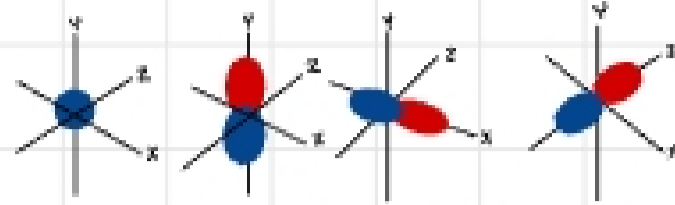


**Quantum mechanics**

Wave equation = 1 proton + 1 electron



Wave functions = ways to solve wave equation

Each wavefunction is a function of spatial location

Wave functions:  $\psi_1, \psi_2, \psi_3, \dots$

$\psi_2$  has a special meaning. It indicates the probability of

**Electron density and atomic orbitals**

Finding an electron in that location. Therefore a 3 dimensional plot of  $\psi^2$  will look like

A positive value doesn't imply a positive charge. The value of  $\psi(+\dots)$  is a mathematical convention that

refers to the phase of a wave.  $\psi^2$  (describes the electron density as a function of location) will always be a (+) #.

At a node, where  $\psi = 0$  the electron density ( $\psi^2$ ) will also be zero. This means no electron density at the node.

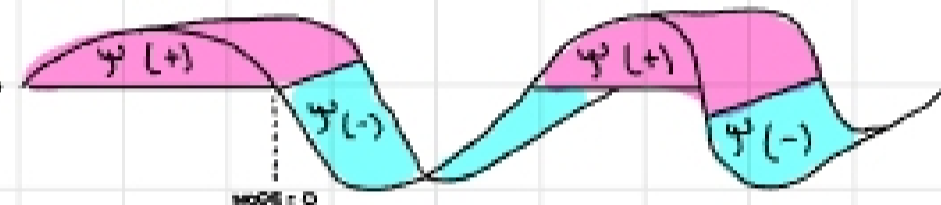
Electrons are lowest in energy when they occupy the first orbital occupied orbital = cloud, clouds are different shapes

and sizes. An electron cloud is NOT comprised with billions of particles, it is a single entity, which is occupied by electron density

which is called an atomic cloud. Phases of atomic orbitals wave = wave function, value is dependent on location

Locations above the average level have a positive ( $\psi$ ) and

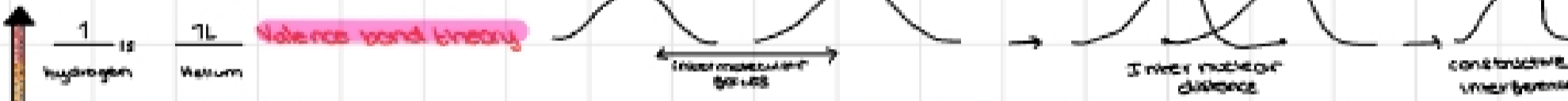
average wave



Locations below are negative ( $\psi$ ), locations where ( $\psi = 0$ ) are called nodes!

Paufli principle → lower energy orbital filled first. Pauli exclusion principle each orbital can hold a max of two electrons that have

opposite spins. Hund's Rule → when dealing w/ p orbitals, one electron is placed in each degenerate orbital first, before electrons are paired.



Constructive interference → produces waves with larger amplitude. Destructive interference results in waves cancelling each other, which is a node.

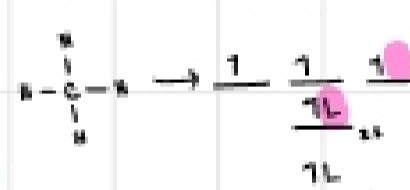
Valence bond theory → a bond is showing electron density between two atoms as a result of constructive interference of their orbitals.

sigma ( $\sigma$ ) bond →

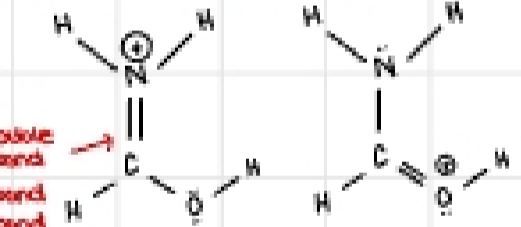


orbital cross section

1.10 Hybridized atomic orbitals Nitrate and  $sp^2$  hybridization →



**LECTURE TWO NOTES**



Relationship between the two is → Resonance forms

VSEPR theory  
Valence Shell Electron Pair theory

Constitutional isomers: same molecular formula but different connectivities

Isomers: molecules that share the same molecular formula and arrangement but differ from one another in 3-dimensional space

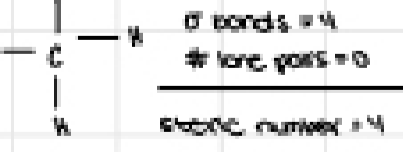
Resonance forms: another way of drawing Lewis dot structures for a given compound

Steric number: number of groups surrounding an atom

- Bonds atoms

- lone pairs

Examples - 1 steric # = 4



Hybridization of  $CH_3^+$




	0 lone pairs	1 lone pair	2 lone pairs	3 lone pairs	4 lone pairs
2					
3					
4					
5					
6					

1.6

**Bond line structures:** simplify the drawing process of a structure and make it easier to read.

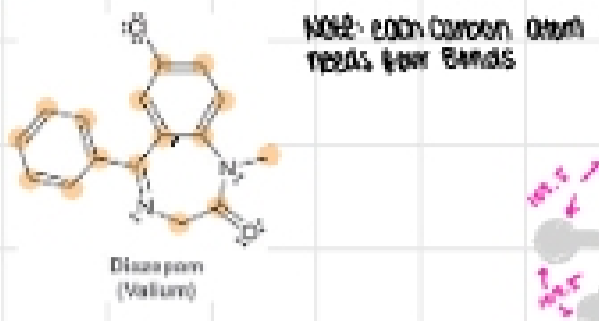


Bond lines are zigzags, each corner is a carbon atom.

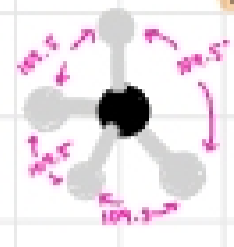
Examples with 6 carbon atoms (  ) Double bonds are shown with two lines, triple bonds are with three.



practice problem: identify the number of carbon atoms:



NOTE: triple bonds are linear rather than zig zag because of linear geometry



1.11

**Predicting molecular geometry: VSEPR theory**

**tetrahedral geometry:** the geometry of an atom with 4 bonds separate by  $109.5^\circ$

**trigonal pyramidal geometry:** molecular geometry with one atom at the apex and 3 atoms at the corners of a trigonal base

**Bent geometry:** two  $\sigma$  bonds and two lone pairs with a steric number of 4

**trigonal planar geometry:** three hybridized, all bond angles are  $120^\circ$ , 3 valence electrons.

**linear geometry:** has two valence electrons, each is used to form a  $\sigma$  bond.



1.13

**Intermolecular forces:** attractive forces between molecules

All intermolecular forces are electrostatic.

The electrostatic interactions for neutral molecules

are classified as dipole-dipole interactions, hydrogen

bonding, fleeting dipole-dipole interactions

NOTES

Induction is caused by the presence of an electronegative atom

1 debye =  $10^{-18}$  esu-cm. example: C-Cl bond length =  $1.772 \times 10^{-8}$  cm  
 $\mu = e \times d$   
 $= (4.8 \times 10^{-10} \text{ esu}) \cdot (1.772 \times 10^{-8} \text{ cm})$   
 $= 8.51 \times 10^{-18} \text{ esu-cm}$

$\rightarrow 8.51 \times 10^{-18} / 3.33 \times 10^{-30} = 2.55 \text{ D}$

pce 3 notes

electronegativity differences result in polar bonds

induction  $\rightarrow$  dipole moment  $\rightarrow$  units of debye (D)

double bonds are more

the amount of partial charge. the distance one ( $\delta^+$ ) and ( $\delta^-$ ) are separated.

polar than carbon-carbon.

For molecules with more than one polar bond, the molecular dipole moment

is the vector sum of the individual bond dipoles.



most negative ( $\delta^-$ )



most positive ( $\delta^+$ )