Alkanones.

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LECTURE IX

- **HYBRIDISATION OF CARBON**
  - **sp^3**
  - **sp^2**
  - **sp**
  - **ELECTRONIC CONFIGURATION**
  - **ORBITALS**
  - **SIGMA BONDS VS PI-BONDS**

OBJECTIVES: At the end, you should be able to…

- Write the electronic configuration of simple atoms including Carbon
- Explain hybridisation using carbon
- Differentiate between an atomic orbital and a molecular orbital
- Identify & explain d/f hybridisation types in simple moleucles
- Differentiate between sigma bonds and pi bonds

WHAT IS AN ORBITAL

- **An orbital** is **a mathematical approximation** of the region in space where there is **the highest probability** of finding an electron at any given point in time

- **An atomic orbital** is an orbital of electrons associated with **an atom** of a free element

- **Molecular orbital** belongs to molecules formed by the atoms

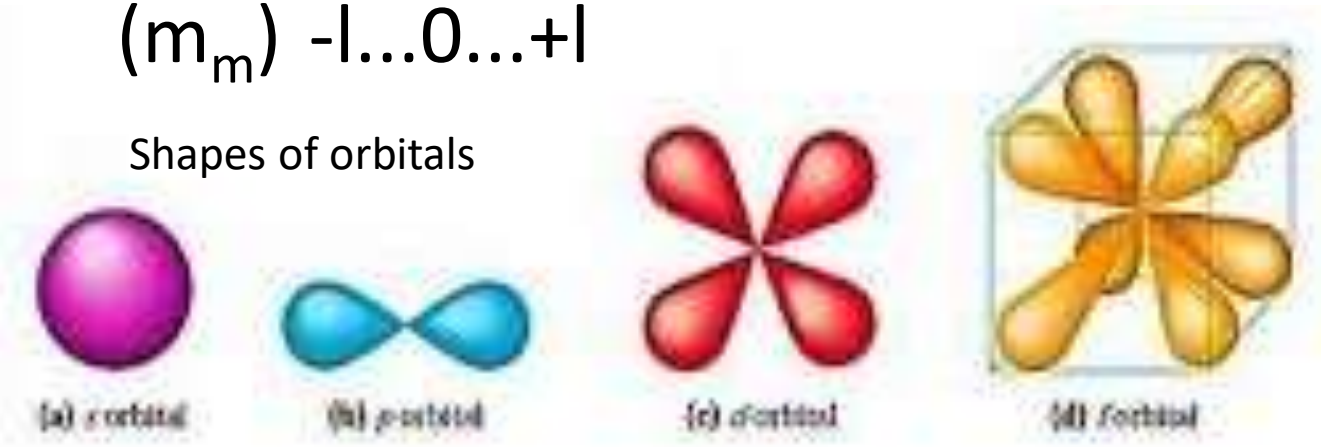
ELECTRONIC CONFIGURATION

Recall

- Principal quantum number (n) 1,2,3,4,5...etc
- Azimuthal quantum number (l) **s,p,d,f**
- Spin quantum number (m_s) $+1_{/2}$ or $-1_{/2}$
- Magnetic quantum number (m_m) -l...0...+l

More in CHM 102

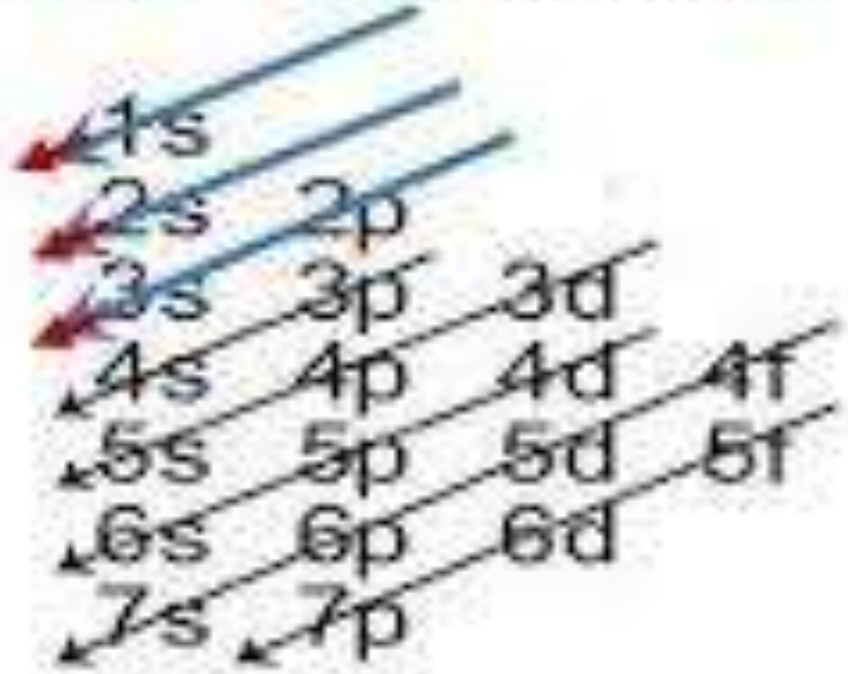
Shapes of orbitals



Electron Configuration Chart

s holds up to 2 p holds up to 6 d holds up to 10

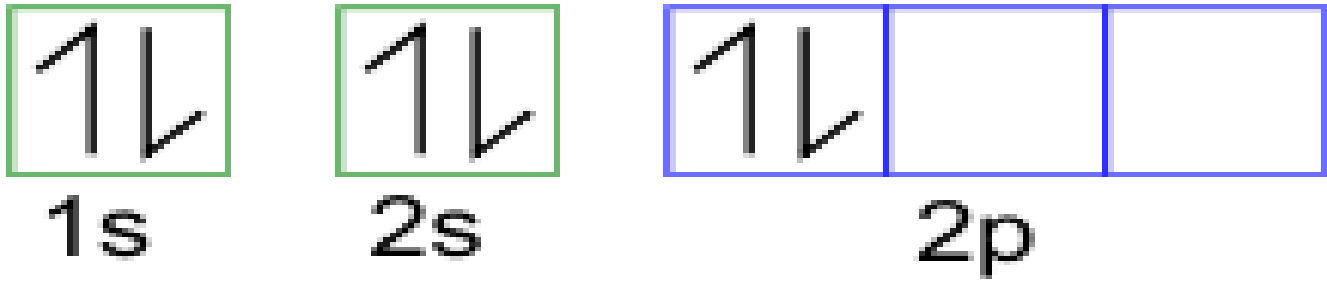
6
C
Carbon
12.01



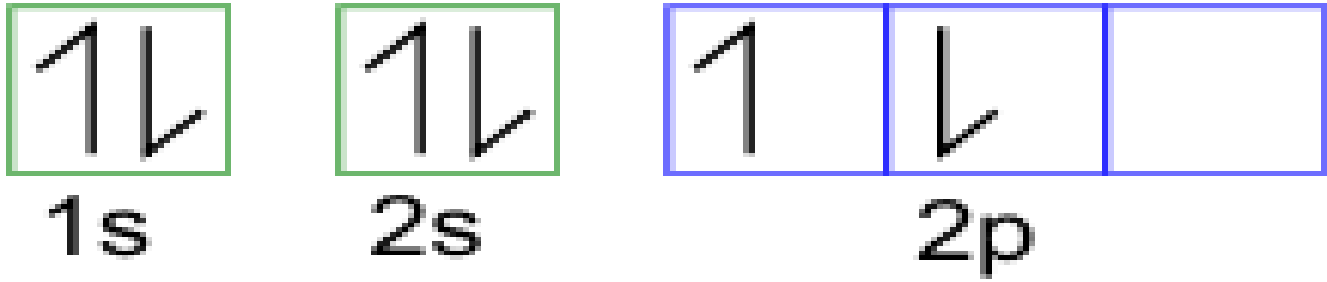
$1s^2\ 2s^2\ 2p^2$

ELECTRONIC CONFIGURATION: Rules

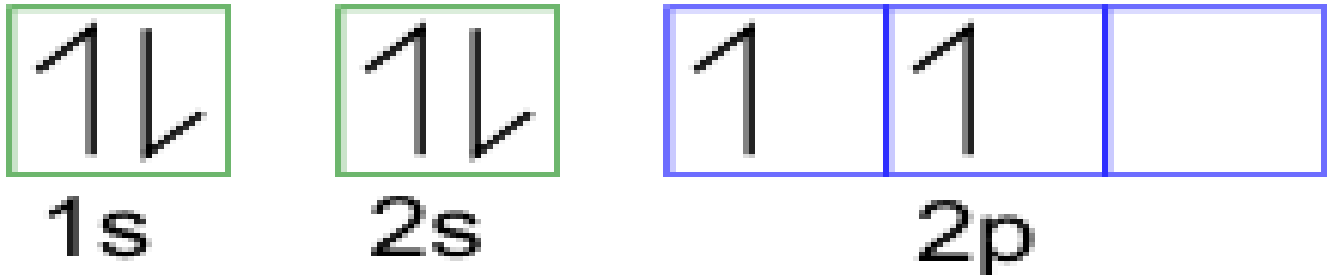
- Aufbau principle



- Hund's Rule



- Pauli's exclusion principle

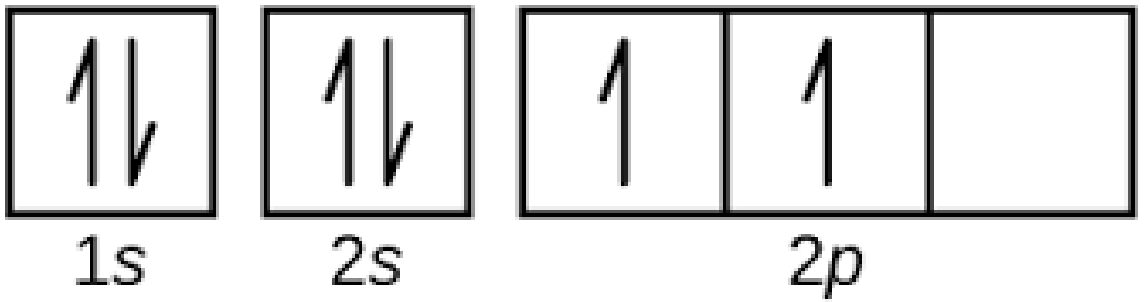


ELECTRONIC CONFIGURATION OF CARBON

$^{12}_{6}C$

- i.e Atomic Number = 6; Mass Number = 12

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



ELECTRONIC CONFIGURATION: Examples

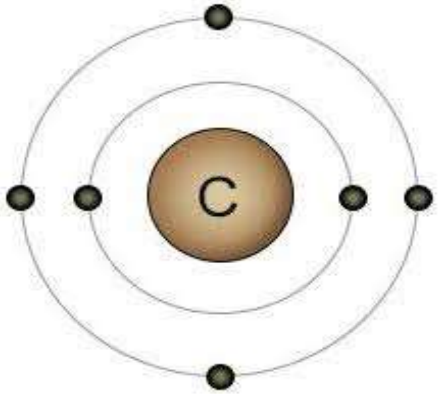
Q

- Write the electronic configurations of…

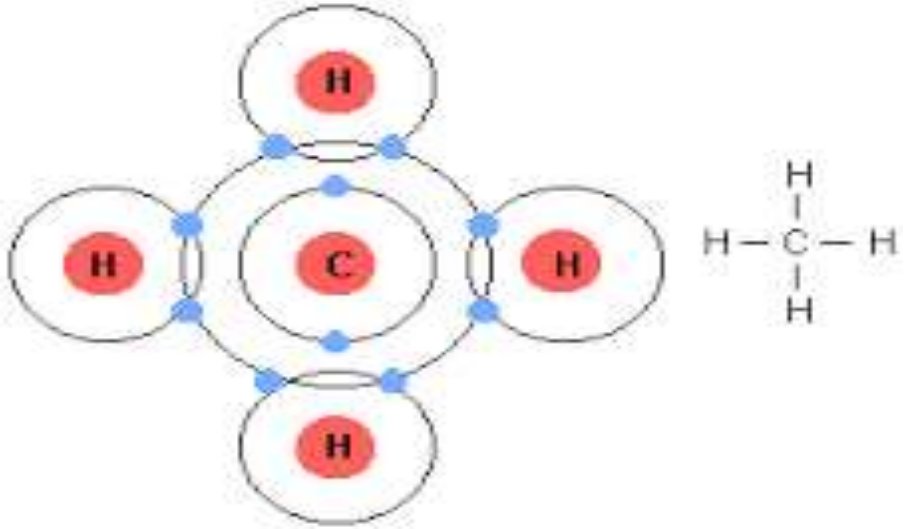
- N
- O
- S^{2-}

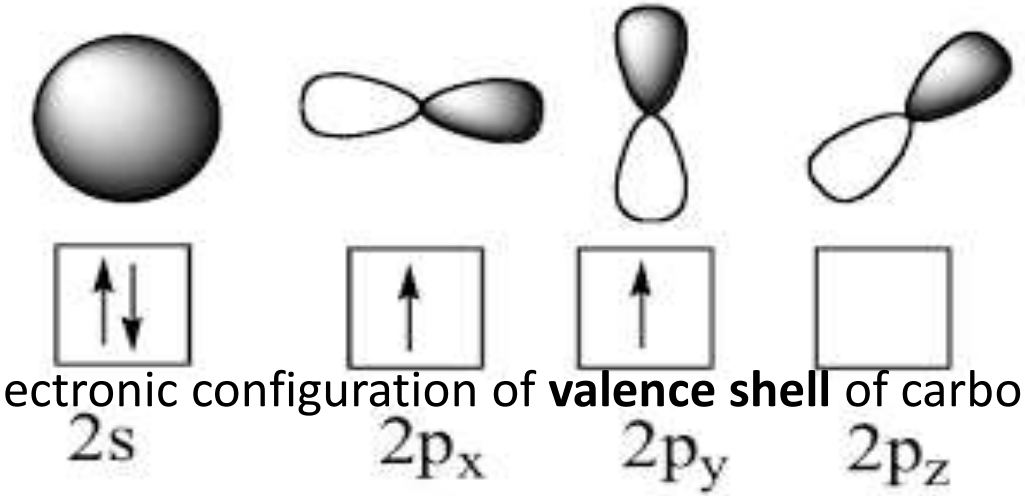
QUESTIONS???

VALENCE SHELLS



- **Valence shell** ➔ Outermost shell in an atom
- **Valence electrons** ➔ Outermost electrons in an atom
  - **$1s^2$ $2s^2$ $2p^2$**
- They are the ones **involved in chemical bonding**



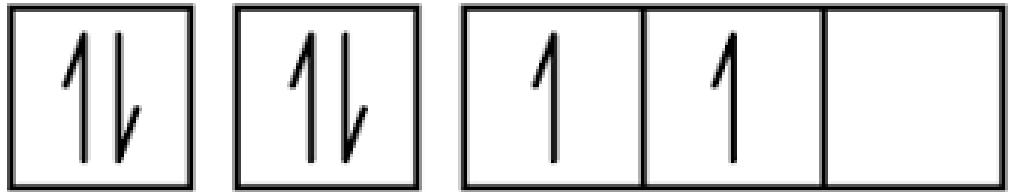


Electronic configuration of **valence shell** of carbon

HYBRIDISATION OF CARBON

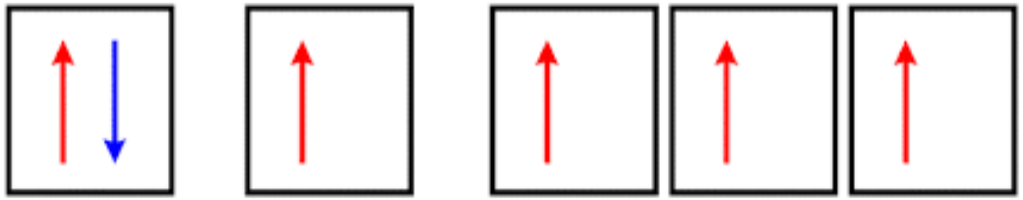
- Hybridisation is the **mixing** of *half-filled valence atomic orbitals* of similar *energy* to form identical ***hybrid orbitals***
- But for valence shell orbitals to become all half-filled (i.e. one electron each), **excitation** must happen

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



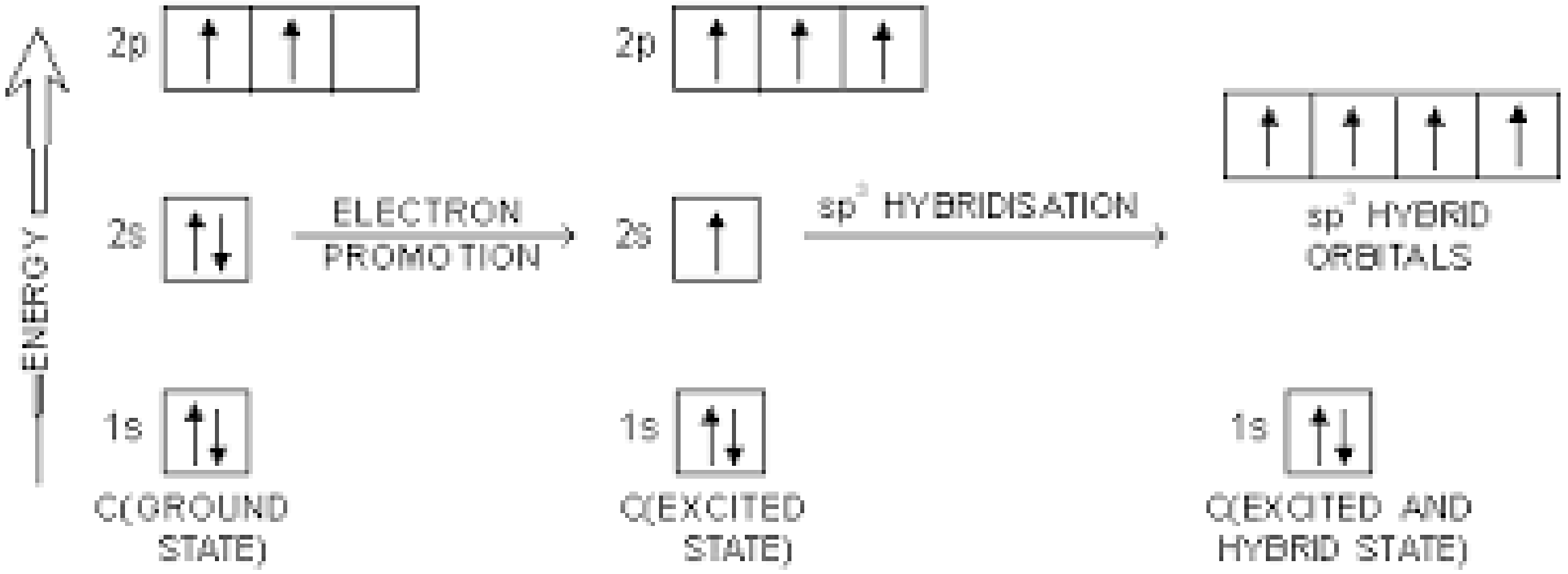
Ground State

Becomes
$1s^2$ $2s^1$ $2p^3$



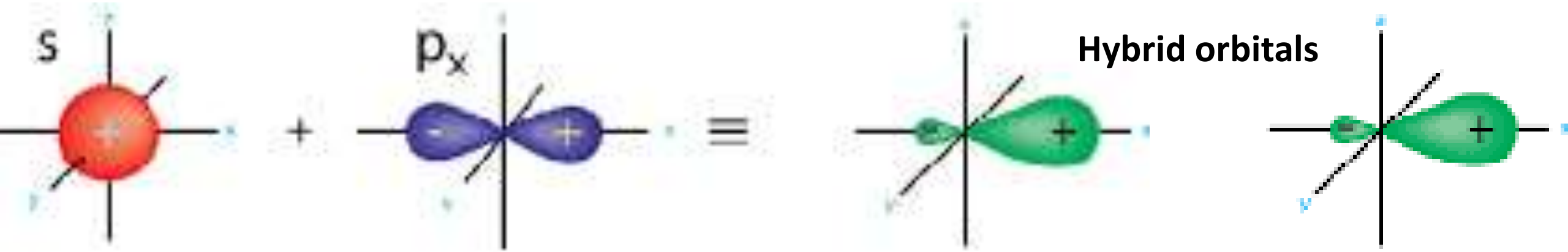
Excited State

HYBRIDISATION OF CARBON



HYBRIDISATION OF CARBON

- The hybrid orbitals formed are identical to one another
  - **i.e. Same shapes, same energies**
  - **Totally d/f from the un-hybridised orbitals that formed them**
- Total number of hybrid orbitals formed = Total number of unhybridised orbitals **mixed**

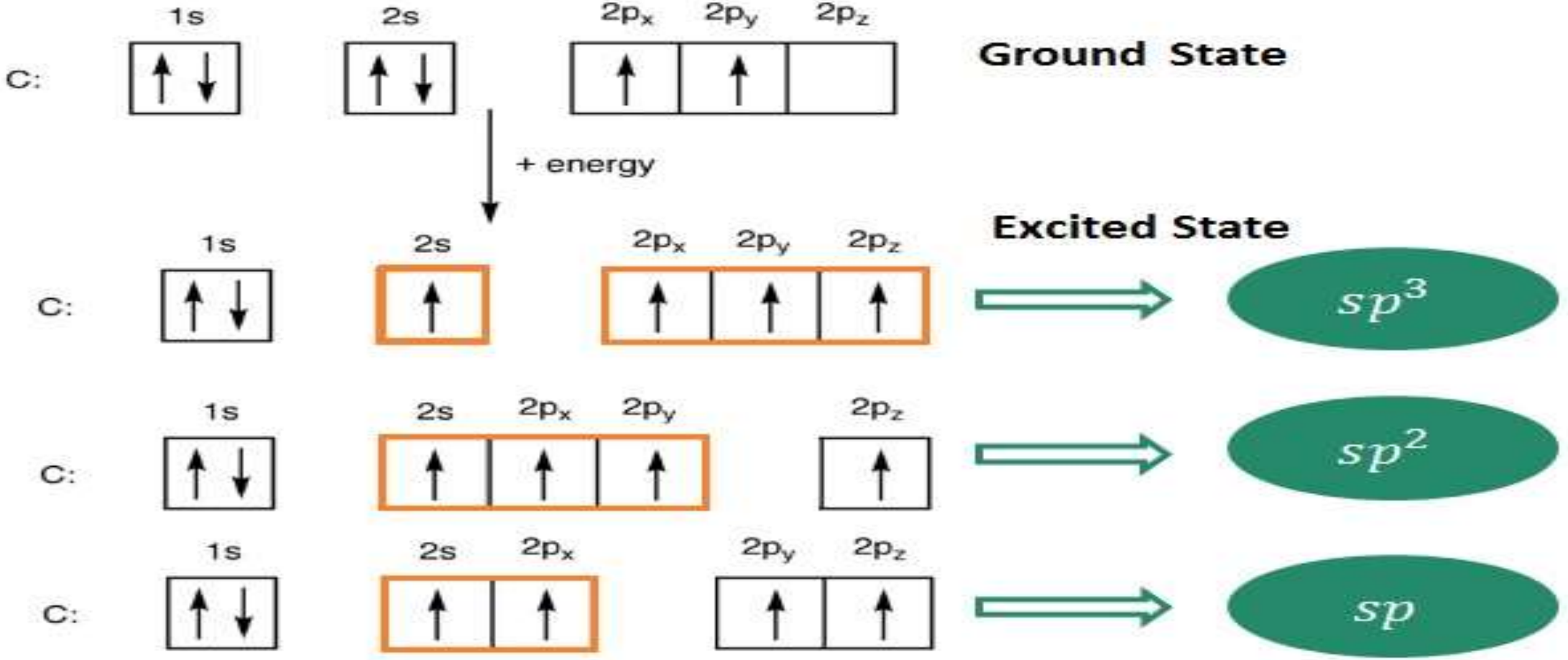


HYBRIDISATION OF CARBON: Types

- Hybridisation is v*ery Important in Organic Chemistry b/c* **Carbon must hybridise b4 bonding**

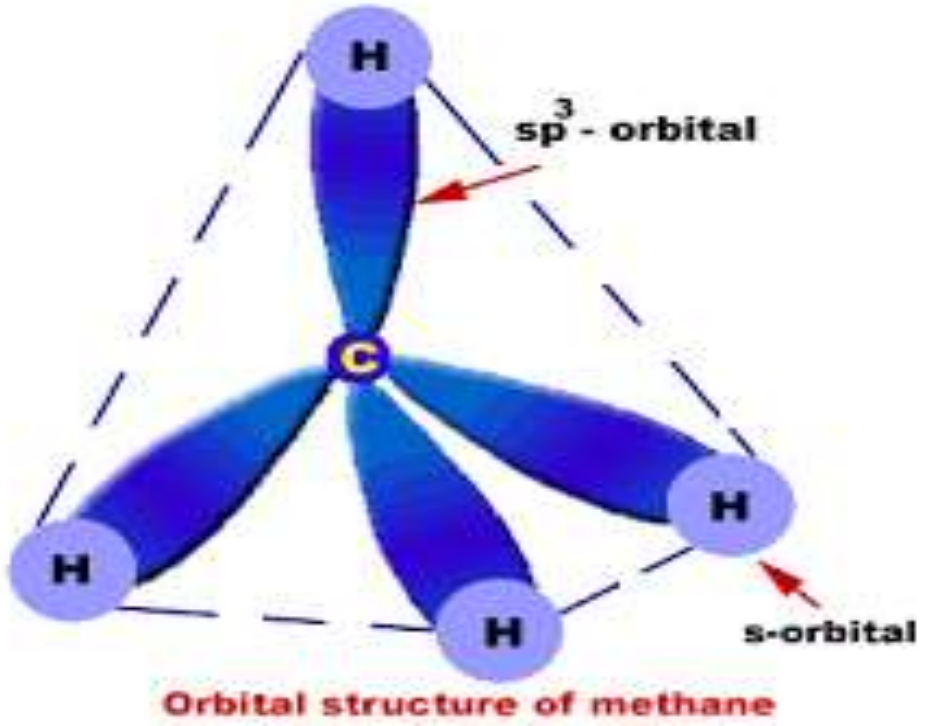
- **There are three (3) types! (sp^3, sp^2 and sp hybridisations)**
  - **Depending on how may p-orbitals mixed with the 's'**
- ***sp^3*** = One **s** + Three **p orbitals** mixed
- ***sp^2*** = One **s** + Two **p** mixed *(one unhybridised p-orbitals left)*
- ***sp*** = One **s** + One **p** mixed *(two unhybridised p-orbitals left)*

HYBRIDISATION OF C: 3 Types, sp^3, sp^2 & sp

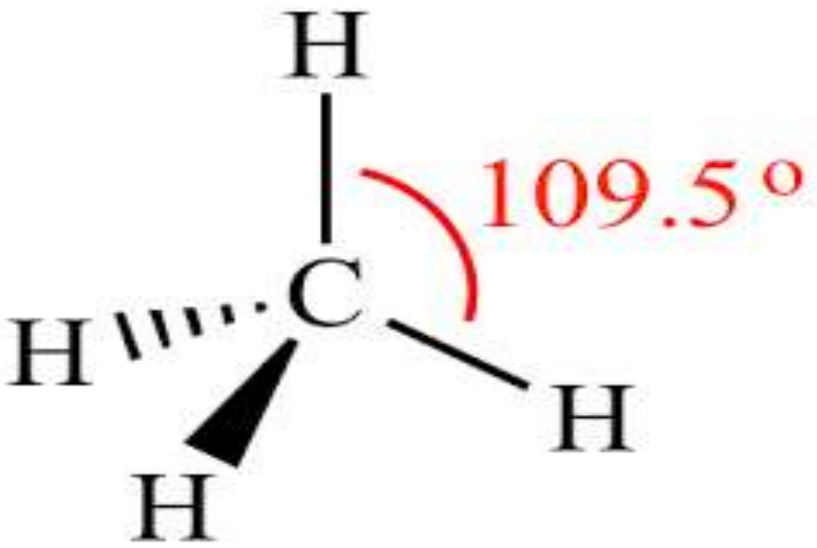


QUESTIONS???

TYPES: sp^3 HYBRIDISATION IN METHANE (CH_4)



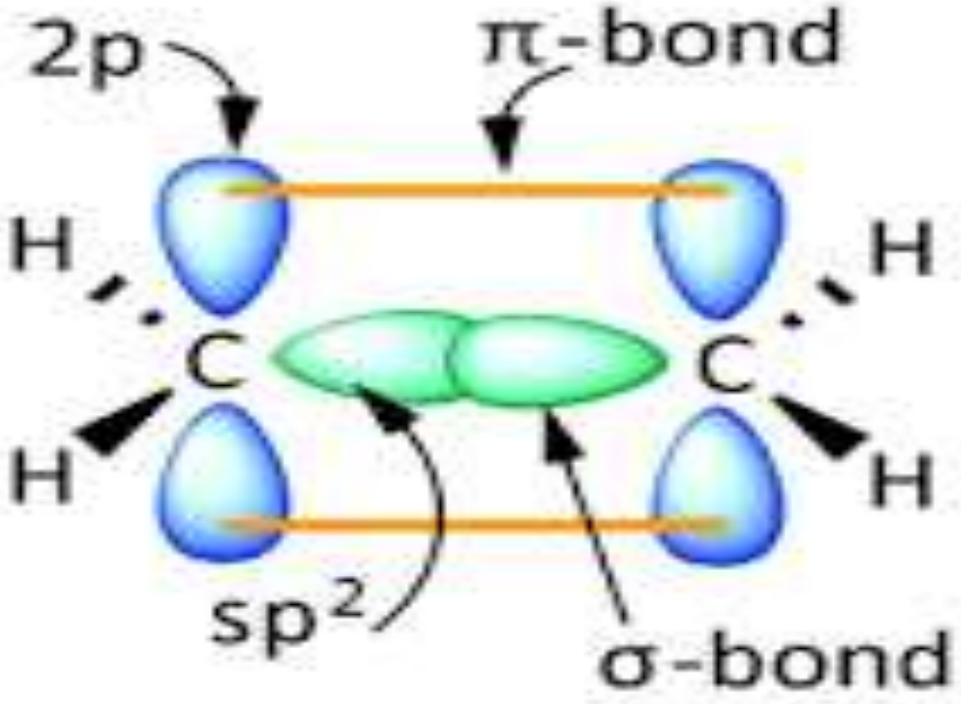
Orbital structure of methane



Four (4) C-H SIGMA bonds are formed

- **A SIGMA BOND (σ)** is formed by direct **(Head to Head) overlap of HYBRIDISED ORBITALS**
- **All single bonds are sigma bonds!!!**

TYPES: sp^2 HYBRIDISATION IN ETHENE (C_2H_4)

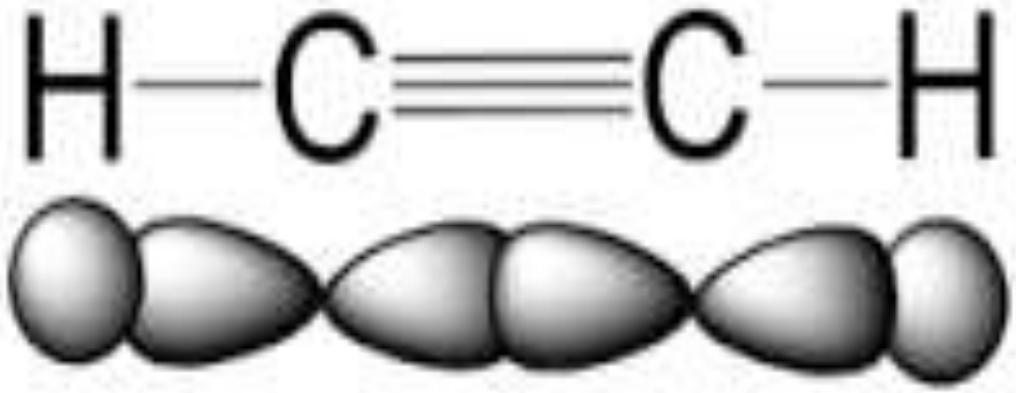


1. Four (4) C-H SIGMA bonds are formed

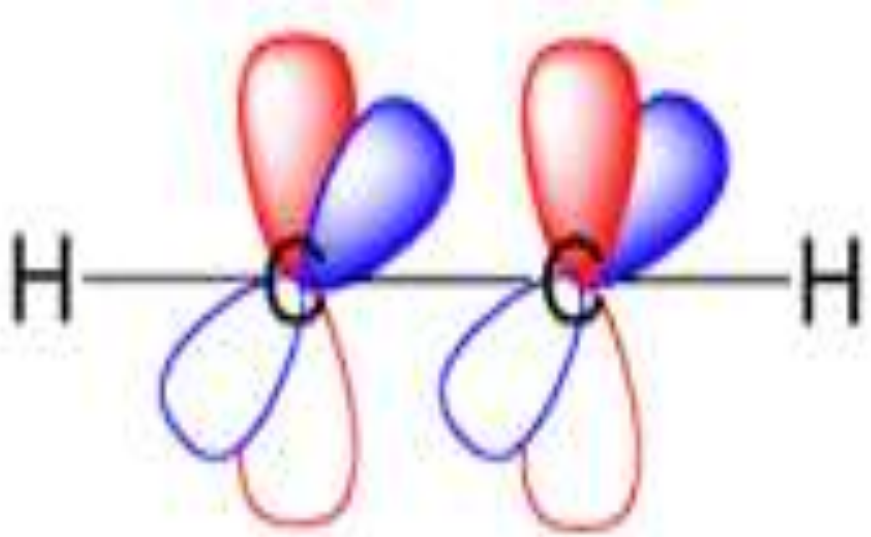
2. One C-C sigma bond & One C-C Pi-bond

- **A Pi-BOND** is formed by indirect **(side to side) interaction of two UN-hybridised orbitals**
- Every double bond is made of **one sigma (σ) bond** & **one pi-bond (π)**

TYPES: sp HYBRIDISATION IN ETHYNE (C_2H_2)



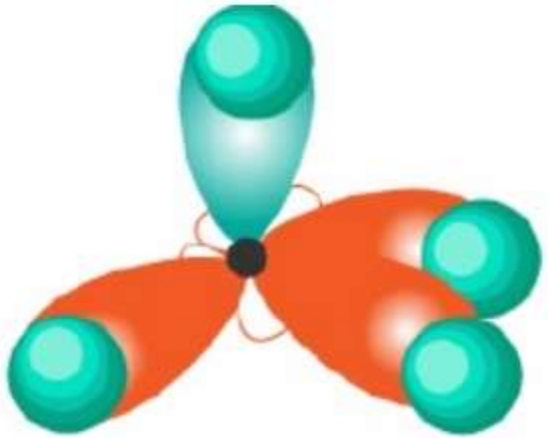
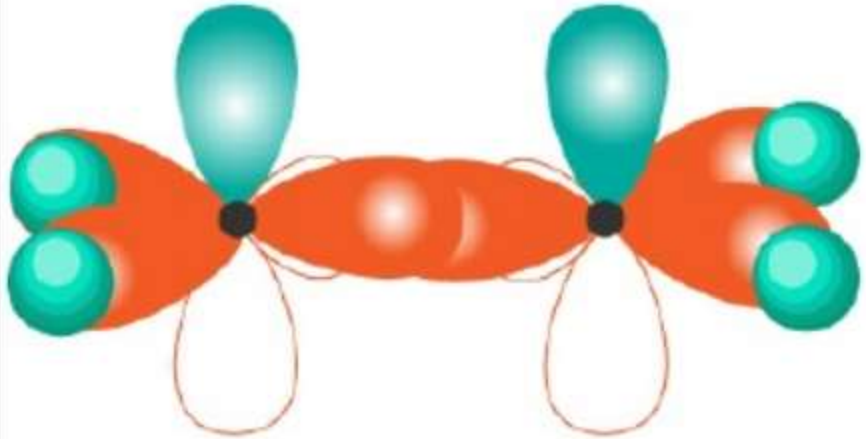
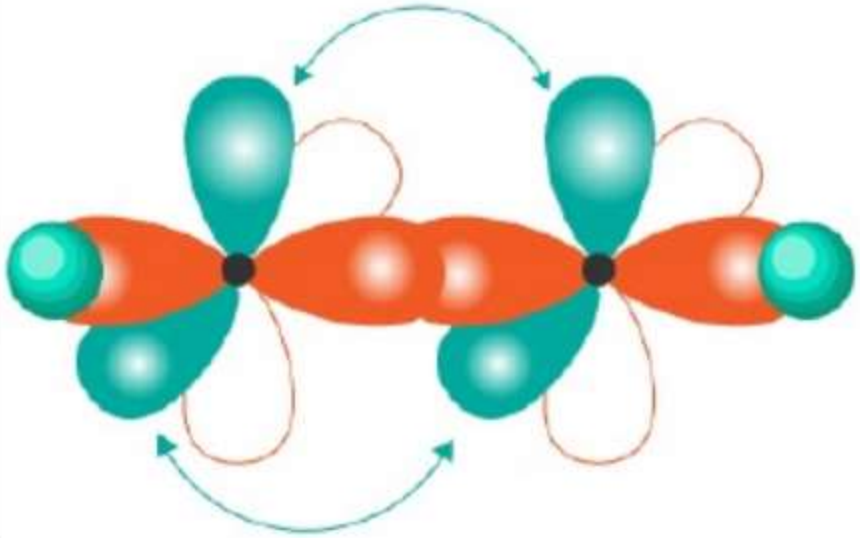
σ bonding framework



Two (2) C-H SIGMA bonds are formed
One (1) C-C SIGMA bond &
Two C-C PI-bonds

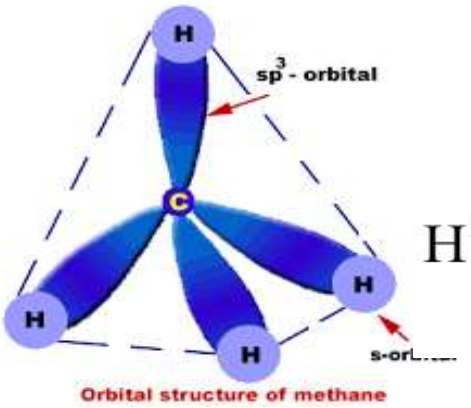
- Every triple bond is made of **one sigma (σ) bond** and **two pi-bonds (π)**

HYBRIDISATION OF CARBON: Examples

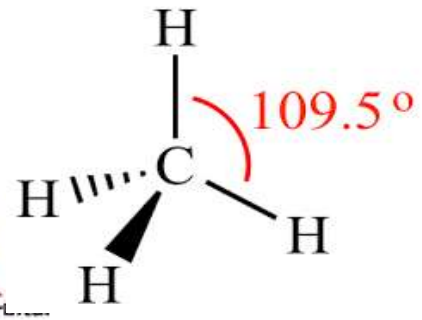
$CH_4(sp^3)$	$CH_2 = CH_2(sp^2)$	$HC \equiv CH(sp)$
		
4 C-H sigma bonds	4 C-H sigma bonds One C-C sigma bond, one C-C **pi-bond**	2 C-H sigma bonds One C-C sigma bond, **Two** C-C **pi-bonds**

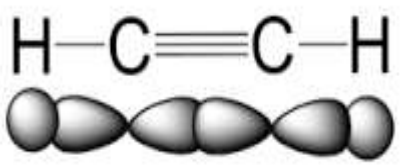
HYBRIDISATION OF CARBON: Properties

Hybridization	Structure	Bond Angle	Example
sp^3	Tetrahedral	109.5°	CH_4(methane)
sp^2	Trigonal Planar	120°	$CH_2 = CH_2$(ethene)
sp	Linear	180°	$HC \equiv CH$(acetylene)

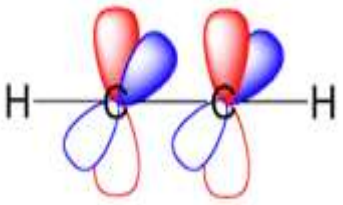


Orbital structure of methane

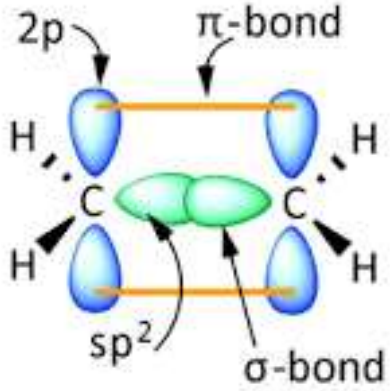


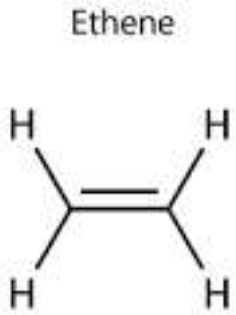


σ bonding framework



π overlap





SIGMA (σ) BONDS vs PI (π) BONDS

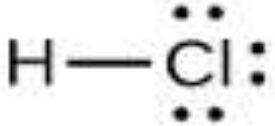
1. Sigma bonds are **stronger** than pi bonds. Pi-bonds can be easily broken
   - Hence molecules w/ **Pi-bonds are more reactive** (C_2H_2>C_2H_4>C_2H_6)

2. Sigma bond can exist alone (i.e. as single bonds)
   - Pi-bonds only exist with a sigma bond to make double/triple bonds

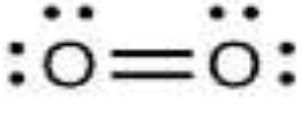
3. Sigma bonds can be formed by both hybridized &unhybridised orbitals
   - Pi-bonds are only formed by unhybridised orbitals

4. Electron density in sigma bonds is within the plane of the bond
   - Electron density in pi bonds is above &below the plain of the bond

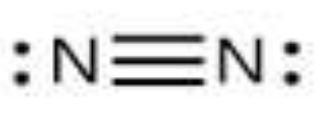
Tutorial IV



One σ bond
No π bonds



One σ bond
One π bond

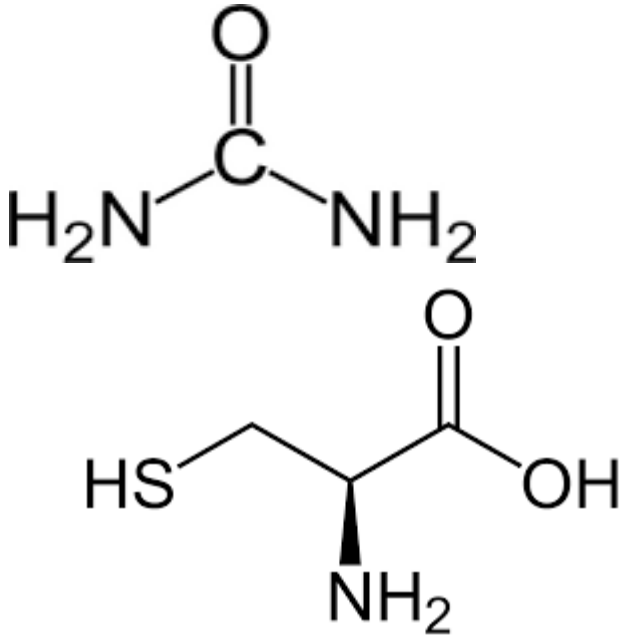


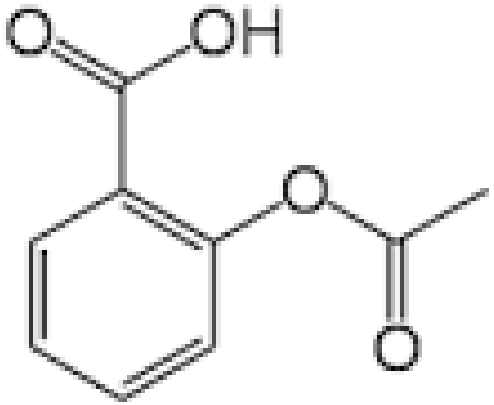
One σ bond
Two π bonds

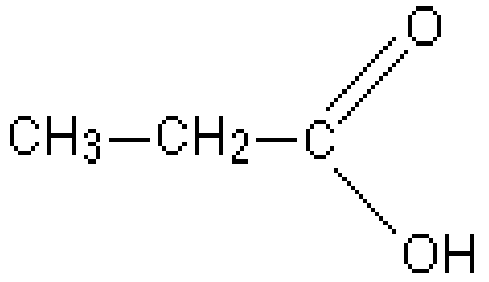
Q

- **Given this;**

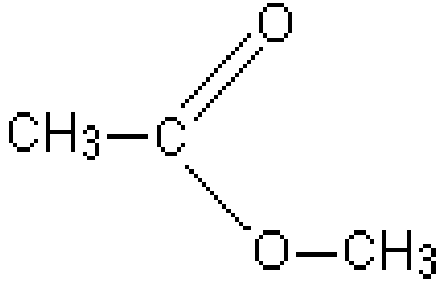
How many σ & π bonds are in the compounds below???







propanoic acid



methyl ethanoate

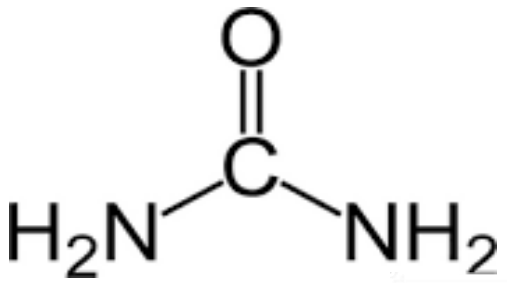
Tutorial IV

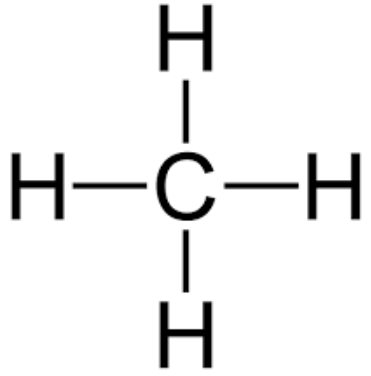
Hybridization	Structure	Bond Angle	Example
sp^3	Tetrahedral	109.5°	CH_4(methane)
sp^2	Trigonal Planar	120°	$CH_2 = CH_2$(ethene)
sp	Linear	180°	$HC \equiv CH$(acetylene)

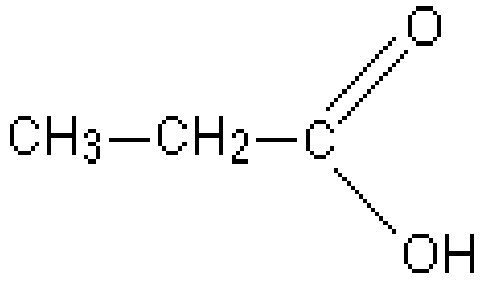
Q

- **Given this;**

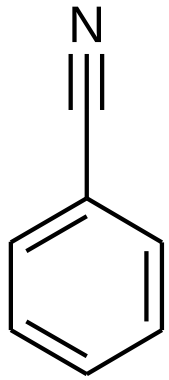
What are the hvbridisation states of the Carbon atoms in these molecule?



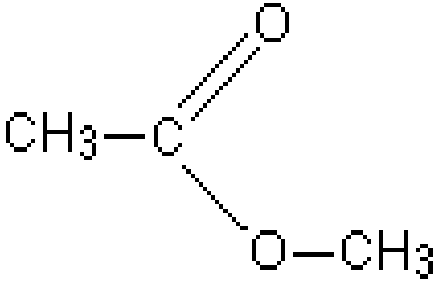




propanoic acid



benzonitrile



methyl ethanoate


Question