Chemistry Lecture 1 – Atoms, Molecules and Quantum Mechanics

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Atoms

- Nucleus (protons, neutrons) + electrons
- Elements written as ${}^{A}_{Z}X$
  - A = *mass number* = protons + neutrons
  - Z = *atomic number* = protrons
  - X = element symbol (i.e. Mg)
- *Isotopes*: same atomic number (same # protons), diff mass number (diff # neutrons)
- *Atomic weight/molar mass*: from periodic table, defined in amu or g/mol (when do we use?)
  - # moles = # grams / molecular weight
- *Ion*: diff # electrons than protons, so has a charge (+ cation, - anion)
- Size differences:
  - For same element: cations are smaller than neutral, anions are larger than neutral
  - For same # electrons: smaller with higher atomic number b/c of more attractive force from protons

Periodic Table

- *Period*: horizontal row
- *Group/Family*: vertical column, numbered 1-18 or IA-VIIIA, IIIB-IIB
- Types of elements
  - *Metals*:
    - Tend to lose electrons to form positive ions
    - Ductile, malleable, thermal/electrically conductive, luster (shiny)
    - Generally solids @ room temperature except mercury
    - Usually form ionic oxides
  - *Transition metals*: in the sunken area of the periodic table (section B groups)
  - *Nonmetals*: tend to gain electrons to form negative ions, usually form covalent oxides
  - *Metalloids*: between a metal and a nonmetal
- Groups/Families
  - *Alkali metals* (Group 1A): low melting point, form 1^{+} cations, react strongly with most nonmetals including water (to form hydroxides and hydrogen gas)
  - *Alkaline earth metals* (Group 2A): higher melting point, less reactive than 1A, form 2^{+} cations
  - Group 4A: can form four covalent bonds with nonmetals. C can form strong pi bonds, everything else can form two additional bonds for a total of 6
  - Group 5A: can form three covalent bonds. N can form strong pi bonds, everything else can form two additional bonds for a total of 5
  - *Chalcogens* (Group 6A): oxygen and sulfur most important, both can make strong pi bonds. Oxygen reacts with metals to form metal oxides. Pure sulfur is S_8
  - *Halogens* (Group 7A): F, Cl, Br, I. All exist as diatomic molecules and like to gain electrons
  - *Noble gases* (Group 8A): nonreactive, normally found in nature as isolated atoms
- *Diatomic molecules*: H, O, N, Cl, Br, I, F
- Small atoms can form *pi bonds*, large atoms (3^{rd} period or above) have d orbitals so can form more than 4 bonds

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Periodic Trends
- *Ionization energy*: energy it takes to remove an electron
- *Electronegativity*: tendency to attract an electron in a bond
- *Electron affinity*: willingness of an atom to accept an additional electron
- Start with E: (energy of ionization, electron affinity, electronegativity) increase going LEFT-RIGHT, BOTTOM-TOP
- Don't start with E: (atomic radius, metallic character) increase going RIGHT-LEFT, TOP-BOTTOM

SI
- *Units*: kg, m, s, A, K, cd, mol
- *Prefixes*: mega/kilo/deci/centi/milli/micro/nano/pico/femto

Molecules: separate and distinct units made of atoms
- *Empirical formula*: relative number of atoms of one element to another
- *Molecular formula*: exact number of atoms per molecule
- <u>Calculating percent composition by mass</u>
  - For each atom, find weight of atom in molecule / total molecular weight
- <u>Calculating empirical formula from percent mass</u>
  - Assume a 100 gram sample, multiply by % masses to find # grams of each element
  - Find # moles of each element from the # grams
  - Divide by smallest # of moles to get empirical formula (might have to multiply by a factor to make all numbers integers)
  - If we want the molecular formula, have to use (given) total molecular weight

Bonds
- *Covalent bond*: shares electrons; electrons closer to more electronegative atom
- *Bond dissociation energy/bond energy*: energy it takes to break a bond
  - Higher bond energy = lower bond length
  - Double bonds have higher bond energy (lower length), triple bonds even higher/lower
- *Compound*: substance made from two or more elements

Naming compounds
- *Ionic*: cation + anion
  - Cations usually just name of element
  - Metals with more than one possible charge (i.e. copper) called copper (I) or copper (II)
  - Anions of elements end in -ide
  - Polyatomic anions containing oxygen end in -ite or -ate (also hypo- -ite and per- -ate)
- *Acids*: named after anion
  - Acids of elements = hydro- element -ic
  - Oxyacds = anion name -ic/-ous acid
- *Binary molecular compounds* (2 elements): leftmost/lowest, then other one w/ prefixes

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Chemical reactions

- *Physical vs chemical changes*: chemical when molecular structure is changed
- Remember to balance all equations!
- Limiting reagent: what will get used up first
  - Find # moles available of each reactant
  - Look at ratios between coeffs in balanced equation to find out what gets used up first
- Theoretical vs actual yield
  - Theoretical is what's predicted by equation, actual is what you get in an experiment
  - *Percent yield*: $\%\ \text{yield} = \frac{\text{actual yield}}{\text{theoretical yield}} \cdot 100\%$
- Types of Reactions
  - *Combination*: A + B → C
  - *Decomposition*: C → A + B
  - *Single displacement*: A + BC → B + AC
  - *Double displacement*: AB + CD → AD + CB

Quantum Mechanics

- Quantum numbers
  - *Principal quantum number* n: shell level
  - *Azimuthal quantum number* l: subshell/orbital shape: s, p, d, f. Can range from 0 to $n - 1$
  - *Magnetic quantum number* m_l: which orbital; ranges from $-l$ to $+l$
  - *Electron spin quantum number* m_s: $-1/2$ or $+1/2$
- *Pauli exclusion principle*: no two electrons can have the same set of quantum numbers
- *Hund's rule*: one electron will go into each available orbital before any orbital has 2 electrons
- *Aufbau principle*: electrons look for an available orbital with the lowest energy state

  1s → 2s → 2p → 3s → 3p → 4s → 3d → 4p → 5s → 4d → 5p → 6s → 4f → 5d → 6p …
- *Electron configuration*:
  - Br = $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^5$ = [Ar] $4s^2 3d^{10} 4p^5$
  - Exceptions: $4s^2 3d^4 \rightarrow 4s^1 3d^5$, $4s^2 3d^9 \rightarrow 4s^1 3d^{10}$
  - For ions, make sure you have the right number of electrons
- *Heisenberg uncertainty principle*: we can never be sure about both the position and the momentum of a particle

$$\Delta x \Delta p \geq \frac{\hbar}{2}$$

Electromagnetic Energy

- *Planck's quantum theory*: electromagnetic energy is quantized in discrete increments
- For a photon, $E = hf$ and $\lambda = h/mv$
- Emission spectra:
  - Electrons have specific quantized energy levels that are unique for each atom
  - When a photon of the right wavelength hits the atom, it can excite an electron to a higher energy level
  - After a while, the electron drops from the high energy level releasing another photon
  - If you use a wide spectrum of light, you can see what wavelength of photons are released to identify the material
- Photoelectric effect:
  - Electrons can be ejected from metal by shining light on it
  - The light energy must be greater than the work function Φ of the metal
  - The kinetic energy of ejected electron $= hf - \Phi$