Chapter 2 Atoms, Molecules, and Ions (Chapter 2 and Section 4.1 in OpenStax)

John Dalton's Atomic Theory (four postulates from1805)
- An atom is the smallest particle with a chemical identity.
  Its identity is retained during chemical reactions.
- An element is matter which is only one type of atom. Each element has an atomic symbol.
- Each atom in the element is chemically identical and, he believed, had a characteristic mass.
  This is only partially true, as his original theory did not account for isotope masses.
- A compound is matter with two or more types of atoms in fixed integer proportions.
  If proportions change, then a different compound is formed (e.g., CO and CO_2)
- A chemical reaction is a rearrangement of atoms present in reactants.
  It is a chemical change that transforms reactants into products.

J.J. Thomson
- J.J. Thomson discovered the electron (e^{-1}) in 1897.
  This showed that atoms were not indivisible, but contained smaller particles.
- He allowed "cathode rays" from a cathode (–) to pass
  through a circular anode (+) with a hole in the center.
- He also used a set of charge plates beyond the anode
  to bend the beam towards the (+) anode plate.
- The cathode rays were independent of the cathode material.
- Thomson concluded that they were composed
  of particles that are present in all matter.
- He also found the e^{-1}'s mass to charge ratio (kg/coulomb) in 1907.

Robert Millikin
- Robert Millikin found both charge and mass of the e^{-1} in 1909.
- With his oil drop experiment, he placed oil droplets in a chamber between
  the (+) anode plate on top and the (–) cathode plate on the bottom.
- He observed the difference in velocity between droplets that fell
  when the plates were uncharged and rose when they were charged.
- He found the electron's charge = 1.6×10^{-19} coulombs.
  That allowed him to find $m_e = 9.109 \times 10^{-31}$ kg.
- m_e is less than 1/1800 (or 0.05 %) of the mass of a hydrogen atom.

Ernest Rutherford
- Ernest Rutherford discovered the atomic nucleus in 1911.
- He showed that 99.95% of the atomic mass is concentrated
  into a very small space, which we call the nucleus.
- He aimed alpha radiation at gold foil. Most of the particles passed
  directly through it, but 1 in 8000 particles were deflected and scattered.
- The relatively small portion deflected was caused by
  the concentration of the atomic mass in the nucleus.

Nuclear Structure and Isotopes

- The nucleus is composed primarily of protons and neutrons.
- The proton (p^{+1}) has a + charge equal in magnitude to that of e^{-1}.
- The proton has a much larger mass than the electron: (m_p) = 1800(m_e).
- The atomic number (Z) is the number of p^{+1} and determines the atomic identity, that is, which element the atom is.
- The neutron (n^0) has no charge, and its mass is 0.1% greater than that of p^{+1}.
- The mass number (A) is the combined sum of protons and neutrons.
- Atoms of an element all have the same Z, but can have a different number of neutrons.
- Isotopes are atoms of an element with same Z, but with different A's. An atom with a particular number of neutrons is also called a nuclide.
- The atomic weight on the periodic table is the weighted average of all isotopes. It is the sum of each isotope mass times its natural abundance (decimal fraction).
- The precise isotope mass and natural abundance can both be found with a mass spectrometer.
- The atomic mass unit (amu) is equal to exactly 1/12 the mass of a single ^{12}C atom.
- In a mass spectrometer, atoms are first ionized, and then are accelerated and deflected by a magnetic field towards a detector. The detector calculates the exact mass and counts the total number of atoms (abundance) for each isotope.
- Amount of deflection is a function of the mass to charge ratio (where charge is usually +1).

Ex 2.02 Atomic Weight of Cr (Z=24) on Periodic Table

A	Exact Mass(amu)		Abundance		Product (amu)
50	49.9461	×	0.04346	=	2.171
52	51.9405	×	0.83789	=	43.520
53	52.9407	×	0.09501	=	5.030
54	53.9389	×	0.02366	=	1.276
Sum					51.997 amu

Periodic Table

- D. Mendeleev and J. Lother Meyer found in 1869 that elements could be ordered in horizontal rows, called periods, so that elements in the same column, or group, had similar physical and chemical properties.
- The modern periodic table has 18 groups, which are sometimes split into 8 main groups (A) in the outer columns and 10 transition groups (B) in the inner columns.
- Also, the bottom of the modern periodic table has two small rows, called inner transition groups, which contain heavier elements that do not fit into the A and B columns.

Elements can be categorized by three types

- Metals are on the left (and lower) side of the periodic table. They are hard and ductile. They have luster and conduct electricity.
- Nonmetals are on right (and upper) side of the periodic table. Typically, they are brittle if solid (many are fluids) and electrically nonconductive.
- Metalloids are in the middle right of the periodic table, touching the staircase line. They have properties intermediate to metal and nonmetal. That is, they have some luster and are electrical semiconductors.

Ionic Compounds (generally metal plus nonmetal for binary compounds)

- An ion is a charged particle composed of one or more atoms.
  Ions are positive (cation) if e^{-1}'s are lost and negative (anion) if e^{-1}'s are gained.
- An ionic compound is composed of cations and anions together. It is neutral and has no overall charge. The total sum of all of the ions' charges is zero for the compound's formula.
- Solid ionic compounds are crystals with a regular 3D arrangement of alternating ions.
  The crystal contains only ions, and does not contain separate discrete molecules.
  Its formula unit gives the proportions, but not any structural information.

Naming Ionic Compounds

- Chemical nomenclature is a systematic method for naming chemical substances.
- Inorganic Compounds are generally composed of elements other than C.
- Ionic Compounds are inorganic and are named as the cation followed by the anion.

Rules for Predicting Ions' Charges:

1. Main group (-A) metals normally form monatomic cations.
   The charge is often the same as the Roman group number, such as Na^{+1} in Group I-A.
2. Some main group metals with large atomic numbers have more than one ion.
   Most common charges are Roman group number and Roman group number minus 2.
3. Most transition metals also have more than one ion. See page 2 of link.
4. Nonmetallic elements normally form anions.
   Their charge is typically the Roman group number minus 8, such as Cl^{-1} in Group VII-A.

Naming Monatomic Ions

1. Name cation as full element name if there is only one possible charge (Na^{+1} is sodium ion).
2. If more than one cation exists for an element, follow the full element's name with the charge in Roman numerals inside parentheses, such as iron(II) for Fe^{+2} and iron(III) for Fe^{+3}.
   An older naming system uses Latin stems followed a suffix.
   The suffix is -ous for the lower charge and -ic for the higher charge.
   For instance, iron(II) is ferrous, and iron(III) is ferric.
3. For monatomic anions, follow stem name for element with -ide, such as oxide or chloride.

Polyatomic Ions

- Polyatomic ions have a charge and consist of two or more atoms bonded together.
  See page 3 of link.
- They are primarily anions, but there are two polyatomic cations:
  Ammonium is NH_4^{+1} and mercury(I) is Hg_2^{+2}
- Oxoanions contain oxygen along with another element.
  Oxygen atoms in the oxoanions almost always have a –2 oxidation number.
  The ion names are ordered by oxidation number of the other atom:
  hypochlorite (ClO^{-1}), chlorite (ClO_2^{-1}), chlorate (ClO_3^{-1}), and perchlorate (ClO_4^{-1})
- Hydrogen can be attached to oxoanions as well:
  monohydrogen phosphate (HPO_4^{-2}) and dihydrogen phosphate ($H_2PO_4^{-1}$)
- Use thio- prefix if an O is replaced by an S:
  sulfate (SO_4^{-2}) and thiosulfate ($S_2O_3^{-2}$)

Ex 2.03 a. Cross over charges for Ca^{+2} and O^{-2} to obtain Ca_2O_2. Then, simplify to CaO.
b. Cross over charges for Al^{+3} and S^{-2} to obtain Al_2S_3.

Ex 2.04 a. Ca_3P_2 is calcium phosphide b. $CoSO_4$ is cobalt(II) sulfate
Ex 2.05 a. iron(III) chromate is $Fe_2(CrO_4)_3$ b. tin(IV) oxide is SnO_2

Molecular Substances

- Generally, all of the atoms in a molecule are nonmetals.
- A molecule is a finite arrangement of atoms chemically bonded together.
  The molecule has particular chemical bonds, as well a 3D structure.
- The formula is a type of notation using atomic symbols followed by integer subscripts.
- The molecular formula shows the proportions of each atom.
  The structural formula shows how atoms are bonded together.
  A molecular model can be constructed by ball-and-stick or (more realistic) space-filling.
- Molecules can have as few as two atoms (Cl_2) or as many as thousands.
  Polymers, for instance, are large macromolecules, composed of many monomer units.
- An organic compound is a molecule containing carbon atoms.
  Originally (over 300 yrs ago), the term organic meant of biological origin.
  An organic compound was first synthesized in a laboratory in 1828 by Friedrick Wöhler.
  He created urea, $CO(NH_2)_2$, from ammonia (NH_3) and cyanic acid (HNCO).
- Hydrocarbons are the simplest organic compounds, containing H and C only.
- A functional group is a specific portion of a molecule.
  It generally gives the molecule a predictable characteristic behavior.
  For instance, an OH group converts a hydrocarbon into an alcohol (ROH).
  The COOH group converts a hydrocarbon to a carboxylic acid (RCOOH).
  An O atom connecting two hydrocarbon groups creates an ether (ROR).
- Organic compounds usually have systematic names that
  include functional groups as well as the hydrocarbon portion.

Naming Binary Molecular Compounds (with two elements only)

1. Name and write formula with elements in the conventional order:
   B Si C As P N H Te Se S I Br Cl O F
   The general order on the periodic table is left-to-right first, and then bottom-to-top.
   Essentially, the more metallic element is first.
2. Use the full element name for the first element.
3. Use the stem name followed by -ide, such as nitride, for the second element.
4. Add prefixes to each element to denote number of each atom.
   Mono is generally omitted from first atom.
   Use di- for 2, tri- for 3, tetra- for 4, etc.

Ex 2.06 Determining Names from Formulas
N_2O_5 is dinitrogen pentoxide P_4O_{10} is tetraphosphorus decoxide

Ex 2.07 Determining Formulas from Names
trisulfur dichloride is S_3Cl_2 tetraphosphorus pentasulfide is P_4S_5

Ex 2.08 Determining Names from Molecular Models
N_2O_4 is dinitrogen tetroxide (periodic table order is left to right)
I_2Cl_6 is diiodine hexachloride (periodic table order is bottom to top)

Acids and their Anions

- An acid usually has the H^{+1} cation combined with an anion in the formula (H_nX).
- A binary acid is named as hydrogen stem-ide if it is a pure compound (s, l, or g), and named as hydro-stem-ic acid if it is in aqueous solution (aq).
- An oxoacid (H_nXO_m) contains one or more hydrogen ions with an oxoanion. Often, more than one compound is possible.
- The lower oxidation number on X (has lower m) is hydrogen stem-ite or stem-ous acid. The higher oxidation number on X (has higher m) is hydrogen stem-ate or stem-ic acid.

Ex 2.09 Determine the Anion Name in $H_2SeO_{3(aq)}$ (Selenous Acid)

- For the anion name, replace "ous" with "ite" to get selenite.
- $H_2SeO_{3(s)}$ is hydrogen selenite, and it contains the selenite ion, SeO_3^{-2}.
- This is similar to sulfurous acid, $H_2SO_{3(aq)}$, and the sulfite ion, $SO_3^{-2}{}_{(aq)}$, except that for sulfur the "ur" is dropped to get sulfate.

Hydrates of Ionic Compounds

- A hydrate is a solid compound which contains water bound inside the crystal.
- Water molecules are chemically bonded to the ions in the crystal.
- Depending on the substance, the water may be easily added or removed, often by altering the temperature. Heating tends to drive away the water.
- Follow dry compound's formula with $\bullet xH_2O$, where x is an integer, such as $CuSO_4\bullet 5H_2O_{(s)}$.
- Follow dry compound's name with prefix-hydrate, such as copper(II) sulfate pentahydrate.
- When water has been removed, remove hydrate from the name, and use the prefix anhydrous. For example, $CuSO_{4(s)}$ is anhydrous copper(II) sulfate, which has a white color.
- When water vapor contacts anhydrous copper(II) sulfate, it becomes a blue-colored hydrate:

$$CuSO_{4(s)} + 5H_2O_{(g)} \rightarrow CuSO_4\bullet 5H_2O_{(s)}$$

Ex 2.10 Determine the name of $CoCl_2\bullet 6H_2O_{(s)}$

- Co^{+2} is cobalt(II), and Cl^{-1} is chloride.
- There are six (hexa) waters of crystallization (hydrate).
- So the name for this hydrate is cobalt(II) chloride hexahydrate.

Chemical Reactions (Equations and Balancing)

- The chemical equation is a symbolic representation of the compounds involved.
- The reactants are the starting materials, on the left side of the arrow.
- The products are to the right of the arrow.
- Temperature, catalysts, solvents, and other conditions may be placed above or below arrow.
- A balanced equation has the **same number** of each atom on both sides of the equation.
- Start by balancing an atom which occurs in only one substance for each side of the equation.
- Change **only** stoichiometric coefficient (big numbers before formula).
- Do **not** change subscripts (little numbers) in chemical formulas.
- This reaction is balanced so that each side has one C atom, four H atoms, and four O atoms:

$$1CH_4 + 2O_2 \rightarrow 1CO_2 + 2H_2O$$

Ex 2.12

a. $1Na_2O + 1Zn(OH)_2 \rightarrow 1ZnO + 2NaOH$

b. $2Al_2S_3 + 9O_2 \rightarrow 2Al_2O_3 + 6SO_2$

c. $4H_3PO_3 \rightarrow 3H_3PO_4 + 1PH_3$