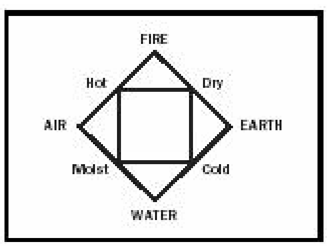
SUBAREA I. ATOMIC STRUCTURE AND THE PROPERTIES OF MATTER

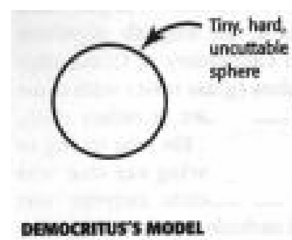
COMPETENCY 1.0 UNDERSTAND THE VARIOUS MODELS OF ATOMIC STRUCTURE, THE PRINCIPLES OF QUANTUM THEORY, AND THE PROPERTIES AND INTERACTIONS OF SUBATOMIC PARTICLES.

Skill 1.1 Identifying major features of models of atomic structure (e.g., Bohr, Rutherford, Heisenberg, Schrödinger) and the supporting evidence for these models (e.g., gold foil experiment, emission spectra)

Our current understanding of atomic structure and the nuclear atom took over two thousand of years and the work of many individuals, often thinking outside of the box.

The concept of the atom can be traced back to the ancient Greek philosophers but may have actually originated with the founder of Buddhism, Gutama who said, “Death is actually the disaggreation of atoms” on his deathbed.





Atoms created quite a controversy in the Greek forum. Two opinions existed; those who believed that matter was continuous followed Aristotle and Plato and those who believed that matter was not continuous followed Leucippetius. Leucippitus believed that a fragment of matter existed that could not be divided and still retain properties of that matter. A student of Leucippetius, Democritus, named the smallest piece of matter atomos, Greek for indivisible.

> *"sweet or sour, hot or cold by convention, existing are only atoms and void"*

Aristotle and Plato had reputations of being very wise and knowledgeable men and so most people believed them. Aristotle did not like the randomness of Democritus’ ideas. He preferred a more ordered matter. Therefore, the idea of atoms and those who believed in their existence had to go underground.

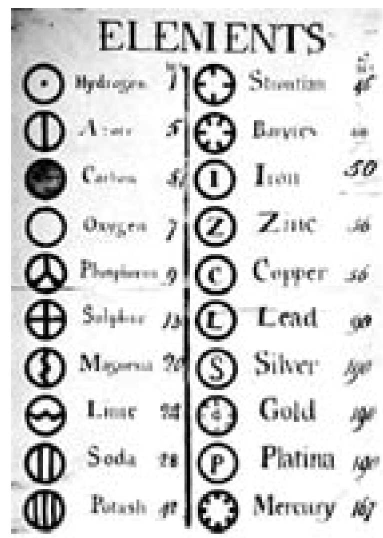
Epicuious created a school and society for those who believed in atoms. Titus Leucritius wrote *de Rurum Natura* in 55 B.C. This poem described the nature of atoms. In the poem there is reference to some phrases of Parmenidis which bear a striking resemblance to what is now known as the law of mass conservation.

> *"the content of the universe was never before more or less condensed than it is today"*

Dalton

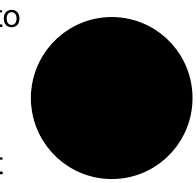
The existence of fundamental units of matter called atoms of different types called elements was proposed by ancient philosophers without any evidence to support the belief. Modern atomic theory is credited to the work of **John Dalton** published in 1803-1807. Observations made by him and others about the composition, properties, and reactions of many compounds led him to develop the following postulates:

1) Each element is composed of small particles called atoms.
2) All atoms of a given element are identical in mass and other properties.
3) Atoms of different elements have different masses and differ in other properties.
4) Atoms of an element are not created, destroyed, or changed into a different type of atom by chemical reactions.
5) Compounds form when atoms of more than one element combine.
6) In a given compound, the relative number and kind of atoms are constant.



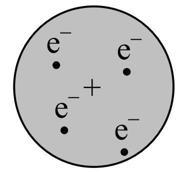
Dalton's table of atomic symbols and masses

Dalton determined and published the known relative masses of a number of different atoms. He also formulated the law of partial pressures. Dalton's work focused on the ability of atoms to arrange themselves into molecules and to rearrange themselves via chemical reactions, but he did not investigate the composition of atoms themselves. **Dalton's model of the atom** was a tiny, indivisible, indestructible **particle** of a certain mass, size, and chemical behavior, but Dalton did not deny the possibility that atoms might have a substructure.



Prior to the late 1800s, atoms, following Dalton's ideas, were thought to be small, spherical and indivisible particles that made up matter. However, with the discovery of electricity and the investigations that followed, this view of the atom changed.

Thomson



Joseph John Thomson, often known as **J. J. Thomson**, was the first to examine this substructure. In the mid-1800s, scientists had studied a form of radiation called "cathode rays" or "electrons" that originated from the negative electrode (cathode) when electrical current was forced through an evacuated tube. Thomson determined in 1897 that **electrons have mass**, and because many different cathode materials release electrons, Thomson proposed that the **electron is a subatomic particle**. **Thomson's model of the atom** was a uniformly positive particle with electrons contained in the interior. This has been called the "plum-pudding" model of the atom where the pudding represents the uniform sphere of positive electricity and the bits of plum represent electrons. For more on Thomson, see http://www.aip.org/history/electron/jjhome.htm.

Planck

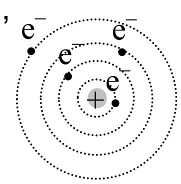
Max Planck determined in 1900 that **energy is transferred by radiation in exact multiples of a discrete unit of energy called a quantum**. Quanta of energy are extremely small, and may be found from the frequency of the radiation, *v*, using the equation:

$$\Delta E = h\nu$$

where *h* is Planck's constant and $h\nu$ is a quantum of energy.

Rutherford

Ernest Rutherford studied atomic structure in 1910-1911 by firing a beam of alpha particles at thin layers of gold leaf. According to Thomson's model, the path of an alpha particle should be deflected only slightly if it struck an atom, but Rutherford observed some alpha particles bouncing almost backwards, suggesting that **nearly all the mass of an atom is contained in a small positively charged nucleus**. **Rutherford's model of the atom** was an analogy to the sun and the planets. A small positively charged nucleus is surrounded by circling electrons and mostly by empty space. Rutherford's experiment is explained in greater detail in this flash animation: http://www.mhhe.com/physsci/chemistry/essentialchemistry/flash/ruther14.swf.

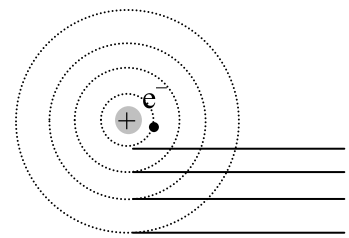


Bohr

Niels Bohr incorporated Planck's quantum concept into Rutherford's model of the atom in 1913 to explain the **discrete frequencies of radiation emitted and absorbed by atoms with one electron** (H, He^{+}, and Li^{2+}). This electron is attracted to the positive nucleus and is closest to the nucleus at the **ground state** of the atom. When the electron absorbs energy, it moves into an orbit further from the nucleus and the atom is said to be in an electronically **excited state**. If sufficient energy is absorbed, the electron separates from the nucleus entirely, and the atom is ionized:

$$H \rightarrow H^{+} + e^{-}$$

The energy required for ionization from the ground state is called the atom's **ionization energy**. The discrete frequencies of radiation emitted and absorbed by the atom correspond (using Planck's constant) to discrete energies and in turn to discrete distances from the nucleus. **Bohr's model of the atom** was a small positively charged nucleus surrounded mostly by empty space and by electrons orbiting at certain discrete distances ("shells") corresponding to discrete energy levels. Animations utilizing the Bohr model may be found at the following two URLs: http://artsci–ccwin.concordia.ca/facstaff/a–c/bird/c241/D1.html and http://www.mhhe.com/physsci/chemistry/essentialchemistry/flash/linesp16.swf.



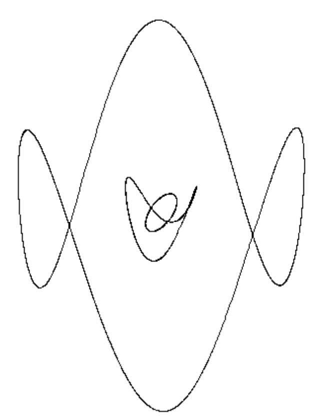
Bohr's model of the atom didn't quite fit experimental observations for atoms other than hydrogen. He was, however, on the right track. DeBroglie was the first to suggest that possibly matter behaved like a wave. Until then, waves were understood as having properties such as wavelength, frequency and amplitude while matter had properties such as mass and volume. DeBroglie's suggestion was quite unique and interesting to scientists.

De Broglie

Depending on the experiment, radiation appears to have wave-like or particle-like traits. In 1923-1924, Louis de Broglie applied this **wave/particle duality to all matter with momentum**. The discrete distances from the nucleus described by Bohr corresponded to permissible distances where standing waves could exist. **De Broglie's model of the atom** described electrons as **matter waves in standing wave orbits** around the nucleus. The first three standing waves corresponding to the first three discrete distances are shown in the figure. De Broglie's model may be found here: http://artsci-ccwin.concordia.ca/facstaff/a-c/bird/c241/D1-part2.html.

Heisenberg

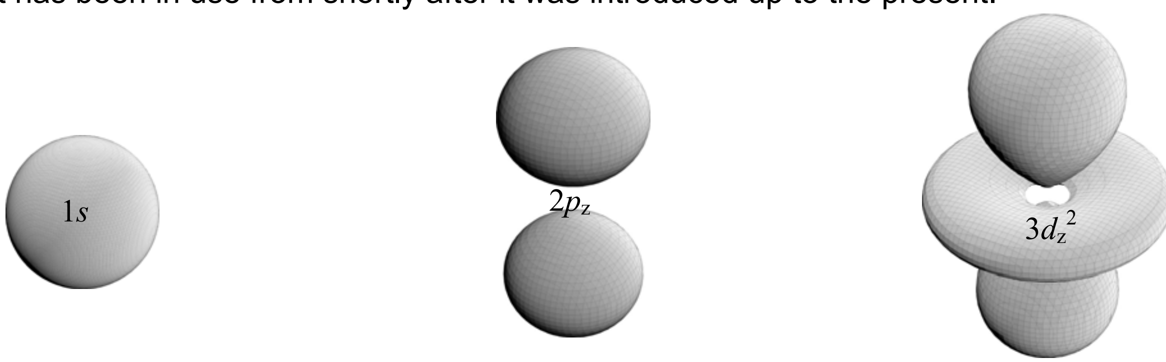
The realization that both matter and radiation interact as waves led Werner Heisenberg to the conclusion in 1927 that the act of observation and measurement requires the interaction of one wave with another, resulting in an **inherent uncertainty** in the location and momentum of particles. This inability to measure phenomena at the subatomic level is known as the **Heisenberg uncertainty principle**, and it applies to the location and momentum of electrons in an atom. A discussion of the principle and Heisenberg's other contributions to quantum theory is located here: http://www.aip.org/history/heisenberg/.



Schrödinger

When Erwin Schrödinger studied the atom in 1925, he replaced the idea of precise orbits with regions in space called **orbitals** where electrons were likely to be found. **The Schrödinger equation** describes the **probability** that an electron will be in a given region of space, a quantity known as **electron density** or Ψ^2. The diagrams below are surfaces of constant Ψ^2 found by solving the Schrödinger equation for the hydrogen atom 1*s*, $2p_z$ and $3d_0$ orbitals. Additional representations of solutions may be found here: http://library.wolfram.com/webMathematica/Physics/Hydrogen.jsp.

Schrödinger's model of the atom is a mathematical formulation of quantum mechanics that describes the electron density of orbitals. It is the atomic model that has been in use from shortly after it was introduced up to the present.



This model explains the movement of electrons to higher energy levels when exposed to energy. It also explains the movement of electrons to lower energy levels when the source of energy has disappeared. Accompanying this drop in energy level is the emission of electromagnetic radiation (light as one possibility).

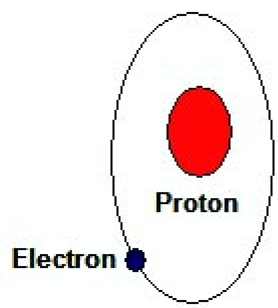
Using Plank's equation, the frequency of that electromagnetic radiation, EMR, can be determined, radiation caused by the movement of matter.

The union of deBroglie's, Planck, Heisenberg, Schrodinger and Bohr's ideas lead to the development of the wave-mechanical view of the atom. The solution to Schrodinger's equation provides for 3 quantum numbers. This added to Pauli's idea that no two electrons could have the same solution set for Schrodinger's equation (known as Pauli exclusion principle) provides four quantum numbers that describe the most probable orbital for an electron of a given energy or the quantum mechanical model of the atom.

Skill 1.2 Identifying the characteristics of protons, neutrons, and electrons and the contribution each makes to atomic number, mass number, and the formation of ions

Atomic theory basically states that atoms are the smallest unit of matter that retains the properties of a substance. While they were considered for some time to be the smallest, indivisible type of matter, they are in fact composed of subatomic particles, including protons, neutrons, and electrons. The nucleus of the atom is very small in relationship to the atom and much of the atom is actually empty space. Within the nucleus are positively charge protons and uncharged neutrons. Thus, the nucleus has a net positive charge. Electrons circle the nucleus and carry a negative charge.

Atoms differ depending upon the element. The simplest atom is hydrogen, which has one proton and one electron that are attracted to each other due to an electrical charge. The spinning force of the electron keeps the electron from crashing into the proton and keeps the electron always moving.



Hydrogen Atom

This is the hydrogen atom, abbreviated H. It has a single neutron and single rotating electron.

The **nucleus** is the center of the atom. The positive particles inside the nucleus are called **protons.** The mass of a proton is about 2,000 times that of an electron. The number of protons in the nucleus of an atom is called the **atomic number**. All atoms of the same element have the same atomic number.

Neutrons are another type of particle in the nucleus. Neutrons and protons have about the same mass, but neutrons have no charge. Neutrons were discovered because scientists observed that not all atoms in neon gas have the same mass. They had identified isotopes. **Isotopes** of an element have the same number of protons, but have different masses. Neutrons explain the difference in mass. They have mass but no charge.

The mass of matter is measured against a standard mass such as the gram. Scientists measure the mass of an atom by comparing it to that of a standard atom. The result is relative mass. The **relative mass** of an atom is its mass expressed in terms of the mass of the standard atom. The isotope of the element carbon is the standard atom. It has six (6) neutrons and is called carbon-12. It is assigned a mass of 12 atomic mass units (amu). Therefore, the **atomic mass unit (amu)** is the standard unit for measuring the mass of an atom.

The **mass number** of an atom is the sum of its protons and neutrons. For any element, there are various isotopes, distinguished by their varying number of neutrons. The **atomic mass** of an element is a weighted (by natural abundance- see Skill 1.3) average of the mass numbers of its isotopes.

The following table summarizes the terms used to describe atomic nuclei:

Term	**Example**	**Meaning**	**Characteristic**
Atomic Number	# protons (p)	same for all atoms of a given element	Carbon (C) atomic number = 6 (6p)
Mass number	# protons + # neutrons (p + n)	changes for different isotopes of an element	C-12 (6p + 6n) C-13 (6p + 7n)
Atomic mass	average mass of the isotopes (weighted by abundance)	usually not a whole number	atomic mass of carbon equals 12.011

Skill 1.3 Analyzing the relationship between atomic mass and the relative abundance of different isotopes of a particular element

The atomic mass of an element is the mass of an atom of the element at rest. Relative atomic mass, also called atomic weight and average atomic mass, is the average of the atomic masses of all isotopes of a given element, adjusted for isotopic abundance. Thus, the atomic weight given for each element on the periodic table is not a round number because it is an average value that takes the relative abundance of isotopes into consideration.

Isotopes of an element vary in the number of neutrons in the nucleus. For example, nitrogen exists in two isotopes, N-14 and N-15. In other words, some nitrogen atoms have a mass of 14 while others have a mass of 15. The atomic weight of nitrogen is 14.007 (as listed in the periodic table). Thus, we can determine the approximate relative abundance of the two nitrogen isotopes as follows.

$$14(x) + 15(1 - x) = 14.007$$
$$14x + 15 - 15x = 14.007$$
$$15 - x = 14.007$$
$$x = 15 - 14.007$$
$$x = 0.993$$

The relative abundance of the N-14 isotope is x, 99.3%. The relative abundance of the N-15 isotope is 1 – x, 0.7%.

Skill 1.4 Analyzing an atom's electron configuration

<u>Quantum numbers</u>

The quantum-mechanical solutions from the Schrödinger Equation utilize three quantum numbers (n, l, and m_l) to describe an orbital and a fourth (m_s) to describe an electron in an orbital. This model is useful for understanding the frequencies of radiation emitted and absorbed by atoms and chemical properties of atoms.

The **principal quantum number *n*** may have positive integer values (1, 2, 3, …). n is a measure of the **distance** of an orbital from the nucleus, and orbitals with the same value of n are said to be in the same **shell**. This is analogous to the Bohr model of the atom.

The **azimuthal quantum number** may have integer values from 0 to n-1. It describes the angular momentum of an orbital. This determines the orbital's **shape**. Orbitals with the same value of n and l are in the same **subshell.** Subshells are usually referred to by the principle quantum number followed by a letter corresponding to l as shown in the following table:

Azimuthal quantum number l	0	1	2	3	4
Subshell designation	*s*	*p*	*d*	*f*	*g*

The **magnetic quantum number m_l or m** may have integer values from $-l$ to l. m_l is a measure of how an individual orbital responds to an external magnetic field, and it often describes an orbital's **orientation**. A subscript—either the value of m_l or a function of the *x*-, *y*-, and *z*-axes—is used to designate a specific orbital. Each orbital may hold up to two electrons.

The **spin quantum number m_s or s** has one of two possible values: –1/2 or +1/2. m_s differentiates between the two possible electrons occupying an orbital. Electrons moving through a magnet behave as if they were tiny magnets themselves spinning on their axis in either a clockwise or counterclockwise direction. These two spins may be described as $m_s = -1/2$ and $+1/2$ or as down and up.

The **Pauli exclusion principle** states that **no two electrons in an atom may have the same set of four quantum numbers** and provides this forth quantum number, m_s.

The following table summarizes the relationship among n, l, and m_l through n=3:

n	l	Subshell	m_l	Orbitals in subshell	Maximum number of electrons in subshell
1	0	1*s*	0	1	2
2	0	2*s*	0	1	2
	1	2*p*	–1, 0, 1	3	6
3	0	3*s*	0	1	2
	1	3*p*	–1, 0, 1	3	6
	2	3*d*	–2, –1, 0, 1, 2	5	10

<u>Subshell energy levels</u>
In single-electron atoms (H, He^{+}, and Li^{2+}) above the ground state, subshells within a shell are all at the same energy level, and an orbital's energy level is only determined by n. However, in all other atoms, multiple electrons repel each other. Electrons in orbitals closer to the nucleus create a screening or **shielding effect** on electrons further away from the nucleus, preventing them from receiving the full attractive force of the nucleus. **In multi-electron atoms, both *n* and *l* determine the energy level of an orbital**. In the absence of a magnetic field, **orbitals in the same subshell with different m_l all have the same energy** and are said to be **degenerate orbitals**.

The following list orders subshells by increasing energy level:
1*s* < 2*s* < 2*p* < 3*s* < 3*p* < 4*s* < 3*d* < 4*p* < 5*s* < 4*d* < 5*p* < 6*s* < 4*f* <5*d* < 6*p* < 7*s* < 5*f* < …

This list may be constructed by arranging the subshells according to *n* and *l* and drawing diagonal arrows as shown below:

1*s*				
2*s*	2*p*			
3*s*	3*p*	3*d*		
4*s*	4*p*	4*d*	4*f*	
5*s*	5*p*	5*d*	5*f*	5*g*
6*s*	6*p*	6*d*	6*f*	6*g*
7*s*	7*p*	7*d*	7*f*	7*g*
8*s*	8*p*	8*d*	8*f*	8*g*

Skill 1.5 Demonstrating knowledge of how atomic spectra relate to the quantum properties of atoms, including how spectra are used for identifying elements and determining their electron configuration

Atomic spectra are the patterns of light emitted by a particular element resulting from the energy released when excited electrons fall to lower energy levels. When we heat a sample of gas made up of atoms of a single element, the electrons become excited and jump to higher energy levels within their atoms. Over time, these electrons fall back to their original energy levels, releasing photons of light in the process. When the emitted light passes through a spectrum, it separates into distinct wavelengths. We can identify and record the wavelengths in the visible spectrum by noting their different colors. Thus, each element has a characteristic banding pattern consisting of a different number of emissions and different color emissions.

The arrangement of electrons in distinct orbitals or energy levels within an atom allows for the identification of elements by atomic spectra. Because each element has a different number and pattern of electrons, each element has a different atomic spectrum.