Organic chemistry background I

Organic compounds

- **Definition**
  - Any member of compounds containing carbon
  - Exception: carbonates (HCO_3^- and CO_3^{2-}), simple carbon oxides (CO and CO_2), carbides*, cyanides (CN^-)

    ** carbides: compound composed of carbon and a less electronegative element*

    (ex: CaC_2, CSi, WC)

- **Makeup of organic molecules**
  - Millions of organic compounds exist due to the ability of carbon to form up to four stable carbon-carbon bonds
  - Unlimited kinds of *carbon skeletons* can be made
  - Elemental composition: C, H, O, N, S, P, halogens
  - Heteroatoms: elements in an organic molecule other than C and H

Description of a compound

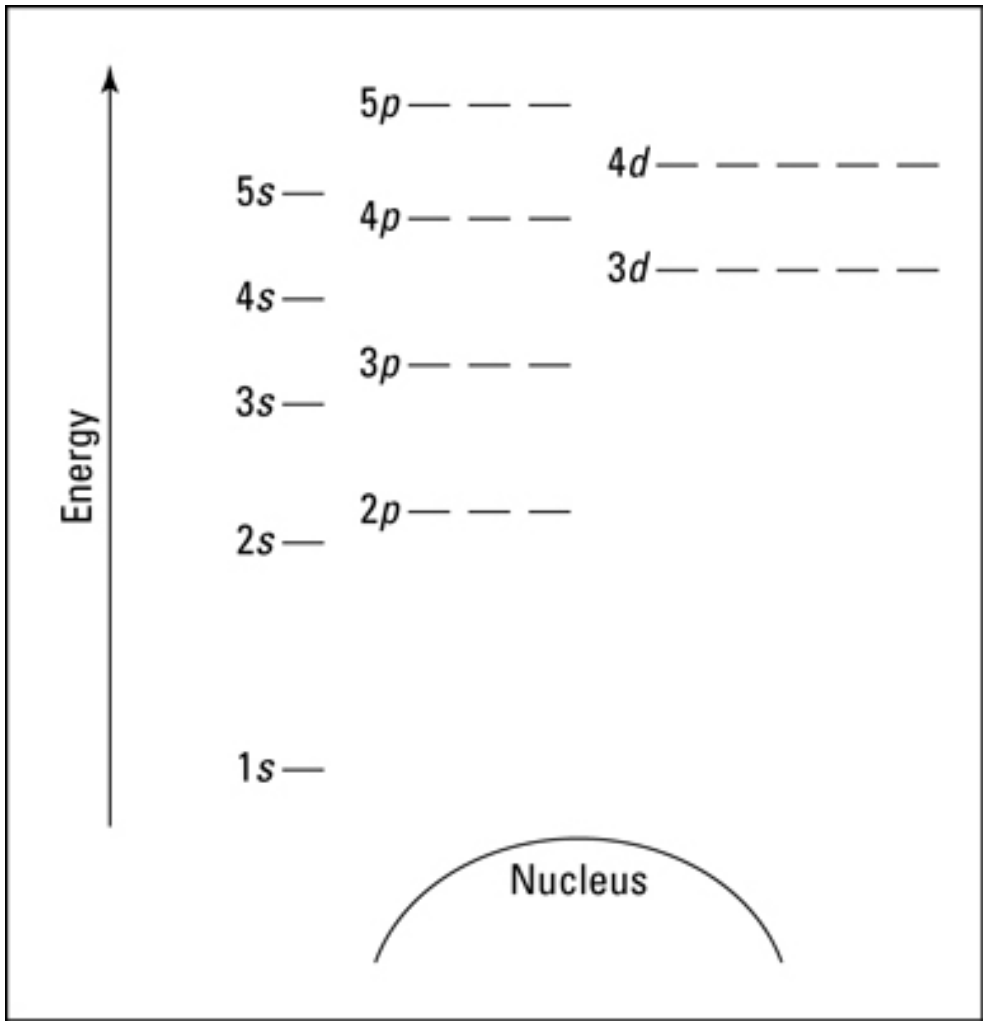
- **Elemental composition**: which elements the compound contains
- **Molecular formula**: how many atoms of each of the elements are present in one molecule
- **Molecular mass**: sum of the masses of all atoms present in the molecule
- **Molecular structure (constitution)**: the exact connection of the atoms constituting the molecule
- **Molecular geometry**: the 3-D arrangement of the atoms

Electron shells of elements

- Atoms containing **“filled shells”** are stable
  - Noble gases: He, Ne, Ar, Kr, Xe, Rn

- Atoms in organic molecules have **tendencies to attain filled-shell conditions** by gaining, losing, or most importantly, **sharing electrons**

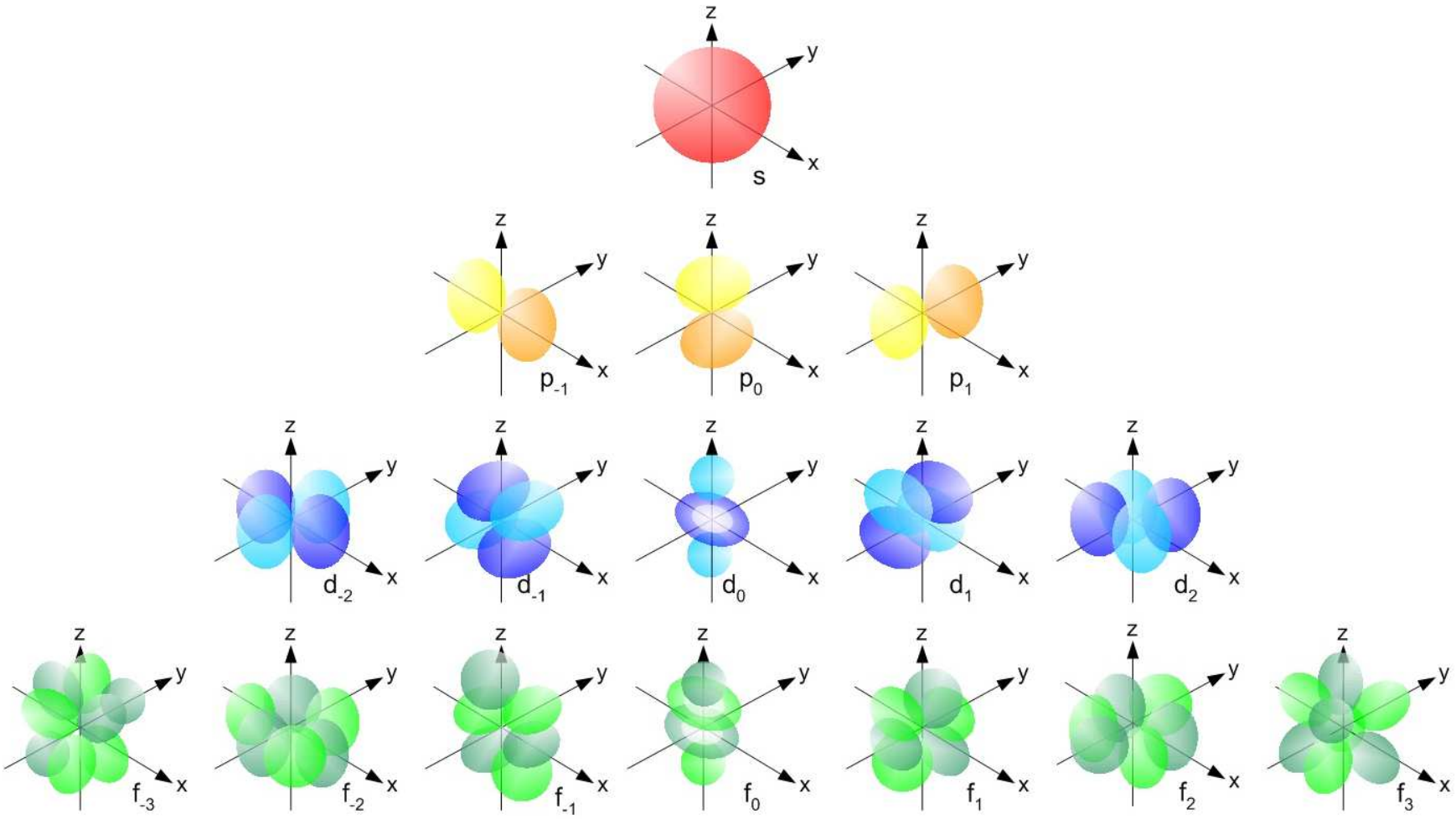
Orbital energy levels



http://www.dummies.com

- 1st shell (K-shell): holds 2 electrons ($1s^2$)
- 2nd shell (L-shell): holds 8 electrons ($1s^2\ 2s^2\ 2p^6$)
- 3rd shell (M-shell): holds 18 electrons ($1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^{10}$), but a stable configuration is reached when the shell is filled with 8 electrons ($1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6$)

Orbital diagrams



http://www.khanacademy.org

Electron shells of elements

source: EOC text

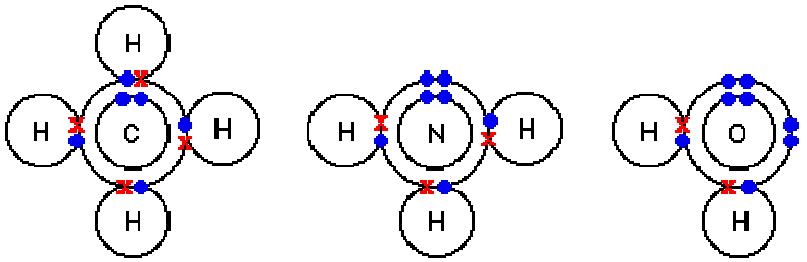
Name	Element[a]		Mass[b] (u)	Number of Electrons in Shell					Net Charge of Kernel[c]	Number of Covalent Bonds Commonly Occurring in Organic Molecules
	Symbol	Number		K	L	M	N	O		
Hydrogen	H	1	1.008	1					1+	1
Helium	He	2		2					0	
Carbon	C	6	12.011	2	4				4+	4
Nitrogen	N	7	14.007	2	5				5+	3,(4)[d]
Oxygen	O	8	15.999	2	6				6+	2,(1)[e]
Fluorine	F	9	18.998	2	7				7+	1
Neon	Ne	10		2	8				0	
Phosphorus	P	15	30.974	2	8	5			5+	3,5
Sulfur	S	16	32.06	2	8	6			6+	2,4,6,(1)[e]
Chlorine	Cl	17	35.453	2	8	7			8+	1
Argon	Ar	18		2	8	8			0	
Bromine	Br	35	79.904	2	8	18	7		7+	1
Krypton	Kr	36		2	8	18	8		0	
Iodine	I	53	126.905	2	8	18	18	7	7+	1
Xenon	Xe	54		2	8	18	18	8	0	

[a] The underlined elements are the noble gases. [b] Based on the assigned atomic mass constant of u=atomic mass of $^{12}C/12$; abundance-averaged values of the naturally occurring isotopes. [c] Kernel: the portion of an atom excluding the outer shell electrons. [d] Positively charged atom. [e] Negatively charged atom.

Covalent bond

- Octet rule: atoms tend to combine in such a way that each atom has 8 electrons in its outer (valence) shell

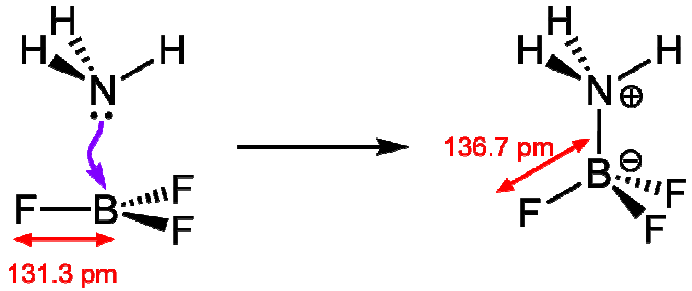
- Covalent bond
  - Atoms complete their outer-shell octet by sharing a pair of electrons, in most cases one electron contributed by each of the two bonded atoms
  - Each atom feels it has both of the shared electrons
  - The electron pairs are localized between the two positive atomic nuclei; the electrostatic attraction of these nuclei to these electrons holds the atoms together

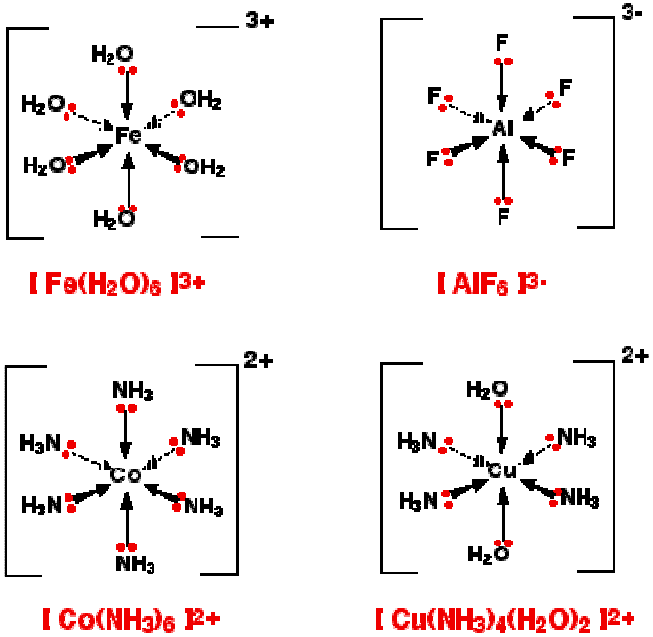


http://www.chemguide.co.uk

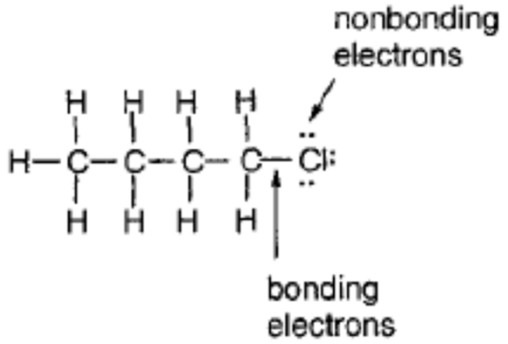
Covalent bond

- Coordinate bond
  - A kind of a covalent bond in which the two electrons derive from the same atom
  - One atom donates a lone pair of electrons (Lewis base) and the other atom accepts the electron pair (Lewis acid)





Drawing molecular structures

(1) 

(2) $H_3C-CH_2-CH_2-CH_2-Cl$

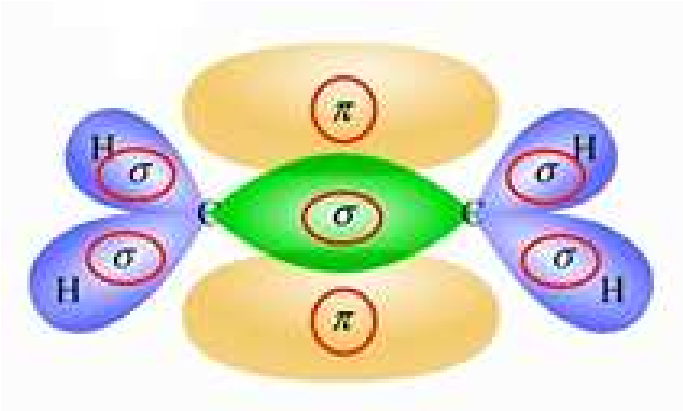
(3) $H_3CCH_2CH_2CH_2Cl$

(4) 

Double and triple bonds

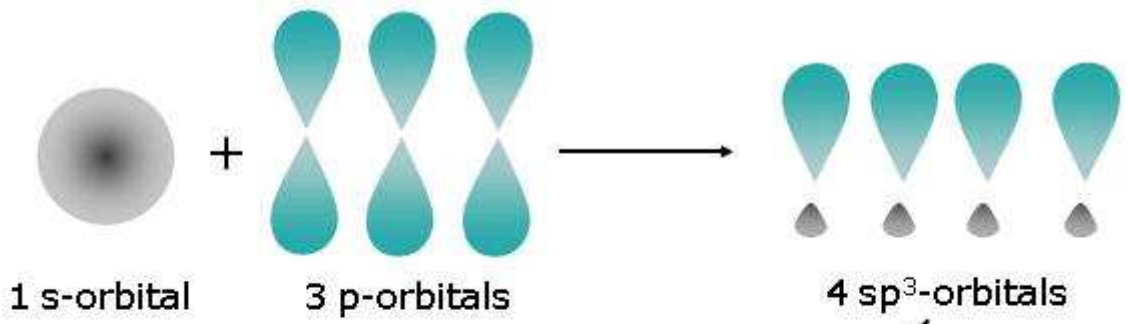
- Atoms with more than one missing electrons in their outer shells may form double or triple bonds

- Single covalent bond is a sigma (σ) bond; double and triple bonds contain one σ bond and π bond(s)
  - σ bond: a covalent bond in which orbital overlap of the bond is concentrated along the axis joining the two nuclei
  - π bond: a covalent bond formed by overlap of parallel p orbitals (generally weaker than the σ bonds)



http://chemistryistorture.blogspot.kr/2013/03/red-high-density-valence-bond-theory-so.html

Orbital hybridization



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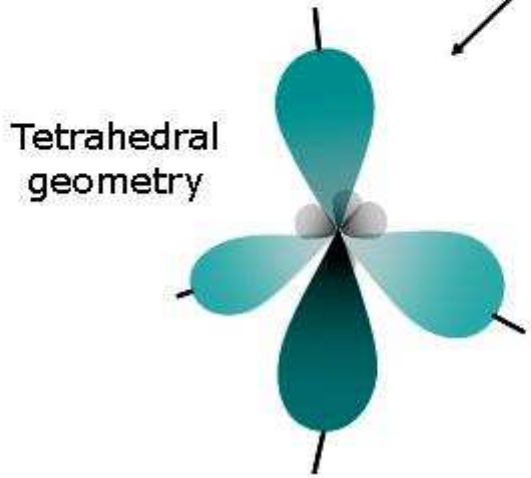
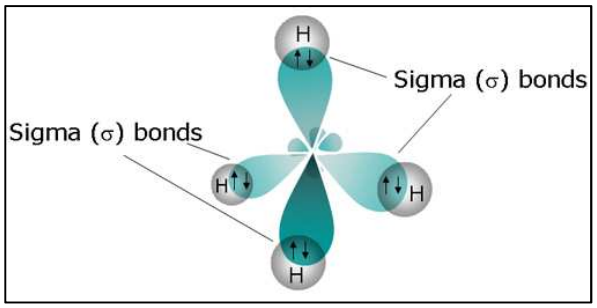


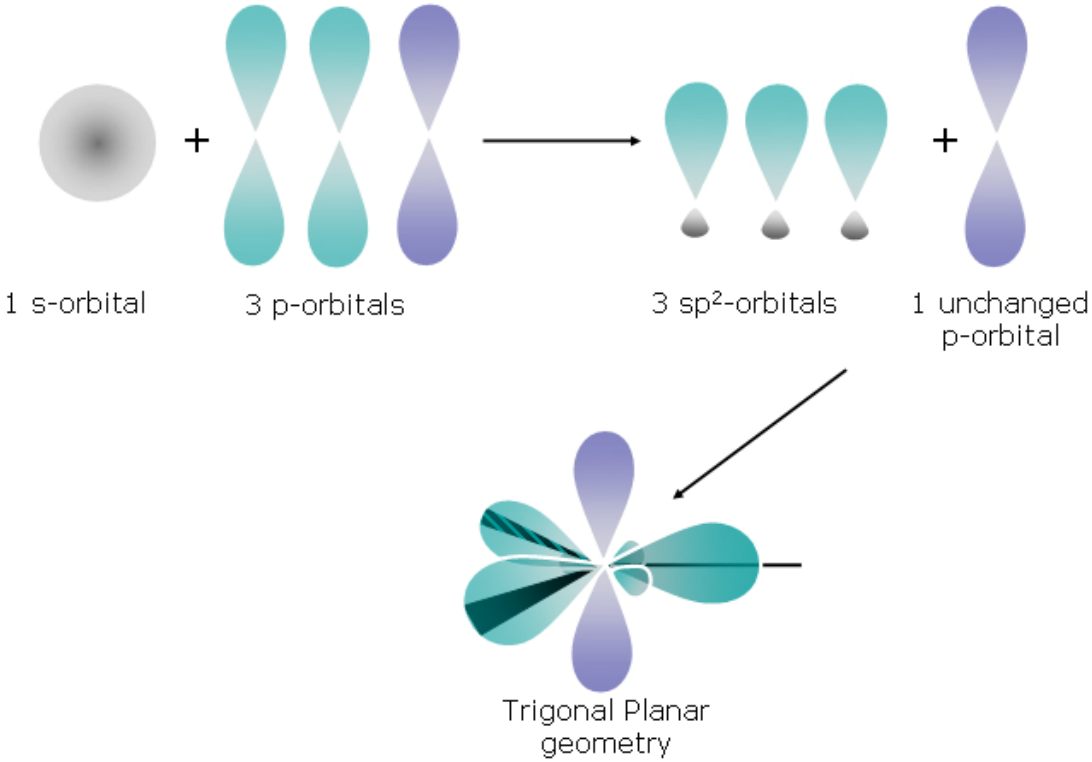
sp3 hybridization

methane



http://magic.piktochart.com

Orbital hybridization



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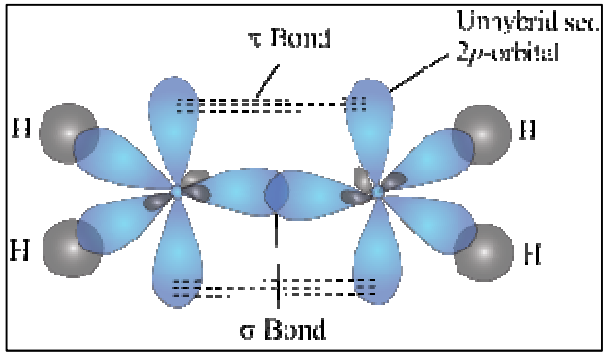
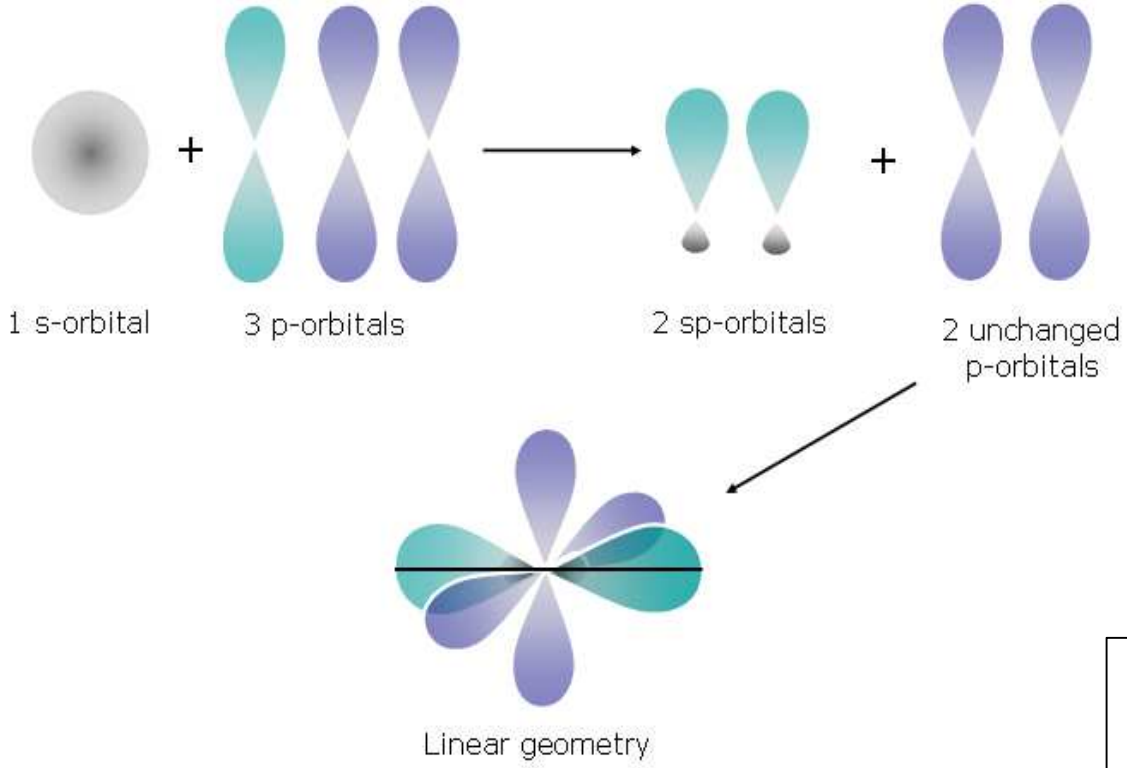
sp2 hybridization

ethene (ethylene)



http://www.meritnation.com

Orbital hybridization



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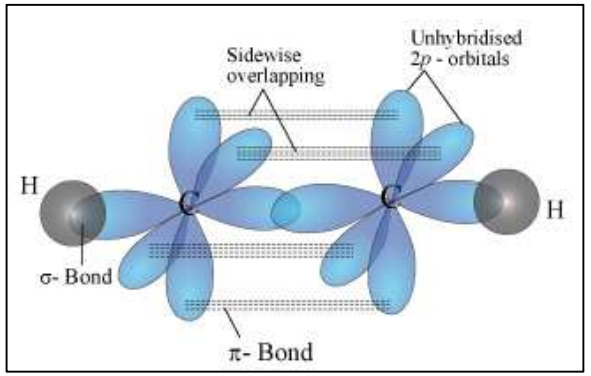
sp hybridization

ethyne (acetylene)



http://www.meritnation.com