Inorganic Pharmaceutical Chemistry

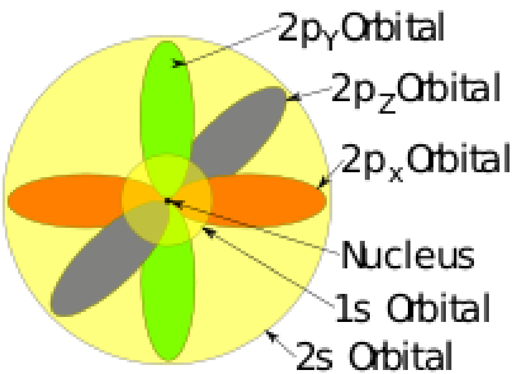
Pharmaceutical Chemistry

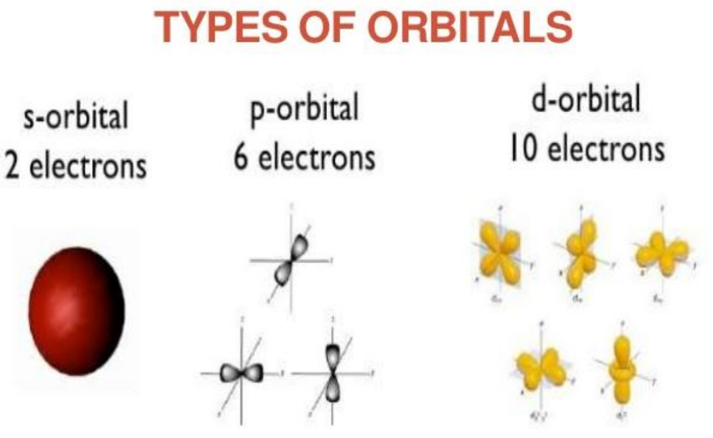
Lecture 1:

Atomic and Molecular Structure

Third Stage

Semester 1





The Periodic Table

Key: 0.98 — Pauling electronegativity; 3 — Atomic number; Li — Element; 6.941 — Atomic weight (^{12}C)

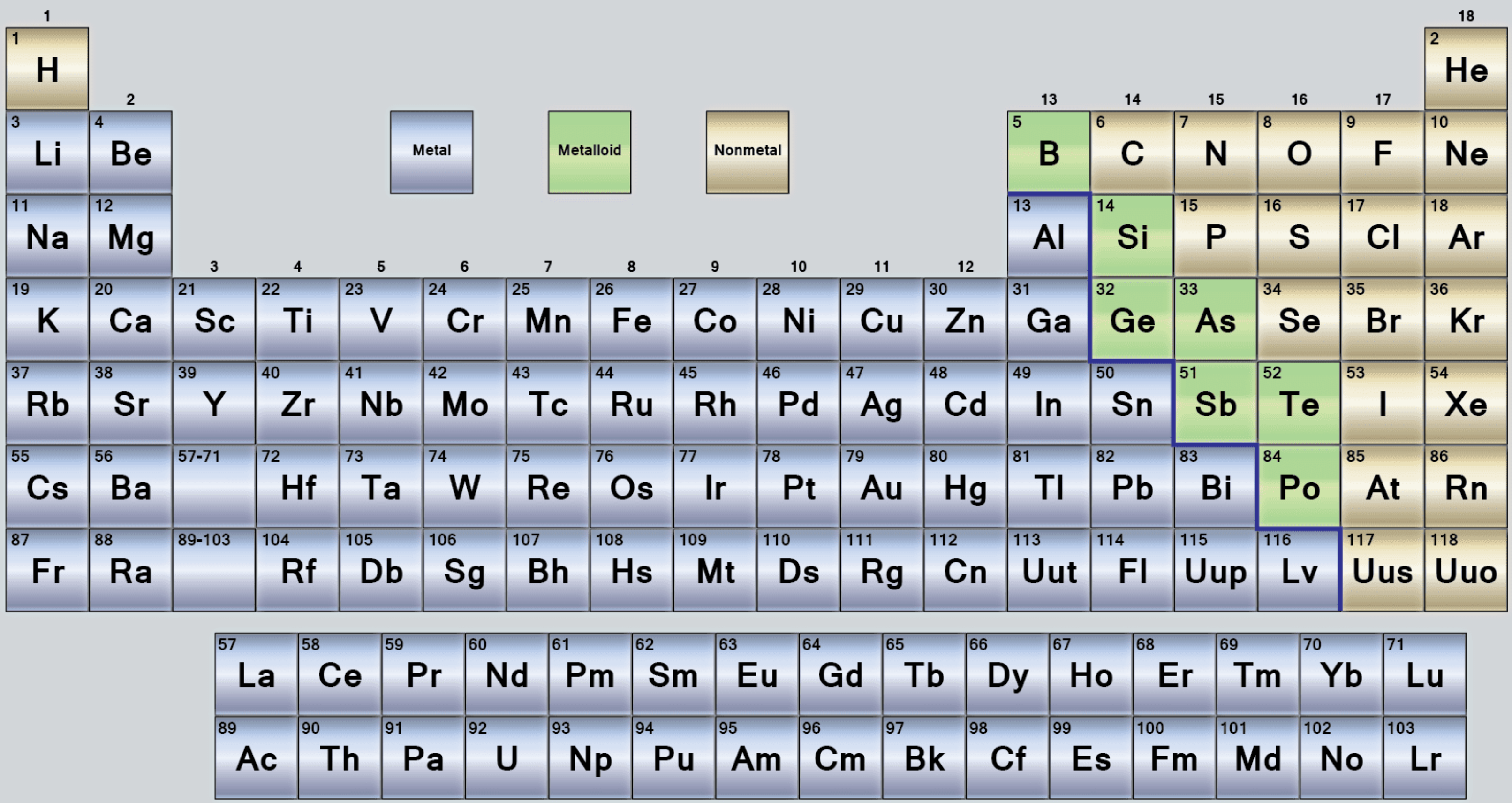
1 2.20 H 1.008	2 He 4.003

Group: 3 4 5 6 7 8 9 10 11 12 — d transition elements

Group 1	Group 2	3	4	5	6	7	8	9	10	11	12	Group 13	Group 14	Group 15	Group 16	Group 17	Group 18
3 0.98 Li 6.941	4 1.57 Be 9.012											5 2.04 B 10.811	6 2.55 C 12.011	7 3.04 N 14.007	8 3.44 O 15.999	9 3.98 F 18.998	10 Ne 20.179
11 0.93 Na 22.990	12 1.31 Mg 24.305											13 1.61 Al 26.98	14 1.90 SI 28.086	15 2.19 P 30.974	16 2.58 S 32.054	17 3.16 Cl 35.453	18 Ar 39.948
19 0.82 K 39.102	20 1.00 Ca 40.08	21 Sc 44.956	22 Ti 47.90	23 V 50.941	24 Cr 51.996	25 Mn 54.938	26 Fe 55.847	27 Co 58.933	28 Ni 58.71	29 Cu 63.546	30 Zn 65.37	31 1.81 Ga 69.72	32 2.01 Ge 72.59	33 2.18 As 74.922	34 2.55 Se 78.96	35 2.96 Br 79.909	36 Kr 83.80
37 0.82 Rb 85.47	38 0.95 Sr 87.62	39 Y 88.906	40 Zr 91.22	41 Nb 92.906	42 Mo 95.94	43 Tc (99)	44 Ru 101.07	45 Rh 102.91	46 Pd 106.4	47 Ag 107.87	48 Cd 112.40	49 1.78 In 114.82	50 1.96 Sn 118.69	51 2.05 Sb 121.75	52 2.10 Te 127.60	53 2.66 I 126.90	54 Xe 131.30
55 0.79 Cs 132.91	56 0.89 Ba 137.34	57 La 138.91	72 Hf 178.49	73 Ta 180.95	74 W 183.85	75 Re 186.2	76 Os 190.2	77 Ir 192.22	78 Pt 195.09	79 Au 196.97	80 Hg 200.59	81 2.04 Ti 204.37	82 2.32 Pb 207.19	83 2.02 Bi 208.98	84 Po (210)	85 At (210)	86 Rn (222)
87 Fr (223)	88 Ra 226.025	89 Ac 227.0	104 Rf (261)	105 Db (262)	106 Sg (263)	107 Bh	108 Hs	109 Mt	110 Uun	111 Uuu	112 Unb						

58 Ce 140.12	59 Pr 140.91	60 Nd 144.24	61 Pm (147)	62 Sm 150.35	63 Eu 151.96	64 Gd 157.25	65 Tb 158.92	66 Dy 162.50	67 Ho 164.93	68 Er 167.26	69 Tm 168.93	70 Yb 173.04	71 Lu 174.97
90 Th 232.04	91 Pa (231)	92 U 238.03	93 Np (237)	94 Pu (242)	95 Am (243)	96 Cm (247)	97 Bk (247)	98 Cf (249)	99 Es (254)	100 Fm (253)	101 Md (253)	102 No (256)	103 Lw (260)

- Elements on the left and middle are METALS (except Hydrogen)
- Elements on the right are NONMETALS
- METALLOIDS form the narrow stair-step area between metals and nonmetals.
- The last group (18) to the right are NOBLE GASES



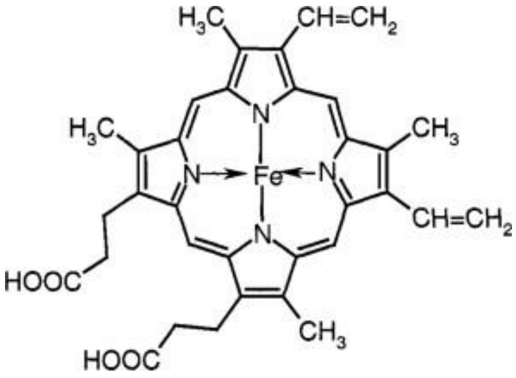
A metalloid is an element that has properties that are intermediate between those of metals and nonmetals. Metalloids can also be called semimetals.

- **Medicinal inorganic chemistry** can be broadly defined as the area of research concerned with metal ions and metal complexes and their clinical applications.

- Metals such as **arsenic** have been used in clinical studies more than 100 years ago, whilst **silver**, **gold** and **iron** have been involved in 'magic cures' and other therapeutic applications for more than **5000 years**.

- Many metal ions play a vital role in living organisms. Metal ions are also involved in a variety of processes within the human body, such as the oxygen transport or the formation of the framework for our bones.

- Haemoglobin is an iron-containing metallo-protein which carries oxygen from the lungs to the various tissues around the human body.



Haemoglobin

- **Calcium** (Ca) ions are a vital component of our bones. Elements such as copper (Cu), zinc (Zn) and manganese (Mn) are essential for a variety of catalytic processes

- Nevertheless, metals are very often perceived as **toxic elements**. Very often, the toxicity of a metal in a biological environment depends on the **concentration** present in the living organism.

- Some metal ions are **essential for life**, but concentrations too high can be highly toxic whilst too low concentrations can lead to deficiency resulting in disturbed biological processes.

Classification of the Elements

Metals

- Lustrous, malleable, ductile, electrically conducting solids at room temperature

Nonmetals

- Often gases, liquids, or solids that do not conduct electricity appreciably

Metalloids

- Elements, alloys or compounds that possess some of the characteristics of metals and some of nonmetals

- Metallic elements combine with nonmetallic elements to give compounds that are typically hard, non-volatile solids
- When combined with each other, the nonmetals often form volatile molecular compounds
- When metals combine (or simply mix together) they produce alloys that have most of the physical characteristics of metals

Electronic Structure of Atoms

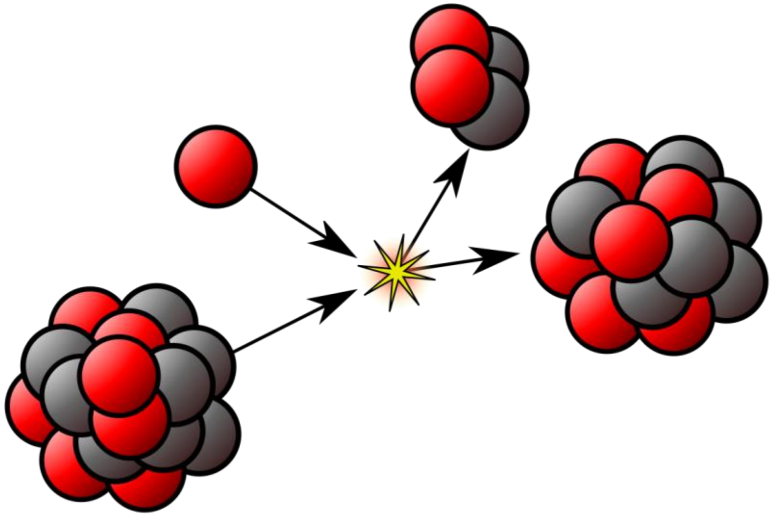
- The fundamental unit of all matter is the **atom**.

- The various chemical and physical properties of matter are determined by its elemental composition.

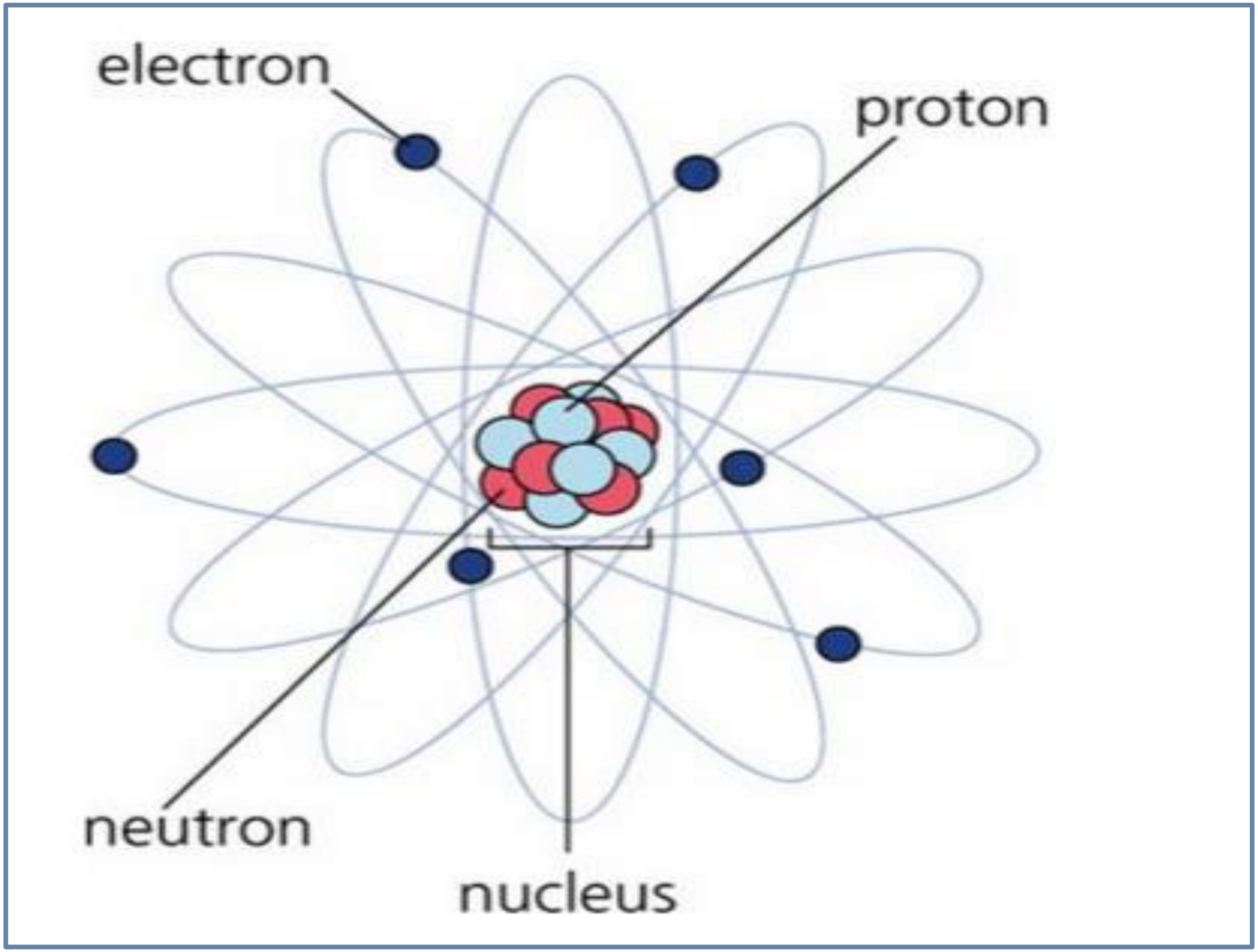
- Elements are composed of like atoms and their isotopes.
- **Subatomic particle: Any of various units of matter below the size of an atom.**
- To predict the properties of matter, molecules, or elements, it is important to understand the structure of atoms.

Subatomic Particles:

- Atoms are composed of a central nucleus surrounded by electrons which occupy discrete regions of space.
- The nucleus is considered to contain two types of stable particles which comprise most of the mass of the atom.
- These particles are "held" within the nucleus by various "nuclear forces."

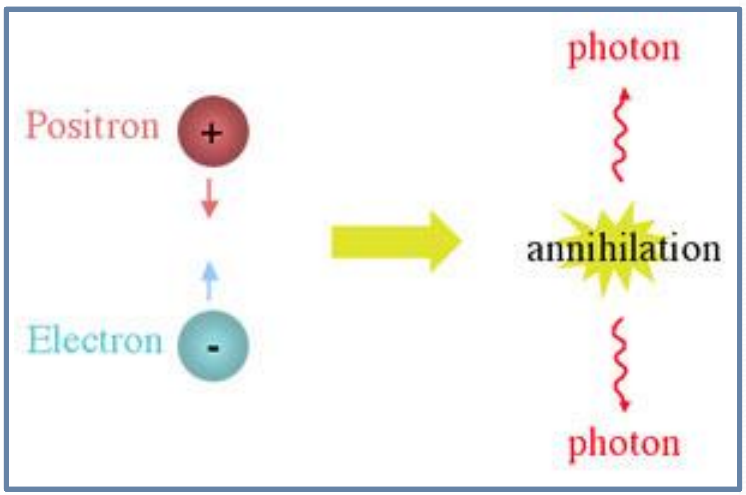


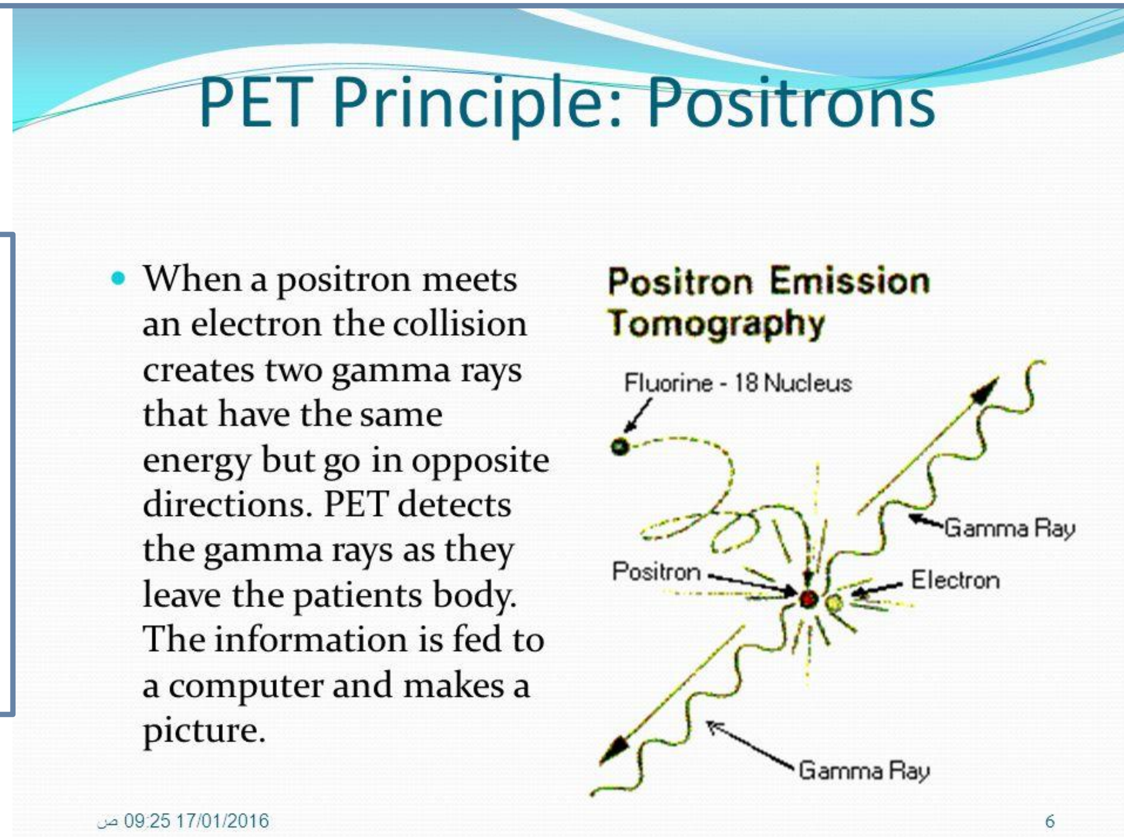
Subatomic Particles:



Positron

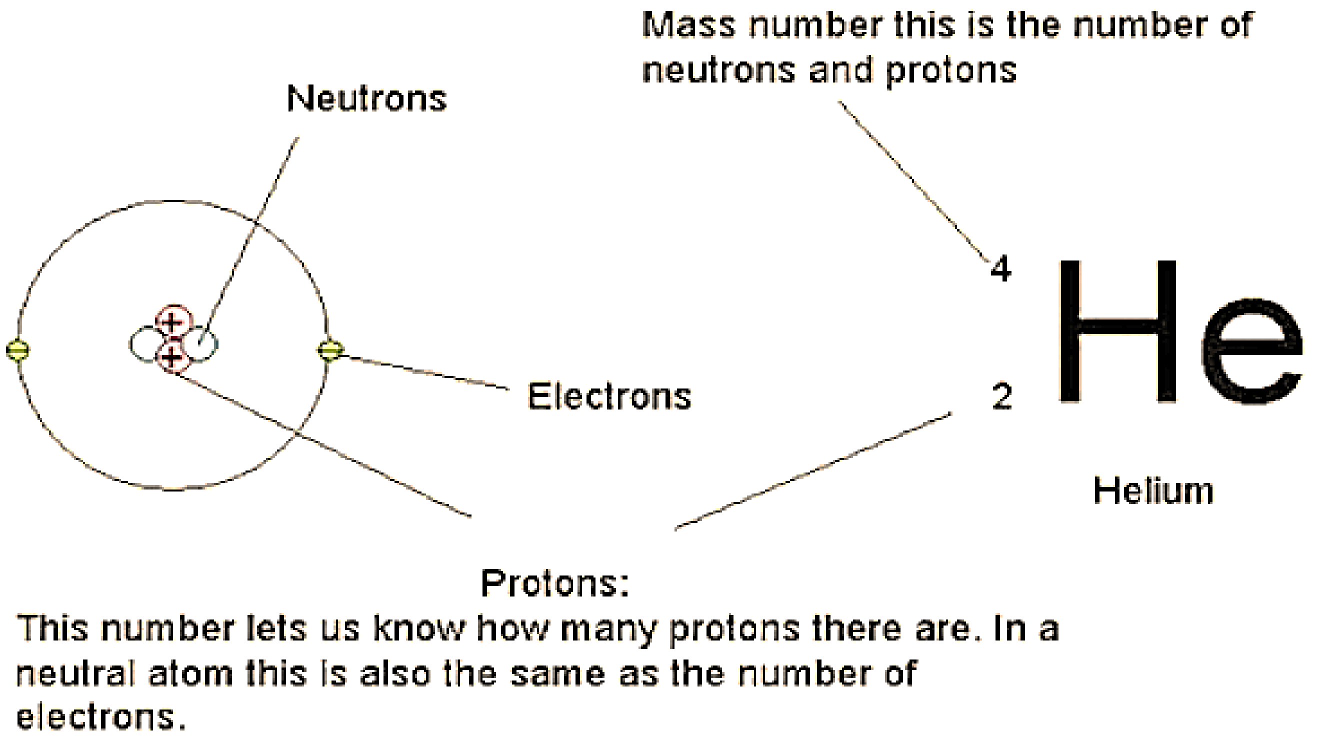
The positron or antielectron is the antiparticle or the antimatter counterpart of the electron. The positron has an electric charge of +1 e, a spin of 1/2 (the same as the electron), and has the same mass as an electron. When a positron collides with an electron, annihilation occurs.





Subatomic Particles:

- The sum of the masses of the protons and neutrons accounts for most of the **atomic mass "weight"** of the element, and the number of protons is equal to the atomic number.



$$^{A}_{Z}E$$

E = element symbol

A = number of protons + number of neutrons = mass number
Z = number of protons = number of electrons = atomic number

Figure 1.3 *Shorthand writing of element symbol*

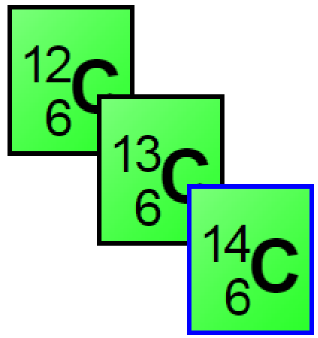
$^{1}_{1}H$	$^{2}_{1}H$	$^{3}_{1}H$
Protium	Deuterium	Tritium

Figure 1.4 *Isotopes of hydrogen*

- *Atoms of the same element can have different numbers of neutrons; the different possible versions of each element are called* ***isotopes****. The numbers of protons and electrons are the same for each isotope, as they define the element and its chemical behaviour.*
- For example, the most common isotope of hydrogen called protium has no neutrons at all. There are two other hydrogen isotopes: deuterium, with one neutron, and tritium, with two neutrons

Subatomic Particles:

- Isotopic forms of a particular element differ in the number of neutrons, and, therefore, in the atomic mass.
- Do isotopes have the same atomic number?



	protons	neutrons	mass number
^{12}C	6	6	12
^{13}C	6	7	13
^{14}C	6	8	14

Isotopes vs. Allotropes

Isotopes - atoms of the same element with different numbers of neutrons

- different compounds with the same formula

Allotropes - different forms of an element

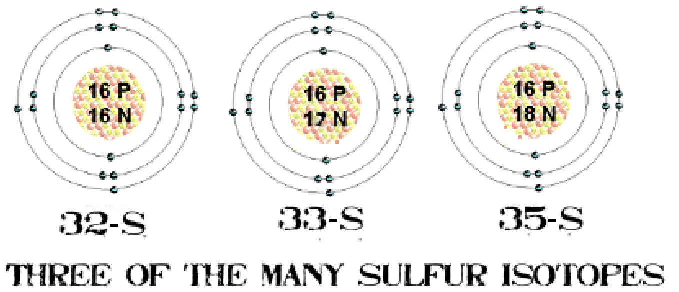
Carbon exhibits both

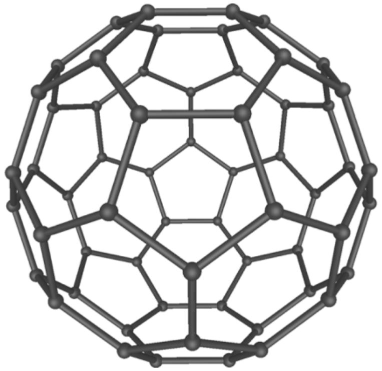
Isotopes: C-12 C-13 C-14

Allotropes: graphite, diamond, and fullerenes

$^{35}_{17}Cl$ $^{37}_{17}Cl$

Chlorine-35 Chlorine-37





Heisenberg principle:

- Also known as *Uncertainty principle.*
- Introduced first in 1927, by the German physicist Werner Heisenberg, it states that the more precisely the position of some particle is determined, the less precisely its momentum [mass. Velocity] can be known, and vice versa. (only for small objects like electrons)
- Thus, it is necessary to discuss the "location" of electrons in atoms and molecules in terms of probability.

Atomic Orbitals

- Atomic orbitals are defined as **discrete volumes of space** about the nucleus that the electrons are placed in.
- The electrons (contained within the boundaries of these orbitals) are described by a set of four numbers called quantum numbers.
- The four quantum numbers set the probability limits within which an electron can be found.
- The **first three** quantum numbers refer to some property of the **space or orbital**, while the fourth quantum number describes the spin of the electron.

The four quantum numbers

1. The Principal Quantum Number (n).

2. The Suborbital Quantum Number (l).

3. The Magnetic Quantum Number (m_ℓ).

4. The Spin Quantum Number (m_s).

The Principal Quantum Number (n):

- *Quantum theory states that electrons in atoms exist in discrete* ***energy levels****.*

- *The energy associated with the electron* ***increases as it location farther from the nucleus****.*

- *The principal quantum number describes the relative positions of these energy levels and their distance from the nucleus.*

- *The values of this number are integers(اعداد صحيحه) n = 1, 2, 3, …*
- *When n = 1 the electron is found in the energy level closest to the nucleus.*

The Suborbital Quantum Number*(l)*:

- *Also called the "angular quantum number," can be any value in the range 0 , 1, 2 , ... **n - 1**.*
- *The secondary quantum number divides the shells into smaller groups of orbitals called sub shells (sublevels).*
- *Usually, a letter code is used to identify (l) to avoid confusion with (n).*

l =	0	1	2	3
Letter =	s	p	d	f

The Suborbital Quantum Number*(l):*

For example: when n = 1, (l) can only equal 0; meaning that shell n = 1 has only an s orbital (l = 0). when n = 3, (l) can equal 0, 1, or 2; meaning that shell n = 3 has s, p, and d orbitals.

Another example : the sub shell with n=2 and (l)=1 is the 2p subshell; if n=3 and l=0, it is the 3s subshell, and so on.

The following figure shows the shapes of the s, p, and d orbitals.

The **standard electron configuration pattern** is as follows:

$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 5s^2 4d^{10} 5p^6 6s^2 4f^{14} 5d^{10} 6p^6 7s^2 5f^{14} 6d^{10}$

The Suborbital Quantum Number*(l)*:

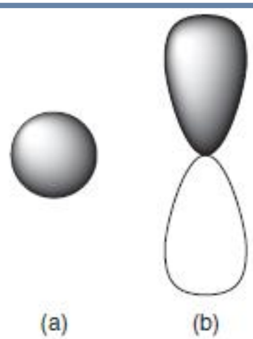


Figure 1.6 Boundary surfaces of (a) s-orbital and (b) p-orbital

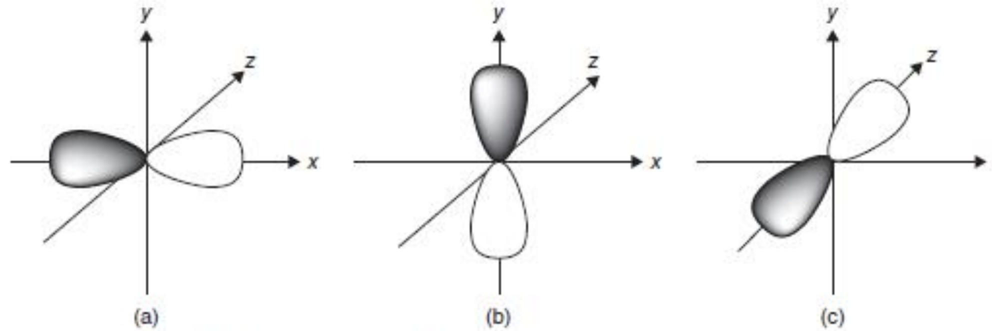


Figure 1.7 Orientation of (a) p_x-orbital, (b) p_y-orbital and (c) p_z-orbital

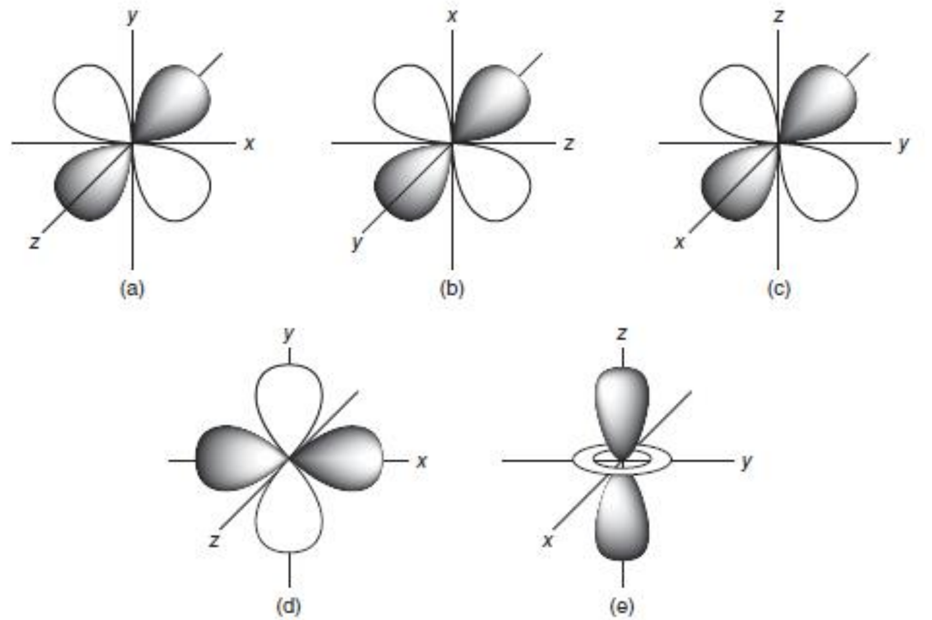
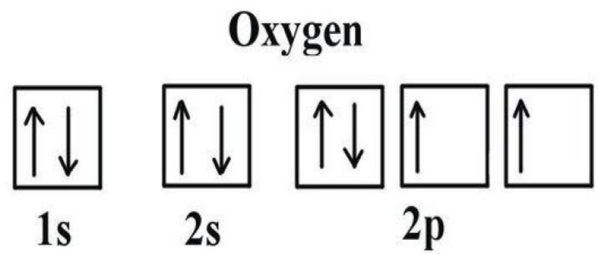


Figure 1.8 Boundary surfaces of five d orbitals: (a) d_{xy}, (b) d_{xz}, (c) d_{yz}, (d) $d_{x^2-y^2}$ and (e) d_{z^2} [10] (Reproduced with permission from [10]. Copyright © 2009, John Wiley & Sons, Ltd.)

The Magnetic Quantum Number (mℓ):

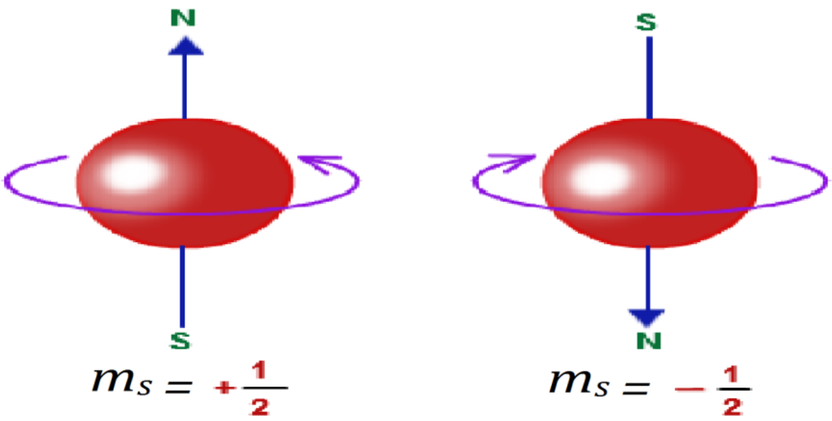
- *Basically, this number describes the spatial orientation of the orbital.*
- *The allowed values are restricted by the value of (l) and can be positive or negative integer:*
- *(l) = 0, 1, 2, 3   Where s=0, p=1, d=2, f=3*
- *mℓ = (-3, -2, -1, 0, +1,+2, +3)*
- *s= 0*
- *p= (-1, 0, +1) e.g. mℓ for oxygen = -1*
- *d= (-2, -1, 0, +1,+2)*
- *f= (-3, -2, -1, 0, +1,+2, +3)*

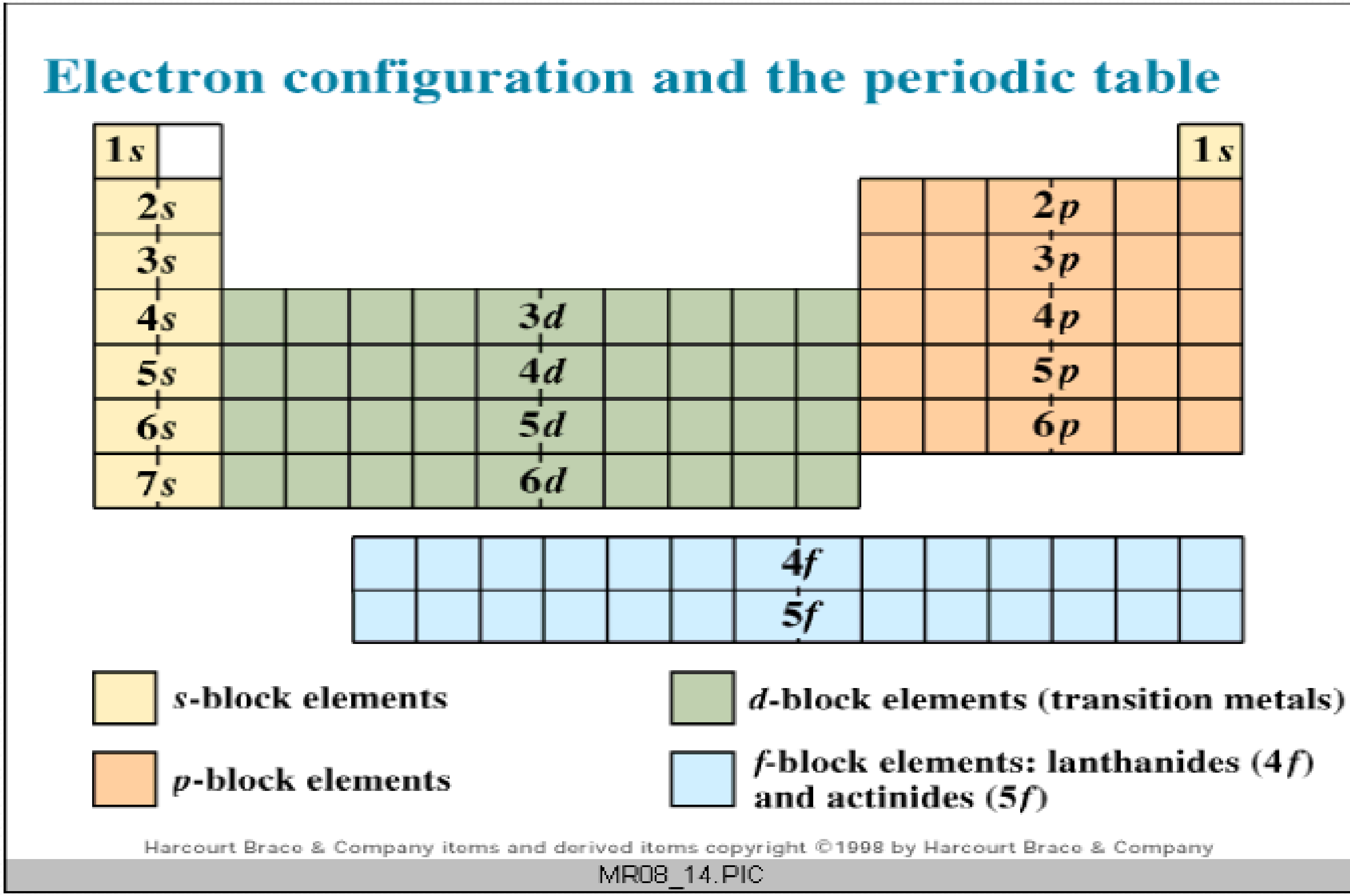


s – 1 orbital
p – 3 orbitals (x, y, z)
d – 5 orbitals (xy, yz, xz, $x^2 - y^2$, z^2)
f – 7 orbitals ($y^3 - 3yx^2$, $5yz^2$-yr^2, x^3-$3xy^2$, zx^2-zy^2, xyz, $5xz^2$-$3xr^2$, $5z^3$-$3zr^2$)

The Spin Quantum Number (m_s):

- *Specifies the orientation of the spin axis of an electron.*
- *The spin quantum number describes the direction the electron is spinning in a magnetic field either clockwise or counter clockwise.*
- *Only two values are allowed: +1/2 or -1/2.*
- *For each subshell, there can be only two electrons, one with a spin of +1/2 and another with a spin of –1/2.*




Electron configuration and the periodic table
1s
1s
2s
3s
4s
5s
6s
7s
3d
4d
5d
6d
2p
3p
4p
5p
6p
4f
5f
s-block elements
p-block elements
d-block elements (transition metals)
f-block elements: lanthanides (4f) and actinides (5f)
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