**Quantitative analysis of organic compound (from last class)**

1. Calculation of % composition:

% of C = $\frac{2.82 \text{ mg of C}}{4.34 \text{ mg}}$ = 65.1 %

% of H = $\frac{0.383 \text{ mg of H}}{4.34 \text{ mg}}$ = 8.83 %

% of O = 100% - 65.1% - 8.83% = 26.1 %

2. Determining the empirical formula:

- Definition: empirical formula is ratio of atoms to each other in a molecular formula
- Three steps to calculate the empirical formula:
  - i) divide each percentage (%) by the atomic weight of element → crude ratio
  - ii) divide all crude ratio by the smallest crude ratio → refined ratio
  - iii) Multiply the refined ratio by an integer value to get integral ratio

| % Composition | Crude ratio | Refined ratio | Integral ratio |
|---|---|---|---|
| 65.1 % C | 65.1 / 12.0 = 5.42 | 5.42 / 1.63 = 3.34 | 3.34 x 3 = 10 |
| 8.83 % H | 8.83 / 1.01 = 8.76 | 8.76 / 1.63 = 5.39 | 5.39 x 3 = 16 |
| 26.1 % O | 26.1 / 16.0 = 1.63 | 1.63 / 1.63 = 1.00 | 1.00 x 3 = 3 |

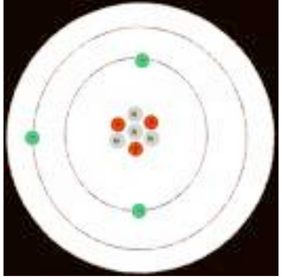
From the integral ratio, the empirical formula is $C_{10}H_{16}O_3$. Since the molecular weight is given as 184 g/mol, the molecular formula is also $C_{10}H_{16}O_3$.

Note: suppose the molecular weight is given as 368 g/mol, then the molecular formula is obtained by multiplying the integral ratios by a factor of 2 and it would be $C_{20}H_{32}O_6$.

---

**Atomic theory:**

- Neil 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

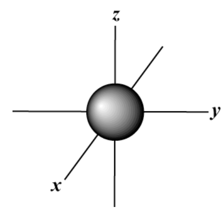
- de Broglie (1924) – his 12 page PhD thesis won him the Nobel prize
    - he proposed that ordinary "particles" such as electrons and protons could behave as both particles and waves (wave-particle duality)

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

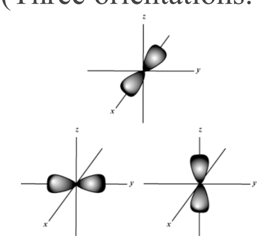
For hydrogen (H) atom: >95% of electron density is found within 1Å = $10^{-8}$ cm

**Orbitals:**

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



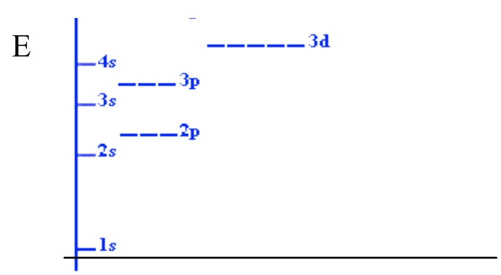

2. p-orbital - dumbbell-shaped (Three orientations: placed on the x, y and z-axis)



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

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

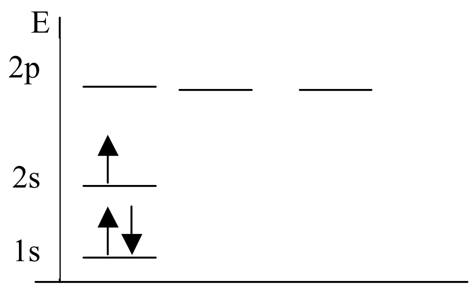
**Energy (E) level diagram for an atom:**



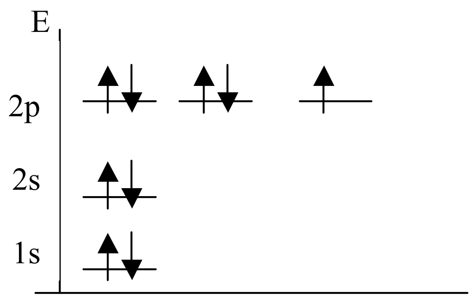
**Rules for filling electron – AUFBAU rule:**

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

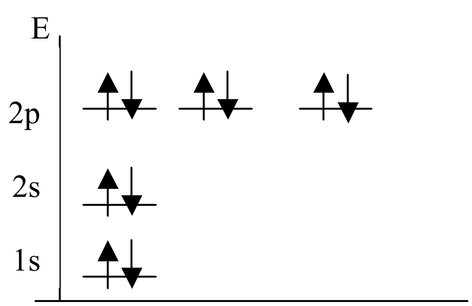
Lithium (Li)




Fluorine (F)




Neon (Ne)

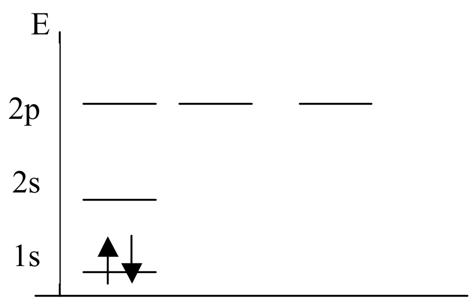



- all elements want inert gas configuration (e.g. Ne) and from above diagram both Li and F are unhappy with unfilled orbitals (not in inert gas configuration)

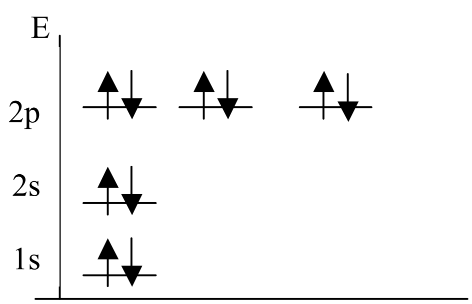
- Li could lose 1$e^-$ from 2s orbital to be isoelectronic to He (as $Li^+$) and F could gain 1$e^-$ to be isoelectronic to Ne (as $F^-$)

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

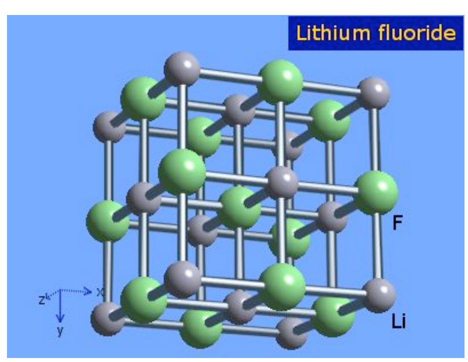
$Li^+$




$F^-$



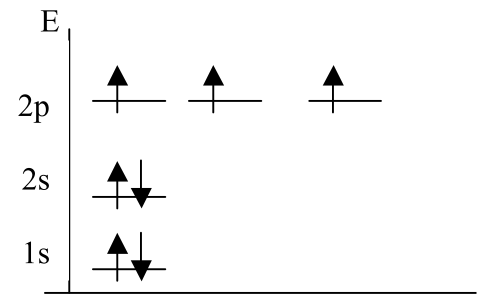

- in space these ions would be attracted to each other
- in solution they might be separated due to solvation (e.g. water would surround)
- in solid, they would form a crystalline solid structure



**Electronic configuration of carbon (C):**

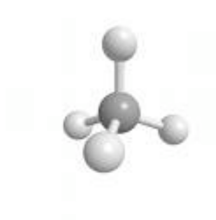
- atomic number = 6
- atomic weight = 12
- other isotopes of carbon
    - $^{13}C$ ($6p^+$, 7n) is a stable isotope, 1% natural abundance
    - $^{14}C$ ($6p^+$, 8n) is radioactive, $t_{1/2}$ = 5700 yrs, $^{14}C$ dating of organic material

Carbon (C)




- need to gain or lose $4e^-$ to get inert gas configuration
- so, carbon makes 4 bonds to share $4e^-$ (covalent bonding)

**Methane, $CH_4$:**



- tetrahedral geometry
- electron density is equidistance from nucleus
- four covalent bond between the carbon atom and the hydrogen atoms
- the angle between two H-atoms = 109˚

**Hybridization:**

- mixing of atomic orbitals (with wrong geometry for bonding) to form the hybrid orbitals that have correct geometry for bonding

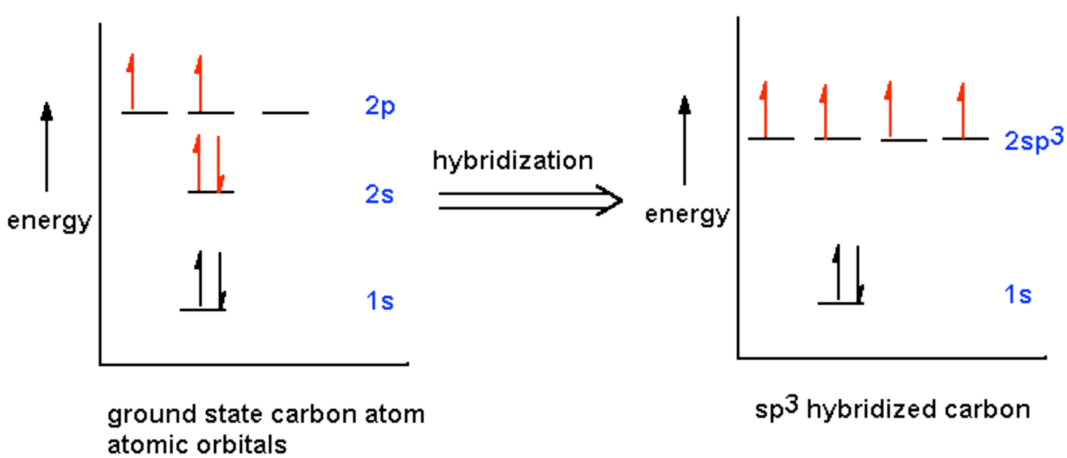



Figure: Hybridization of 2nd shell s orbibtals (one) and p orbitals (three) of carbon

- the 2s orbital and 2p orbitals of carbon are mixed (hybridized) to form the four degenerate $sp^3$ orbitals
- note: $sp^3$ comes from the fact that one s-orbital and three p-orbitals are mixed
- once the hybrid orbitals are formed, four hydrogen atoms can share the four electrons of the outer (bonding) shell of carbon to form four covalent bonds
- now, carbon is isoelectronic to neon and hydrogen is isoelectronic to helium