Gas Law: (different kinds of units for pressure and volume can be used provided the value of the gas constant is adjusted to those units)

PV = nRT P=Pressure in mmHg (or atm)
V=Volume in L
n=moles
T=temperature in °K; °K and °C are same size but 0 °K (absolute zero) = minus 273 °C

$$R \text{ is a constant } \frac{0.082\ L \cdot atm.}{Mol\ .\ °K}$$

Conceptual example: Ammonia gas (NH_3)
MW: 17 g/mol [(14 for N) + (3 for 3 x H)]
Liquid state occupies ~15 mL but gaseous state occupies ~22.4 L!

Sample Question- What volume will 3 mL of N_2 gas occupy at standard pressure and temperature (STP)?

Standard Pressure is 1 atmosphere (atm) or 760 mm Hg; Standard temperature is 273 °K

$$\frac{P_1V_1}{P_2V_2} = \frac{nRT_1}{nRT_2} \quad \text{divide equations to give} \quad \frac{P_1V_1}{P_2V_2} = \frac{T_1}{T_2}$$

P_1 = 760 mmHg T_1 = 273 °K
P_2 = 750 mmHg T_2 = 298 °K V_2 = 3 mL

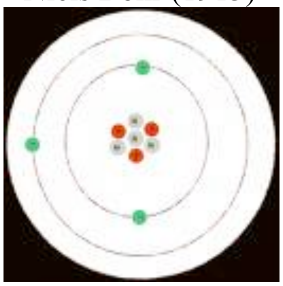
Solve for V_1

$$V_1 = \frac{T_1P_2V_2}{T_2P_1} = \frac{(273\ °K)(750\ mmHg)(3\ mL)}{(298\ °K)(760\ mmHg)}$$

= 2.71 mL is the answer

Atomic theory:

- Niels Bohr (1913) – won his Nobel prize for his atomic theory – NOT fully correct



- the neutrons and protons occupy a dense central region called the nucleus
- the electrons orbit the nucleus much like planets orbiting the Sun

- De Broglie (1924) – his 12 page PhD thesis won him the Nobel prize - he proposed that ordinary “particles” such as electrons and protons could behave as both particles and waves (wave-particle duality)

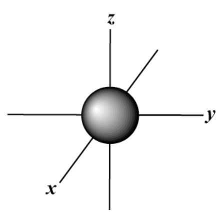
- the orbitals of an atom are described by wave functions (mathematical equations) – they have no direct physical meaning but when squared, provide electron density
- ψ (psi) = orbital
- ψ^2 = (orbital)^2 = electron density distribution

Note. Often the electron density distribution is called an “orbital” by chemists

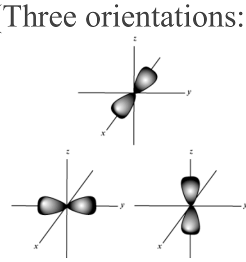
For hydrogen (H) atom: >95% of electron density is found within 1Å = 10^{-8} cm of the nucleus

Orbitals:

1. s-orbital - spherical shaped (electron density)



2. p-orbital - dumbbell-shaped (Three orientations: placed on the x, y and z-axis)

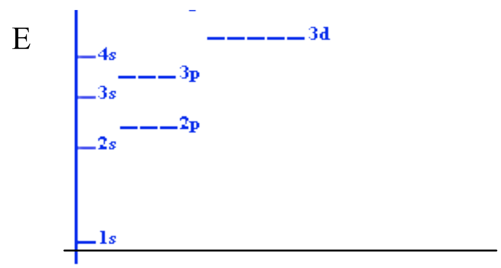


Basic principles:
- like charges repel each other
- unlike charges attract each other
- atoms want to be in inert gas electron configuration (isoelectronic with inert gas)

Atoms	Protons (+)	Neutrons	1s electrons	2s electrons	2p electrons
H	1	0	1		
He	2	2	2		
Li	3	3	2	1	

Abbreviation of electron - e^-

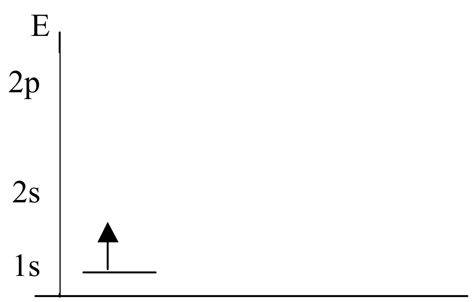
Energy (E) level diagram for an atom:



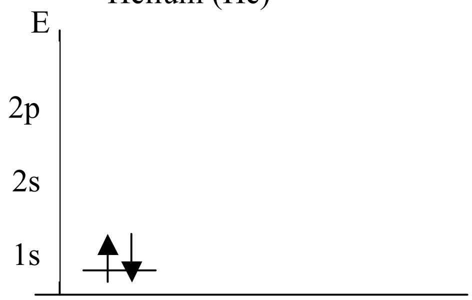
Rules for filling electron – AUFBAU rule (Build up Principle):

- add electron to lowest energy orbital available
- Pauli Exclusion principle: maximum two electrons per orbital (each having opposite spin quantum number)
- fill 1 electron into each orbital of same energy (degenerate orbital), then add second electron - Hund rule

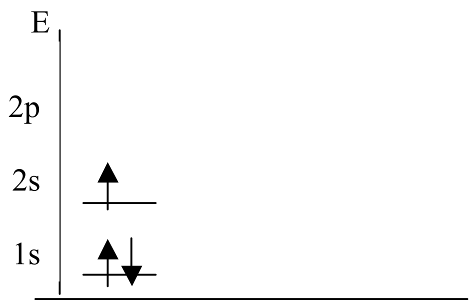
Hydrogen (H)



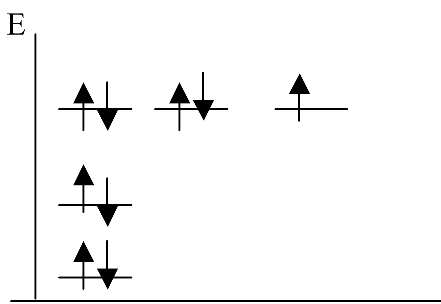
Helium (He)



Lithium (Li)



Fluorine (F)



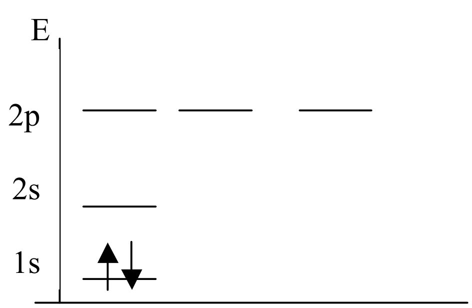
- all elements want inert gas configuration (e.g. Ne) and from above diagrams both Li and F are unhappy with unfilled orbitals (not in inert gas configuration)

Bonding - Ionic

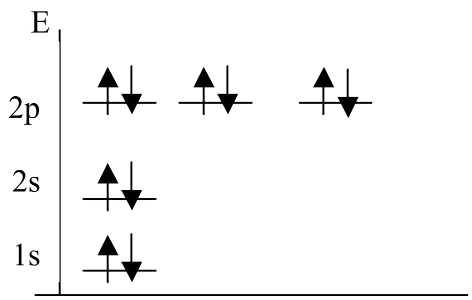
- isoelectronic = same electron configuration
- Li could lose 1e$^-$ from 2s orbital to be isoelectronic to He (as Li^+) and F could gain 1e$^-$ to be isoelectronic to Ne (as F^-)

$$Li^o \quad + \quad F^o \quad \rightarrow \quad Li^+ \quad + \quad F^-$$

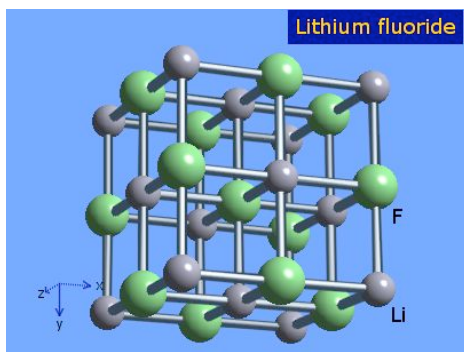
Li^+ (cation)



F^- (anion)



- in space these ions would be attracted to each other
- in solution they might be separated due to solvation (e.g. water would surround)
- in solid, they would form a crystalline solid structure



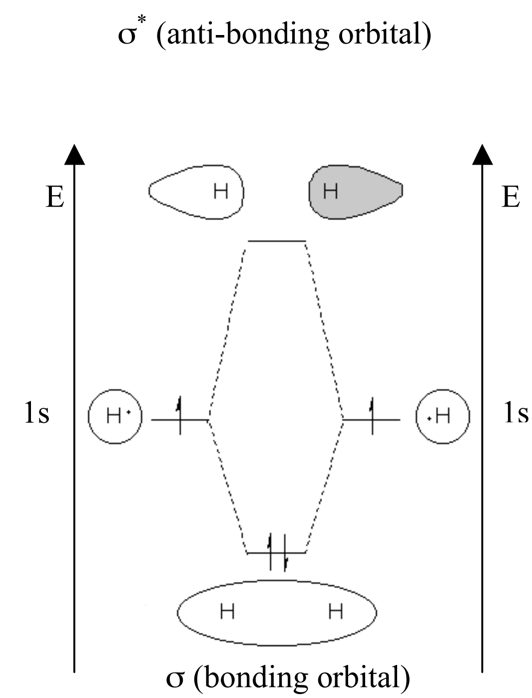
Bonding – Covalent and hybridization

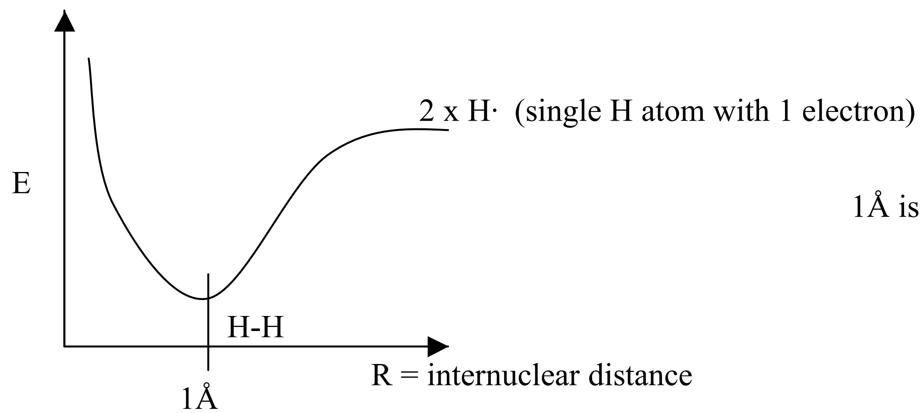
Energetics of Forming Bonds

Linear Combination of Atomic Orbitals (LCAO)

- Gives molecular orbitals (MO)
- Overlap of s atomic orbitals (AO) → gives sigma(σ) MO (cylindrical symmetry)
- Difference between AO and MO → AO present on an atom while MO present between two atoms when bond is formed.
- In terms of strength → σ bond is stronger than a π bond. But a double bond is stronger than a single bond because double bonds contain two bonds (σ-bond + π-bond).

(eg.) H_2



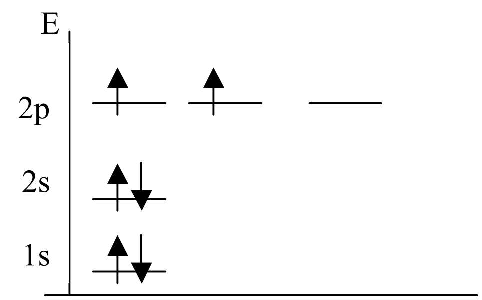


1Å is the average H-H bond distance

Electronic configuration of carbon (C):

- atomic number = 6
- atomic weight = 12 (also has 6 neutrons)
- other isotopes of carbon
    - ^{13}C ($6p^+$, 7n) is a stable isotope, 1.1 % natural abundance
    - ^{14}C ($6p^+$, 8n) is radioactive, $t_{1/2}$ = 5700 yrs, ^{14}C dating of organic material

Carbon (C)



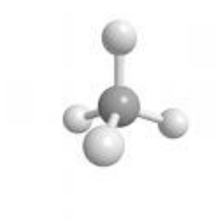
- need to gain or lose $4e^-$ to get inert gas configuration – but this gives unfavourable charge buildup:

- C^{4+} isoelectronic with He

- C^{4-} isoelectronic with Ne

- so, carbon makes 4 bonds to share $4e^-$ (covalent bonding)

Methane, CH_4:



- tetrahedral geometry
- for any 2 bonds electron density is equidistant from nucleus
- four covalent bond between the carbon atom and the hydrogen atoms
- the angle between two H-atoms = 109°