Ministry of Higher Education and Scientific Research

Al-Muthanna University

Inorganic Pharmaceutical chemistry

For the 3rd year students of the «faculty of Pharmacy»

Lecture (2)

Atomic structure part 2

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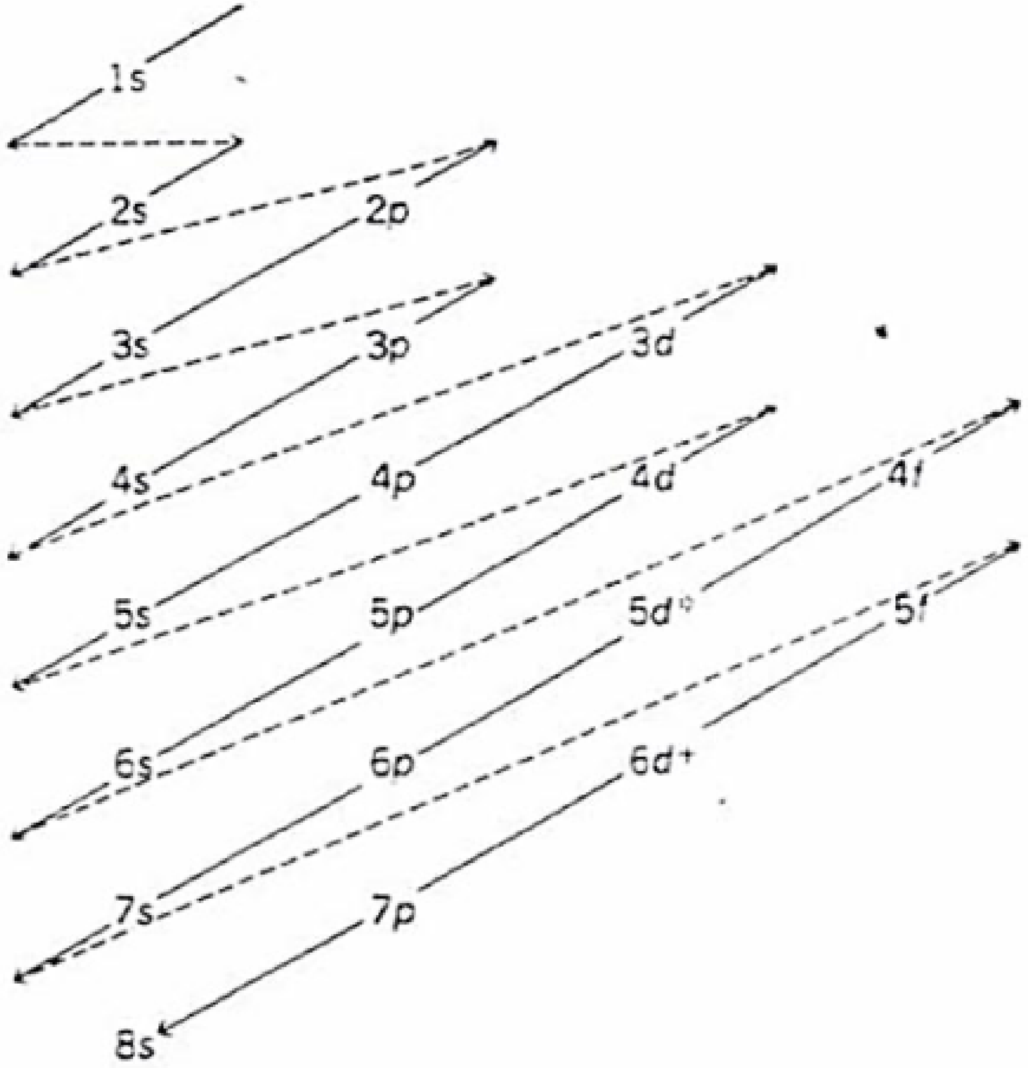
Electronic configuration

Element	Total Electrons	Orbital Diagram 1s	2s	2p			3s	Electron Configuration
H	1	↑						$1s^1$
He	2	↑↓						$1s^2$
Li	3	↑↓	↑					$1s^2\,2s^1$
Be	4	↑↓	↑↓					$1s^2\,2s^2$
B	5	↑↓	↑↓	↑				$1s^2\,2s^2\,2p^1$

A schematic representation of the order in which orbitals are filled.



Quantum Numbers

- The early quantitative description of electronic structure came from Niels Bhor in 1913, and involve a planetary picture of the atom. Electrons were considered as particles which revolve around the nucleus in stationary planar orbits and which had definite energies.
- In the 1920s the theory of quantum mechanics for the description of ultra-small particles was developed as was quantum theory of atomic structure.
- The electrons are placed in discrete volumes of space about the nucleus, these volumes of pace are referred to by the term atomic orbitals, and the electrons contained within their boundaries are described by a set of four numbers called the Quantum Numbers:

Quantum Numbers

The relation of a particular electron to the nucleus can be described through a series of four numbers, called the Quantum Numbers.

- The first three of these numbers describe

1-The energy (Principle quantum number).

2-Shape (Angular momentum quantum number).

3-orientation of the orbital (magnetic quantum number).

4-The fourth number represents the "spin" of the electron (spin quantum number).

1. The principal Quantum Number (n):

Describe the energy level on which the orbitals resides (the energy associated with the electron increases as it located farther from nucleus).
The integer value of n = 1, 2, 3, …, ∞ All orbitals that have the same value of n are said to be in the same shell (level).

2. The suborbital quantum number or the angular quantum number (ɭ):

Describe the shape of the orbitals or the electron cloud.
This number can assume integer values limited by the corresponding value of n.
ɭ = 0 , 1, 2 , ... (n – 1) It divides the shells into smaller subshells.

Value of l	0	1	2	3
Type of orbital	s	p	d	f

Example:

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

The orbitals have points with zero probability of finding an electron. These are called nodes and the nodal planes pass through the nucleus of the atom.

3. The magnetic quantum number (m_l):

- Specifies the orientation in space of an orbital of a given energy(n) and shape l The value of m_l = …, - 1, 0 , + 1, …

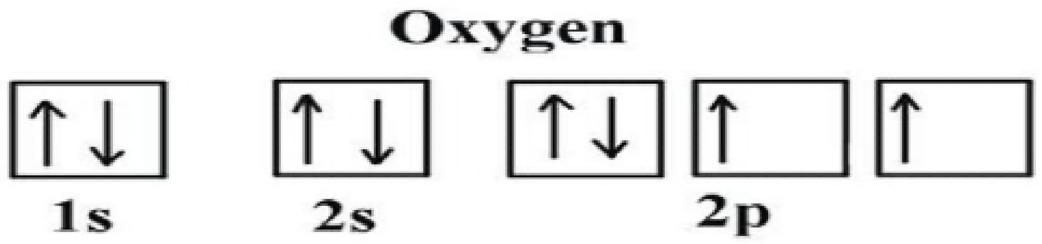
This number divides the subshells into individual orbitals which hold the electrons. there are $2l$ +1 orbitals in each subshell.

- For example, if the value of l = 1 (p orbital), you can write three values for this number: –1, 0, and +1.

This means that there are three different p subshells for a particular orbital.

The subshells have the same energy but different orientations in space.

- (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)



4. The spin quantum number (ms):

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.

Only two values are allowed: +1/2 or –1/2

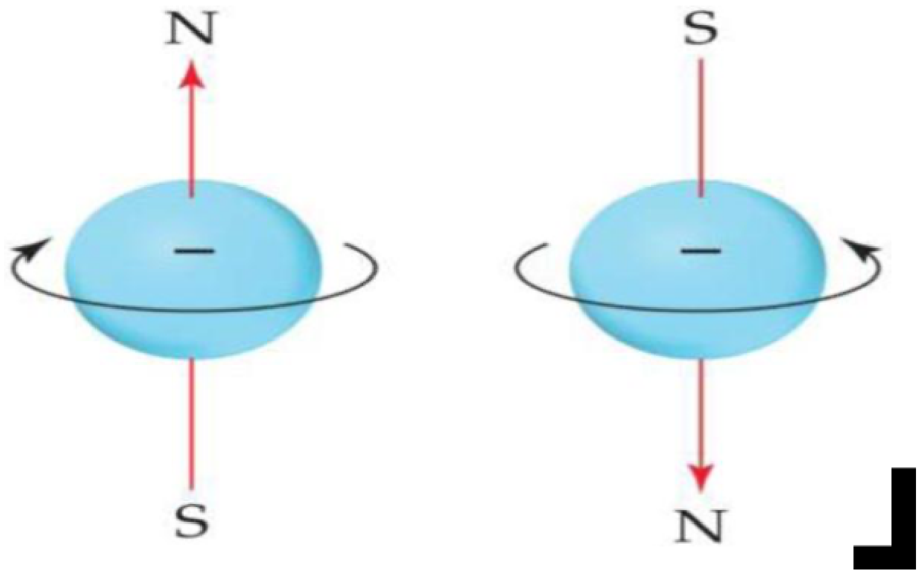


Table 1-1 Values of Quantum Numbers and Orbital State

Quantum Numbers			Orbital
n	*l*	m_l	
1	0	0	1*s*
2	0	0	2*s*
	1	+1, 0, -1	$2p_x$, $2p_y$, $2p_z$
3	0	0	3*s*
	1	+1, 0, -1	$3p_x$, $3p_y$, $3p_z$
	2	+2, +1, 0, -1, -2	$3d_{xy}$, $3d_{xz}$, $3d_{yz}$, $3d_{x^2-y^2}$, $3d_{z^2}$
4	0	0	4*s*
	1	+1, 0, -1	$4p_x$, $4p_y$, $4p_z$
	2	+2, +1, 0, -1, -2	$4d_{xy}$, $4d_{xz}$, $4d_{yz}$, $4d_{x^2-y^2}$, $4d_{z^2}$
	3	+3, +2, +1, 0, -1, -2, -3	4*f*

Ionization

- - When an atom gains an electron, it becomes negatively charged (more electrons than protons) and is called an anion.
- - In the same way that nonmetal atoms can gain electrons,
- - metal atoms can lose electrons and they become positively charged cations.
- - Cations are always smaller than the original atom.
- - Conversely, anions are always larger than the original atom.

$$Co^0 \xrightarrow{-2e^-} Co^{2+}$$

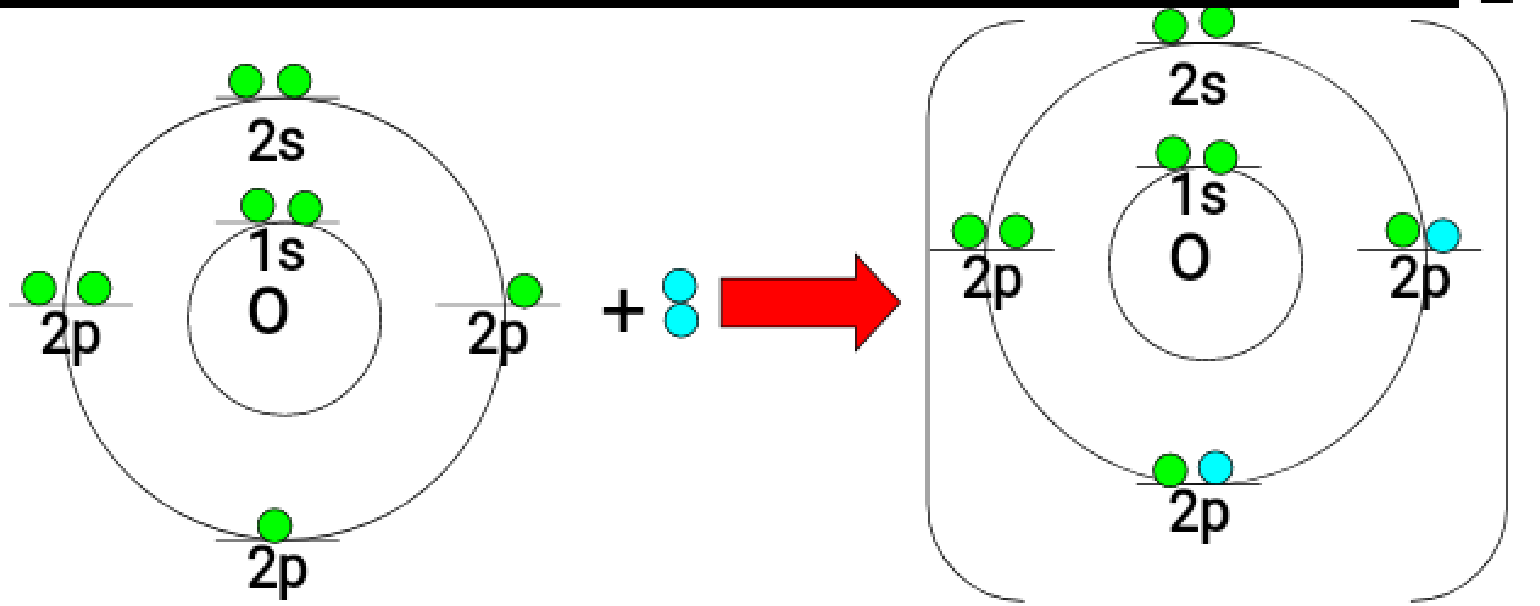
$$Na^0 \xrightarrow{-1e^-} Na^+$$

$$O \xrightarrow{+2e^-} O^{2-}$$

$$Mg^0 \xrightarrow{-2e^-} Mg^{2+}$$

$$Ga \xrightarrow{-3e^-} Ga^{3+}$$

ANION = atom with a NEGATIVE charge



$O + 2e^{-}$ □ O^{2-}

Oxidation states

- The elements of boron family have $2s^2$ $2p^1$ configuration which means that they have 3 valance electron available for bond formation. By loosing these electrons they are accepted to show +3 oxidation states in there compounds.

The Periodic Law

- When elements are arranged in order of increasing atomic number,
  there is a periodic repetition of their physical and chemical properties.

- Horizontal rows = periods There are 7 periods

- Vertical column = group (or family) Similar physical & chemical prop. Identified by number & letter (IA, IIA)

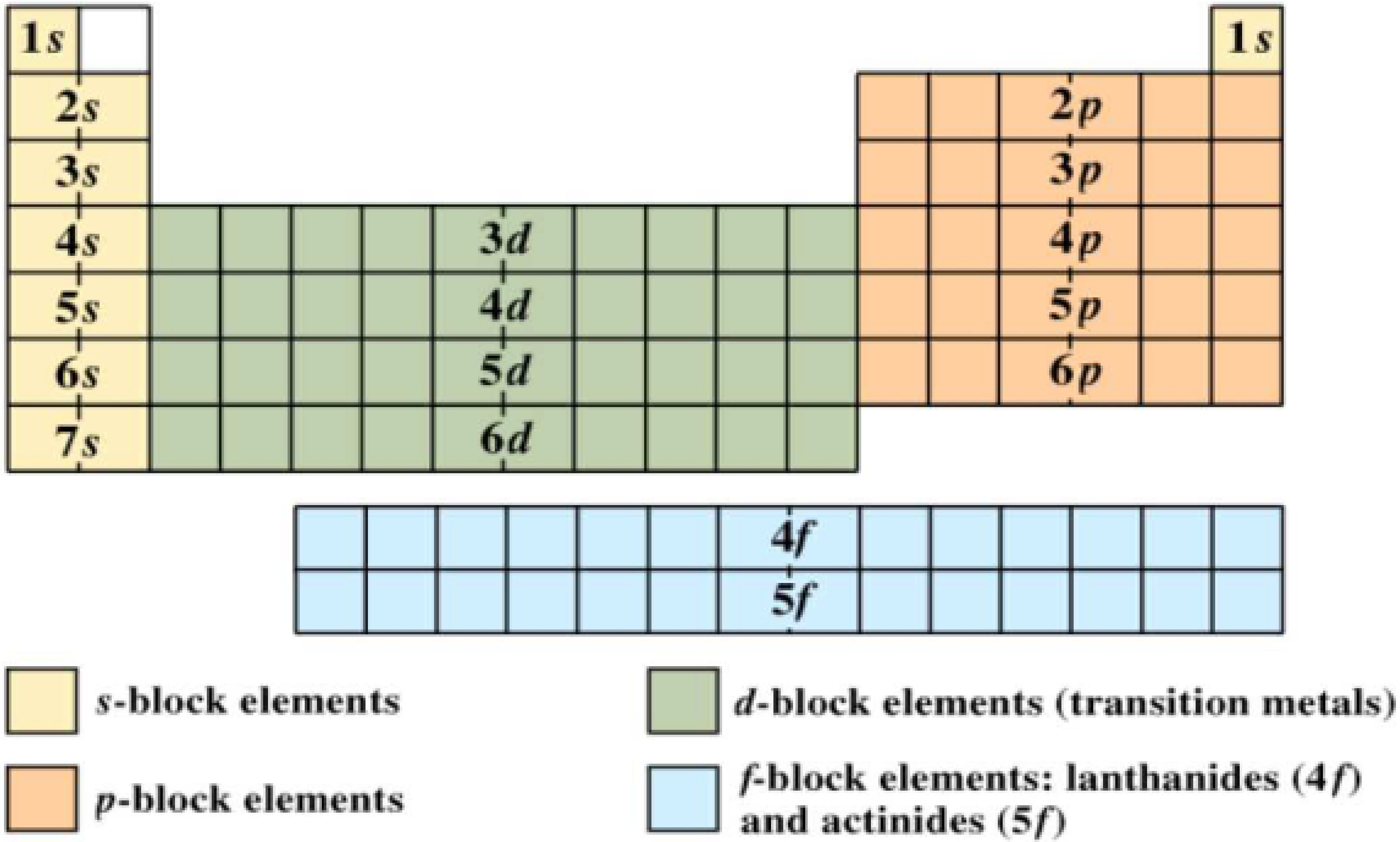
Periodic table of the elements

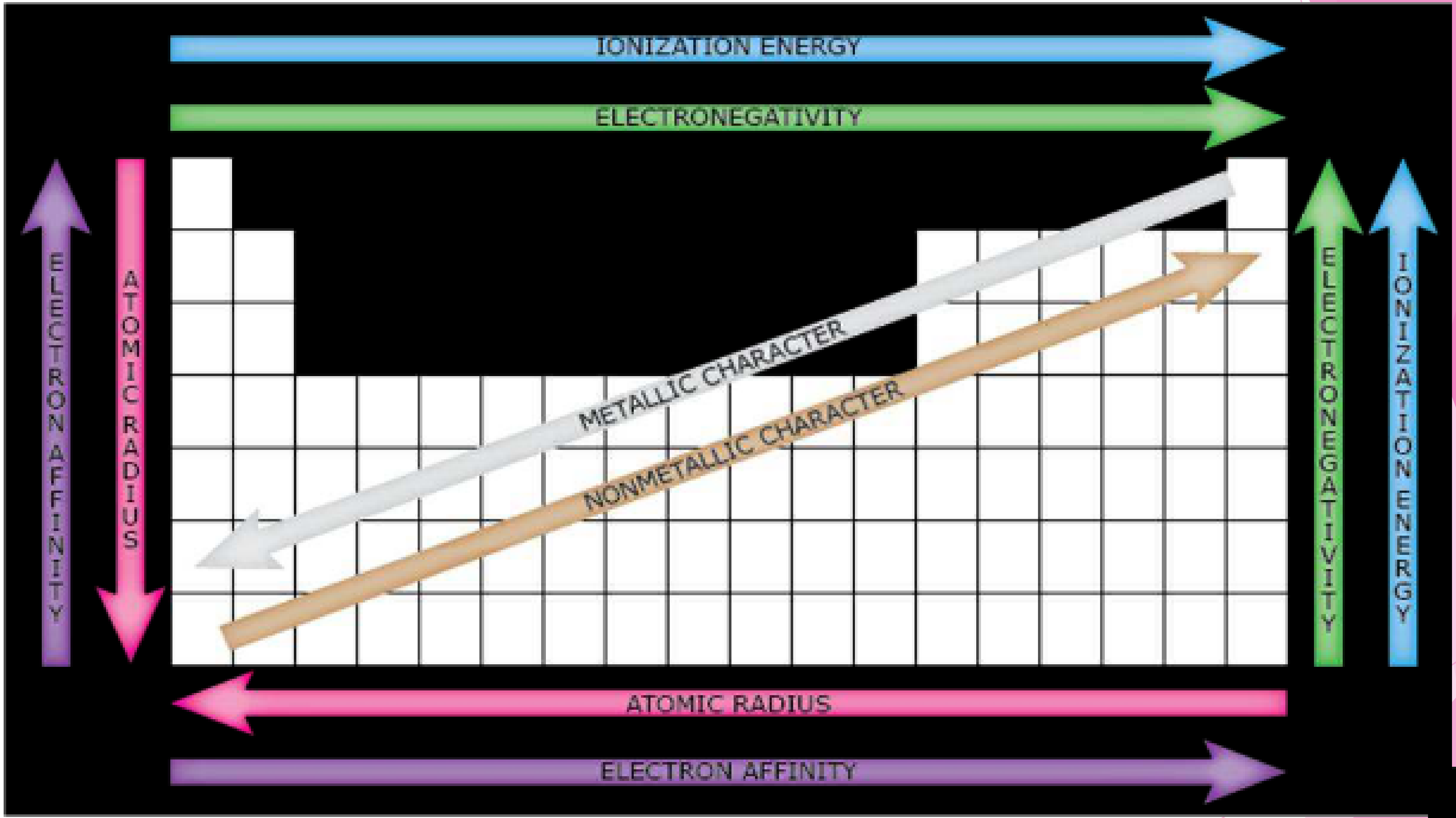
- Alkali metals
- Alkaline-earth metals
- Transition metals
- Other metals
- Other nonmetals
- Halogens
- Noble gases
- Rare-earth elements (21, 39, 57–71) and lanthanoid elements (57–71 only)
- Actinoid elements

period \ group	1*	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	1 H																	2 He
2	3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
3	11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
4	19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
5	37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
6	55 Cs	56 Ba	57 La	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
7	87 Fr	88 Ra	89 Ac	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Nh	114 Fl	115 Mc	116 Lv	117 Ts	118 Og

lanthanoid series	6	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu
actinoid series	7	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr

Electron configuration and the periodic table




IONIZATION ENERGY
ELECTRONEGATIVITY
ELECTRON AFFINITY
ATOMIC RADIUS
METALLIC CHARACTER
NONMETALLIC CHARACTER
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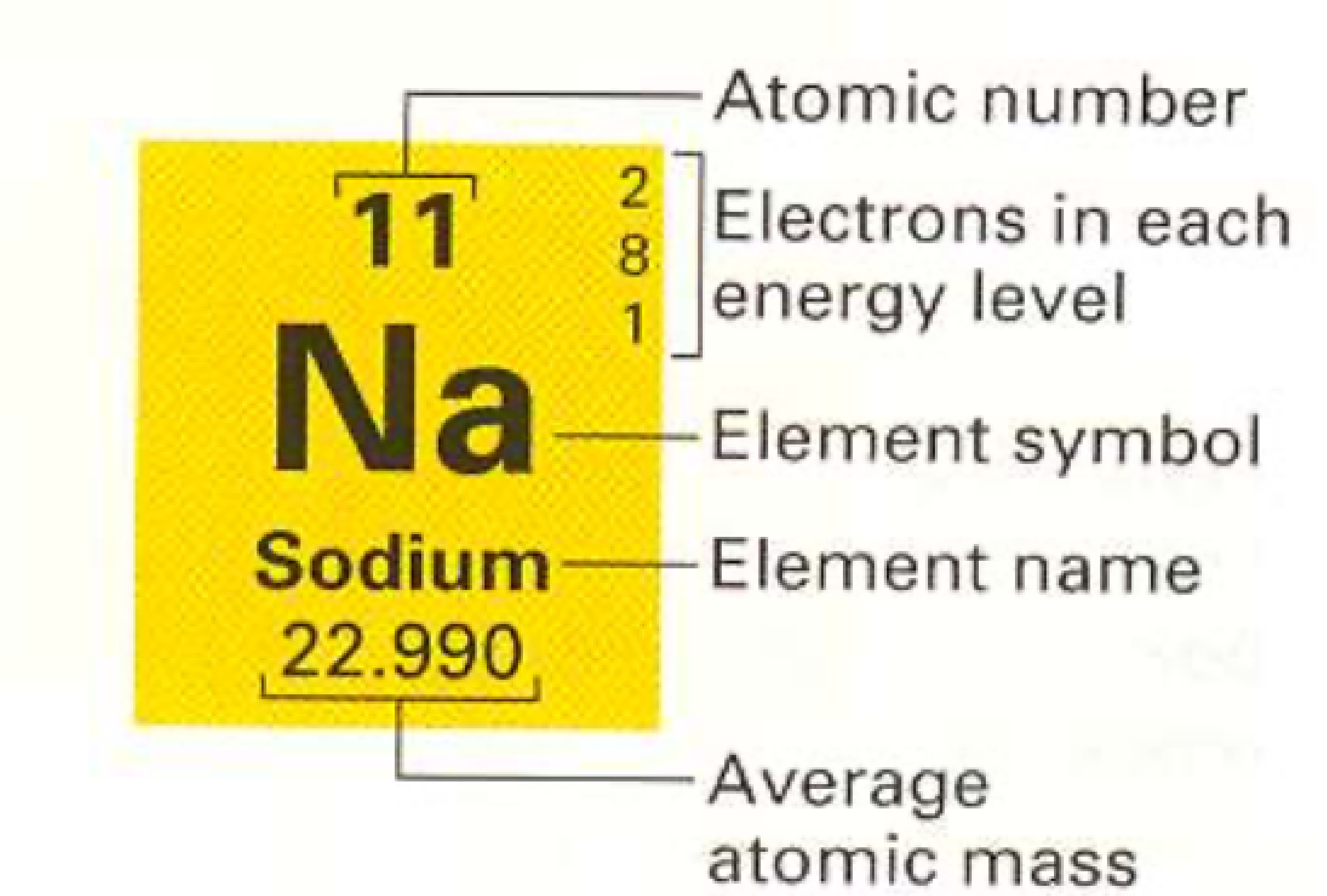
Classifying the Elements

Classify elements based on electron configuration



Best Regards!

Thank you!