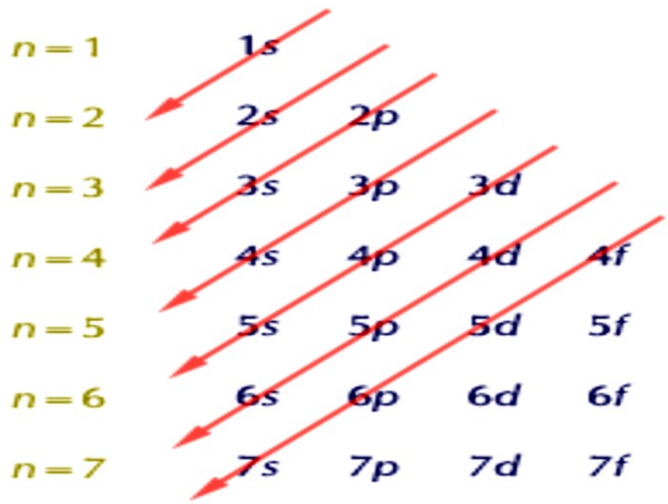
1. INTRODUCTION TO ORGANIC CHEMISTRY

- Organic chemistry is a subject of chemistry concerned with compounds that contain element Carbon. e.g methane CH_4, Ethyne CH ≡ CH, ethanol CH_3CH_2OH etc.
- The name organic chemistry reflects the old belief that organic compounds could be produced only by living organisms. e.g., glucose ($C_6H_{12}O_6$), Starch, sucrose, urea etc.

Electronic Configuration of Carbon



Total number of electrons = Atomic number.

Atomic number of Carbon = 6 = $6e^-$

Electron configuration = $1S^2 2S^2 2P^2$

– Low energy to high energy orbitals

1s (2)

2s (2)

2p (6)

3s (2)

3p (6)

4s (2)

3d (10)

4p (6)

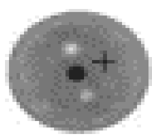
5s (2)

Catenation

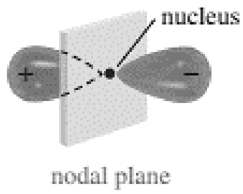
- Catenation is the linkage of atoms of the same element into long chains.
- Catenation occurs most readily in carbon, which forms covalent bonds with other carbon atoms not only with single bonds (C – C), but also with multiple bonds (C = C or C $\equiv$ C).
- Sulfur and silicon are the elements next most inclined to catenation, but they are far inferior to carbon.

Hybridization

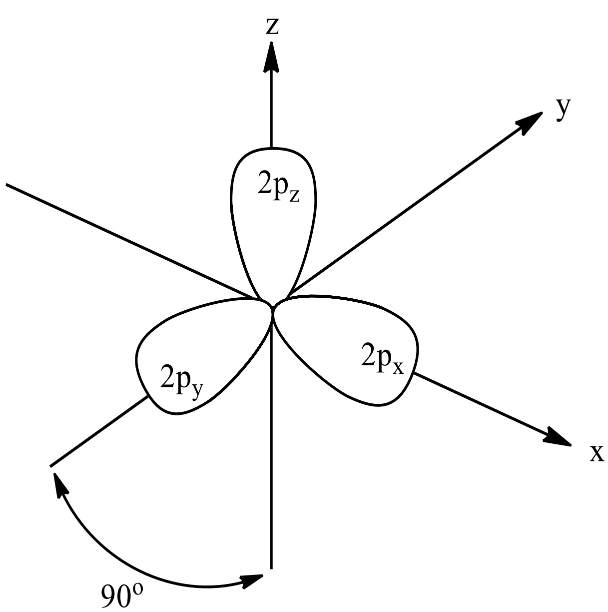
- An orbital is a region in space of an atom where there is a high probability to find an electron.
- The shape of an s orbital is that of a sphere with the nucleus at the center.



- The shape of each p orbital is approximately that of a dumbell or lobe-shaped object, with the nucleus directly between the two lobes.



- The three 2p orbitals are mutually perpendicular and are designated $2p_x, 2p_y$ and $2p_z$.



p-orbitals

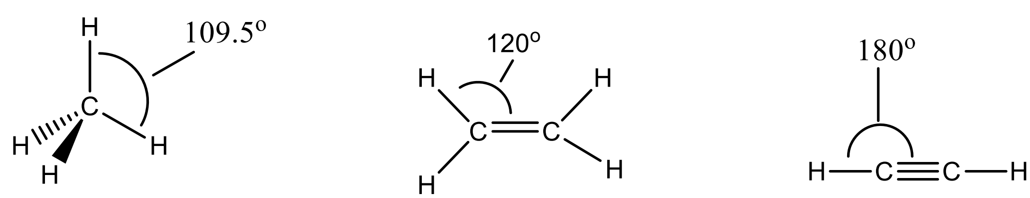
- **Hybridization -** It is the term applied to the mixing of atomic orbitals in an atom to generate a set of hybrid orbitals.

Hybrid Orbitals

- These are atomic orbitals obtained when two or more non-equivalent orbitals of the same atom combine in preparation for covalent bond formation.

Hybridization of Atomic Orbitals

- The formation of covalent bonds with second - period elements present a problem while formation of covalent bonds between two hydrogen atoms is straight forward.
- In forming covalent bonds, all period two elements use 2s and 2p atomic orbitals.
- The three 2p atomic orbitals are at angles of 90° to one another and if atoms of second - period elements used these orbitals to form covalent bonds, the bond angles around each would be approximately 90°.
- However, bond angles of 90° are rarely observed in organic molecules. What is observed instead, are bond angles of approximately 109. 5° in molecules with single bonds only, 120° in molecules with double bonds and 180° in molecules with triple bonds.



- To account for these observed bond angles, Pauling proposed that atomic orbitals combine to form new orbitals, called <u>hybrid</u> <u>orbitals</u>.

Hybridization of Carbon (sp, sp^2 and sp^3)

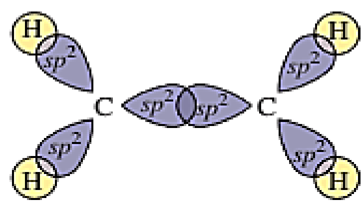
To be discussed in lecture two.

General rule of predicting hybridization of orbitals and bond angles.

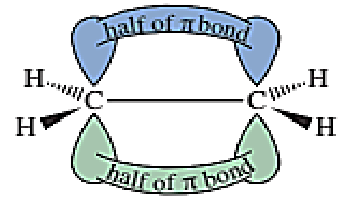
- Rule 1: Both sigma bonding electrons and lone pairs can occupy hybrid orbitals. The number of hybrid orbitals on an atom is determined by adding the number of sigma bonds and the number of lone pairs of electrons on that atom.
- Rule 2: Use the hybridization and geometry that give the widest possible separation of the calculated number of bonds and lone pairs.

HYBRID ORBITALS	HYBRIDIZATION	GEOMETRY	APPROXIMATE BOND ANGLES
2 3 4	S+P = SP S+P+P = SP^2 S+P+P+P=SP^3	LINEAR TRIGONAL PLANAR TETRAHEDRAL	180^O 120^O 109.5^O

- Rule 3: If two or three pairs of electrons form a multiple bond between two atoms, the first bond is a sigma bond formed by a hybrid orbital. The second bond is a Pi bond and the third bond of a triple bond is another Pi bond.

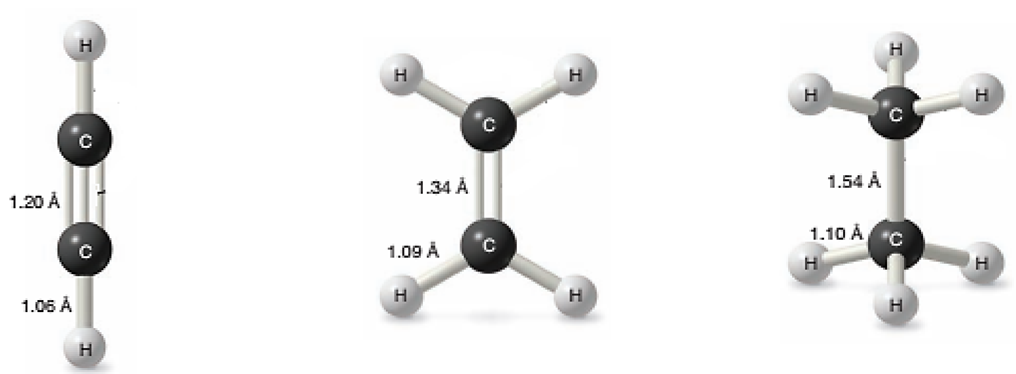


σ bond framework



π bond

Bond lengths of ethyne, ethene and ethane



- The shortest C–H bonds are associated with those carbon orbitals with the greatest s character.

sp → 50% s

sp^2 → 33% s

sp^3 → 25% s