2.1 - Falsely Positive? The Chemistry of Drugs in Sport

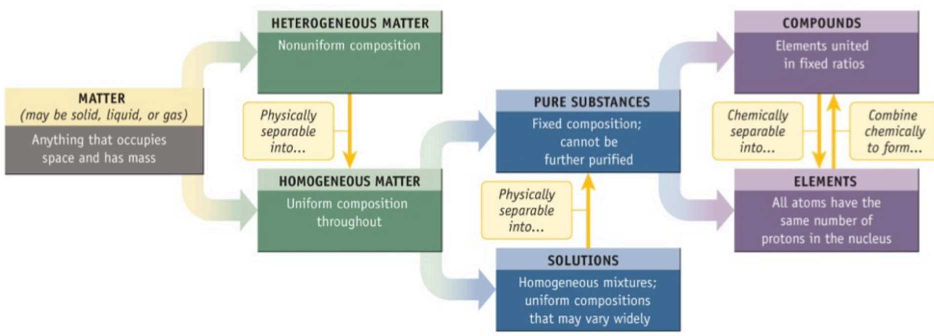
- Can classify performance-enhancing drugs by origin
  - naturally produced in humans through transformation of substances in diet (endogenous)
  - introduced in body from external source, laboratory synthesis (exogenous substances)
  - some substances are both and therefore harder to detect (i.e. steroid testosterone)

- Methods of detecting drugs, like THG (tetrahydrogestrinone), through urine or blood tests using techniques like gas chromatography and mass spectrometry
  - chromatography to separate compounds and spectrometer to analyze and tell mass and structure of molecules
  - in case of endogenous and exogenous substances mix use isotope ratio mass spectrometry
    - after compounds separated, they're burned and carbon-12 and carbon-13 are detected
    - 1% of carbon are C13 naturally, exogenous substances have lower amounts --> starting material used to synthesize them are plants w/ low C12 content (i.e. soy)
    - endogenous substances made from cholesterol (from metabolizing plants and animal protein); slightly higher C13 levels

2.2 - Classifying Matter

- Matter can be classified in many ways:
  - State/phase - solid (rigid shape, fixed volume), liquid (fixed volume but fluid; take the shape of their container), gas (fluids, fill up container they're in), plasma (ionized gases in medium w/ charged particles)

- Kinetic-molecular model of matter used to understand the different phases --> all matter made of constantly moving small particles
  - solids: closely packed, regular array, vibrate rapidly in fixed position
  - liquids and gases: fluid b/c particles not fixed in specific place and move past each other
    - in gases molecules or atoms far apart and move v. quick and collide w/ each other and container
  - higher the temp, faster the movement --> energy of motion (kinetic energy) acts to overcome force of attraction therefore change of state is particles moving so fast they move past each other out of certain positions



Homogenous and Heterogenous Mixtures:

- Mixtures are portions of matter w/ 2 or more chemical substances (referred to as constituents/components)
  - homogenous mixture: uniform, same properties throughout (i.e. air, gasoline, soft drinks)
  - heterogenous mixture: constituents are non-uniform (i.e. ramen, blood)

Pure Substances and Mixtures:

- Pure substances are homogenous, they're forms of matter that contain one constituent
  - substances single pure forms of matter; sometimes mixtures are referred to as substances (mixtures of substances)
  - substance --> water, copper, sugar

2.3 - Three Levels of Operation: Observable, Molecular, Symbolic

- observable level: direct observations from the human eye
  - move on to molecules, atoms, and ions (their arrangement and movement) to understand what was directly seen
- molecular level: particles that cannot be seen
- symbolic level: using words, equations, symbols to communicate ideas

2.4 - Elements and Their Atoms

- Atoms are building blocks of matter, there are different atoms that differ in amount of neutrons, protons, and electrons which are called elements (all atoms in an element are 1 type)
    - atoms of one element cannot be changed into atoms of another (unless unclear transformations are applied)
    - 118 known elements, 90 found in nature, others have been synthesized

- Difference from 1 substance to another:
    - which types of atom
    - relative numbers of each type of atom
    - how the atoms are arranged in relation to each other

2.5 - Compounds

- Compounds diff from substances of the elements they're made from; unique set of properties
    - chemical compounds - substances whose molecules or ions are made of 2 or more diff elements in fixed and definite proportions
        - endless combinations, more than 20 million compounds known, half a million added each year
        - mixture of elements (properties of mixed elements remain observable) vs. chemical compound (diff properties from elements that make it up individually)

Chemical Formulas of Compounds:

- Chemical formula represents composition of compound --> indicates relative numbers of atoms of each element in a sample

2.6 - Chemical Reactions, Chemical Change

- After a chemical reaction we may not be left with the same substances we had prior, but we'll always have the same amount of atoms (maybe rearranged differently)
    - reactants - substances present before reaction
    - products - new substances formed during reaction
        - all can be represented by chemical equation

Chemical and Physical Properties of Substances:

- Differences between substances described in chemical and physical properties
    - chemical properties describe characteristic behaviour in reactions w/ substances (chemical transformation into new substances)
    - physical properties describe colour, state, melting point, boiling point, density etc.

2.7 - Protons, Electrons, and Neutrons: Ideas about Atomic Structure

- Atoms of all elements made of same 3 subatomic particles
    - protons - pos. electrical charge
    - neutrons - electrically neutral
    - electrons - neg. electrical charge

- Mass of protons and neutrons greater than electrons
    - protons + neutrons = small nucleus (basically contains most of the mass of the atom)
        - electrons surround nucleus and occupy mod of the volume of the atom
        - number of electrons around nucleus same as the number of protons in nucleus (therefore atom has 0 electrical charge)

Element Identity and Atomic Number:

- All atoms of an element have the same number of protons in the nucleus (therefore same number of electrons); this is the atomic number (Z)

2.8 - Isotopes of Elements

- Most elements have 2 or more types of atom w/ diff numbers of neutrons
    - atoms of the same element w/ diff numbers of neutrons are isotopes
        - b/c mass of atom depends on mostly protons and neutrons, diff isotopes have diff masses

Isotope Identity and Mass Number:

$^{A}_{Z}E$

- Mass number (*A*) is the sum of protons and neutrons in the atoms of an isotope --> A = Z + # of neutrons

- some isotopes are specially named, like hydrogen's (protium, deuterium, and tritium) --> 2nd is heaviest and 3rd doesn't exist naturally

Isotope Abundance:

- Natural abundance of isotopes influenced by environmental conditions (climate, soil) not only biological pathways
- Proxy measurement --> the measurement of temp through the indirect measurement of isotope ratios of water
- The % abundance of an isotope of an element is the % of atoms of that isotope in relation to the total number of atoms of all the isotopes of the element

$$\textit{Percent abundance} = \frac{\textit{number of atoms of the isotope}}{\textit{total number of atoms of the element}} \times 100\%$$

2.9 - Relative Atomic Masses of Isotopes of and Atomic Mass Units

- Relative atomic mass of an atom of an isotope of any element is its mass on a scale in which the mass of a carbon-12 atom is exactly 12

- Sometimes atomic mass units (u) are used to express masses of atomic particles (carbon-12 atom has mass of 12 u)

$$A_r(^{16}O) = \frac{\text{Mass of an } ^{16}O \text{ atom}}{\text{Mass of a } ^{12}C \text{ atom}} \times 12 = 1.33291 \times 12 = 15.99492$$

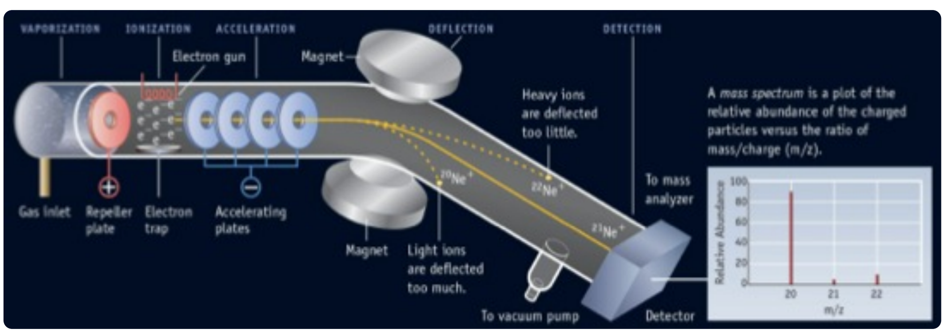
Absolute and relative masses of subatomic particles:

Particle	MASS: Grams	MASS: Atomic Mass Units	Charge	Symbol
Electron	9.109383×10^{-28}	0.0005485799	−1	$^{0}_{-1}e$ or e^-
Proton	1.672622×10^{-24}	1.007276	+1	$^{1}_{1}p$ or p^+
Neutron	1.674927×10^{-24}	1.008665	0	$^{1}_{0}n$ or n^0

* These values and others in the book are taken from the National Institute of Standards and Technology website at http://physics.nist.gov/cuu/Constants/index.html

Measuring Atomic Mass and Isotope Abundance:

- Mass spectrometer used to know the relative atomic masses and abundances of isotopes
    - also used to find identity of molecules of substances
- Steps of mass spectrometer:
    - gas sample of element put into chamber
    - molecules or atoms in sample converted to ions (charged particles, b/c loss of electron)
    - beam of ions directed through magnetic field, paths of ions is deflected (degree of deflection depends on ratio mass/charge)
    - lighter ions are deflected more, separated ion beams detected as electric current at end of chamber and current is measured
    - measurement related to number of ions of a particular mass, therefore related to abundance of ion
    - b/c isotopes of element have diff masses, mass spectrum will show one peak per isotope



2.10 - Atomic Weights of Elements

- Atomic weight of an element is the average relative atomic mass of a representative sample of its atoms, taking into account the relative abundances of its isotopes (unit less numbers b/c average of ratios)
- Atomic weights of unstable (radioactive) elements changing b/c % abundance of isotopes changing
- Atomic weight for some elements with stable isotopes are not constants of nature, can vary according to fraction of an element's stable isotopes

EXAMPLE: Atomic weight of boron

$A_r(^{10}B)=10.0129$; $A_r(^{11}B)=11.0093$;

$$\textit{Atomic weight of B} = \frac{19.91}{100} \times 10.0129 + \frac{80.09}{100} \times 11.0093 = 10.81$$

2.11 - Amount of Substance and Its Unit of Measurement: The Mole

- In order to account for how much of a certain substance is obtained (for products and reactants) it is important to define a convenient amount of matter that contains a known number of particles
  - unit of measurement is mole; unit of quantity (amount of substance/n)
  - a mole of atoms of an element is the amount whose mass in grams is numerically equal to its atomic weight
    - one mole of all substances contain the same number of particles, regardless of the identity of the particles
- Chemical amount and amount are interchangeable
- The best estimate for how many specified particles are in 1 mole of a substance is Avogadro's constant (N_A) = 6.0221415 x 10^23

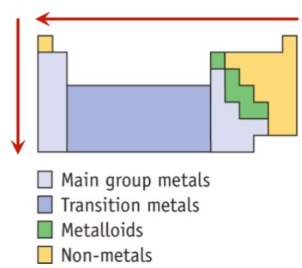
Changing Definitions:

- Units of measurement are arbitrary and subject to change as more knowledge is accumulated over time; IUPAC (international union of pure and applied chemistry) and other organizations work to handle these changes and provide evidence/reason for doing so
- Definition of atomic weight went from hydrogen (being exactly 1) to oxygen (being exactly 16) and is now on carbon (being exactly 12)
- A mol is the amount of a substance that contains 6.02214179 x 10^23 mol ^-1 specified elementary entities --> new def'n of mol based on uncertainty of measurement of a mole of a substance being the number of atoms in 12.00 g of carbon-12 (although not officially changed)

Molar Mass:

- Molar mass (M) is the mass (in g) of 1 mole of any element --> measured in g/mol
Amount to mass: mass (g) = amount (mol) X molar mass (g/mol) --> m = n x M
Mass to amount: amount (mol) = mass (g)/ molar mass (g/mol) --> n = m/M

2.12 - The Periodic Table of Elements



Language of the Periodic Table:

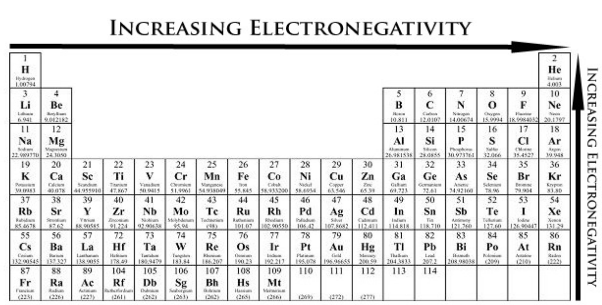
- Elements w/ similar chemical and physical properties arranged in vertical columns --> groups
  - groups 1,2, and13 - 18 are the main group elements
  - groups 3 to 12 are transition metals
- More metallic as you go across the periods to the left and as you go down the group
- All of group 18 are gases at room temp
  - w/ exception of carbon in the form of graphite non-metals don't conduct electricity
  - bromine is liquid at room temp
- Metalloids/semi-metals hard to distinguish as either

Developing the Periodic Table:

- Table originally developed from experimental observations of chemical and physical properties (Mendeleev)
  - periodicity was discovered, periodic occurrence of elements w/ similar properties
- Moseley discovered that wave lengths of x-rays emitted by given elements were related to the atomic number of the element
  - helped in developing the law of chemical periodicity

EXTRA: PERIODIC TRENDS (http://chemwiki.ucdavis.edu/Inorganic_Chemistry/Descriptive_Chemistry/Periodic_Trends_of_Elemental_Properties/Periodic_Trend)

1) Electronegativity measures an atom's tendency to attract and form bonds with electrons. This property exists due to the electronic configuration of atoms. Most atoms follow the octet rule (having the valence, or outer, shell comprise of 8 electrons). Because elements on the left side of the periodic table have less than a half-full valence shell, the energy required to gain electrons is significantly higher compared with the energy required to lose electrons. As a result, the elements on the left side of the periodic table generally lose electrons when forming bonds. Conversely, elements on the right side of the periodic table are more energy-efficient in gaining electrons to create a complete valence shell of 8 electrons. The nature of electronegativity is effectively described thus: the more inclined an atom is to gain electrons, the more likely that atom will pull electrons toward itself.

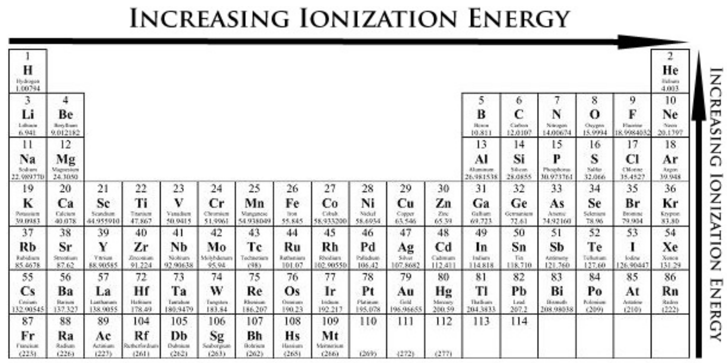


- **From left to right across a period of elements, electronegativity increases.** If the valence shell of an atom is less than half full, it requires less energy to lose an electron than to gain one. Conversely, if the valence shell is more than half full, it is easier to pull an electron into the valence shell than to donate one.
- **From top to bottom down a group, electronegativity decreases.** This is because atomic number increases down a group, and thus

there is an increased distance between the valence electrons and nucleus, or a greater atomic radius.

- **Important exceptions of the above rules include the noble gases, lanthanides, and actinides.** The noble gases possess a complete valence shell and do not usually attract electrons. The lanthanides and actinides possess more complicated chemistry that does not generally follow any trends. Therefore, noble gases, lanthanides, and actinides do not have electronegativity values.
- **As for the transition metals, although they have electronegativity values, there is little variance among them across the period and up and down a group.** This is because their metallic properties affect their ability to attract electrons as easily as the other elements.

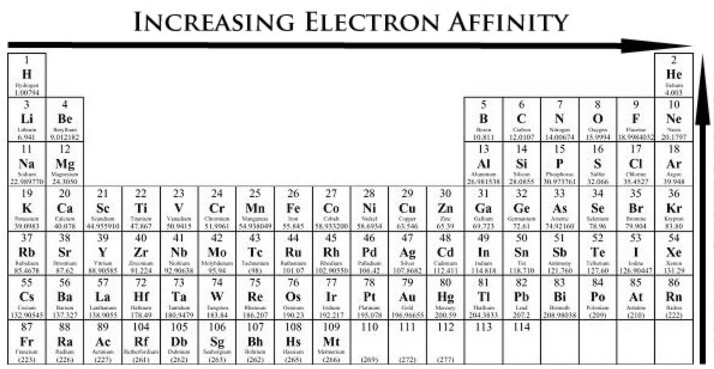
2) Ionization energy is the energy required to remove an electron from a neutral atom in its gaseous phase. Conceptually, ionization energy is the opposite of electronegativity. The lower this energy is, the more readily the atom becomes a cation. Therefore, the higher this energy is, the more unlikely it is the atom becomes a cation. Generally, elements on the right side of the periodic table have a higher ionization energy because their valence shell is nearly filled. Elements on the left side of the periodic table have low ionization energies because of their willingness to lose electrons and become cations. Thus, ionization energy increases from left to right on the periodic table.



Another factor that affects ionization energy is *electron shielding*. Electron shielding describes the ability of an atom's inner electrons to shield its positively-charged nucleus from its valence electrons. When moving to the right of a period, the number of electrons increases and the strength of shielding increases. As a result, it is easier for valence shell electrons to ionize, and thus the ionization energy decreases down a group. Electron shielding is also known as *screening*.

- The ionization energy of the elements within a period generally ***increases*** from left to right. This is due to valence shell stability.
- The ionization energy of the elements within a group generally ***decreases*** from top to bottom. This is due to electron shielding.
- The noble gases possess very high ionization energies because of their full valence shells as indicated in the graph. Note that heliu, has the highest ionization energy of all the elements.

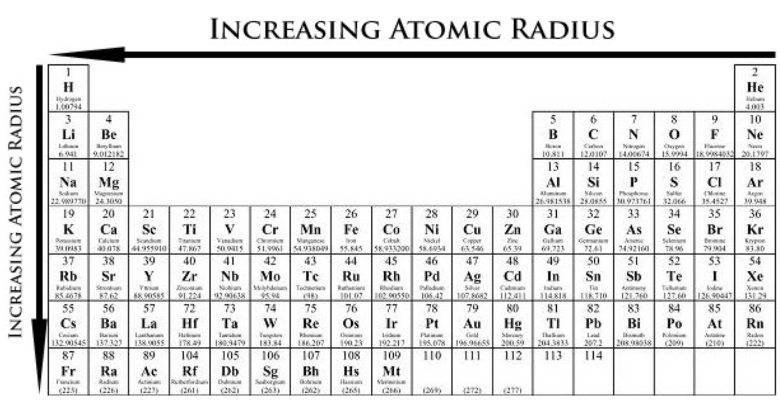
3) electron affinity is the ability of an atom to accept an electron. Unlike electronegativity, electron affinity is a quantitative measurement of the energy change that occurs when an electron is added to a neutral gas atom. The more negative the electron affinity value, the higher an atom's affinity for electrons.



Electron affinity generally decreases down a group of elements because each atom is larger than the atom above it (this is the atomic radius trend, discussed below). This means that an added electron is further away from the atom's nucleus compared with its position in the smaller atom. With a larger distance between the negatively-charged electron and the positively-charged nucleus, the force of attraction is relatively weaker. Therefore, electron affinity decreases. Moving from left to right across a period, atoms become smaller as the forces of attraction become stronger. This causes the electron to move closer to the nucleus, thus increasing the electron affinity from left to right across a period.

- Electron affinity ***increases** from left to right* within a period. This is caused by the decrease in atomic radius.
- Electron affinity ***decreases** from top to bottom* within a group. This is caused by the increase in atomic radius.

4) atomic radius is one-half the distance between the nuclei of two atoms (just like a radius is half the diameter of a circle). However, this idea is complicated by the fact that not all atoms are normally bound together in the same way. Some are bound by covalent bonds in molecules, some are attracted to each other in ionic crystals, and others are held in metallic crystals. Nevertheless, it is possible for a vast majority of elements to form covalent molecules in which two like atoms are held together by a single covalent bond. The covalent radii of these molecules are often referred to as atomic radii. This distance is measured in picometers. Atomic radius patterns are observed throughout the periodic table.



Atomic size gradually decreases from left to right across a period of elements. This is because, within a period or family of elements, all electrons are added to the same shell. However, at the same time, protons are being added to the nucleus, making it more positively charged. The effect of increasing proton number is greater than that of the increasing electron number; therefore, there is a greater nuclear attraction. This means that the nucleus attracts the electrons more strongly, pulling the atom's shell closer to the nucleus. The valence electrons are held closer towards the nucleus of the atom. As a result, the atomic radius decreases.
Down a group, atomic radius increases. The valence electrons occupy higher levels due to the increasing quantum number (n). As a result, the valence electrons are further away from the nucleus as 'n' increases. Electron shielding prevents these outer electrons from being attracted to the nucleus; thus, they are loosely held, and the resulting atomic radius is large.

- Atomic radius ***decreases*** *from left to right* within a period. This is caused by the increase in the number of protons and electrons across a period. One proton has a greater effect than one electron; thus, electrons are pulled towards the nucleus, resulting in a smaller radius.
- Atomic radius ***increases*** *from top to bottom* within a group. This is caused by electron shielding.

2.13 - IUPAC Periodic Table of the Isotopes

- Atomic weights should not be considered as constants of nature; the natural abundance of stable isotopes varies w/ geographic location
  - isotopes are not present in the same ration in different compounds and therefore depending on where element is found its atomic weight will vary
  - conventional atomic weight is the single number IUPAC lists on the periodic table b/c for commercial and some calculation purposes a single number rather than interval is needed

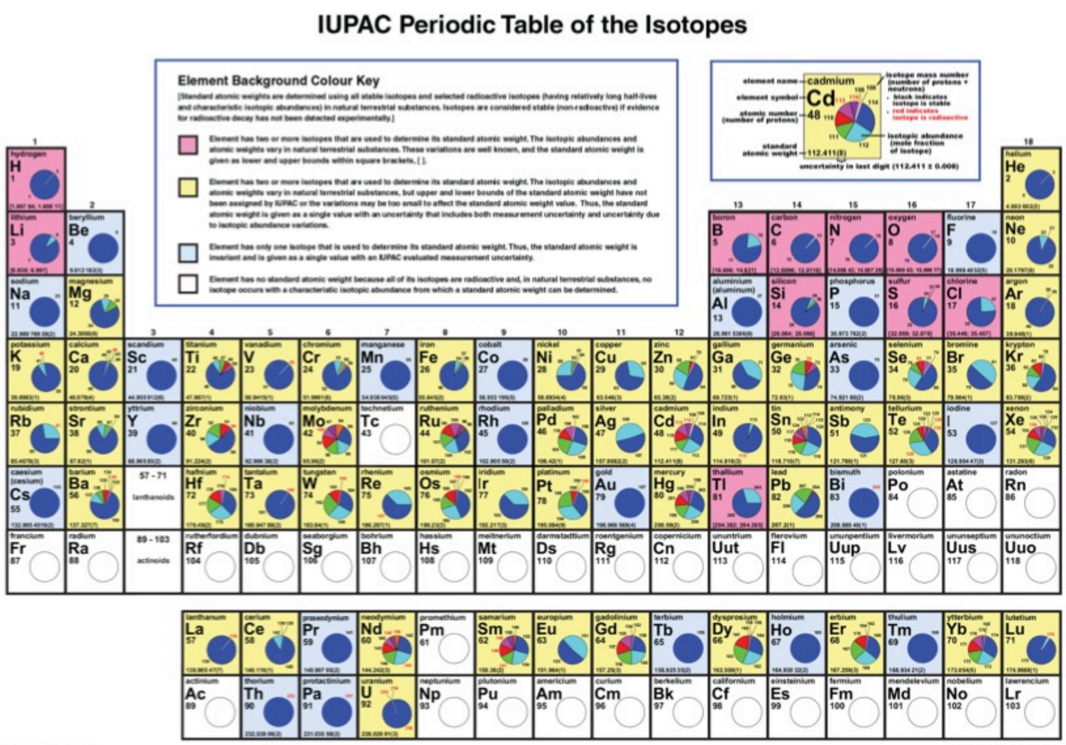


FIGURE 2.15 IUPAC Isotopic Periodic Table of the Elements

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- Atomic weights for some important elements (in pink in table above) should not be thought as constants of nature b/c natural abundance of their stable isotope varies due to processes like diff biochemical pathways, environmental, and climatic conditions
--> therefore IUPAC created this periodic table of isotopes for emphasis