Atomic Structure and Properties

1.1 Moles and Molar Mass

Avogadro's number: $\mathrm{N_A} = 6.022 \times 10^{23}\ \mathrm{mo}^{-1}$

Quantitative connection between the mass of a substance and the number of particles that the substance contains: $n = \frac{m}{M}$

Finding the formula mass for a compound:

1. Count atoms in chemical formula
2. Find atomic mass of each element on the periodic table
3. Multiple atomic by atomic mass to find mass per element
4. Sum results to find total formula mass

The mass of each sample is equal to the formula mass of the substance's particles in units of grams. This is the mass of one mole, or the molar mass.

$$\begin{gathered}
Sucrose:\ \mathrm{C_{12}H_{22}O_{11}} \\
----\\
Finding\ formula\ mass \\
\begin{array}{ll}
1. & 12\,C,\ 22\ H,\ 11\ O \\
2. & C:\ 12.01u,\ H:\ 1.01u,\ O:\ 16.00u \\
3. & C:\ 12 \cdot 12.01u = 144.12u \\
 & H:\ 22 \cdot 1.01u = 22.22u \\
 & O:\ 11 \cdot 16.00u = 176.00u \\
4. & 144.12 + 22.22 + 176.00 = 342.3u
\end{array} \\
----\\
Formula\ mass:\ 342.3u \\
Molar\ mass:\ 342.3\ g/mol
\end{gathered}$$

1 mole = molar mass in grams

Molar mass units: u

Example: 1 mole of Carbon = 12 grams of carbon

1.2 Mass Spectroscopy of Elements

The mass spectrum of a sample containing a single element can be used to determine the identity of the isotopes of that element and the relative abundance of each isotope in nature. The average atomic mass of an element can be estimated from the weighted average of the isotopic masses using the mass of each isotope and its relative abundance.

Reading a Mass Spectroscopy Graph

- Each bar represents an isotope
- Height of bar represents relative abundance
- x axis: mass in amu
- y axis: percent abundance in nature

Finding Average Isotopic Mass

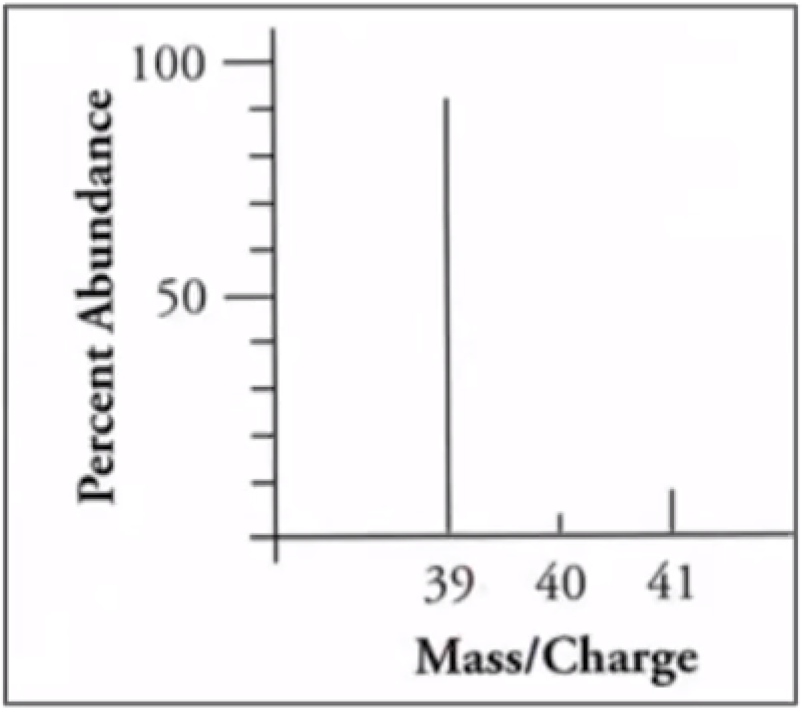
1. Multiply relative abundance by isotopic mass
2. Sum everything together

3 Types of Questions on the Exam:

- Estimate atomic mass from mass spectrum
- Identify element from mass spectrum
- Identify isotope from mass spectrum

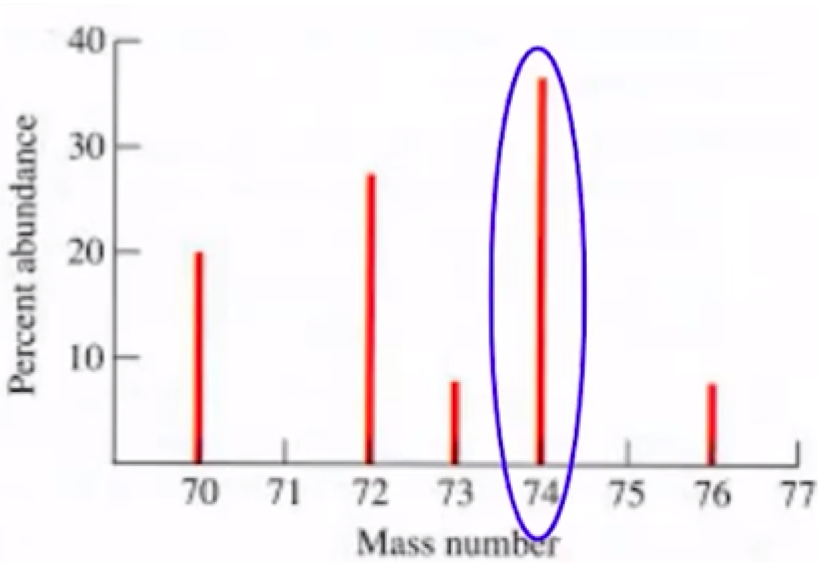
Example Problem

1. Identify the element.



Answer: You can visualize that the atomic mass is about 39. It is obviously potassium when looking at a periodic table

2. Identify the element and the number of neutrons represented by the peak at 74 amu.



Answer: You can visualize tha tthe atomic mass is between 72 and 73, which is Germainium. Germainium has 31 protons. Do 74-32 which is 42. There are 42 neutrons.

1.3 Elemental Composition of Pure Substances

Some pure substances are composed of individual molecules, while others consist of atoms or ions held together in fixed proportions as described by a formula unit. According to the law of definite proportions, the ratio of the masses of the constitute elements in any pure sample of that compound is always the same. In other words, the elements present and the ratio of those elements' atoms is the same for every sample in the compound. This also means that there is a constant mass ratio of elements in every compound.

The chemical formula that lists the lowest whole number ration of atoms of the elements int he compound is the empirical formula.

Example: H_2O always has a 2:1 ratio

Finding Percent Composition by Mass

1. Find the total mass of the compound
2. Divide the mass of each element by the total mass

Empirical Formula vs. Chemical (Molecular) Formula

Empirical formula: the lowest whole number ratio of atoms of each element in a compound

Chemical (molecular) formula: the actual number of atoms of each element in a compound

If different compounds have the smallest whole number ratio of atoms, the composition by mass of those compounds is the same (same empirical formula = same percent composition by mass).

Find the Empirical Formula

1. Convert percent to grams (if needed)
2. Convert grams to moles
3. Divide by the lowest number of moles
4. Multiple each number so that all are whole numbers (if needed)
5. Use the mole ratio to write the empirical formula

3 Types of Questions on the Exam:

- Straightforward mass or percent composition data –> empirical formula
- Combustion analysis: burning a sample of O_2 and analyzing products to determine relative amounts of C and H
- Hydrate analysis: heating hydrated ionic solid and analyzing mass change to determine mole ratio of water to anhydrous solid

1.4 Composition of Mixtures

While pure substances contain molecules or formula units of a single type, mixtures contain molecules or formula units of two or more types, whose relative proportions can vary. This means that it contains more than one type of particle. They have variable compositions depending hon the pure substances they contain and the relative amounts of those substances, which an be determined through elemental analysis. Example: solution

Elemental composition of a mixture can be used to determine the relative amounts of the pure substances that compose it.

1.5 Atomic Structure and Electron Configuration

The atom is composed of negatively charged electrons and a positively charged nucleus that is made of protons and neutrons. Coulomb's law is used to calculate the force between two charged particles. If the particles have opposite charges, then it will be a force of attraction. If the charges are the same, it will be a force of repulsion.

$$F \propto \frac{q_1 q_2}{r^2}$$

> *$\propto$ = proportional to*
>
> *q_1 = electrical charge on particle 1*
>
> *q_2= electrical charge on particle 2*

> *On the AP test, we will only by making quantitative comparisons. We will not be plugging numbers in.*
>
> *If q_x is larger, then the force of attraction/repulsion is greater.*
>
> *If distance (r) is greater, then the force of attraction/repulsion is less.*

Electrons can be thought of as being in "shell (energy levels)" and "subshells (sublevels)," as described by the electron configuration. Inner electrons are called core electrons, and outer electrons are called valence electrons. The electron configuration is explained by quantum mechanics, s delineated in the Aufbau principle and exemplified in the periodic table of the elements.

> *Aufbau principle: electrons will fill up the lowest energy orbitals 1st*

The relative energy required to remove an electron from different subshells of an atom or ion or from the same subshell in a different atoms or ions (ionization energy) can be estimated through a qualitative application of Coulomb's law. This energy is related to the distance from the nucleus and the effective (shield) charge of the nucleus.

As you move right on the periodic table, elements get higher and higher ionization energies because there are more and more protons that have a large attractive force. Removing an electron from a complete valence shell takes significantly more ionization energy than removing an electron from a non-complete valence shell.

^DOUBLE CHECK

1.6 Photoelectron Spectroscopy

The energies of the electrons in a given shell can be measured experimentally with photoelectron spectroscopy (PES). The position of each peak int he PES spectrum is related to the energy required to remove an electron form the corresponding subshell, and the height of each peak is (ideally) proportional to the number of electrons in that subshell.

Relating PES to Coulomb's Law

The way that the graph is set up, the peak furthest to left is closest to the nuclei. However, just stating this does not justify it using Coulomb's law.

> *Coulomb's law states that there is an inversely proportional relationship between distance and binding energy. The closer an electron is to the nucleus, the higher the attraction will be. Since (insert peak) has the highest binding energy, these electrons must be closes to the nucleus.*

1.7 Periodic Trends

The organization of the periodic table is based on the recurring properties of the elements and explained by the pattern of electron configurations and the presence of completely or partially filled shells (and subshells) of electrons in atoms.

> *Trend: The number of shells increases as you move down.*

> *Trend: The radius size decreases as you move right. (larger charge on particles = greater attraction = electrons closer to nucleus)*

Trends in atomic properties within the periodic table (periodicity) can be qualitatively understood through the position of the element in the periodic table, Coulomb's law, the shell model, and the concept of shielding/effective nuclear charge. These properties include:

- Ionization energy
- Atomic and ionic radii
- Electronegative
- Electron affinity

The periodicity is useful to predict/estimate values of properties in the absence of data.

Ionization Energy

This is the energy required to remove an electron from an atom and is tied to the atomic radius.

> *Trend: IE increases as you move up and to the right and decreases as you move down and to the left.*

Larger Atomic Radii

- Weaker attraction between valence electrons and the nucleus
- Smaller ionization energy

Smaller Atomic Radii

- Stronger attraction between valence electrons and the nucleus
- Large ionization energy

Electronegativity

This is the ability of an atom in a molecule to attract shared electrons to itself. Noble gases do not have electronegativity values because they largely do not share electrons with other elements.

> *Trend: Electronegativity increases as you move up and to the right and decreases as yo move down and to the left*

Larger Atomic Radii

- Weaker attraction due to a greater distance between the nucleus of one atom and the valence electrons of another atom
- Smaller electronegativity

Smaller Atomic Radii

- Stronger attraction due to a smaller distance between the nucleus of one atom and the valence electrons of another atom
- Larger electronegativity

Common Mistake

~~Atom X has a small radius because it is more electronegative (WRONG)~~

Atom X has a high electronegativity due to a small atomic radius (CORRECT)

Electron Affinity

This is the energy change when an atom gains an electron to form a negativity charged ion. It can be endothermic (gain energy) or exothermic (lose energy).

> *Trend: EA increases as you move up and to the right and decreases as you move down and to the left.*

Metals

- Easier to lose electrons because the nucleus doesn't have a strong attraction to valence electrons
- Adding electron is endothermic or slightly exothermic, electron affinity is positive or negative

Nonmetals

- Easier to gain electrons because the nucleus has a stronger attraction to valence electrons
- Adding electrons is exothermic, electron affinity is negative

1.8 Valence Electrons and Ionic Compounds

Valence electrons are the S and P electrons in the highest energy level. The likelihood that two elements will form a chemical bond is determined by the interactions between the valence electrons and the nuclei of elements. Elements in the same column of the periodic table tend to form analogous compounds. Typical charges of atoms in ionic compounds are governed by their location of the periodic table and the number of valence electrons.