

1

Structure of Atoms

*"I have discovered something
very interesting."*

W. C. Roentgen (Nov. 8, 1895)

The fifty years following Roentgen's discovery of x-rays saw remarkable changes in physics that literally changed the world forever, culminating in a host of new products from nuclear fission. Discovery of the electron (1897) and radioactivity (1898) focused attention on the makeup of atoms and their structure as did other discoveries. For example, in 1900, Planck introduced the concept that the emission (or absorption) of electromagnetic radiation occurs only in a discrete amount where the energy is proportional to the frequency, ν , of the radiation, or

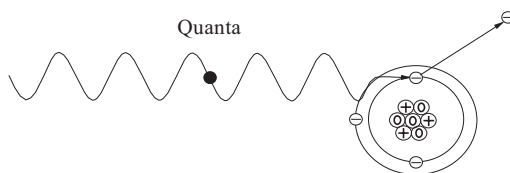
$$E = h\nu$$

where h is a constant (Planck's constant) of nature; its value is

$$h = 6.1260693 \times 10^{-34} \text{ J s or } 4.13566743 \times 10^{-15} \text{ eV s}$$

Planck presumed that he had merely found an ad hoc solution for blackbody radiation, but in fact he had discovered a basic law of nature: any physical system capable of emitting or absorbing electromagnetic radiation is limited to a discrete set of possible energy values or levels; energies intermediate between them simply do not occur. Planck's theory was revolutionary because it states that the emission and absorption of radiation must be discontinuous processes, i.e. only as a transition from one particular energy state to another where the energy difference is an integral multiple of $h\nu$. This revolutionary theory extends over 22 orders of magnitude from very long wavelength radiation such as radio waves up to and including high energy gamma rays. It includes the energy states of particles in atoms and greatly influences their structure.

Einstein (in 1905) used Planck's discrete emissions (or quanta) to explain why light of a certain frequency (wavelength) causes the emission of electrons from the surface of various metals (the photoelectric effect). Light photons clearly have no rest mass, but behaving like a particle, a photon can hit a bound electron and "knock" it out of the atom.



The kinetic energy of the ejected electrons is $KE = h\nu - \phi$.

Example 1–1. Light with a wavelength of 5893 \AA produces electrons from a potassium surface that are stopped by 0.36 volts. Determine: a) the maximum energy of the photoelectron, and b) the work function.

Solution. a) The maximum energy KE_{max} of the ejected photoelectrons is equal to the stopping potential of 0.36 eV .

b) the work function is the energy of the incident photon minus the energy given to the ejected electron, or

$$\begin{aligned}\phi &= [4.13566743 \times 10^{-15} \text{ eV s}] (3 \times 10^8 \text{ m/s}) / 5.893 \times 10^{-10} \text{ m}] - 0.36 \text{ eV} \\ &= 1.7454 \text{ eV}.\end{aligned}$$

A. H. Compton used a similar approach to explain x-ray scattering as interactions between “particle-like” photons and loosely bound (or “free”) electrons of carbon (now known as the Compton effect). Energy and momentum are conserved and the calculated wavelength changes agreed with experimental observations.

1.1

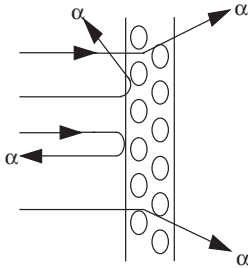
Atom Constituents

Atoms consist of protons and neutrons (discovered in 1932 by Chadwick) bound together to form a nucleus which is surrounded by electrons that counterbalance each proton in the nucleus to form an electrically neutral atom. Its components are: a) *protons* which have a reference mass of about 1.0 and an electrical charge of $+1$; b) *electrons* which have a mass about $1/1840$ of the proton and a (-1) electrical charge; and c) *neutrons* which are electrically neutral and slightly heavier than the proton. The number of protons (or Z) establishes the identity of the atom and its mass number (A) is the sum of protons and neutrons (or N) in its nucleus. Electrons do not, and, according to the uncertainty principle, cannot exist in the nucleus, although they can be manufactured and ejected during radioactive transformation. Modern theory has shown that protons and neutrons are made up of quarks, leptons, and bosons (recently discovered), but these are not necessary for understanding atoms or how they produce radiant energy.

Four forces of nature determine the array of atom constituents. The *electromagnetic force* between charged particles is attractive if the charges (q_1 and q_2) are of opposite signs (i.e. positive or negative); if of the same sign, the force F will be

repulsive and quite strong for the small distances between protons in the nucleus of an atom. This repulsion is overcome by the *nuclear force* (or strong force) which is about 100 times stronger; it only exists in the nucleus and only between protons and neutrons (there is no center point towards which nucleons are attracted). The weak force (relatively speaking) has been shown to be a form of the electromagnetic force; it influences radioactive transformation; and the gravitational force, though present, is negligible in atoms.

The nucleus of an atom containing Z protons is essentially a charged particle (with charge Ze) that attracts an equal number of electrons that orbit the nucleus some distance away. Thomson theorized that each negatively charged electron was offset by a positively charged proton and that these were arrayed somewhat like a plum pudding to form an electrically neutral atom. This model proved unsatisfactory for explaining the large-angle scattering of alpha particles by gold foils as observed by Rutherford and Geiger-Marsden. Such large deflections were due to the electromagnetic force between a positively charged nucleus (Ze) at the center of the atom and that of the alpha particle ($2e$).



The force for such deflections is inversely proportional to the distance r between them, or

$$F = k \frac{q_1 q_2}{r^2} = k \frac{(2e)(Ze)}{r^2},$$

which yields a value of r of about 10^{-15} m which Rutherford proposed as the radius of a small positively-charged nucleus surrounded by electrons in orbits about 10^{-10} m in size. This model had a fatal flaw: according to classical physics the electrons would experience acceleration, v^2/r , causing them to continuously emit radiation and to quickly (in about 10^{-8} s) spiral into the nucleus.

In 1913, Niels Bohr explained Rutherford's conundrum by simply declaring (postulate I) that atoms are stable and that an electron in its orbit does not radiate energy, but only does so when it experiences one of Planck's quantum changes to an orbit of lower potential energy (postulate III) with the emission of a photon of energy

$$h\nu = E_2 - E_1$$

And, that the allowed stationary states for orbiting electrons (postulate II) are those for which the orbital angular momentum, L , is an integral multiple of $h/2\pi$, or:

$$L = n \frac{h}{2\pi}$$

where $n = 1, 2, 3, 4, \dots$, represents the principal quantum number for discrete, quantized energy states. Since $L = mvr$, the calculated radius of the first (or when $n = 1$) electron orbit for hydrogen (the simplest atom) was found to be 0.529×10^{-8} cm, which agreed with experiment. Postulate III is apparently based on Planck's quantum hypothesis, but postulate II appeared to be arbitrary even though it worked, at least for hydrogen. It would only be explained by de Broglie's hypothesis some 13 years later (see below).

Bohr assumed that electrons orbiting a nucleus moved in circular orbits under the influence of two force fields: the coulomb attraction (a centripetal force) provided by the positively charged nucleus and the centrifugal force of each electron in orbital motion at a radius, r_n , and velocity, v_n . These forces are equal and opposite each other, or:

$$\frac{mv_n^2}{r_n} = k \frac{q_1 q_2}{r_n^2}$$

where r_n can be calculated from postulate II. And, since q_1 and q_2 are unity for hydrogen

$$r_n = \frac{(nh)^2}{(2p)2kmq^2} = n^2 r_1$$

where $n = 1, 2, 3, 4, \dots$ and r_1 is the radius of the first orbit of the electron in the hydrogen atom, the so-called Bohr orbit. And since the quantum hypothesis limits values of n to integral values, the electron can only be in those orbits which are given by:

$$r_n = r_1, 4r_1, 9r_1, 16r_1, \dots$$

These relationships can be used to calculate the total energy E_n of an electron in the n th orbit where the sum of its kinetic and potential energy is

$$E_n = \frac{mv_n^2}{2} + \left(-\frac{ke^2}{r_n} \right)$$

$$E_n = -\frac{1}{n^2} \frac{(2\pi)^2 k^2 q^4 m}{2h^2} = -\frac{1}{n^2} \times 13.58 \text{ eV}$$

which is the binding energy of the electron in hydrogen and is in perfect agreement with the measured value of the energy required to ionize hydrogen. For other values of n , the allowed energy levels of hydrogen are:

$$E_n = -\frac{E_1}{4}, -\frac{E_1}{9}, -\frac{E_1}{16}, \dots$$

where $E_1 = -13.58$ eV. These predicted energy levels can be used to calculate the possible emissions (or absorption) of electromagnetic radiation and their wavelengths for hydrogen. When Bohr did so for $n = 3$ he obtained the series of wavelengths measured by Balmer, and since the theory holds for $n = 3$, Bohr postulated that it should also hold for other values of n , and the corresponding wavelengths were soon found providing dramatic proof of the theory.

In 1926, Louis de Broglie postulated that if Einstein's and Compton's assignment of particle properties to waves was correct, why shouldn't the converse be true; i.e., that particles have wave properties such that an electron (or a car for that matter) has a wavelength, associated with its motion, or

$$\lambda = \frac{h}{p} = \frac{h}{mv}$$

and that as a wave it has momentum, p , with the value:

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

This simple but far-reaching concept was later proved by Davisson and Germer who observed diffraction (a wave phenomenon) of electrons (clearly particles) from a nickel crystal. De Broglie's wave/particle behavior of electrons also opened the door to description of the dynamics of particles by wave mechanics, perhaps the most revolutionary development in physics since Einstein's special theory of relativity.

Simple though it appears, de Broglie's hypothesis has consequences as significant as Einstein's equivalence of mass and energy ($E = mc^2$) which are related to each other through c^2 , a large constant of proportionality; in de Broglie's equations, the wavelength, and the momentum p of a particle are related to each other through Planck's constant, a very small one.

1.2

Structure, Identity, and Stability of Atoms

The identity of an atom is determined by the number and array of protons and neutrons in its nucleus. An atom with one proton is defined as hydrogen; it has one orbital electron for electrical neutrality. Deuterium (or hydrogen-2) also con-

tains one proton and one electron but also a neutron and is quite stable; tritium (hydrogen-3) with one proton and one electron has a second neutron which causes it to be unstable, or radioactive. These three are isotopes of hydrogen.

Two protons cannot be joined to form an atom because the repulsive electromagnetic force between them is so great that it even overcomes the strongly attractive nuclear force. If, however, a neutron is present, the distribution of forces is such that a stable nucleus is formed and two electrons will then join up to balance the two plus (+) charges of the protons to create a stable, electrically neutral atom of helium so defined because it has two protons. Its mass number (A) is 3 (2 protons plus 1 neutron) and is written as helium-3 or ${}^3\text{He}$. Because neutrons provide a cozy effect, yet another neutron can be added to obtain ${}^4\text{He}$ which still has two electrons to balance the two positive charges. This atom is the predominant form (or isotope) of helium on earth, and it is very stable (this same atom, minus the two orbital electrons, is ejected from some radioactive atoms as an alpha particle, i.e., a charged helium nucleus). Helium-5 (${}^5\text{He}$) cannot be formed because the extra neutron creates a very unstable atom that breaks apart very fast (in 10^{-21} s or so). But, for many atoms an extra neutron(s) is easily accommodated to yield one or more isotopes of the same element, and for some elements adding an extra neutron (or proton) to a nucleus only destabilizes it; i.e., it will often exist as an unstable, or radioactive, atom. Such is the case for hydrogen-3 (${}^3\text{H}$, or tritium) and carbon-14 (${}^{14}\text{C}$). Elements are often identified by name and mass number, e.g., hydrogen-3 (${}^3\text{H}$) or carbon-14 (${}^{14}\text{C}$).

Three protons can be assembled with three neutrons to form lithium-6 (${}^6\text{Li}$) or with four neutrons, lithium-7 (${}^7\text{Li}$). Since lithium contains three protons, it must also have three orbital electrons, but because the first orbit can only hold two electrons (there is an important reason for this which is explained by quantum theory) the third electron occupies another orbit further away.

1.3

Chart of the Nuclides

As shown in Figure 1-1, a plot of the number of protons versus the number of neutrons increases steadily for heavier atoms because extra neutrons are necessary to distribute the nuclear force and moderate the repulsive electrostatic force between protons. The heaviest element in nature is ${}^{238}\text{U}$ with 92 protons and 146 neutrons; it is radioactive, but very long-lived. The heaviest stable element in nature is ${}^{209}\text{Bi}$ with 83 protons and 126 neutrons. Lead with 82 protons is much more common in nature than bismuth and for a long time was thought to be the heaviest of the stable elements; it is also the stable endpoint of the radioactive transformation of uranium and thorium, two primordial naturally occurring radioactive elements (see Chapter 6).

The *chart of the nuclides* contains basic information on each element, how many isotopes it has (atoms on the horizontal lines) and which ones are stable (shaded) or unstable (unshaded). A good example of such information is shown in

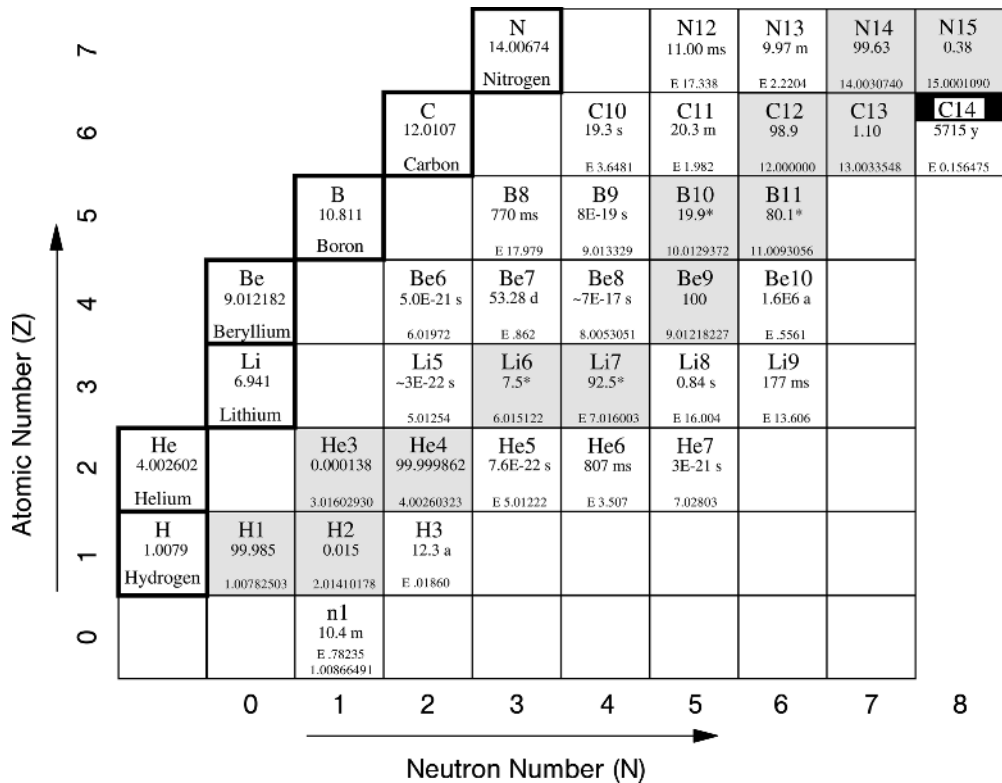


Fig. 1-1 Part of the chart of the nuclides.
(*Nuclides and Isotopes*, 16th Edition, KAPL, Inc, 2002.)

Figure 1-2 for four isotopes of carbon (actually there are 8 measured isotopes of carbon but these 4 are the most important). They are all carbon because each contains 6 protons, but each has a different number of neutrons, hence they are distinct isotopes with different weights. ^{12}C and ^{13}C are shaded and thus are stable, as are the two shaded blocks for boron (5 protons) and nitrogen (7 protons) also shown in Figure 1-2. The nuclides in the unshaded blocks (e.g., ^{11}C and ^{14}C) are unstable simply because they don't have the right array of protons and neutrons to be stable (we will use these properties later to discuss radioactive transformation). The dark band at the top of the block for ^{14}C denotes that it is a naturally-occurring radioactive isotope, a convention used for several other such radionuclides. The block to the far left contains information on naturally abundant carbon: it contains the chemical symbol, C, the name of the element, and the atomic weight of natural carbon, or 12.0107 grams/mole, weighted according to the percent abundance of the two naturally occurring stable isotopes. The shaded blocks contain the atom percent abundance of ^{12}C and ^{13}C in natural carbon at 98.90 and 1.10 atom percent, respectively; these are listed just below the chemical symbol. Similar information is provided for all of the elements in the chart of the nuclides.

<div>C</div> <div>12.0107</div> <div>Carbon</div> <div><div><div><div></div></div><div><div></div></div></div><div><div><div></div></div><div><div></div></div></div></div> <div><div><div></div></div><div><div></div></div></div> <div><div><div></div></div><div><div></div></div></div> <div><div><div></div></div><div><div></div></div></div> <div><div><div></div></div><div><div></div></div></div> <div><div><div></div></div><div><div></div></div></div> <div><div><div></div></div><div><div></div></div></div> <div><div><div></div></div><div><div></div></div></div> <div><div><div></div></div><div><div></div></div></div> <div><div><div></div></div><div><div></div></div></div> <div><div><div></div></div><div><div></div></div></div> <div><div><div></div></div><div><div></div></div></div> <div><div><div></div></div><div><div></div></div></div> <div><div><div></div></div><div><div></div></div></div> <div><div><div></div></div><div><div></div></div></div> 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Fig. 1-2 Excerpt from the chart of the nuclides for the two stable isotopes of carbon ($Z = 6$) and its two primary radioactive isotopes, in relation to primary isotopes of nitrogen ($Z = 7$) and boron ($Z = 5$). (Adapted from KAPL, 2002.)

1.4

Nuclear Models

The array of protons and neutrons in each element is unique because nature forces these constituents toward the lowest potential energy possible; when they attain it they are stable, and until they do they have excess energy and are thus unstable, or radioactive; e.g. tritium or carbon-14. Descriptions of the dynamics and changes in energy states of nuclear constituents often use a shell model; however, descriptions of fission and other phenomena are best done with a liquid drop model. The exact form of the nuclear force in the nucleus is not yet known nor the structure of potential energy states of its constituents, but a shell model corresponds nicely with the emission of gamma rays from excited nuclei. These emissions are similar to those that occur when orbital electrons change to one of lower potential energy.

The nucleus exhibits periodicities that suggest energy shells not unlike those observed for electron shells. Atoms that have 2, 8, 20, 28, 50, and 82 neutrons or protons and 126 neutrons are particularly stable. These values of N and Z are called magic numbers, and elements with them have many more stable isotopes than their immediate neighbors. For example, Sn ($Z = 50$) has 10 stable isotopes, while In ($Z = 49$) and Sb ($Z = 51$) each have only 2. Similarly, for $N = 20$, there are 5 stable isotones (differing elements with the same N number), while for $N = 19$, there is none, and for $N = 21$, there is only one. The same pattern holds for other magic numbers.

A *nebular model of the atom*, as shown in Figure 1-3, provides an overall description of the atom. In it the electrons are spread as waves of probability over the whole volume of the atom, a direct consequence of de Broglie's discovery of the wave characteristics of electrons and other particles. Electrons are distributed around a nucleus in energy states that are an equal number of de Broglie wavelengths, or $n\lambda$, where n , the principal quantum number, corresponds to energy shells, K, L, M, etc. for $n = 1, 2, 3, \dots$; changes between electron states are quantized with discrete energies. The outer radius of the nebular cloud of electrons is about 10^{-10} m which is some 4 to 5 orders of magnitude greater than the nuclear radius at about one femtometer (10^{-15} m), commonly called one fermi in honor of the great Italian physicist and nuclear navigator, Enrico Fermi. The radius of the nucleus is proportional to $A^{1/3}$ or

$$r = r_0 A^{1/3}$$

where A is the atomic mass number of the atom in question and the constant r_0 has an average value of about 1.3×10^{-15} m, or 1.3 fermi.

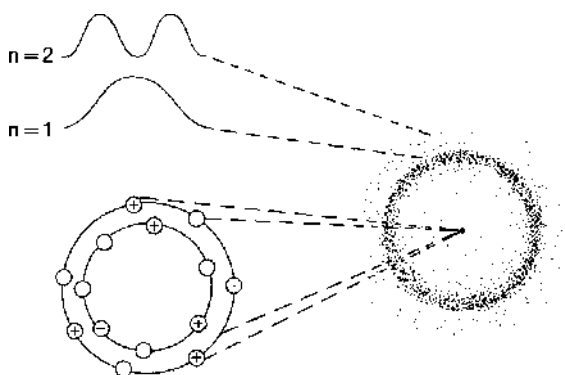


Fig. 1-3 Very simplified model of a nebular atom consisting of an array of protons and neutrons with shell-like states within a nucleus surrounded by a cloud of electrons with three dimensional wave patterns and also with shell-like energy states.

Problems – Chapter 1

- 1-1. How many neutrons and how many protons are there in: a) ^{14}C , b) ^{27}Al , c) ^{133}Xe , and d) ^{209}Bi ?
- 1-2. Calculate the radius of the nucleus of ^{27}Al in meters and fermis.
- 1-3. When light of wavelength 3132 \AA falls on a caesium surface, a photoelectron is emitted for which the stopping potential is 1.98 volts. Calculate the maximum energy of the photoelectron, the work function, and the threshold frequency.

1–4. The work function of potassium is 2.20 eV. What should be the wavelength of the incident electromagnetic radiation so that the photoelectrons emitted from potassium will have a maximum kinetic energy of 4 eV? Also calculate the threshold frequency.

1–5. Calculate the de Broglie wavelength associated with the following:

- a) an electron with a kinetic energy of 1 eV
- b) an electron with a kinetic energy of 510 keV
- c) a thermal neutron (2200 m/s)
- d) a 1500 kg automobile at a speed of 100 km/h.

1–6. Calculate the de Broglie wavelength associated with: a) a proton with 15 MeV of kinetic energy, and b) a neutron of the same energy.