

CH 1010 Chemical Properties, Bonding, and Forces Notes

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1 Systems of Units & Numbers

Chemistry is the study of matter and its properties; making observations, chiefly quantitative ones, is critical. To make quantitative measurements, we need a number and a unit. For instance, you can't just say that something is "5", you have to say that it's "5 centimeters" or "5 kPa", because the number is meaningless without the unit.

The two main systems of units are the English system, used in the United States and one or two obscure places, and the metric system, used everywhere else. The English system is rarely if ever used for scientific purposes since there is no systematic relationship between units — unlike the metric system, you can't define a unit of force in terms of other fundamental units, for instance, at least not directly and easily. Since units need a base value, we define units either in terms of each other or in terms of some fundamental value. For example, there is a metal alloy sphere in storage somewhere that is the defined value of a kilogram, while a meter can be defined as the amount of time it takes for light to travel a certain distance in a vacuum. Since sometimes you might need to convert between different systems of units, there are scalar values and formulas that can be used to convert between units. 1 inch is 2.54 cm, for example, and you can convert from degrees Celsius to degrees Fahrenheit by doing $F(c) = (9/5)c + 32$.

1.1 Significant Figures

Significant figures are also an important factor in taking measurements. This value is usually determined by the device used to take a measurement. If you use a scale to measure a weight, but it doesn't show the tenths place for its output, you can't claim to have a number of significant figures down to the tenths.

To determine significant figures, there are a few rules:

1. Nonzero integers always count as significant.
2. Leading zeros that precede nonzero digits do not count as significant.
3. Captive zeros are zeros between nonzero digits, and always count as significant.
4. Trailing zeros are zeros at the right end of the number, and are significant only if the number contains a decimal point.
5. Exact numbers, or numbers with an infinite number of significant figures, are given by counting (e.g. 8 molecules) or from definitions (e.g. 2π).

Sometimes you might need to express a value with a number of significant figures greater than it seemingly has. For example, the number 2200 has 2 significant figures on its own, so to express it with 3 you would write it in scientific notation as $22.0 \cdot 10^2$.

When performing operations involving significant figures, special considerations must be taken. When multiplying or dividing measurements, the result should have the same number of significant figures as the measurement with the lowest significant figure count. However, when adding or subtracting, the result has the same number of **decimal places** as the measurement with the lowest number of decimal places. For example, doing $2.345 + 0.07 + 2.9975$ yields 5.4125, but with the correct number of decimal places it's only 5.41. For another example, adding 5.9 to 2.221 yields 3.679 in exact numbers, but to correct for the number of decimal places you should round it up to 3.7.

1.2 Uncertainty

All measurements have some degree of uncertainty. Precision is the degree of agreement (reproducibility) among several measurements of the same quantity, while accuracy is how close the measurement is to the true value. Usually, the more precise a measurement is, the more accurate it is, but this isn't always the case. Sources of error can be either random or systematic, where random error has equal probability of being too high or too low, and systematic error is where the measurement is always either too high or too low. Random error can come from simple variations in measurement or uncontrollable external conditions, but systematic error is often the fault of the researcher, e.g. an uncalibrated instrument or a faulty experiment design.

2 Matter

Matter is defined as anything that takes up space and has mass. Matter always has volume, which is the amount of space it takes up, and mass, or the quantity of matter. Unlike weight, an object always has the same mass, regardless of where it is in the universe. Weight is actually a force, given as the measure of attraction of gravity for the object. Weights can actually vary at different latitudes, by as much as 0.5%.

Matter also has *state*, usually either solid, liquid, or gas. Solids always have definite shape and volume, liquids have definite volume but no definite shape, and gasses neither definite shape nor definite volume. Solids are as they are because of strong bonds between molecules that keep molecules rigidly in place. Liquids have no similar structure, but the intermolecular forces are still strong enough to keep everything in one place. Finally, (ideal) gasses have no force of any kind between their particles. When a substance normally exists as a gas, it's called a gas, but other substances in gas form are called *vapors*, ex. water vapor and carbon dioxide gas.

Matter can be classified even further into different types. If the matter is a pure substance (no variable composition), it's usually either an element or a compound. If the matter is a mixture (variable composition), it can be said to be either heterogeneous (imperfect mixture) or homogeneous (the same phase mixed together such that the two are indistinguishable). For example, helium is an element, water is a compound, water+sand is a heterogeneous mixture, and bronze is a homogeneous mixture. It's important to note that pure substances always have definite and unchanging properties, while the properties of a mixture may vary. Also noteworthy is that elements cannot be broken down into similar substances (although with a little nuclear magic you *might* be able to split their atoms!).

2.1 Properties of Matter

Properties of matter can be broken down into physical properties and chemical properties. Physical properties are properties observed or measured without changing the identity of the substance, such as melting point, density, or color. Chemical properties are the abilities of a substance to change into another substance, such as iron's ability to react with oxygen to form rust (iron oxide). Properties can be said to be either extensive or intensive — either the property depends on the amount of the substance (mass, volume, energy, ...), or it doesn't (density, temperature...), respectively.

These properties can be exploited for the purposes of certain operations. For example, you can separate some mixtures by boiling away the solvent, leaving only the solute behind (e.g. boil the water out of salt water, leaving only the salt), or you can use differing boiling points among liquids in a fractional distillation process. Another such process is chromatography, involving a mobile phase (liquid or gas) and a stationary phase (solid). Separation occurs because the components of the mixture have different affinities for the two phases, and so they move through the system at different rates as a result. Common applications include paper chromatography, liquid chromatography, and column chromatography.

There are three fundamental chemical laws:

1. **Law of conservation of mass** — matter is neither created nor destroyed in chemical reactions.
2. **Law of definite proportions** (or law of constant composition) — different samples of the same compound contain the same elements in the same proportions by mass.
3. **Law of multiple proportions** — when two elements combine to form more than one compound, the weights of one element with a fixed weight of another are related to each other in a ratio of small whole numbers. For example, H and O form H_2O_2 and H_2O . If you have 2 grams of hydrogen and 16 grams of oxygen in H_2O , you must have 32 grams of oxygen in H_2O_2 .

3 Atomic Structure

Atomic structure concerns the identity and arrangement of subatomic particles, or protons, neutrons, and electrons.

The original model of the atom was proposed by J.J. Thompson based on his early cathode ray experiments, and was called a *plum pudding model*. Under his model, the atom was a positive cloud in which

electrons with dispersed. Millikan's oil drop experiment was able to show that electrons have a negative charge. However, Rutherford's experiment was able to disprove the plum pudding model. Rutherford's experiment involved shooting alpha particles through a sheet of gold; if the plum pudding model held, no particles would be deflected, but since some were, there must be some positively charged object deflecting them — the nucleus.

So, atoms are made of a positive nucleus composed of protons and neutrons (also known as “nucleons”), with electrons “orbiting” the nucleus, held in orbit by the difference in charge between the two. Neutrons and protons have about the same mass, but electrons are actually a few orders of magnitude less massive. Neutrons have no charge, but protons and electrons have exactly the opposite charge, so you can find an atom's charge by simply subtracting the two numbers. If an atom has more electrons than protons, it is negatively charged, and vice versa.

3.1 Quantum-Mechanical Model

This requires a little bit of background.

Electromagnetic Radiation encompasses all forms of energy on the EM spectrum, including light, infrared, radio waves, microwaves, X-rays, and gamma rays. Light itself travels at about $2.99 \cdot 10^6$ m/s. Light has wave-like properties, including wavelength λ (distance between two consecutive peaks or troughs), frequency f (number of waves/cycles per second that pass a given point), and speed, which in a vacuum is given by the constant c . These are all related together by the simple formula $c = f\lambda$.

The electromagnetic spectrum contains all possible wavelengths, the, with longer wavelengths on the right and shorter wavelengths on the left. The shorter the wavelength, the higher the energy — this is one of many reasons why it's a bad idea to get hit by gamma rays, which have by far the shortest wavelength.

Quantum model of light Light's wave-like, among other interesting properties, cannot be explained by classical physics. It also can't explain the black body effect, wherein hotter objects emit shorter wavelengths of light with higher amount of energy. It also can't explain the photoelectric effect, where electrons are ejected from the surface of certain metals exposed to light of at least a certain minimum frequency (the threshold frequency).

The solution to these problems is to *quantize* light — this idea was actually formulated by Planck, and used by Einstein to explain the photoelectric effect. Under this model, light can be viewed as a stream of particles called “photons”, where the energy of a photon is given by its frequency in combination with some other data points, like Planck's constant.

Where this comes into play for atoms is in atomic spectra. When an element is vaporized and thermally or electrically excited, it emits certain light. This emitted light, when passed through a narrow slit and refracted by a prism, results in a line spectrum. In fact, these spectra are generated by electrons jumping from one energy level to the next, but there will be more on that later. The point is, these atomic spectra form a unique fingerprint for an element. Hydrogen has the simplest line spectrum with only four lines, at 410.1 nm, 434.1 nm, and two others that I didn't have the time to write. That shows that in hydrogen atoms, the sole electron may have only one of four different energy levels. Related terms:

- Absorption spectrum — distribution of wavelengths or frequencies of radiation absorbed.
- Emission spectrum — distribution of wavelengths or frequencies of radiation emitted (release of excess energy)
- Continuous spectrum — contains light of all wavelengths, like a rainbow.
- Line spectrum — contains radiation of only specific wavelengths.
- Ground state — the lowest possible energy state for an electron to be in.
- Excited state — when an atom has excess energy.

Bohr's Model of the Atom Bohr's model is based on calculations involving the energy levels available to the electron in the hydrogen atom. Under this model, the electron orbits in a circle around the nucleus, and moves closer or further from the nucleus depending on its energy level — higher energy levels mean higher orbits. These energy levels are given by $E = -2.178 \cdot 10^{-18} J(Z^2/n^2)$ where n is the integer number of the orbit and Z is the nuclear charge. Note that this *only* works for the hydrogen atom, it never worked for other atoms.

Quantization of Energy Based on this, we can conclude that energy is quantized; that is, values are restricted to only certain values. Furthermore, there is a certain wave-particle duality — matter and energy are *not* distinct here. A relevant formula (de Broglie?) is:

$$\lambda = \frac{h}{mu}$$

...where h is Planck's constant ($6.626 \cdot 10^{-24}$ J s), m is the mass of the particle in kg, and u is the speed in m/s. Also, $E = hv = \frac{hc}{\lambda}$ where E is energy of the particle and h is Planck's constant. Note that by Heisenberg's principle it is impossible to know the velocity and position of a particle at the same time. Anyways, the final quantum mechanical model ends up being:

$$H\Psi = E\Psi$$

...where E is the energy of the atom, H is the Hamiltonian operator (set of mathematical operations), and Ψ is the wave function. No, I don't know what any of this means, and no, I don't have to, it's beyond the scope of this course.

Example Calculate the wavelength of light emitted when an electron in a hydrogen atom goes from level 4 to level 3.

$$\begin{aligned}\Delta E &= -2.178 \cdot 10^{-18} J \left(\frac{1}{n_{final}^2} - \frac{1}{n_{initial}^2} \right) \\ (4, 3) &= -1.059 \cdot 10^{-19} J \\ \lambda &= \frac{hc}{|\Delta E|} \\ &= 1.88 \cdot 10^{-6} m\end{aligned}$$

When the electron jumps from level 5 to level 4, the light produced should be infrared light.

3.2 Notation

When elements are written out, the number above is the atomic mass and the number below is the atomic number (i.e. proton count). For example, ${}^1_1\text{H}$ is hydrogen with one proton and one electron, but no neutrons. Two other isotopes (same atomic number but different mass number) are ${}^2_1\text{H}$ and ${}^3_1\text{H}$, which have 1 and 2 neutrons, respectively. The average atomic mass is based on the weighted average mass of the element across all isotopes. For example, the average atomic mass of nitrogen is 14.01 and its atomic number is 7, which means that on average nitrogen has only 7 neutrons, but there exist isotopes in some small amount that have more than 7 neutrons. Nitrogen is with 8 neutrons, for example, is still nitrogen and is has all the same chemical properties, but for some very select purposes it behaves differently. On the right side of the element is the charge, which is an important chemical property. This is denoted by putting a superscript with either a + or a -, and the magnitude of the charge. For instance, H^+ is hydrogen missing one electron (giving it a positive charge), otherwise known as just a proton. If the element is neutral, there is no right superscript.

So, to write the complete symbol for an element, combine all values together, to get something like: ${}^2_1\text{H}^-$ (for one isotope of hydrogen). This usually isn't necessary unless one of the values has changed. For example, for ${}^{116}\text{Cd}$ we don't really need to write out the atomic number (48) since it's implied by the fact that this element is Cd (Cadmium). However, for an element with 34 protons, 45 neutrons, and 36 electrons, we would still write out ${}^{79}_{34}\text{Se}^{2-}$

4 Quantum Stuff

4.1 Quantum Numbers

Schrodinger's equation states:

$$H\Psi = E\Psi$$

Many wave functions (orbitals) satisfy this. Each orbit is characterized by different quantum numbers that describe different properties:

4.1.1 Principle Quantum Number n

n gives you the orbit shell of the electron; lower numbers mean lower orbits and lower energies. The orbit size increase will decrease over time as the energy increases.

4.1.2 Azimuthal Quantum Number l

l defines the shape of the orbital (subshells), and ranges from 0 to $n - 1$. When $l = 0$, the orbit is an s-type, and it's a p-type, d-type, and f-type for $l = 1, 2, 3$, respectively. Here, $ns < np < nd < nf$. For a given l , a larger n means higher energy, as does a larger l mean higher energy.

4.1.3 Magnetic quantum number m_l

m_l defines atomic orbitals, or the orientation of the orbital in space. Values of m_l range from $-l$ to l . For a given l , the number of possible m_l values is equal to the number of orbitals in the subshell. In general, s orbitals are spherical, p orbitals are dumbbell-shaped, d orbitals have two different fundamental shapes, and f orbitals are complex.

When referencing p orbitals, it's necessary to say which axis the orientation is in. For instance, $2P_x$.

4.1.4 Spin quantum number m_s

m_s is for electrons spin, and can only have two values: parallel spins (same m_s) or opposite spins (different m_s). Electrons occupying the same orbital are paired — they have opposite spins.

4.1.5 Examples

- For $n=1$, $l=1$, the atom has 1 orbital and at most 2 electrons.
- For $n=2$, the outer shell has 3 orbitals and 6 electrons, so the atom can have at most 8 electrons
- For $n=3$, the outer shell has 5 orbitals and 10 electrons, so the atom can have at most 18 electrons
- For $n=4$, the outer shell has 7 orbitals and 14 electrons, so the atom can have at most 32 electrons.

In general n^2 will give you the total number of orbitals, so just multiply that by two to get the number of electrons: $2n^2$. Remember, these quantum numbers apply to the electrons themselves, not the atoms.

4.2 Electron Configurations

s subshells can have 2 electrons, p subshells can have 6 electrons, d subshells can have 10 electrons, and f subshells can have 14 electrons. When you're trying to distribute, note that the total number of electrons in an atom is n^2 , the maximum number of electrons per orbital is 2, and no two electrons may have the same set of 4 quantum numbers.

For an atom in its ground state, electrons are found in the energy shells, subshells, and orbitals that produce the lowest energy for the atom. That is, populate the lowest energy shells with electrons before the others. This is the Aufbau principle.

Here are some examples:

- Hydrogen — one electron, and the lowest energy shell available is e, so this should be written as $1s^1$.
- Helium — two electrons, so fill the first shell and call it $1s^2$.
- Lithium — three electrons but the first shell is filled, so the configuration is $1s^2 2s^1$.
- Beryllium — four electrons, $1s^2 2s^2$
- Oxygen — eight electrons, $1s^2 2s^2 2p^4$.
- Sodium — eleven electrons, $1s^2 2s^2 2p^6 3s^1$

This is called a complete electron distribution. There's also another way to represent these, using shorthand involving the noble gas. For instance, the whole series $1s^2 2s^2 2p^6$ can be represented as [Ne], since it's the noble gas in the previous period. So, you can write out Sodium's electron configuration as [Ne] $3s^1$.

The order of filling (when each gets filled) is 1s, 2s, 2p, 3s, 3p, 4s, 3d, 4p, 5s, 4d, 5p, 6s, 4f, 5d, 6p, 7s, 5f, 6d, 7p. You might notice that there are some discrepancies here, but these can be explained away using the periodic table. The first two groups on the periodic table are called the "s-block" elements, since their outermost shells are always *s* shells. The block of elements on the right, from Boron to Neon, are called the p-block elements for similar reasons, and the low space in the middle (from Selenium to Zinc) are the d-block elements. Finally, the elements at the very bottom, the Lanthanides and the Actinides, are the f-block elements.

Using this information, it should be trivial to find the electron configuration of arbitrary elements using the periodic table. The period number tells you what shell you're on, the group number tells you the number of electrons in the outermost shell. Just note that the d-block (transition elements...) start out at 3d, not 4d as it would seem based on the period number. Similarly, the f-block starts off at 4f.

Naturally, there are a few exceptions. Chromium isn't actually [Ar] $4s^2 3d^4$, it's actually $4s^1 3d^5$ (something about how this is more stable). The same goes for Molybdenum, which is [Kr] $5s^1 4d^5$. Copper is also an exception, at [Ar] $4s^1 3d^{10}$, and Silver has the same configuration (just with different shell numbers).

5 Element Properties

At the highest level, elements can be categorized into metals and nonmetals. Anything left of the diagonal line on most tables (with the exception of hydrogen) is a metal. Metals are hard, lustrous, ductile, shiny, and make for good conductors. They also can form alloys, they have high boiling points, high thermal conductivity, and they tend to lose electrons (forming positively charged ions called cations). Non-metals have exactly the opposite properties of the metals — they're usually soft, dull, brittle, sometimes gasses or liquids, and they tend to gain electrons (forming negatively charged ions called anions). Along the line itself exist the metalloids, which have properties in between that of metals and non-metals. Silicon, boron, arsenic, antimony, tellurium are among the metalloids (also known as semi-metals). Not all metals are the same, though — some metals, called the active metals, are extremely reactive, such as lithium or caesium. The other metals are far less reactive, and are called inactive metals.

The periodic table's layout isn't randomly chosen, it's based on electron shells and chemical properties. Elements in the same column are said to be in the same group or family, and have similar properties. Rows are called periods, and share little other than the fact that electrons are added to the same shell as you progress to the right. As an example, lithium a reactive metal shares a lot in common with caesium, a *very* reactive metal. In fact, lithium and caesium both belong to the group *alkali metals*, the group one to the right contains the *alkaline earth metals*, the gasses all the way to the right are called the *noble gasses*, the elements in the group one to the left from there are the *halogens*, and the group one to the left of that contains the *chalcogens* (?). Everything in the middle (the "low" section of the periodic table) are called the transition elements, and the bottom two rows (separate from the others) are the inner transition elements; the upper row contains the lanthanides, the lower row contains the actinides. The transition elements are generally of commercial importance (copper, iron, nickel, gold, silver, etc.), while the inner transition elements aren't (with the possible exceptions of ^{235}U , used for reactors and blowing things up, and ^{241}Am , used for ionization-type smoke detectors).

Elements properties are often determined (in part) by their valence electrons, or the electrons in the outermost shell. For example, sodium's full configuration is $1s^2 2s^2 2p^6 3s^1$, but only the $3s^1$ contains the valence electrons. d shells are not considered in the s/p blocks, nor are f shells; both are considered part of the core. In any case, these valence electrons are usually the ones involved in the formation of ions, and are exchanged or shared in chemical bonds. As the nucleus's proton count increases, it generally gets harder to lose valence electrons, since it has a greater influence on them. This helps explain why the alkali elements are so willing to lose electrons, while the halogens readily accept them.

Relevant here is Hund's rule of maximum multiplicity. For degenerate orbitals, the lowest energy is attained when the number of electrons with the same spin is maximized. Electrons pair only after each orbital in a subshell is occupied by a single electron (here, degenerate means same energy). So, if you have a 3p subshell, start by filling from -1 on to 1, and only move on to opposite spin once there are no more orbitals to fill. If there are unpaired electrons, the configuration is said to be paramagnetic, while atoms with only paired electrons are called diamagnetic. When losing electrons, electrons are lost from the lower l value shells first, so s electrons are always the first to go. For example, the four quantum numbers for the electron lost when a potassium atom forms a +1 ion are 4, 0, 0, $-\frac{1}{2}$ (down spin is always first by convention).

5.1 Periodic Trends & Properties

Elements that are in the same group all have similar electron configurations. The shell numbers might be different, but the valence electrons are the same. As you go down a group, more shells get added, so the atom's radius increases, which can help change some properties. Atomic size also increases as you progress left in a period, since there are fewer protons in the nucleus to exert a force on the electrons. When it comes to determining which atoms are bigger than others, always look to group before period. When forming ions, ionic radius increases as you go down a group. Cations (positive ions) are smaller than their parent items, and vice versa for anions. Ionic size decreases as charge increases for different cations of a given elements. In an isoelectronic series, look to the number of protons alone (more protons means smaller radius).

Ionization energy is the amount of energy required to remove an electron from a gaseous atom to form a gaseous ion. It generally increases across a period and decreases down a group. Second and third ionization energies are what it takes to remove an electron from a 1+ and 2+ ion, respectively. In general: the more protons an atom has, the more difficult it is to remove an electron, and the further out the electrons are, the easier it is.

Electron affinity is the energy released when a gaseous atom adds an electron and becomes an ion. It decreases along periods and increases along groups. Metallic behavior is relevant here, as metals are much more willing to share electrons.

5.2 Average atomic mass

Average atomic mass is not an integer number, despite that by all rights it should be. This is because isotopes have different masses, and are in fact naturally occurring. In reality, these masses can be calculated using mass spectrometers, which work by vaporizing a material, ionizing the gas, accelerating it, then deflecting it with a magnetic field. Heavier particles won't be deflected as much as lighter elements, so this difference in deflection amount can be used to calculate mass.

So, the atomic mass (also known as the atomic weight) is obtained from the weighted average of the isotopic masses of all isotopes present in nature for an element.

Example An element has two naturally occurring isotopes. Isotope 1 has a mass of 120.9038 amu and a relative abundance of 57.4%, and isotope 2 has a mass of 122.9042 amu. Find the atomic mass of this element and, by comparison to the periodic table, identify it.

To calculate this, simply take $120.9038 \cdot 0.574 + 122.9042 \cdot (1 - 0.574) = 121.8$. This element most closely matches Antimony.

Example 2 Gallium has two naturally occurring isotopes, Gallium 59 and Gallium 81, with masses of 68.9257 amu and 70.9249, respectively. Calculate the abundances of these isotopes of gallium, given the atomic weight of gallium to be 69.723 amu.

To find one of the abundances, solve $68.9257x + 70.9249(1 - x) = 69.723$ to get $x = .6012$.

6 Compounds & Bonding

To form molecules, bonds between atoms are necessary. All compounds can be classified into ionic or molecular (covalent) bonds. In the former, an electron (or many) are transferred, for example between sodium and chlorine. In the latter, electrons are shared.

6.1 Ionic compounds

Ionic bonds involve the transfer of electrons, and are based on the attraction between two oppositely charged ions. Ionic compounds are mostly solid, and generally have a structure of rows of alternating ions. They usually resist denting and bending, they conduct when melted, and have high melting/boiling points, but they are usually brittle.

Binary ionic compounds are composed of a metal and a nonmetal, e.g. NaCl. Another option is a metal and a polyatomic ion (ex. NaNO_3) and a metal. Polyatomic ions are ions composed of multiple atoms, for instance NH_4^+ . For regular ions, the alkali metals lose 1 electron as do the alkaline earth metals, elements in further groups generally gain electrons. The noble gasses, however, are completely stable and inert, and consequently don't form bonds with anything (they have no need to gain or lose an electron).

When two separated gaseous ions come together to form a solid ionic compound, a massive amount of energy is released, called *lattice energy*. This energy can be found using Coulomb's law $k \frac{Q_1 Q_2}{r^2}$ where k is Coulomb's constant, each Q is an ion charge, and r is the distance between the ions (related to the ionic radius). Large ion charges and smaller distances lead to more stable ionic compounds. For example, the lattice energy of LiCl is -834 kJ/mol (exothermic reaction energies are negative by convention), whereas CsCl has a lattice energy of closer to -600 kJ/mol. However, in general, the ion charge is generally more important. So despite that NaF has a smaller bond distance, its lattice energy of -910 kJ/mol is much lower than Ca_2O_2 's lattice energy of -3414 kJ/mol. Examples:

- $\text{LiF} > \text{CsF}$
- $\text{NaBr} > \text{NaI}$
- $\text{BaCl}_2 < \text{BaO}$
- $\text{Na}_2\text{SO}_4 < \text{CaSO}_4$
- $\text{KF} < \text{K}_2\text{O}$
- $\text{Li}_2\text{O} > \text{Na}_2\text{S}$

6.1.1 Naming

To name an ion, a few rules need to be established. For naming purposes only, form the Type I metal group from the alkali metals, the alkaline earth metals, Aluminum (+3), Zinc (+3), Cadmium (+3), and Silver (+1). These metals do not need the charge included as part of their name in the compound. For these metals, the name is just the name of the element plus the word "ion". For Type II metals, which can have more than one kind of charged ion (ex. Fe^{2+}), add the charge in roman numerals after, e.g. Iron (III). For monoatomic ions, add "-ide" to the end and append the word "ion". For instance, Se^{2-} is a Selenide ion. More example:

- Na_2O — Sodium oxide
- CsF — Cesium fluoride
- NiO^{2-} —Nickle (II) oxide

To immediately identify ionic compounds, just look to the first element in the name. If it's a metal and it's bound to a non-metal, the compound is ionic.

6.2 Molecular/Covalent Compounds

Molecular bonding involves covalent bonds, or the sharing of electrons. To identify these compounds by name, look to the composing elements — if they're nonmetals, the compound is covalent.

6.3 Polyatomic Oxide Ions

These ions are named based on the number of oxygens. If there are four, it's a "per-ate", e.g. NO_4 is pernitrate. If there are three, it's "-ate", e.g. NO_3 is nitrate. If there are two, it's -ite, e.g. NO_2 is nitrite. Finally, if there's only one, it's "hypo-ite", e.g. NO is hyponitrite. The charge is also important, somehow, since SeO_4^{2-} is actually Selenate, so if the charge is greater than -1 the name is downgraded by one increment (?). Similarly, SiO_2^{2-} is Silicite. More examples:

- AsO_3^{3-} — Arsenite ion
- Hypoiodite ion — IO^-

6.4 Chemical Formulas

Chemical formulas are the simplest way of representing a molecule or formula unit. The symbols of the atoms indicate the type of atoms present and the subscripts indicate the relative number of atoms or molecules. For instance, $\text{Mg}(\text{BrO}_3)_2 \cdot 6\text{H}_2\text{O}$ is a complicated molecule.

This exposes the need for a naming system for ionic compounds where polyatomic ions are involved. Ionic compounds follow the same rules as with regular binary ionic compounds. The metal/cation is always written first; if the metal is a type II metal, the charge must be shown in parentheses as a roman numeral. The polyatomic ion name is then placed after the metal name. Here are some examples:

- $\text{Ba}_3(\text{PO}_4)_2$ — Barium phosphate
- CuSO_4 — Copper (II) sulfate
- NaHCO_3 — Sodium hydrogen carbonate (commonly called sodium bicarbonate)
- NaH_2PO_4 — Sodium dihydrogen phosphate
- $\text{Hg}_2(\text{NO}_2)_2$ — Mercury (I) nitrite
- CoCl_2 — Cobalt (II) chloride

Ionic compounds with a specific number of water molecules associated each formula unit are called *hydrated*. The number is shown after a centered dot, and in the name is indicated in the systematic name with a prefix in front of "hydrate". Examples:

- NH_4BrO_3 — Ammonium bromate
- $\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$ — Copper (II) sulfur pentahydrate
- PF_5 — Phosphorus pentafluoride
- $\text{Sn}(\text{ClO}_4)_4$ — Tin (IV) perchlorate
- $\text{Hg}_2(\text{IO}_3)_2$ — Mercury (I) iodate
- $\text{Cr}_2(\text{CO}_3)_3$ — Chromium (III) carbonite
- CS_2 — Carbon disulphate
- $(\text{NH}_4)_2\text{O}$ — Ammonium oxide
- $\text{MgSO}_4 \cdot 6\text{H}_2\text{O}$ — Magnesium sulfate hexahydrate
- Cd_3N_2 — Cadmium nitride
- $\text{Ba}(\text{HCO}_3)_2$ — Barium hydrogen carbonate

6.5 The Mole

In a chemistry context, a mole isn't an animal, it's a quantity — specifically, $6.022 \cdot 10^{23}$. The number isn't random, it's defined as the amount of matter that contains as many objects as the number of atoms in exactly 12 grams of ^{12}C . So, the molar mass of an atom in amu is then numerically the same as the mass of one mole of that atom in grams. For example, the atomic mass of oxygen is 16, so a mole of oxygen will have a mass of 16 grams. Note that this conversion factor of $6.022 \cdot 10^{23} \text{ amu} = 1 \text{ g}$ is an exact number, so there's no worrying over significant figures here. As an example, converting 0.001 grams of carbon into moles relies on the molar mass of carbon (12.01 g). Divide the mass by the molar mass to get the number of moles, then multiply that by $6.022 \cdot 10^{23}$ to get the number of atoms as $5.014 \cdot 10^{19}$ (note: this number does not obey the significant figures rules, realistically there should be only a "5" given).

Moles can also be applied to molecules. The molar mass of a molecule is just the mass in grams of one mole of the substance. The molar mass in grams of any substance is always numerically equivalent to its formula mass in amu, so this conversion is simple enough and no additional complexity is added to the elements-only mole system.

6.6 Bonding Rules & Lewis Dot Diagrams

There are two major rules: the octet rule and the duet rule. Atoms of the main group elements generally try to form bonds to achieve eight outer electrons (octet rule), while atoms on the left side (near helium) bond to try to get only two outer electrons.

This leads to useful diagrams called Lewis dot diagrams, where the electrons are represented as dots around the chemical symbol, in pairs on each of the four sides. The number of dots varies with the number of electrons, but elements in the same group always have the same dot structure. Examples:

- $\cdot \ddot{\text{Cl}} :$
- $\text{Mg} \cdot$
- $\text{K} \cdot$

Lewis structures can be used to show covalent bonds by showing the order and arrangement of valence electrons. Shared electrons are usually represented as a dash. Electrons that are not shared are called nonbonding pairs or lone pairs. For example, $\text{C} - \ddot{\text{O}} :$ shows the Lewis dot structure behind carbon monoxide. Another good example is triple bonded N_2 , written as $\ddot{\text{N}} \equiv \ddot{\text{N}}$. Each bond corresponds to a *pair* of electrons, which is why this might look a little strange. Note that these diagrams only represent the bonds between atoms and the structure involved, they don't necessarily show shape. For instance, H_2O might be drawn with all atoms in a straight line, but in reality the hydrogens do not form a 180° angle.

In case it's needed, there's a good method for figuring these out:

1. Find the total number of valence electrons.
2. Create a skeletal arrangement of atoms. Hydrogen is usually at the periphery, oxygens usually don't bond to each other, and the central atom (the less electronegative atom) is usually the first element in the formula.
3. Create a dash between adjacent atoms to represent bonds. There should be an octet of electrons for each atom, once all bonds are taken into account. Use the total number of valence electrons as counted in the first step to determine whether more bonds should be added or extra electrons should be placed somewhere.

Note that there are a few exceptions to the octet rule, wherein the octet in the outer shell can be exceeded. Carbon, nitrogen, oxygen, and fluorine all strictly follow the octet rule (they simply don't have the capacity to do otherwise), boron always aims for six electrons, but elements in higher periods can sometimes accept them. For example, xenon can accept an additional pair of electrons, letting it form compounds in rare cases despite being a noble gas. Another example is sulfur, which can form sulfur tetrafluoride, for instance. Here, have a list of octet rule exceptions:

1. Odd number of electrons, ex. NO_2
2. Electron-deficient, ex. BF_3
3. Expanded octets (where central atom is a nonmetal in the third, fourth, or fifth period, which have available d orbitals), ex. PF_5 , SF_4 .

It is also possible to have more than one valid Lewis structure if double bonds are next to single bonds; this is called resonance. Resonance forms differ only in the distribution of electrons, not in the arrangement of atoms. The actual structure is the intermediate form, called the resonance hybrid, in which hybrid electron pairs are delocalized resulting in partial bonds. Double headed arrows are used between different resonance forms.

To select the best Lewis structure out of all the resonant forms, look to these formal charges. Formal charges are just the number of electrons minus the number of lone electrons plus half the number of bonding electrons, calculated on an atom-per-atom basis. There are a few rules, in order from most to least importance:

1. Any structure with like charges on adjacent atoms is undesirable.
2. Any structure with a positive formal charge on an oxygen or a fluorine is undesirable (if there is negative formal charge in a structure, it should reside on the most electronegative atom, usually oxygen or fluorine)
3. The structure with formal charges closest to all zero is favored.

This explains why NO_2 is usually written as $\ddot{\text{O}}=\text{N}=\ddot{\text{O}}$, despite that there are two other resonant forms.

6.7 Bonds

Bond length is the distance between the nuclei of two bonded atoms, and bond order is the number of shared electron pairs; for a given pair of atoms, a higher bond order results in a shorter bond length, and thus more energy in the bond. Predictably, this is called bond energy.

Bonds can also have polarity. A normal nonpolar covalent bond involves the equal sharing of electrons, but in a polar bond, electrons spend more time on one atom than the other. This polarity is usually determined by differences in electronegativity — the atom with higher electronegativity will have the electrons more frequently. For instance, when hydrogen is bonded to fluorine, the shared electron pair will spend the majority of its time with fluorine due to its extremely high electronegativity. In general, if the electronegativity difference is 0, the bond is nonpolar covalent, if less than or equal to 0.4 it's mostly covalent, if between 0.4 and 1.7, it's polar covalent, and if greater than 1.7, it's mostly ionic. However, for a molecule for itself to be polar, covalent molecules must have a combination of polar bonds *and* an asymmetric structure or distribution of polar bonds. In symmetrical molecules, the dipoles cancel each other out, creating a nonpolar molecule.

Electronegativity itself is just the ability of an atom to attract shared electrons to itself across a covalent bond. In general, electronegativity increases across a period (proton count increases) but decreases down a group (atomic radius increases). Fluorine is by far the most electronegative element, at electronegativity of 4.0, and is predictably one of the most absurdly reactive elements on the periodic table.

6.8 VSEPR

VSEPR, or **V**alence **S**hell **E**lectron **P**air **R**epulsion theory, is used to predict the shape molecules will take based on the location of spare electron pairs. The gist of it is that spare pairs will orient themselves such that repulsion between them is minimized. This explains why H_2O takes a bent shape: the two lone pairs arrange themselves on the “empty” side of the oxygen, pushing the two hydrogens away.

7 Advanced Bonding & Mechanics

7.1 Valence Bond Theory

For a covalent bond to form, the orbitals of two atoms must overlap. This can explain the covalent bonds present in some simple diatomic molecules like Cl_2 or H_2 . When this happens, electron spins may need to change — in hydrogen, for instance, the spin of the electron is up ($1/2$) by default, so when orbitals overlap one electron must necessarily change its spin to down ($-1/2$). Note that this theory does not explain the formation of bonds and observed geometries of polyatomic molecules like methane (CH_4).

For this reason, there is a *modified* valence bond theory. According to this version, valence atomic orbitals in molecules are different from those in isolated atoms. This process of mixing specific combinations of orbitals is called hybridization; it's performed mathematically and the results are the hybrid orbitals. The two key points are that the number of hybrid orbitals obtained is equal to the number of atomic orbitals mixed, and the type of hybrid depends on the types of the atomic orbitals involved. For example, if you mix an s orbital and two p orbitals, you'll get 3 sp^2 orbitals. As another example, $s + 3p = 4sp^2$, or $s + 3p + d = 5sp^3d$ (note that the coefficients do *not* represent the shell here!). The spatial orientation of hybrid orbitals corresponds with one of the five electron-group arrangements predicted by VSEPR theory. There are also some other consequences here, somehow. If you combine one- s and one- p , you'll get two sp orbitals and two remaining p orbitals... how, I don't know.

Extra electron pairs in a double or triple bond have no effect on the geometry of the molecule; extra electron pairs are not, in fact, located in hybrid orbitals. Bonds are by default sigma bonds, but in double or triple bonds the remaining bonds are formed as pi bonds. Pi bonds are located above and below the original bond axis, and as such are not as strong.

More specifically, sigma bonds are simple end-to-end overlap involving a single lobe; all single bonds are sigma bonds. Sigma bonds allow free rotation. Pi bonding, on the other hand, involves two regions of electron density, one above and one below the main sigma bond. Because of this side-to-side overlap, the free rotation of the atoms with respect to each other is restricted — the pi bond *must* be broken if rotation is to happen. A triple bond would then involve a total of four regions of electron density, one on each of the four sides of the central sigma bond.

7.2 Molecular Bond Theory

Valence bond theory can explain some bonding, but it can't explain molecular shape or any of the magnetic/spectral properties of molecules. To fill in this gap, molecular bond theory was formed, wherein orbitals are delocalized over the entire molecule — into molecular orbitals. The two types of molecular orbitals (MOs) are bonding MOs and antibonding MOs. In the first, there is a constructive interference between AOs, causing increased electron density between two nuclei but overall lower energy. The the second, AOs interfere destructively instead, causing regions of electron density that destabilize the molecule, but result in overall higher energy. Bonding and antibonding MOs are represented as adding and subtracting orbitals, respectively. Antibonding MOs are usually denoted with an asterisk (*) above the name for the bond, ex. σ_{1s}^* .

Diagrams of these MOs can be drawn, according to a few guidelines:

1. The number of MOs formed is equal to the number of AOs combined.
2. Orbitals with similar energy/shape mix more effectively than do those of different energy/shape
3. Orbitals of different n (different sizes/energies) result in less effective mixing
4. An MO can accommodate two electrons.
5. Electrons fill according to Hund's rule
6. The labels on MOs indicate their symmetry, parent atomic orbitals, and bonding/antibonding. An asterisk indicates antibonding, a σ indicates that electron probability is between the two nuclei, and a π indicates that electron probability is above and below the line between nuclei.
7. Bond order is equal to the number of electrons in bonding MOs minus the number of electrons in antibonding MOs, all divided by 2.

7.3 Intermolecular Forces

Intermolecular forces are forces that act between molecules rather than between atoms in a molecule. They're nonbonding and they're much weaker than intramolecular forces (less than 15% as strong as bonding forces in most cases), but they influence the physical properties of the molecule all the same. The main types are ion-dipole, dipole-dipole, hydrogen bonding, and London dispersion forces. As the strength of the intermolecular forces at play increases, boiling/melting point will generally increase. For example, Propane has a very low dipole moment and so has a boiling point of 231 K, while acetonitrile has a much higher dipole moment of 3.9, and consequently has a boiling point of 355 K, despite having a lower molecular weight (?).

Ion-dipole forces are between an ion and the partial charge on the end of a polar molecule. This force increases as the charge of the ion or the magnitude of the dipole moment increases. For example, when NaCl dissolves in water, the ions disassociate, with the positive sodium ions attracted to the negative oxygen atom in water and the negative chlorine ion attracted to the positive hydrogen atoms in water. Ion-dipole forces are the strongest of all the intermolecular forces.

Dipole-dipole forces exist between neutral polar molecules. The positive pole of one molecule is attracted to the negative pole of another, causing a force that is notable but otherwise weaker than ion-dipole forces. The higher the dipole moment, the stronger the dipole-dipole force.

Hydrogen bonding is a special type of dipole-dipole force between hydrogen atoms in a polar bond (particularly HF, HO, and HN), and an unshared electron pair on a nearby atom (usually fluorine, oxygen, or nitrogen). Hydrogen bonding is extremely strong, and largely explains why water (H₂O) has such a high melting and boiling point (not to mention an absurdly high specific heat) despite being such a small and light molecule. Hydrogen bonding is stronger than regular dipole-dipole forces for two main reasons: the hydrogen atom behaves almost like a bare proton when in a highly polar bond (due to the difference in electronegativity), and because its small size allows the unshared electron pair involved approach much closer than would otherwise be possible. As an example of how strong hydrogen bonding is, the two helixes in DNA are held together by hydrogen bonds between nucleotides.

London dispersion forces exist due to temporary dipoles (momentary nonsymmetrical electron distribution) induced in atoms or molecules; as such, *all* molecules are subject to this, although larger atoms are more susceptible. The temporary dipole can in turn induce a similar dipole in a neighboring atom, allowing an exceedingly weak force to briefly exist between the two molecules. All molecules have dispersion forces. The strength depends on two factors: the number of electrons in the atoms that make up the molecule, (as molar mass increases, dispersion forces become stronger), and the polarizability (ease with which electrons are dispersed to form temporary dipoles) of the molecule.

The strongest intermolecular force is ion-dipole, followed by hydrogen bonding, dipole-dipole, and dispersion forces, in that order.

8 Liquids

Solutions A solution is a homogeneous mixture of solvent (the material in larger amount) and solute. The most common solvent is water, which forms aqueous solutions. Solubility is then a measure of how much solute can dissolve in a given solution. If liquids are miscible, they have unlimited solubility in each other, i.e. they can be mixed in any quantity, like CH₃OH and H₂O. The opposite is when liquids are immiscible, or when they have only limited solubility. In general, like dissolves like, so that means polar compounds dissolve polar compounds, and vice versa. This explains why water and octane won't mix, since water is polar and octane is nonpolar, while water and acetone will mix (?).

Surface Tension is a measure of the elastic force on the surface of a liquid. Strong intermolecular forces result in higher surface tensions. In cases of strong enough surface tension or a low enough force, this can even stop foreign objects from breaking through the surface.

Viscosity is a liquid's resistance to flow. It depends on a combination of temperature, intermolecular forces, and molecular complexity. Viscosity decreases with heating but increases with molecular complexity and intermolecular forces. Larger molecules result in more viscous liquids because very large molecules easily become entangled with each other, resisting flow.

Capillarity is the rising of a liquid through a narrow space, even against the pull of gravity. It's caused by competition between intermolecular forces within the liquid (cohesive forces) and those between the liquid and the tube walls (adhesive forces). If adhesion is greater than cohesive forces, you'll get a concave meniscus, such as water in a glass capillary. If cohesive forces are stronger than adhesive forces, you'll see a convex meniscus, like mercury in a glass.