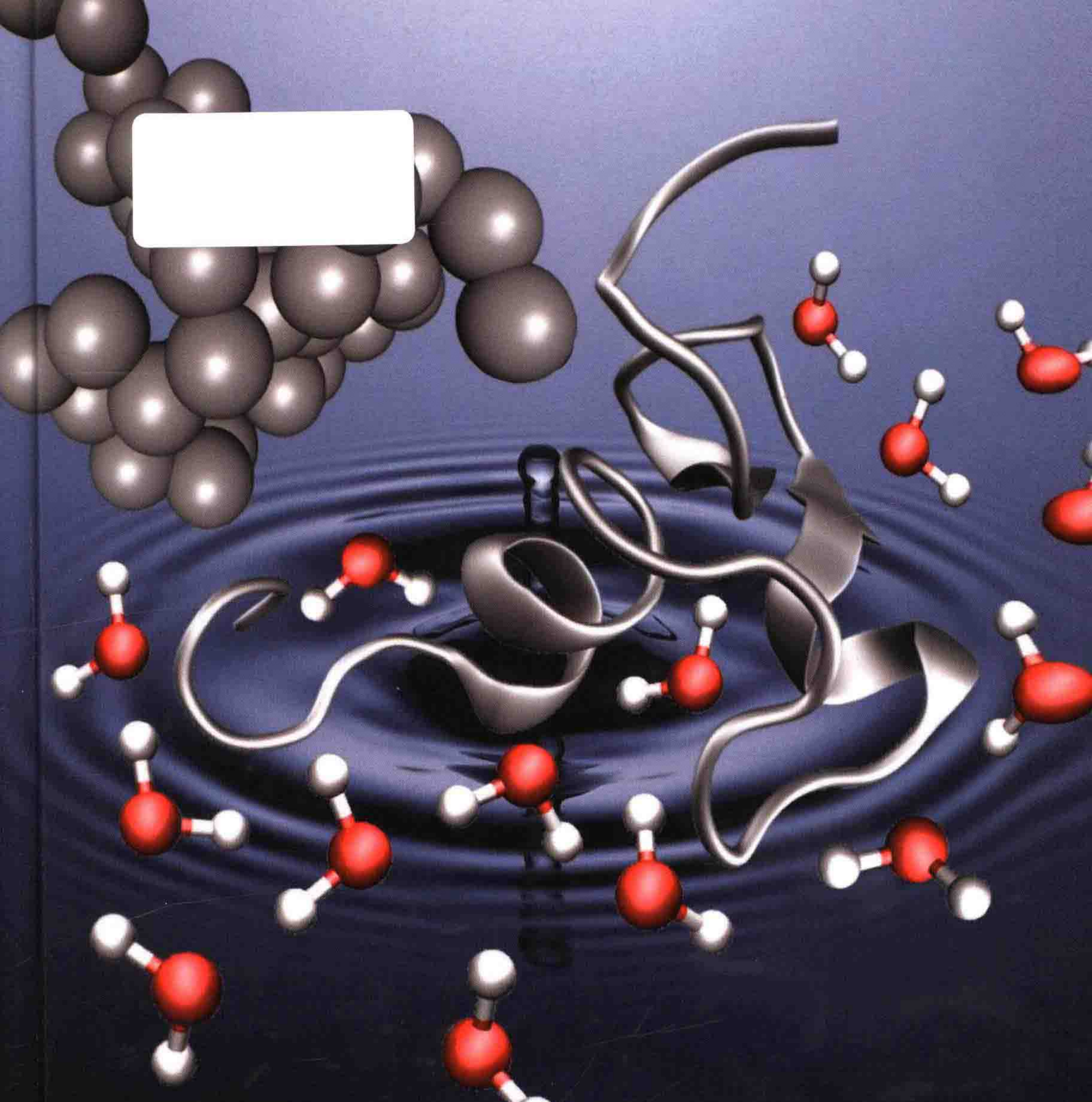

Modeling of Biomolecules and Protein Based Materials

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Modeling of Biomolecules and Protein Based Materials

Preface

Material science is a multidisciplinary field which encompasses all major fields of sciences such as physics, chemistry and biology. As defined by NASA, "Materials science is an extremely broad field that encompasses the study of all materials. Materials scientists seek to understand the formation, structure, and properties of materials on various scales, ranging from the atomic to microscopic to macroscopic. Establishing quantitative and predictive relationships between the way a material is produced, its structure and its properties is fundamental to the study of materials." Materials science though assumed to focus on the study of materials from the macroscopic level actually begins at the atomic scale from bridges, highway building materials to carbon nanotubes. Whatever level material science begins its journey at; its major foundation is the study of structure function relationship of molecules that make up the material. Since centuries mankind has be utilizing the concepts of material science to study and change properties of materials to better suit the needs of human kind. The field of provides information about the structure and composition of materials as and the various ways of processing the materials to better suit our needs. The field of physics provides an in depth knowledge at the atomic level of the materials which can be exploited to better the electronic industry. Materials science also relies heavily on polymer science which is involved in synthesizing new polymeric materials in this century. Materials scientists thus deal with metals, ceramics, and rubber, different kinds of synthetic and natural polymers, superconducting materials, graphite materials, integratedcircuit chips, and fuel cells.

Material science of natural polymers and biomolecules is the main focus of biomaterial research and relies heavily on structure function relationship of the biomolecules. Biomaterial research has led to new innovations in health/medical industry such as a steady state improvement in dental implants and anatomical replacement parts. In addition, biomaterial research in good drug delivery devices, tissue engineering scaffolds and biochips is just beginning to take a leap. It is thus imperitent to expose students with interest in any of the fields of sciences and engineering the vast scope of material science that embraces almost all disciplines of sciences. The 21st century learners are computer literate and are better oriented towards learning using technology. The use of computer modeling as a engaging and explorative tool along with physical hands on modeling can be used to reveal to students that abstract phenomenon's can actually be visualized and understood. For the general biology class wherein you have a diverse array of intellectual abilities, teacher facilitated exposure to computer models of concepts followed by building physical models would be used to emphasize the structure function relationships of molecules.

This book is fed with the information of this subject. This book will be very useful for a wide range of interested groups.

—Editor

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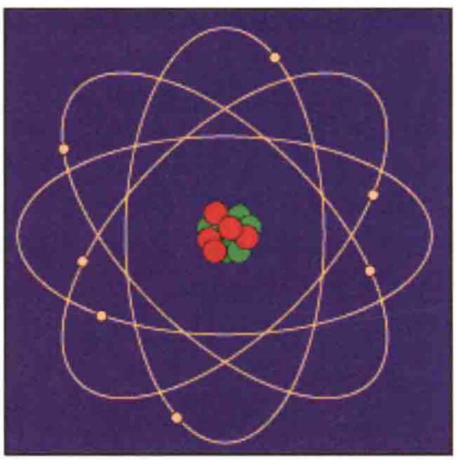
Chapter 1

Introduction

All things are made of a substance called matter. You can think of matter as everything that is not empty space. Many people believe that the space around them is empty space. While this may be true for an astronaut on a space walk, it is not true for us here on earth.



So what kind of matter surrounds you in this "empty" space? Well, one would hope that air would be in the vicinity. Although we can not see the air, it is all around us. Air is made of tiny units of matter, moving rapidly and bouncing off one another and other things. What can make up substances that are so important but invisible?

All matter (including the air we breathe) is composed of very tiny, basic units called atoms. First let us find out what particles make up the atom. An atom is composed of three types of subatomic particles:

- protons,
- electrons,
- and neutrons.

These subatomic particles make up the atoms that make up all matter, both living and nonliving! If everything is made up of atoms, then how can all matter be so different? Atoms can have different numbers of protons, electrons, and neutrons. These different numbers of subatomic particles define the different elements. An element is a pure substance made up of only one kind of atom. Examples of different elements include Hydrogen, Carbon, Sulfur, Oxygen, Nitrogen and Phosphorus. There are many more elements such as Gold, Silver, Mercury or Uranium, but the elements listed first are the ones that generally compose organic matter.

Different elements have very different physical properties or characteristics. Atoms of the same element have the same number of protons, electrons, and neutrons. However, atoms of different elements have different numbers of protons, electrons, and neutrons. All protons are identical to one another, as are all electrons and all neutrons. It is only the number of these subatomic particles that creates the different properties found among the elements. Take Hydrogen and Helium as an example. Hydrogen has one proton and one electron. Helium has two protons, two electrons, and two neutrons. How different are Hydrogen and Helium from each other? They are both gases and they are both lighter than air. However, the Hindenberg blimp that burned in a matter of minutes was filled with Hydrogen, which is extremely flammable. The Goodyear blimp is filled with Helium, which is non-flammable and called an inert, or non-reactive gas. Although the difference in the numbers of protons and electrons is not great between Hydrogen and Helium, these two elements have very different properties.

Atomic Mass and Atomic Number

All elements can be identified by their atomic mass and atomic number. These two values can tell you how many protons, electrons, and neutrons are in any element. The following are examples of the atomic mass and atomic number for the atoms found in several different elements.

- Hydrogen has one proton and one electron. It has an atomic number of one and an atomic weight of one.
- Helium has two protons, two electrons, and two neutrons. It has an atomic number of two and an atomic weight of four.
- Carbon has six protons, six electrons, and six neutrons. It has an atomic number of six and an atomic weight of twelve.

- Oxygen has eight protons, eight electrons, and eight neutrons. It has an atomic number of eight and an atomic weight of sixteen.

Do you see a pattern forming? Electrons are very light compared to the mass of neutrons and protons. Neutrons and protons have approximately the same mass.

Structure of the Atom

Because the number of protons and electrons must be equal in all neutral atoms, the atomic number could represent either the number of protons or electrons.

Scientists have decided that the number of protons represents the atomic number, because the number of electrons may vary when atoms participate in chemical reactions.

The element Hydrogen is unique in that it has no neutrons. Therefore, most of the mass of a Hydrogen atom must come from the proton, because electrons have a tiny mass when compared with protons and neutrons.

The actual atomic mass of each subatomic particle is as follows:

- Proton 1.0073 atomic mass units (amu's)
- Electron 0.00055 atomic mass units (amu's)
- Neutron 1.0087 atomic mass units (amu's).

In practice, we round off the numbers and count the mass of the electron as zero. Atomic weight is equal to the number of protons plus the number of neutrons.

You do not have to memorize all the atomic numbers and atomic weights. They are all on a handy table called the Periodic Table of the Elements, which we will learn to use in this unit. Before going on to the periodic table let's learn more about the parts of the atom.

The Bohr Model

A physicist, Neils Bohr, designed a model for atomic structure. It is called the Bohr model (of course) and is a simple but excellent way to visualize the structure of atoms.

The Bohr Model describes the protons and neutrons located at the centre of the atom, in what we term as the nucleus. The electrons exist around the nucleus in what we call electron shells.

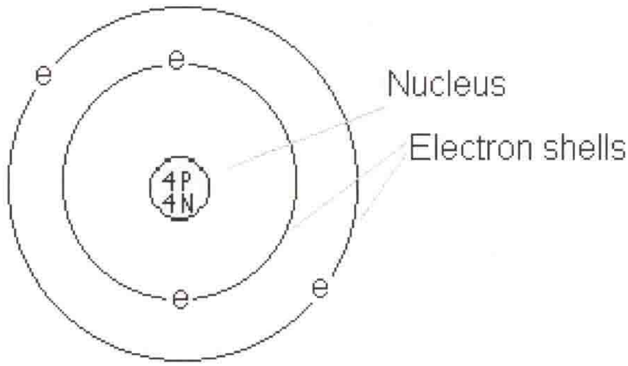


Figure: *Bohr Model of the atom.*

In addition to mass, subatomic particles also have charges. Electrons have a charge of negative one, and protons have a charge of positive one. These positive and negative charges are opposite and exactly equal in strength. For this reason, an atom with one electron and one proton has no net charge. The +1 charge of the proton and the -1 charge of the electron cancel each other out. Neutrons, as their name suggests, are neutral, or uncharged particles. Neutrons contribute mass, but no charge to an atom.

Just like the poles of magnets, the opposite charges on protons and electrons attract one another. This weak nuclear force helps hold the electrons near the nucleus of the atom. You may wonder how all the positively charged protons could possibly exist close together in the nucleus. The protons are of like charge, so why don't the positive charges repel each other? The answer lies in a second fundamental force, called the strong nuclear force.

Atoms of elements must always have the same number of electrons and protons or the elements would be highly reactive and very unstable. If an atom has an unequal number of electrons or protons, it is an ion. Ions can exist only when surrounded by other ions of opposite charge.

The Periodic Table

The periodic table of the elements not only supplies information about the numbers of protons, electrons, and neutrons, but also predicts the reactivity of the atoms of each element. This allows us to predict how different elements will combine to form compounds.

The electrons in atoms interact and form chemical bonds to make different compounds with unique properties. Compounds are formed when the atoms of different elements combine through the sharing of their electrons or the interaction of their charges.

Compounds are represented by a molecular formula. A molecule is the smallest unit of a compound that exhibits the defining characteristics of that compound. The molecular formula uses the abbreviation for each element and represents the proportions of each type of atom in a compound. To start, let us review the molecular formulas of a few common compounds that are probably familiar to you.

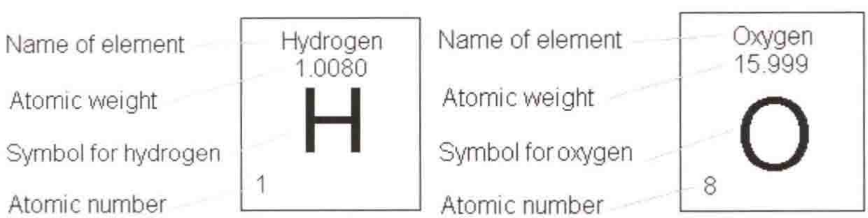
H_2O- water.

NaCl- Sodium chloride (table salt).

The periodic table supplies the information we will need to decipher what the molecular formula of a compound represents, and also how to predict the proportions of elements in a compound.

The periodic table contains the following information:

- Name of Element
- Atomic number
- Symbol of Element
- Atomic weight.



What does the molecular formula of H_2O represent? "H" is the abbreviation for hydrogen, and "O" is the abbreviation for oxygen. The compound water contains two atoms of hydrogen for every one atom of oxygen.

When the atoms of hydrogen and oxygen combine in the above proportions, water is formed. Consider the following molecular formula: H_2O_2. What does this molecular formula represent? This compound has two hydrogens for every two oxygens. Is this compound water?

No! It is a very common disinfectant called Hydrogen Peroxide that can be found at any drug store. Even though the molecular formula is very similar to water the addition of one oxygen gives hydrogen peroxide very different properties when compared to water.

How small are molecules? Can they ever be seen? The most convincing way to demonstrate the relative size of a molecule of water is to find out how many molecules are in about 1 teaspoon of water.

To determine this we need to learn two new concepts. How to calculate the weight of one molecule, and how to use a constant numerical value called Avogadro's number... named after Avogadro of course!

Using the periodic table, let us calculate the molecular weight of water, or the weight of one molecule of H_2O.

Step One: What is the atomic weight of two hydrogens?

Step Two: What is the atomic weight of oxygen?

Step Three: What is the combined weight of two hydrogens and one oxygen? This answer will tell us the molecular weight of H_2O.

Avogadro's number is approximately equal to 6.02×10^{23}. This number tells us how many molecules there are of a substance in a number of grams equal to the molecular weight of that substance. For example, the molecular weight of water is 18, and if you weigh out 18 grams of water in a cup, the cup will contain 6.02×10^{23} molecules of water. If you weigh out the molecular weight of any compound in grams, you will have 6.02×10^{23} molecules of that compound.

Here are some more examples:

The molecular weight of NaCl is 58. Fifty-eight grams of NaCl contains 6.02×10^{23} molecules of NaCl.

The molecular weight of sucrose $C_{12}H_{24}0_{12}$ (table sugar) is 360, and 360 grams of sucrose contains 6.02×10^{23} molecules.

No matter what compound you use, if you weigh out its molecular weight in grams you have 6.02×10^{23} molecules in that amount.

How big is Avogadro's number? Let's put it into perspective. Avogadro's number is approximately 6×10^{23}. One million is a mere 1×10^{6}. Our conclusion? If you had 6×10^{23} dollars you would be MUCH richer than Bill Gates. There are a phenomenal number of molecules in 18 grams of water. Since there are exactly 5 grams of water in a teaspoon, there are 1.673×10^{23} molecules per teaspoon of water. You can see how tiny a molecule must be for so many of them to fit in a teaspoon. There is not a microscope powerful enough to even come close to seeing atoms or molecules.

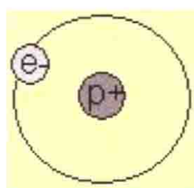
How Compounds Form

We have already touched on the formation of ionic compounds and the sharing of electrons, but now we should discuss this more fully. Atoms of different elements form chemical bonds with one another to produce compounds such as H_2O and NaCl. Electrons present in the atoms of each element are responsible for chemical bond formation. To understand the basics of this process we will reintroduce the Bohr model of the atom in greater detail.

Electrons are constantly on-the-move. They travel so fast and erratically that it is impossible to predict their exact location. This is due to what physicists call the Heisenberg Uncertainty Principle. However, we can say that an electron has a high probability of being found in a certain region around the atom, and this region is what we name the orbital. Electrons do NOT orbit the atom in nice regular circles, like planets orbit the sun. They zip around in random paths around the nucleus like a moth flitting around a light bulb. Electron particles have such a small mass that they behave much like light waves. This may be hard to understand, but don't worry; even the best physicists and chemists have a difficult time understanding the wave-particle nature of electrons.

Electrons with different amounts of energy inhabit orbitals in different electron shells. Physicists have calculated how far each electron shell is from the nucleus of the atom. They have also discovered that the greater the number of electrons in an atom, the more electron shells are necessary to accommodate the electrons.

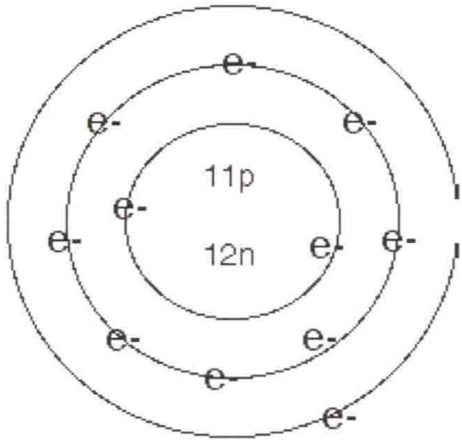
For example, one atom of Hydrogen can be represented by the following Bohr diagram at right. Protons are represented by 1p+, 2p+, 3p+ etc. Electrons are represented by e-.



The dark centre region represents the nucleus that contains the protons and neutrons. The nucleus is responsible for nearly the entire mass of the atom. The area around the nucleus represents the probable location of the one electron in hydrogen. The electron of hydrogen spends most of its time in the first, low energy, electron shell. There is only one orbital in this first electron shell. The orbital is spherically shaped and can hold up to two electrons.

Why is more than one electron shell necessary for atoms with several electrons? Electrons are full of energy, and always trying to stay as far apart from each other as possible. Electrons repel each other because they all have a negative charge. The electron shells closer to the nucleus cover a smaller area and therefore can hold only a certain number of electrons. As electron shells get further from the nucleus of the atom they circumscribe a larger region and can accommodate a larger number of electrons. Each electron orbital has a specified number of electrons it can hold.

What element is represented by the Bohr Model below?



The first electron shell is closest to the nucleus. It can hold up to two electrons. The second electron shell can hold up to eight electrons and the third electron shell can hold anywhere from eight to 18 electrons and so on. Electrons fill the electron shells closest to the nucleus first, and then fill the outer shells accordingly. For example, an atom of Hydrogen (H) with one electron has its electron in the first electron shell. An atom of Helium (He) has two electrons that are both found in the first electron shell. An atom of Lithium (Li) has three electrons, two of which are in the first shell, and the third going into the second electron shell.

The electron orbital configurations quickly become very complex after eight electrons fill the third electron shell. A good general chemistry text can explain the more complicated electron shells, but for our purposes we will examine how electrons are distributed in the first 18 elements of the periodic table. The first three electron shells are filled with two, eight and 18 electrons, respectively. Even though the third shell can hold up to 18 electrons, it can be considered full when it contains eight electrons.

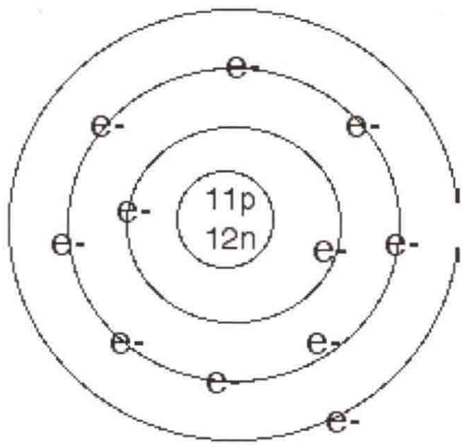
What is the significance of an electron shell being filled? When an electron shell is filled the atom is stable or non-reactive. Let's consider atoms of the elements Hydrogen and Helium once again. Hydrogen, with only one electron in the first shell, is very reactive. It is highly flammable. However, Helium, with two electrons in the first electron shell, is non-reactive. It is called an inert gas.

While all of this is interesting, you may wonder what this has to do with forming compounds. The answer lies in the stability of the outermost electron shell.

Filling the outermost electron shell with electrons makes an atom stable. Atoms combine with other atoms in order to borrow or share electrons. This allows them to fill their outermost electron shell and become stable. A favourite example of many introductory biology textbooks is the compound sodium chloride.

Sodium (Na), atomic number eleven, has eleven electrons. Two are in the first electron shell, eight are in the second electron shell, and one is in the third electron shell. Is the outermost shell filled? How many electrons will it take to fill the third shell?

Bohr model of Sodium:



Chloride (Cl), atomic number 17, has 17 electrons. Two are in the first electron shell, eight are in the second electron shell, and seven are in the third electron shell. Is the outermost shell filled? How many electrons will it take to fill the third shell?

Bohr Model of Chlorine: