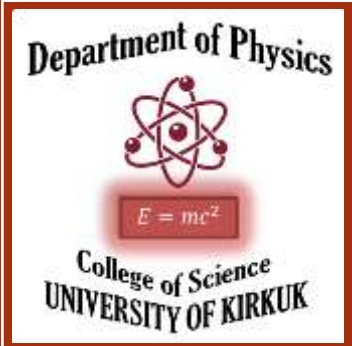

ATOMIC STRUCTURE

Subject: Material Science - Lecture #2

مدرسة المادة : الدكتورة روژه برهان الدين عبدالرحمن

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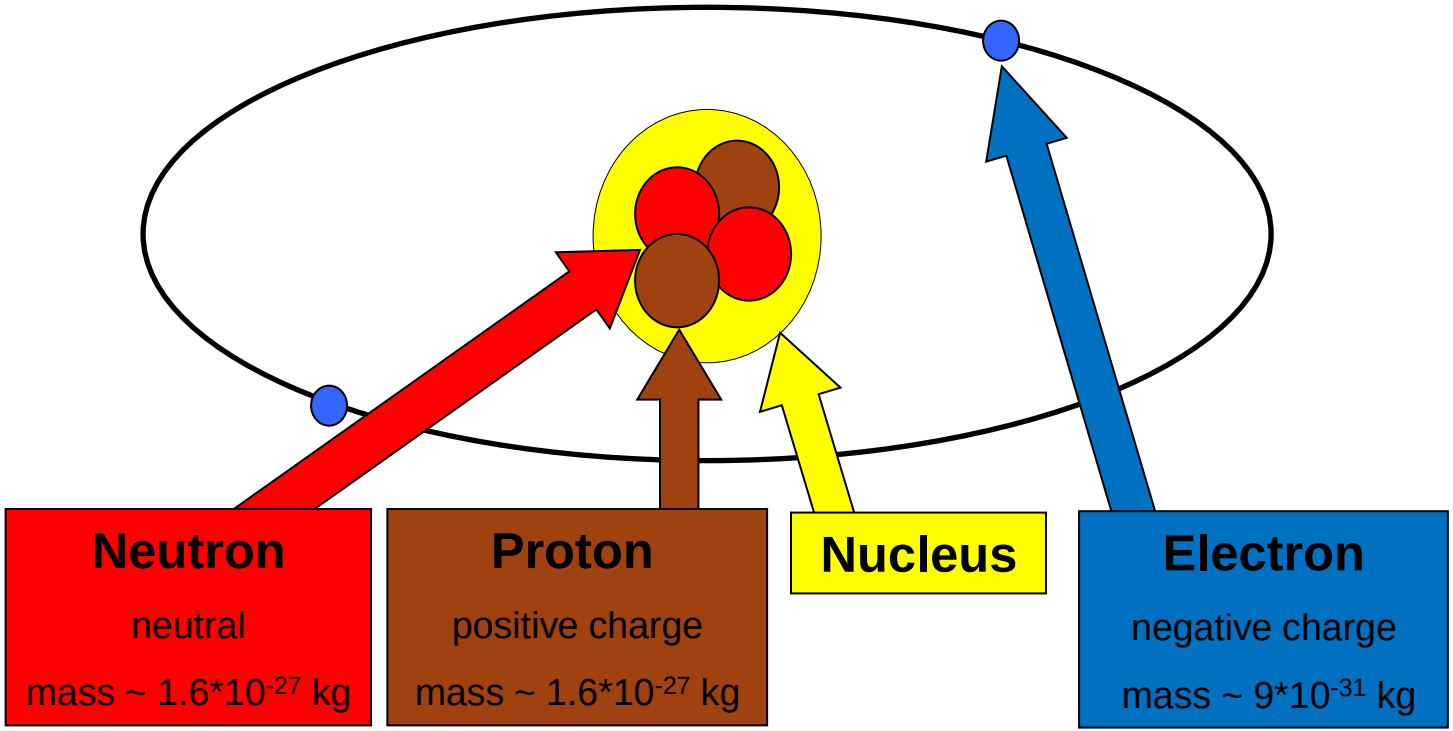
INTRODUCTION

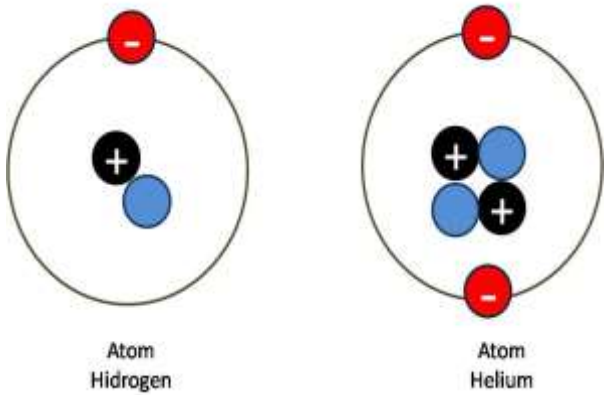
Some of the important properties of solid materials depend on geometric atomic arrangements and also the interactions that exist among constituent atoms or molecules.

Atomic Structure
FUNDAMENTAL CONCEPTS



atomic number (Z) is the number of protons in the nucleus for each chemical element.

- For an electrically neutral or complete atom, the atomic number also equals the number of electrons.

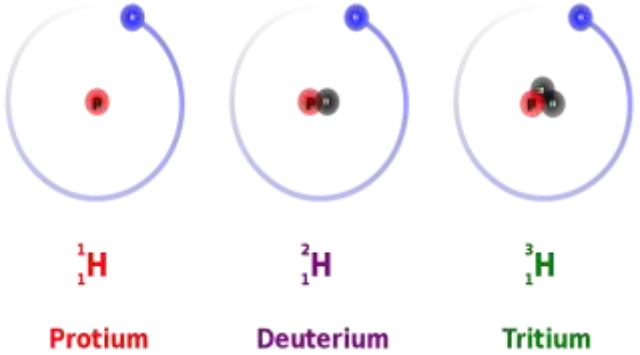


The atomic mass (*A*) is the sum of the masses of protons and neutrons within the nucleus.

$$A \cong Z + N \quad \ldots\ldots\ldots (1)$$

- Although the number of protons is the same for all atoms of a given element, the number of neutrons (N) may be variable. Thus atoms of some elements have two or more different atomic masses, which are called isotopes .

isotopes are elements with the same atomic number but different mass numbers



uranium-235 (U-235) has an AMU of approximately 235, while uranium-238 (U-238) is slightly more massive.

The difference results from the fact that U-238, the most abundant naturally occurring isotope of uranium, has three more neutrons than U-235, an isotope that has been used in nuclear reactors and atomic bombs.

The **atomic weight** of an element corresponds to the weighted average of the atomic masse of the atom's naturally occurring isotopes.

- Atomic weight of carbon is 12.011 amu.
- The atomic weight of an element or the molecular weight of a compound may be specified on the basis of amu per atom (molecule) or mass per mole of material
- The term *atomic mass* is really more accurate than *atomic weight*, we are dealing with masses and not weights. However, atomic weight is, by convention, the preferred terminology.

The **atomic mass unit (amu)** (is a unit measurement for atoms and molecules like the mass of human expressed by kg or Ib) may be used to calculate atomic weight.

For example hydrogen has atomic number of 1 and an atomic mass of 1.00794 amu
According to international union of pure and applied chemistry (IUPAC) 1 amu is defined as $\frac{1}{12}$ of the atomic mass of the most common isotope of carbon , therefore carbon 12 (^{12}C) has a mass of 12 aum (A =12.00000).

Why is carbon the standard?
Carbon is commonly combined with other elements; additionally, the carbon-12 isotope is highly abundant in nature.
After many years of arguing, chemists and physicists agreed that carbon-12 would be the best unit of measurement for atomic masses. Previous standards included hydrogen and oxygen; however, scientists had difficulty using these elements as standards due to the distribution of their isotopes.

In one **mole** of a substance, there are 6.022×10^{23} (Avogadro's number) atoms or molecules.

$$1 \frac{\text{amu}}{\text{atom (or molecule)}} = 1 \frac{\text{g}}{\text{mol}}$$

For example, the atomic weight of iron is

$$55.85 \frac{\text{amu}}{\text{atom}} = 55.85 \frac{\text{g}}{\text{mol}}$$

EXAMPLE

Average Atomic Weight Computation for Cerium

Cerium has four naturally occurring isotopes:
0.185% of $^{136}\mathrm{Ce}$, with an atomic weight of 135.907 amu;
0.251% of $^{138}\mathrm{Ce}$, with an atomic weight of 137.906 amu;
88.450% of $^{140}\mathrm{Ce}$, with an atomic weight of 139.905 amu;
and 11.114% of $^{142}\mathrm{Ce}$, with an atomic weight of 141.909 amu.
Calculate the average atomic weight of Ce.

Solution

The average atomic weight of element M, $\bar{A}_M$, is computed by adding fraction of occurrence atomic weight products for all its isotopes; that is,

$$\bar{A}_M = \sum_i f_{iM} A_{iM} \qquad \ldots\ldots\ldots (2)$$

f_{iM} is the fraction-of-occurrence of isotope i for element M (i.e., the percentage of-occurrence divided by 100).

A_{iM} is the atomic weight of the isotope.

$$\bar{A}_M = f_{^{136}\mathrm{Ce}} A_{^{136}\mathrm{Ce}} + f_{^{138}\mathrm{Ce}} A_{^{138}\mathrm{Ce}} + f_{^{140}\mathrm{Ce}} A_{^{140}\mathrm{Ce}} + f_{^{142}\mathrm{Ce}} A_{^{142}\mathrm{Ce}}$$

$$\bar{A}_M = f_{^{136}\mathrm{Ce}} A_{^{136}\mathrm{Ce}} + f_{^{138}\mathrm{Ce}} A_{^{138}\mathrm{Ce}} + f_{^{140}\mathrm{Ce}} A_{^{140}\mathrm{Ce}} + f_{^{142}\mathrm{Ce}} A_{^{142}\mathrm{Ce}}$$

$$\bar{A}_M = \left(\frac{0.185\%}{100}\right)(135.907\mathrm{amu}) + \left(\frac{0.251\%}{100}\right)(137.906\mathrm{amu}) + \left(\frac{88.450\%}{100}\right)(139.905\mathrm{amu}) + \left(\frac{11.114\%}{100}\right)(141.909\mathrm{amu})$$

$$\bar{A}_M = (0.00185)(135.907\ \mathrm{amu}) + (0.00251)(137.906\ \mathrm{amu}) + (0.8845)(139.905\ \mathrm{amu}) + (0.11114)(141.909\ \mathrm{amu})$$

$$\bar{A}_M = 140.115\ \mathrm{amu}$$

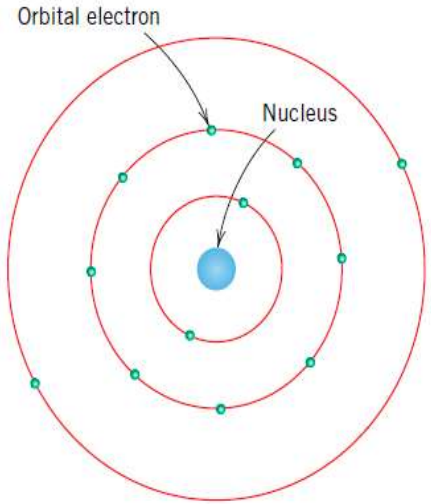
ELECTRONS IN ATOMS

Atomic Models

During the latter part of the nineteenth century, it was realized that many phenomena involving electrons in solids could not be explained in terms of classical mechanics. What followed was the establishment of a set of principles and laws that govern systems of atomic and subatomic that known as **quantum mechanics**.

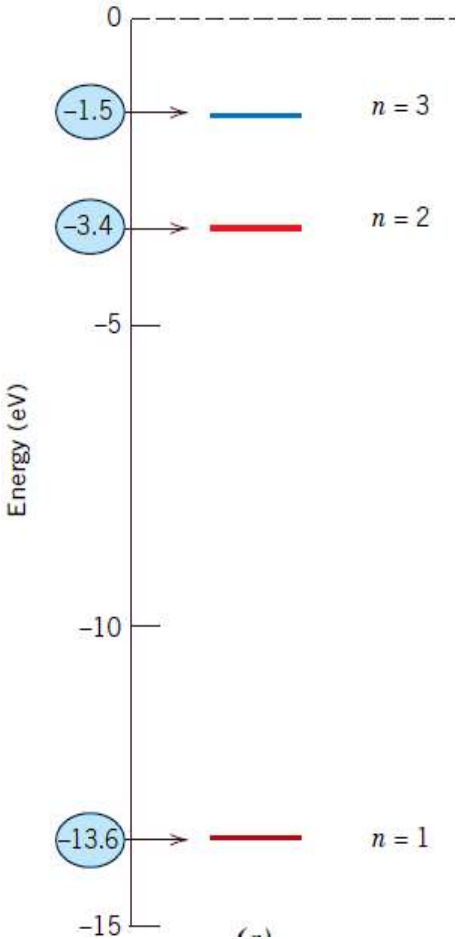
Bohr atomic model in which electrons are assumed to revolve around the atomic nucleus in discrete orbitals, and the position of any particular electron is more or less well defined in terms of its orbital.

- The energies of electrons are quantized that is, electrons are permitted to have only specific values of energy.
- An electron may change energy, but in doing so, it must make a quantum jump either to an allowed higher energy (with absorption of energy) or to a lower energy (with emission of energy).



- The allowed electron energies is associated with energy levels or states.
- The energy states do not vary continuously with energy
- The adjacent states are separated by finite energies.

For example, allowed states for the Bohr hydrogen atom are represented in Figure. These energies are taken to be negative, whereas the zero reference is the unbound or free electron. Of course, the single electron associated with the hydrogen atom fills only one of these states.



- The Bohr model represents an early attempt to describe electrons in atoms, in terms of both position (electron orbitals) and energy (quantized energy levels).
- This Bohr model was eventually found to have some significant limitations because of its inability to explain several phenomena involving electrons.
- A resolution was reached with a **wave-mechanical model**, in which the electron is considered to exhibit both wavelike and particle-like characteristics.

wave-mechanical model an electron is no longer treated as a particle moving in a discrete orbital; rather, position is considered to be the probability of an electron's being at various locations around the nucleus. In other words, position is described by a probability distribution or electron cloud.

Electron energy states for the first three shells of the wave-mechanical hydrogen atom.

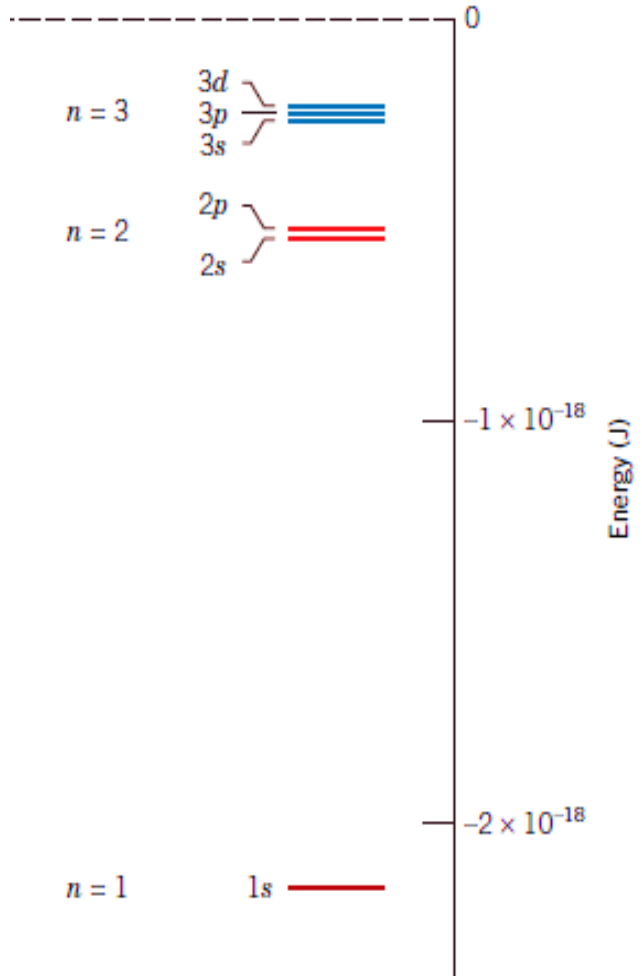
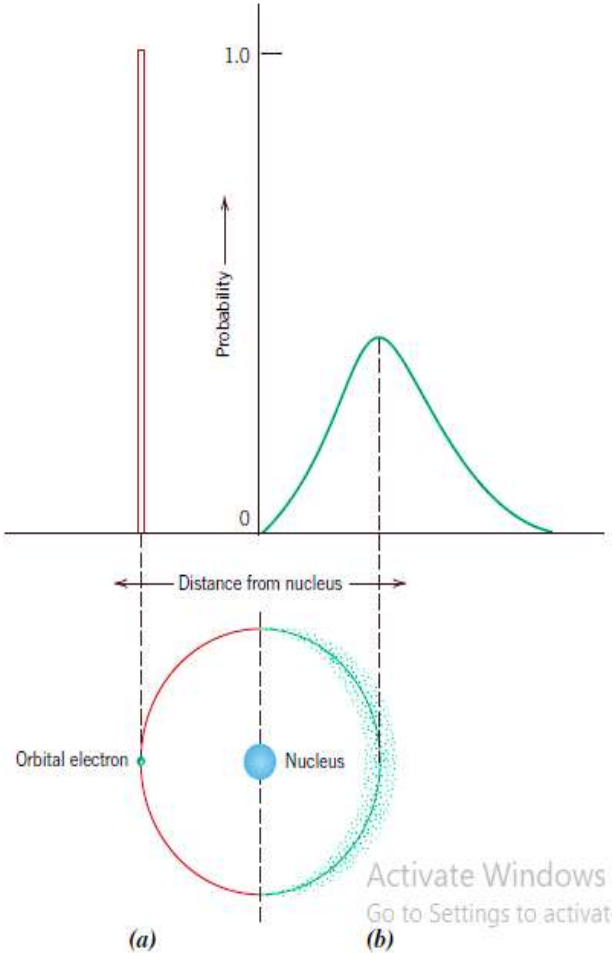


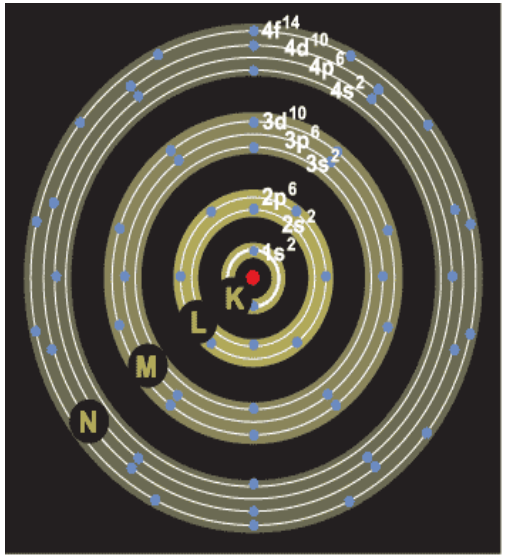
Figure shows comparison of the (a) Bohr and (b) wave mechanical atom models in terms of electron distribution for the hydrogen atom..



Quantum Numbers

In wave mechanics, every electron in an atom is characterized by four parameters called quantum numbers. The size, shape, and spatial orientation of an electron's probability density (or orbital) are specified by three of these quantum numbers.

- Bohr energy levels separate into electron subshells,
- The quantum numbers dictate the number of states within each subshell.
- Shells are specified by a *principal quantum number* n, sometimes these shells are designated by *X-ray notation* by the letters *K*, *L*, *M*, *N*, *O*, and so on, which correspond, respectively, to $n = 1, 2, 3, 4, 5, \ldots,$



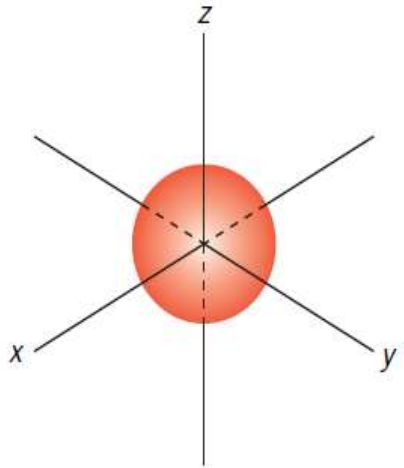
Summary of the Relationships among the Quantum Numbers n, l, m_l and Numbers of Orbitals and Electrons. Note: this quantum number is also associated with the Bohr model

Value of n	*Value of l*	*Values of m_l*	*Subshell*	*Number of Orbitals*	*Number of Electrons*
1	0	0	1*s*	1	2
2	0	0	2*s*	1	2
	1	−1, 0, +1	2*p*	3	6
3	0	0	3*s*	1	2
	1	−1, 0, +1	3*p*	3	6
	2	−2, −1, 0, +1, +2	3*d*	5	10
4	0	0	4*s*	1	2
	1	−1, 0, +1	4*p*	3	6
	2	−2, −1, 0, +1, +2	4*d*	5	10
	3	−3, −2, −1, 0, +1, +2, +3	4*f*	7	14

- The quantum number is related to the size of an electron's orbital (or its average distance from the nucleus).
- The second (or *azimuthal*) quantum number, l, designates the subshell.
- Values of l are restricted by the magnitude of n and can take on integer values that range from $l = 0 \, to \, l = (n - 1)$.
- Each subshell is denoted by a lowercase letter an *s*, *p*, *d*, or *f* related to l values as follows:

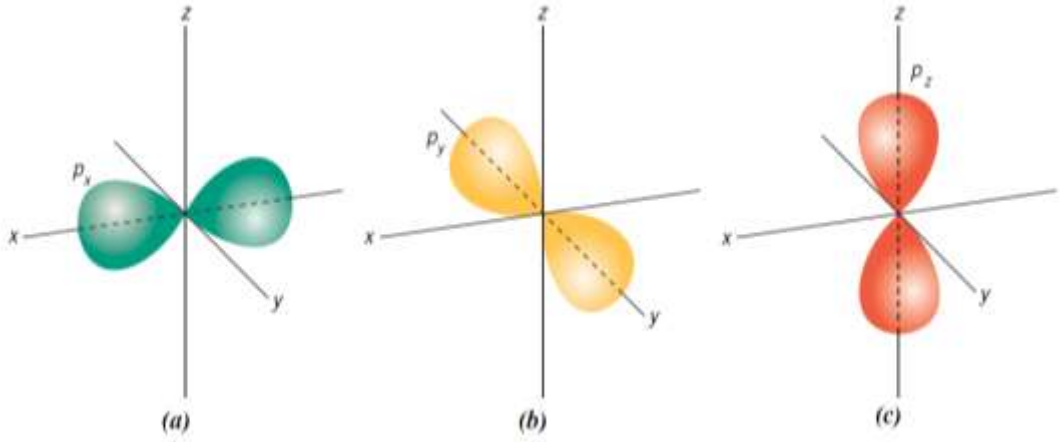
Value of l	*Letter Designation*
0	*s*
1	*p*
2	*d*
3	*f*

electron orbital shapes depend on l.
For example *s* orbitals are spherical and centered on the nucleus.



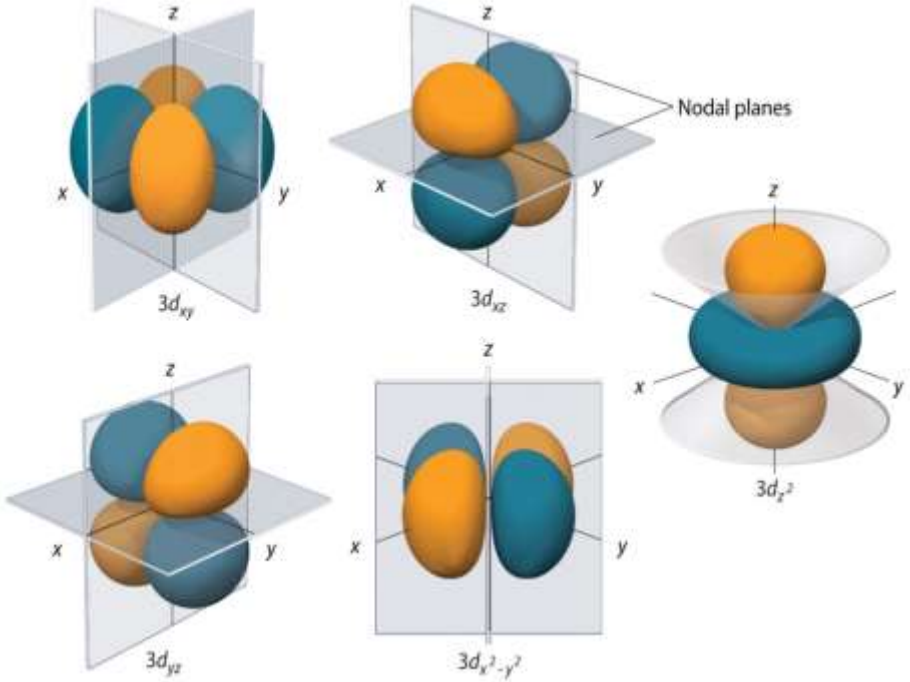
Spherical shape of an *s* electron orbital.

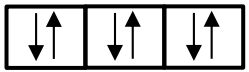
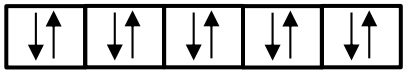
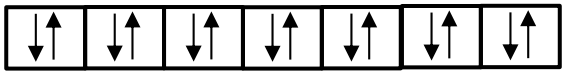
p subshell has three orbitals each has a nodal surface in the shape of a dumbbell (Figure 2.5). Axes for these three orbitals are mutually perpendicular to one another like those of an x-y-z coordinate system; thus, it is convenient to label these orbitals $p_x, p_y \; and \; p_z$.



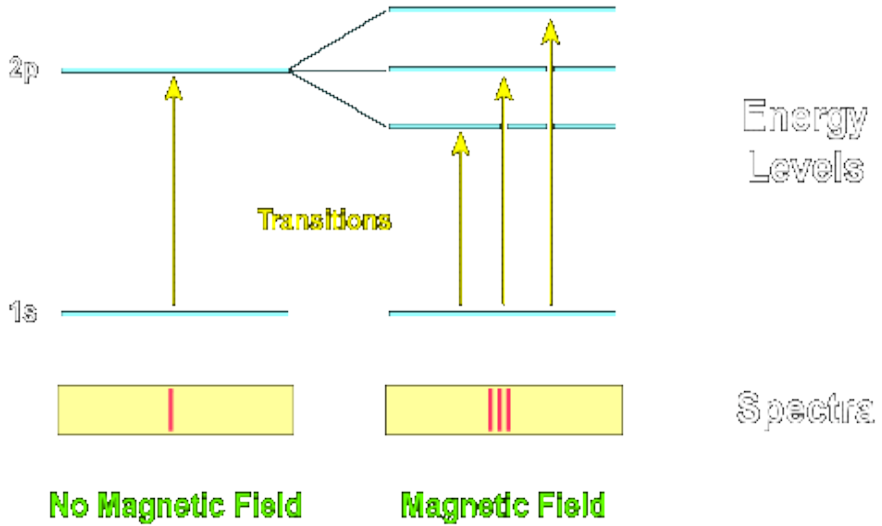
Orientations and shapes of (*a*) p_x, (*b*) p_y, and (*c*) p_z electron orbitals.

Orbital configurations for *d* subshells are more complex.

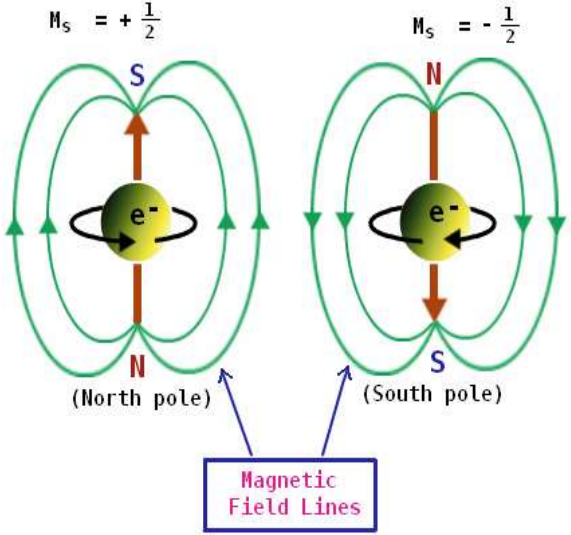


- The number of electron orbitals for each subshell is determined by the third (or magnetic) quantum number, m_l
- m_l can take an integer values between l and $-l$, including 0.
- When $l = 0$, m_l can only have a value of 0 because +0 and -0 are the same. This corresponds to an s subshell, which can have only one orbital  .
- for $l = 1$, m_l can take values of -1, 0, and +1, and three p orbitals  are possible.
- Similarly d subshells have five orbitals  , and f subshells have seven  .

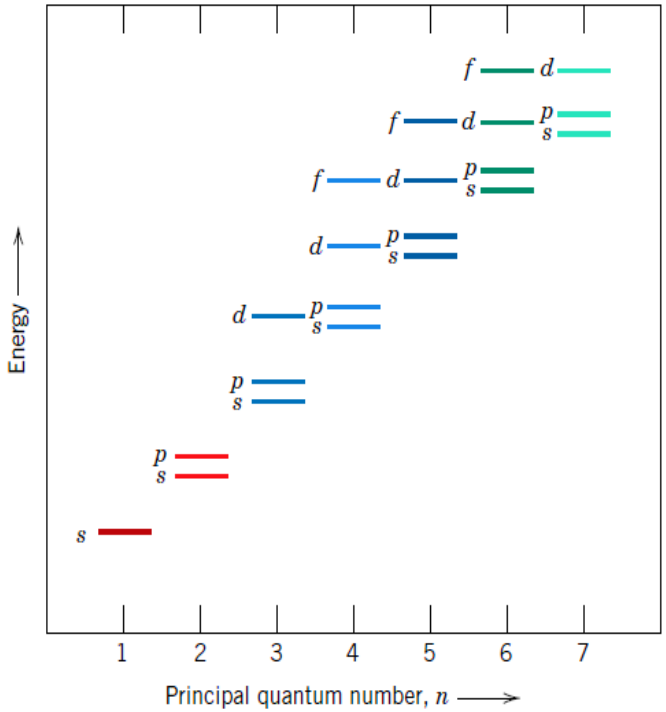
In the absence of an external magnetic field, all orbitals within each subshell are identical in energy.
When a magnetic field is applied, these subshell states split, with each orbital assuming a slightly different energy.



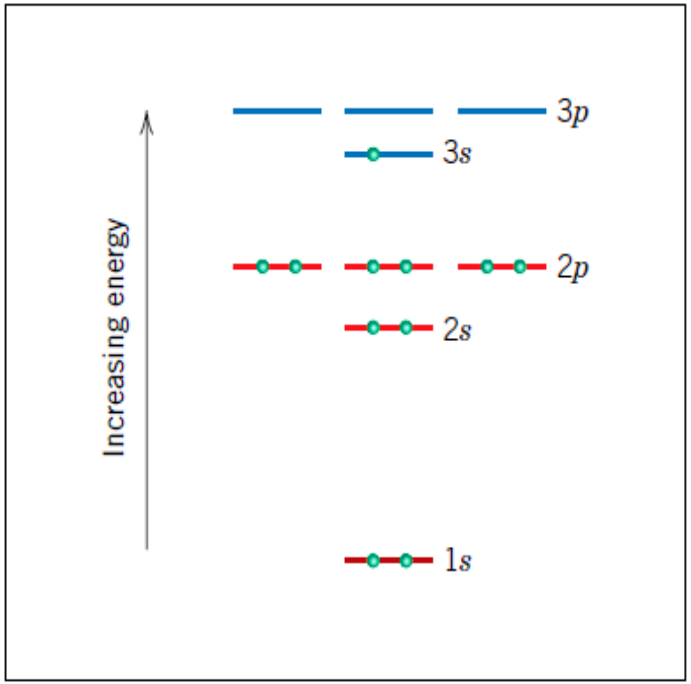
A *spin moment* (m_s) is associated with each electron, which must be oriented either up or down.
The spin moment is the fourth quantum number for which two values are possible: $+\frac{1}{2}$ (for spin up) and $-\frac{1}{2}$ (for spin down)



A complete energy level diagram for the various shells and subshells using the wave-mechanical model is shown in Figure



Schematic representation of the filled and lowest unfilled energy states for a sodium atom (atomic number (Z) of Na =11).



Electron Configurations

- The preceding discussion has dealt with **electron states** values of energy that are permitted for electrons.
- To determine the manner in which these states are filled with electrons, we use the **Pauli exclusion principle**, another quantum-mechanical concept, which stipulates that each electron state can hold no more than two electrons that must have opposite spins.

Thus, s, p, d, and f subshells may each accomodate, respectively, a total of 2, 6, 10, and 14 electrons

- not all possible states in an atom are filled with electrons. For most atoms, the electrons fill up the lowest possible energy states in the electron shells and subshells, two electrons (having opposite spins) per state.
- When all the electrons occupy the lowest possible energies an atom is said to be in its **ground state**. However, electron transitions to higher energy states are possible.
- The **electron configuration** or structure of an atom represents the manner in which these states are occupied. For example, the electron configurations for hydrogen $1s^1$, helium $1s^2$, and sodium $1s^2 2s^2 2p^6 3s^1$

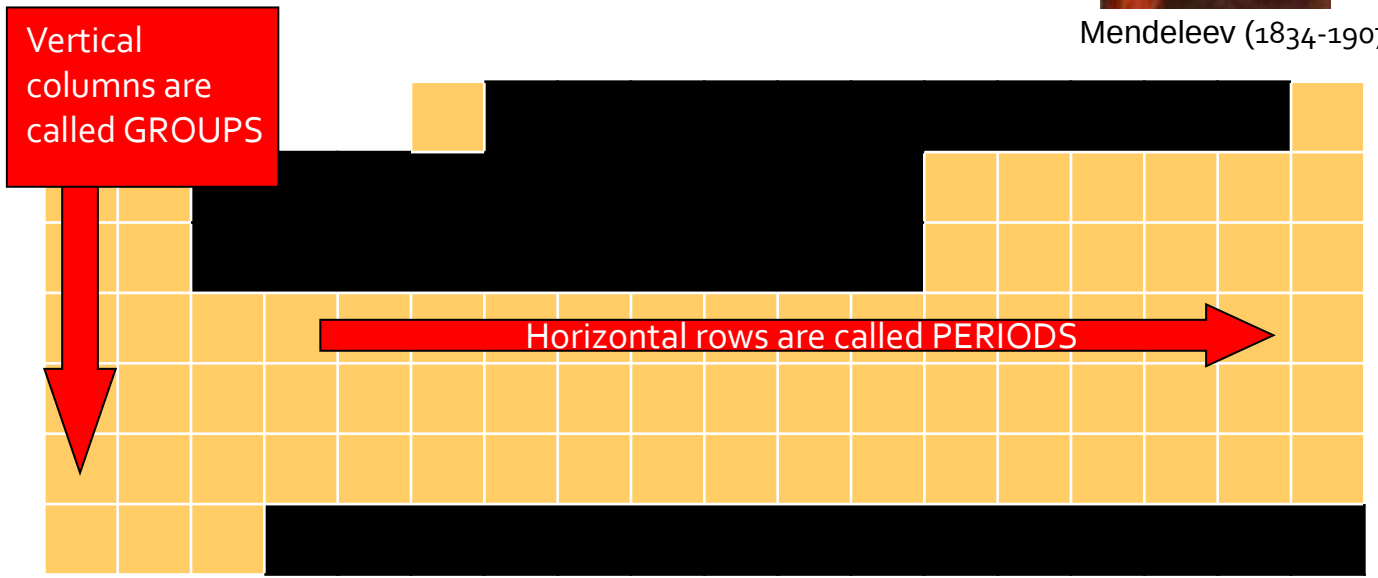
- the **valence electrons** are those that occupy the outermost shell.
- the valence electrons are extremely important they participate in the bonding between atoms to form atomic and molecular aggregates. Furthermore, many of the physical and chemical properties of solids are based on these valence electrons.

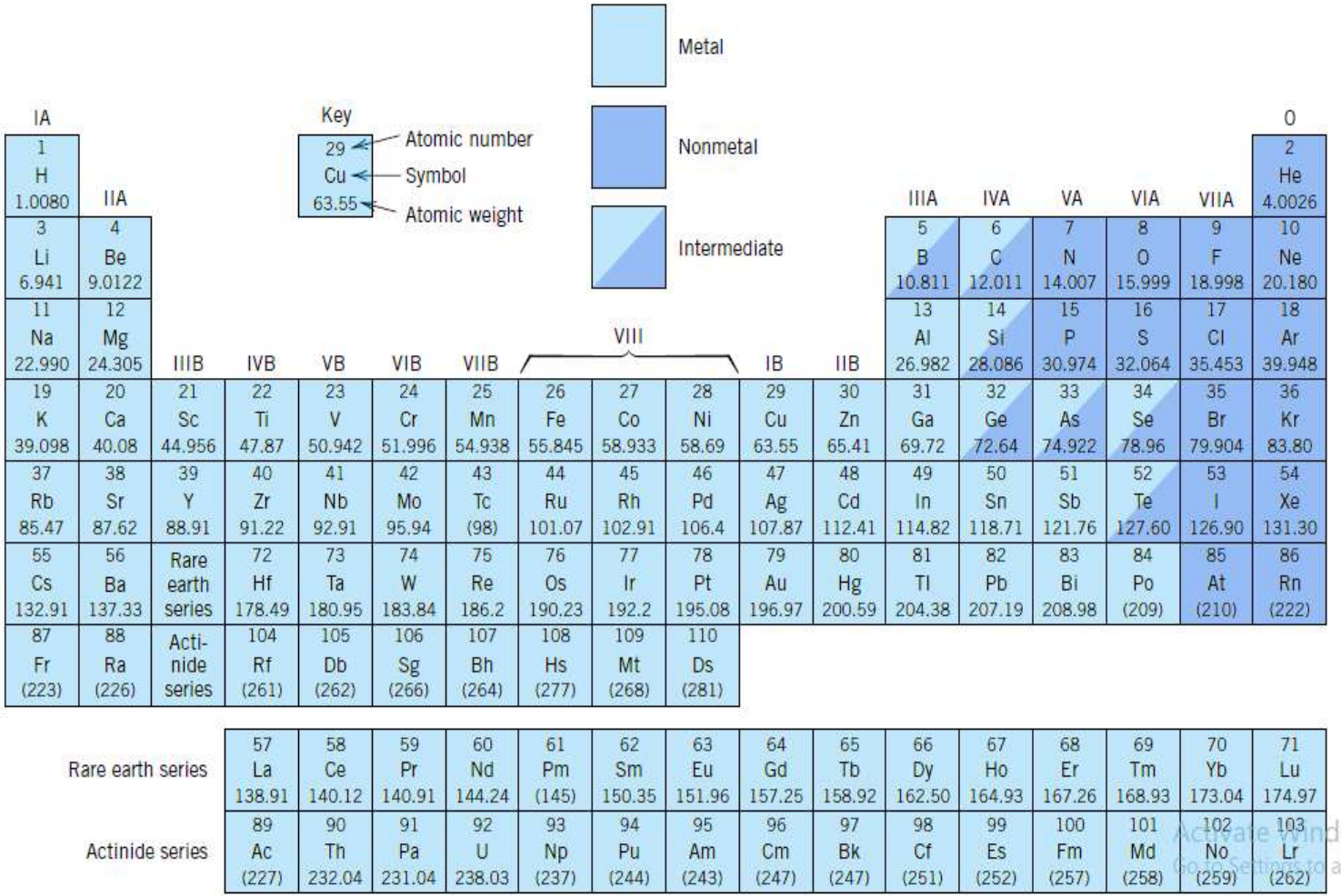
some atoms have what are termed *stable electron configurations* that is, the states within the outermost or valence electron shell are completely filled. this corresponds to the occupation of just the s and p states for the outermost shell by a total of eight electrons, as in neon (Ne, $1s^2 2s^2 2p^6$), argon (Ar, $1s^2 2s^2 2p^6 3s^2 3p^6$), and krypton (Kr, $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6$); one exception is helium (He, $1s^2$). These elements are the inert, or noble, gases, which are virtually unreactive chemically.

THE PERIODIC TABLE

The periodic table arranges all the elements in groups according to their properties.

Mendeleev (1834-1907)

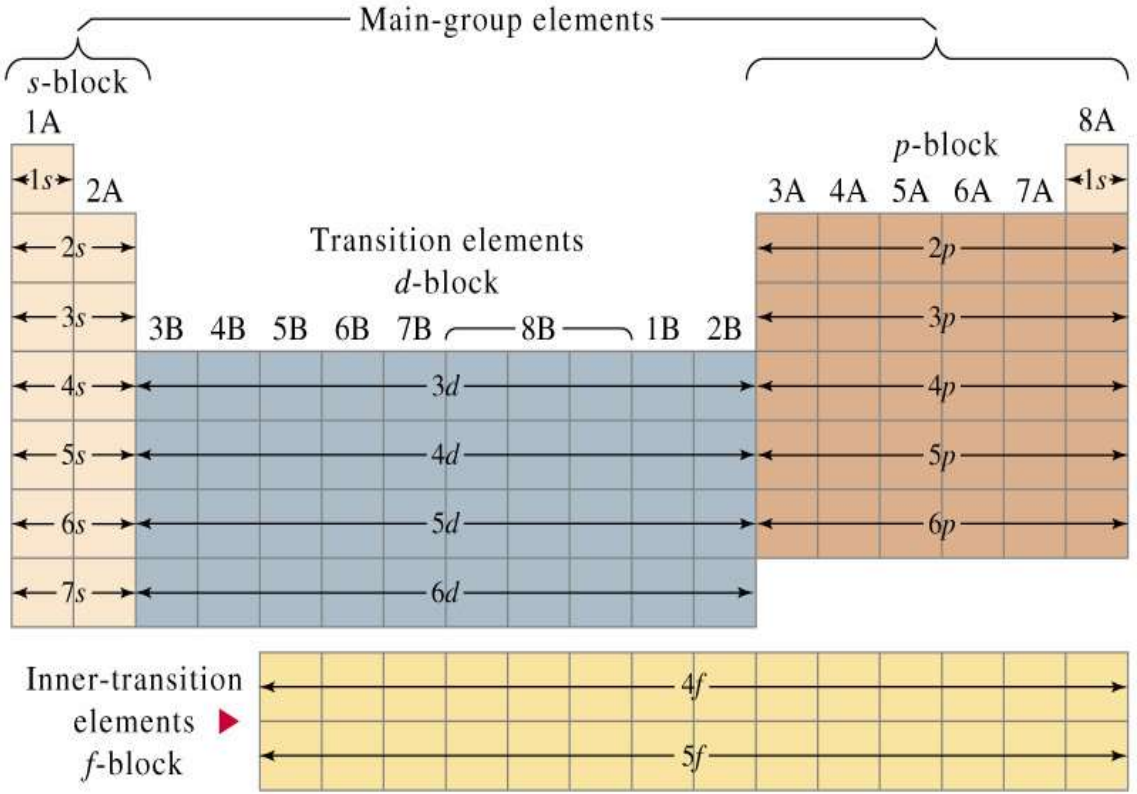




IA												IIIA	IVA	VA	VIA	VIIA	0
1 H 1.0080	IIA																2 He 4.0026
3 Li 6.941	4 Be 9.0122											5 B 10.811	6 C 12.011	7 N 14.007	8 O 15.999	9 F 18.998	10 Ne 20.180
11 Na 22.990	12 Mg 24.305	IIIB	IVB	VB	VIB	VIIB	VIII			IB	IIB	13 Al 26.982	14 Si 28.086	15 P 30.974	16 S 32.064	17 Cl 35.453	18 Ar 39.948
19 K 39.098	20 Ca 40.08	21 Sc 44.956	22 Ti 47.87	23 V 50.942	24 Cr 51.996	25 Mn 54.938	26 Fe 55.845	27 Co 58.933	28 Ni 58.69	29 Cu 63.55	30 Zn 65.41	31 Ga 69.72	32 Ge 72.64	33 As 74.922	34 Se 78.96	35 Br 79.904	36 Kr 83.80
37 Rb 85.47	38 Sr 87.62	39 Y 88.91	40 Zr 91.22	41 Nb 92.91	42 Mo 95.94	43 Tc (98)	44 Ru 101.07	45 Rh 102.91	46 Pd 106.4	47 Ag 107.87	48 Cd 112.41	49 In 114.82	50 Sn 118.71	51 Sb 121.76	52 Te 127.60	53 I 126.90	54 Xe 131.30
55 Cs 132.91	56 Ba 137.33	Rare earth series	72 Hf 178.49	73 Ta 180.95	74 W 183.84	75 Re 186.2	76 Os 190.23	77 Ir 192.2	78 Pt 195.08	79 Au 196.97	80 Hg 200.59	81 Tl 204.38	82 Pb 207.19	83 Bi 208.98	84 Po (209)	85 At (210)	86 Rn (222)
87 Fr (223)	88 Ra (226)	Acti-nide series	104 Rf (261)	105 Db (262)	106 Sg (266)	107 Bh (264)	108 Hs (277)	109 Mt (268)	110 Ds (281)								

Rare earth series	57 La 138.91	58 Ce 140.12	59 Pr 140.91	60 Nd 144.24	61 Pm (145)	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
Actinide series	89 Ac (227)	90 Th 232.04	91 Pa 231.04	92 U 238.03	93 Np (237)	94 Pu (244)	95 Am (243)	96 Cm (247)	97 Bk (247)	98 Cf (251)	99 Es (252)	100 Fm (257)	101 Md (258)	102 No (259)	103 Lr (262)

all elements arrayed in a given column or group have similar valence electron structures, as well as chemical and physical properties. These properties change gradually, moving horizontally across each period and vertically down each column.

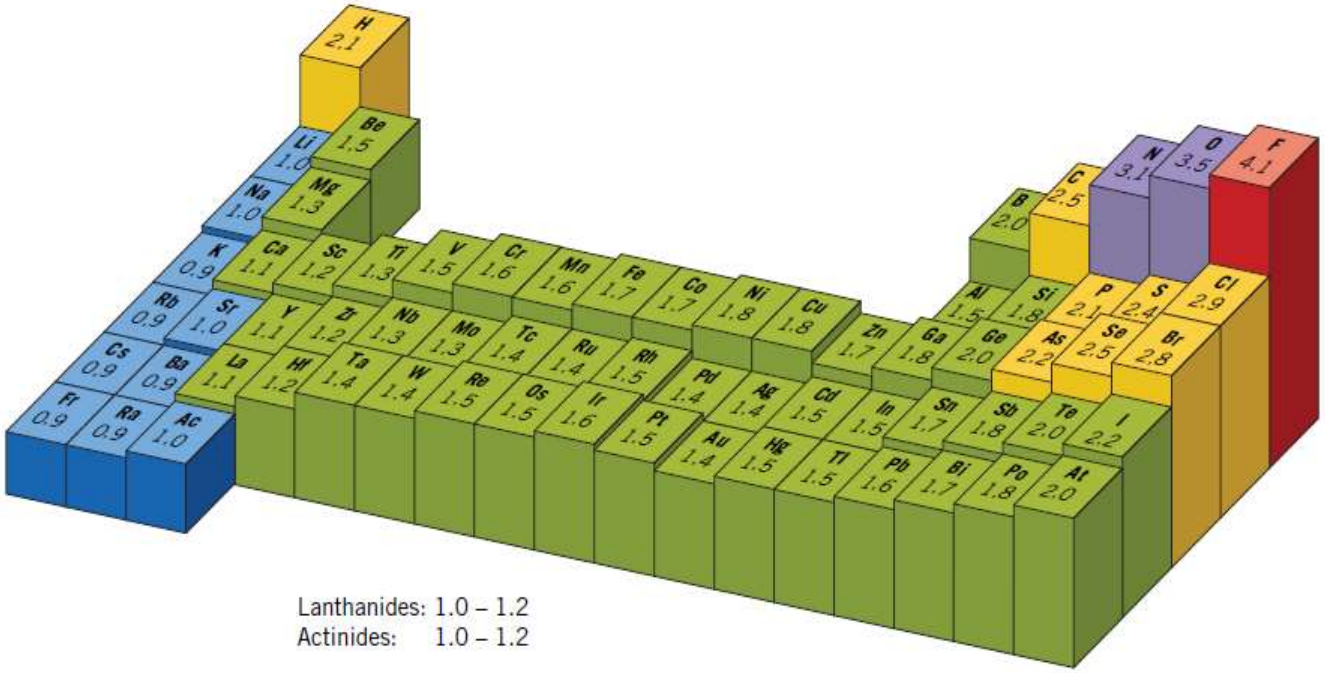


- in Group 0, the rightmost group, are the *inert gases*, which have filled electron shells and stable electron configurations.
- Group VIIA (*halogens*.) and VIA elements are one and two electrons incomplete, respectively, from having stable structures.
- The alkali and the alkaline earth metals (Li, Na, K, Be, Mg, Ca, etc.) are labeled as Groups IA and IIA, having, respectively, one and two electrons in excess of stable structures.

- The elements in the three long periods, Groups IIIB through IIB, are termed the *transition metals,* which have partially filled *d* electron states and in some cases one or two electrons in the next higher energy shell.
- Groups IIIA, IVA, and VA (B, Si, Ge, As, etc.) display characteristics that are intermediate between the metals and nonmetals by virtue of their valence electron structures.

- the elements come under the metal classification sometimes termed **electropositive** elements, indicating that they are capable of giving up their few valence electrons to become positively charged ions.
- the elements situated on the right side of the table are **electronegative**, they readily accept electrons to form negatively charged ions, or sometimes they share electrons with other atoms.

As a general rule, electronegativity increases in moving from left to right and from bottom to top.



The electronegativity values for the elements.

In addition to chemical behavior, physical properties of the elements also tend to vary systematically with position in the periodic table.

- For example, most metals (Groups IIIB through IIB) are relatively good conductors of electricity and heat; nonmetals are typically electrical and thermal insulators.
- Mechanically, the metallic elements exhibit varying degrees of ductility (the ability to be plastically deformed without fracturing. Most of the nonmetals are either gases or liquids, or in the solid state are brittle in nature.

- for the Group IVA elements [C (diamond), Si, Ge, Sn, and Pb], electrical conductivity increases as we move down this column.
- The Group VB metals (V, Nb, and Ta) have very high melting temperatures, which increase in going down this column.

there is not always this consistency in property variations within the periodic table. Physical properties change in a more or less regular manner

Thank you for your attention

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