Chapter 2. Atoms, Molecules, and Ions

Lecture Outline

2.1 The Atomic Theory of Matter

- Greek Philosophers: Can matter be subdivided into fundamental particles?
- Democritus (460–370 BC): All matter can be divided into indivisible *atomos*.
- Dalton: proposed atomic theory with the following postulates:
  - Elements are composed of atoms.
  - All atoms of an element are identical.
  - In chemical reactions atoms are not changed into different types of atoms. Atoms are neither created nor destroyed.
  - Compounds are formed when atoms of elements combine.
- **Atoms** are the building blocks of matter.
- *Law of constant composition*: The relative kinds and numbers of atoms are constant for a given compound.
- *Law of conservation of mass (matter)*: During a chemical reaction, the total mass before the reaction is equal to the total mass after the reaction.
  - Conservation means something can neither be created nor destroyed. Here, it applies to matter (mass). Later we will apply it to energy (Chapter 5).
- *Law of multiple proportions*: If two elements, A and B, combine to form more than one compound, then the mass of B, which combines with the mass of A, is a ratio of small whole numbers.
- Dalton's theory *predicted* the law of multiple proportions.

2.2 The Discovery of Atomic Structure

- By 1850 scientists knew that atoms consisted of charged particles.
- **Subatomic particles** are those particles that make up the atom.
- Recall the law of electrostatic attraction**:** like charges repel and opposite charges attract.

Cathode Rays and Electrons

- Cathode rays were first discovered in the mid-1800s from studies of electrical discharge through partially evacuated tubes (cathode-ray tubes or CRTs).
  - Computer terminals were once popularly referred to as CRTs (cathode-ray tubes).
  - Cathode rays = radiation produced when high voltage is applied across the tube.
- The voltage causes negative particles to move from the negative electrode (cathode) to the positive electrode (anode).
- The path of the electrons can be altered by the presence of a magnetic field.
- Consider cathode rays leaving the positive electrode through a small hole.
  - If they interact with a magnetic field perpendicular to an applied electric field, then the cathode rays can be deflected by different amounts.
  - The amount of deflection of the cathode rays depends on the applied magnetic and electric fields.
  - In turn, the amount of deflection also depends on the charge-to-mass ratio of the electron.
  - In 1897 Thomson determined the charge-to-mass ratio of an electron.
    - Charge-to-mass ratio: 1.76×10^8 C/g.
    - C is a symbol for coulomb.
      - It is the SI unit for electric charge.
- Millikan Oil-Drop Experiment
  - Goal: find the charge on the electron to determine its mass.
  - Oil drops are sprayed above a positively charged plate containing a small hole.
  - As the oil drops fall through the hole they acquire a negative charge.
  - Gravity forces the drops downward. The applied electric field forces the drops upward.
  - When a drop is perfectly balanced, then the weight of the drop is equal to the electrostatic force of attraction between the drop and the positive plate.

- Millikan carried out the above experiment and determined the charges on the oil drops to be multiples of 1.60×10^{-19} C.
- He concluded the charge on the electron must be 1.60×10^{-19} C.

- Knowing the charge-to-mass ratio of the electron, we can calculate the mass of the electron:

$$\text{Mass} = \frac{1.60\times10^{-19}\,\text{C}}{1.76\times10^{8}\,\text{C/g}} = 9.10\times10^{-28}\,\text{g}$$

Radioactivity

- **Radioactivity** is the spontaneous emission of radiation.
- Consider the following experiment:
  - A radioactive substance is placed in a lead shield containing a small hole so that a beam of radiation is emitted from the shield.
  - The radiation is passed between two electrically charged plates and detected.
  - Three spots are observed on the detector:
    1. a spot deflected in the direction of the positive plate,
    2. a spot that is not affected by the electric field, and
    3. a spot deflected in the direction of the negative plate.
  - A large deflection towards the positive plate corresponds to radiation that is negatively charged and of low mass. This is called $\wp$-radiation (consists of electrons).
    - No deflection corresponds to neutral radiation. This is called γ-radiation (similar to X-rays).
  - A small deflection toward the negatively charged plate corresponds to high mass, positively charged radiation. This is called α-radiation (positively charged core of a helium atom)
    - X-rays and γ radiation are true electromagnetic radiation, whereas α- and β-radiation are actually streams of particles--helium nuclei and electrons, respectively.

The Nuclear Atom

- The plum pudding model is an early picture of the atom.
- The Thomson model pictures the atom as a sphere with small electrons embedded in a positively charged mass.
- Rutherford carried out the following "gold foil" experiment:
  - A source of α-particles was placed at the mouth of a circular detector.
  - The α-particles were shot through a piece of gold foil.
  - Both the gold nucleus and the α-particle were positively charged, so they repelled each other.
  - Most of the α-particles went straight through the foil without deflection.
  - If the Thomson model of the atom was correct, then Rutherford's result was impossible.
- Rutherford modified Thomson's model as follows:
  - Assume the atom is spherical, but the positive charge must be located at the center with a diffuse negative charge surrounding it.
  - In order for the majority of α-particles that pass through a piece of foil to be undeflected, the majority of the atom must consist of a low mass, diffuse negative charge -- the electron.
  - To account for the small number of large deflections of the α-particles, the center or **nucleus** of the atom must consist of a dense positive charge.

2.3 The Modern View of Atomic Structure

- The atom consists of positive, negative, and neutral entities (**protons**, **electrons** and **neutrons**).
- Protons and neutrons are located in the nucleus of the atom, which is small. Most of the mass of the atom is due to the nucleus.
- Electrons are located outside of the nucleus. Most of the volume of the atom is due to electrons.
- The quantity 1.602×10^{-19} C is called the **electronic charge**. The charge on an electron is -1.602×10^{-19} C; the charge on a proton is $+1.602 \times 10^{-19}$ C; neutrons are uncharged.
  - Atoms have an equal number of protons and electrons thus they have no net electrical charge.

- Masses are so small that we define the **atomic mass unit**, amu.
  - 1 amu = 1.66054×10^{-24} g.
  - The mass of a proton is 1.0073 amu, a neutron is 1.0087 amu, and an electron is 5.486×10^{-4} amu.
- The **angstrom** is a convenient non SI unit of length used to denote atomic dimensions.
  - Since most atoms have radii around 1×10^{-10} m, we define 1 Å = 1×10^{-10} m.

Atomic Numbers, Mass Numbers, And Isotopes

- **Atomic number** (Z) = number of protons in the nucleus.
- **Mass number** (A) = total number of nucleons in the nucleus (i.e., protons and neutrons).
- By convention, for element X, we write ${}^{A}_{Z}X$.
  - Thus, isotopes have the same Z but different A.
    - There can be a variable number of neutrons for the same number of protons. Isotopes have the same number of protons but different numbers of neutrons.
- All atoms of a specific element have the same number of protons.
  - **Isotopes** of a specific element differ in the number of neutrons.
  - An atom of a specific isotope is called a **nuclide**.
    - Examples: Nuclides of hydrogen include:
      ${}^{1}H$ = hydrogen (protium), ${}^{2}H$ = deuterium, ${}^{3}H$ = tritium; tritium is radioactive.

2.4 Atomic Weights

The Atomic Mass Scale

- Consider 100 g of water:
  - Upon decomposition 11.1 g of hydrogen and 88.9 g of oxygen are produced.
  - The mass ratio of O to H in water is 88.9/11.1 = 8.
  - Therefore, the mass of O is 2 x 8 = 16 times the mass of H.
  - If H has a mass of 1, then O has a *relative mass* of 16.
  - We can measure atomic masses using a mass spectrometer.
  - We know ${}^{1}H$ has a mass of 1.6735×10^{-24} g and ${}^{16}O$ has a mass of 2.6560×10^{-23} g.
  - *Atomic mass units* (amu) are convenient units to use when dealing with extremely small masses of individual atoms.
- 1 amu = 1.66054×10^{-24} g and 1 g = 6.02214×10^{23} amu
- By definition, the mass of ${}^{12}C$ is exactly 12 amu.

Average Atomic Masses

- We average the masses of isotopes to give average atomic masses.
- Naturally occurring C consists of 98.93% ${}^{12}C$ (12 amu) and 1.07% ${}^{13}C$ (13.00335 amu).
- The average mass of C is:
  - (0.9893)(12 amu) + (0.0107)(13.00335 amu) = 12.01 amu.
- **Atomic weight** (AW) is also known as average atomic mass (atomic weight).
- Atomic weights are listed on the periodic table.

The Mass Spectrometer

- A **mass spectrometer** is an instrument that allows for direct and accurate determination of atomic (and molecular) weights.
- The sample is charged as soon as it enters the spectrometer.
- The charged sample is accelerated using an applied voltage.
- The ions are then passed into an evacuated tube and through a magnetic field.
- The magnetic field causes the ions to be deflected by different amounts depending on their mass.
- The ions are then detected.
  - A graph of signal intensity vs. mass of the ion is called a *mass spectrum*.

2.5 The Periodic Table

- The **periodic table** is used to organize the elements in a meaningful way.
- As a consequence of this organization, there are periodic properties associated with the periodic table.
- Rows in the periodic table are called periods.
- Columns in the periodic table are called **groups**.
  - Several numbering conventions are used (i.e., groups may be numbered from 1 to 18, or from 1A to 8A and 1B to 8B).
- Some of the groups in the periodic table are given special names.
  - These names indicate the similarities between group members.
  - Examples:
    - Group 1A: alkali metals
    - Group 2A: alkaline earth metals
    - Group 7A: halogens
    - Group 8A: noble gases
- **Metallic elements**, or **metals**, are located on the left-hand side of the periodic table (most of the elements are metals).
  - Metals tend to be malleable, ductile, and lustrous and are good thermal and electrical conductors.
- **Nonmetallic elements**, or **nonmetals**, are located in the top right-hand side of the periodic table.
  - Nonmetals tend to be brittle as solids, dull in appearance, and do not conduct heat or electricity well.
- Elements with properties similar to both metals and nonmetals are called **metalloids** and are located at the interface between the metals and nonmetals.
  - These include the elements B, Si, Ge, As, Sb and Te.

2.6 Molecules and Molecular Compounds

- A **molecule** consists of two or more atoms bound tightly together.

Molecules and Chemical Formulas

- Each molecule has a **chemical formula**.
- The chemical formula indicates
  1. which atoms are found in the molecule, and
  2. in what proportion they are found.
- A molecule made up of two atoms is called a **diatomic molecule**.
- Different forms of an element, which have different chemical formulas, are known as allotropes. Allotropes differ in their chemical and physical properties. See Chapter 7 for more information on allotropes of common elements.
- Compounds composed of molecules are **molecular compounds**.
  - These contain at least two types of atoms.
  - Most molecular substances contain only nonmetals.

Molecular and Empirical Formulas

- **Molecular formulas**
  - These formulas give the actual numbers and types of atoms in a molecule.
  - Examples: H_2O, CO_2, CO, CH_4, H_2O_2, O_2, O_3, and C_2H_4.
- **Empirical formulas**
  - These formulas give the relative numbers and types of atoms in a molecule (they give the lowest whole-number ratio of atoms in a molecule).
  - Examples: H_2O, CO_2, CO, CH_4, HO, CH_2.

Picturing Molecules

- Molecules occupy three-dimensional space.
- However, we often represent them in two dimensions.
- The **structural formula** gives the connectivity between individual atoms in the molecule.

- The structural formula may or may not be used to show the three-dimensional shape of the molecule.
- If the structural formula does show the shape of the molecule then either a perspective drawing, a ball-and-stick model, or a space-filling model is used.
  - *Perspective drawings* use dashed lines and wedges to represent bonds receding and emerging from the plane of the paper.
  - *Ball-and-stick models* show atoms as contracted spheres and the bonds as sticks.
    - The angles in the ball-and-stick model are accurate.
  - *Space-filling models* give an accurate representation of the 3-D shape of the molecule.

2.7 Ions and Ionic Compounds

- If electrons are added to or removed from a neutral atom, an **ion** is formed.
- When an atom or molecule loses electrons it becomes positively charged.
  - Positively charged ions are called **cations**.
- When an atom or molecule gains electrons it becomes negatively charged.
  - Negatively charged ions are called **anions**.
- In general, metal atoms tend to lose electrons and nonmetal atoms tend to gain electrons.
- When molecules lose electrons, **polyatomic ions** are formed (e.g. SO_4^{2-}, NO_3^-).

Predicting Ionic Charges

- An atom or molecule can lose more than one electron.
- Many atoms gain or lose enough electrons to have the same number of electrons as the nearest noble gas (group 8A).
- The number of electrons an atom loses is related to its position on the periodic table.

Ionic Compounds

- A great deal of chemistry involves the transfer of electrons between species.
- Example:
  - To form NaCl, the neutral sodium atom, Na, must lose an electron to become a cation: Na^+.
  - The electron cannot be lost entirely, so it is transferred to a chlorine atom, Cl, which then becomes an anion: Cl^-.
  - The Na^+ and Cl^- ions are attracted to form an ionic NaCl lattice, which crystallizes.
- NaCl is an example of an **ionic compound** consisting of positively charged cations and negatively charged anions.
  - Important: note that there are no easily identified NaCl molecules in the ionic lattice. Therefore, we cannot use molecular formulas to describe ionic substances.
- In general, ionic compounds are combinations of metals and nonmetals, whereas molecular compounds are composed of nonmetals only.
- Writing empirical formulas for ionic compounds:
  - You need to know the ions of which it is composed.
  - The formula must reflect the electrical neutrality of the compound.
  - You must combine cations and anions in a ratio so that the total positive charge is equal to the total negative charge.
  - Example: Consider the formation of Mg_3N_2:
    - Mg loses two electrons to become Mg^{2+}
    - Nitrogen gains three electrons to become N^{3-}.
    - For a neutral species, the number of electrons lost and gained must be equal.
    - However, Mg can only lose electrons in twos and N can only accept electrons in threes.
    - Therefore, Mg needs to lose six electrons (2x3) and N gains those six electrons (3x2).
    - That is, 3Mg atoms need to form $3Mg^{2+}$ ions (total 3x2 positive charges) and 2N atoms need to form $2N^{3-}$ ions (total 2x3 negative charges).
    - Therefore, the formula is Mg_3N_2.

Chemistry and Life: Elements Required by Living Organisms

- Of the 116 elements known, only about 29 are required for life.
- Water accounts for at least 70% of the mass of most cells.
- Carbon is the most common element in the solid components of cells.
- The most important elements for life are H, C, N, O, P and S (red).
- The next most important ions are Na^+, Mg^{2+}, K^+, Ca^{2+}, and Cl^- (blue).
- The other required 18 elements are only needed in trace amounts (green); they are *trace elements*.

2.8 Naming Inorganic Compounds

- **Chemical nomenclature** is the naming of substances.
- Common names are traditional names for substances (e.g., water, ammonia).
- Systematic names are based on a systematic set of rules.
  - Divided into organic compounds (those containing C, usually in combination with H, O, N, or S) and inorganic compounds (all other compounds).

Names and Formulas of Ionic Compounds

1. Positive Ions (Cations)

- Cations formed from a metal have the same name as the metal.
  - Example: Na^+ = sodium ion.
  - Ions formed from a single atom are called *monoatomic ions*.
- Many transition metals exhibit variable charge.
  - If the metal can form more than one cation, then the charge is indicated in parentheses in the name.
    - Examples: Cu^+ = copper(I) ion; Cu^{2+} = copper(II) ion.
  - An alternative nomenclature method uses the endings **-ous** and **-ic** to represent the lower and higher charged ions, respectively.
    - Examples: Cu^+ = cuprous ion; Cu^{2+} = cupric ion.
- Cations formed from nonmetals end in **-ium**.
  - Examples: NH_4^+ = ammonium ion; H_3O^+ = hydronium ion.

2. Negative Ions (Anions)

- Monatomic anions (with only one atom) use the ending **-ide**.
  - Example: Cl^- is the chloride ion.
- Some polyatomic anions also use the -ide ending:
  - Examples: hydroxide, cyanide, and peroxide ions.
- Polyatomic anions (with many atoms) containing oxygen are called **oxyanions**.
  - Their names end in **-ate** or **-ite**. (The one with more oxygen is called **-ate**.)
  - Examples: NO_3^- is nitr**ate**; NO_2^- is nitr**ite**.
- Polyatomic anions containing oxygen with more than two members in the series are named as follows (in order of **decreasing oxygen**):

• **per-**….**-ate**	example:	ClO_4^-	**per**chlor**ate**
• **-ate**		ClO_3^-	chlor**ate**
• **-ite**		ClO_2^-	chlori**te**
• **hypo-**….**-ite**		ClO^-	**hypo**chlor**ite**

- Polyatomic anions containing oxygen with additional hydrogens are named by adding hydrogen or bi- (one H), dihydrogen (two H) etc., to the name as follows:
  - CO_3^{2-} is the carbon**ate** anion.
  - HCO_3^- is the hydrogen carbonate (or **bi**carbonate) anion.
  - PO_4^{3-} is the phosphate ion.
  - $H_2PO_4^-$ is the **dihydrogen** phosphate anion.

3. Ionic Compounds

- These are named by the cation then the anion.
- Example: $BaBr_2$ = barium bromide.

Names and Formulas of Acids

- Acids are substances that yield hydrogen ions when dissolved in water (Arrhenius definition).
  - The names of acids are related to the names of anions:
  - **-ide** becomes **hydro-**….**-ic** acid; example: HCl **hydro**chlor**ic** acid
  - **-ate** becomes **-ic** acid; $HClO_4$ perchlor**ic** acid
  - **-ite** becomes **-ous** acid. HClO hypochlor**ous** acid

Names and Formulas of Binary Molecular Compounds

- Binary molecular compounds have two elements.
- The most metallic element (i.e., the one to the farthest left on the periodic table) is usually written first. The exception is NH_3.
- If both elements are in the same group, the lower one is written first.
- Greek prefixes are used to indicate the number of atoms (e.g., mono, di, tri).
  - The prefix mono is never used with the first element (i.e., carbon monoxide, CO).
- Examples:
  - Cl_2O is **di**chlorine *mono*xide.
  - N_2O_4 is **di**nitrogen *tetr*oxide.
  - NF_3 is nitrogen *tri*fluoride.
  - P_4S_{10} is **tetra**phosphorus *deca*sulfide.

2.9 Some Simple Organic Compounds

- **Organic chemistry** is the study of carbon-containing compounds.
  - *Organic compounds* are those that contain carbon and hydrogen, often in combination with other elements.

Alkanes

- Compounds containing only carbon and hydrogen are called **hydrocarbons**.
- In **alkanes** each carbon atom is bonded to four other atoms.
- The names of alkanes end in *-ane*.
  - Examples: methane, ethane, propane, butane.

Some Derivatives of Alkanes

- When *functional groups*, specific groups of atoms, are used to replace hydrogen atoms on alkanes, new classes of organic compounds are obtained.
  - **Alcohols** are obtained by replacing a hydrogen atom of an alkane with an –OH group.
  - Alcohol names derive from the name of the alkane and have an *-ol* ending.
    - Examples: methane becomes methanol; ethane becomes ethanol.
  - Carbon atoms often form compounds with long chains of carbon atoms.
    - Properties of alkanes and derivatives change with changes in chain length.
    - *Polyethylene*, a material used to make many plastic products, is an alkane with thousands of carbons.
    - This is an example of a *polymer*.
- Carbon may form *multiple bonds* to itself or other atoms.