

Atoms, Functional Groups,
and Water

Equilibrium and pH

Carbohydrates and
Polysaccharides

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Module 2 / Bonding

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Define, and draw the structure of, a hydrogen bond between any two appropriate molecules.

Recognize and describe a covalent, an ionic, and a hydrogen bond, both structurally and energetically.

Describe the difference between covalent and non-covalent bonds.

Describe the energy associated with breaking covalent and non-covalent bonds.

Describe how water, as a solvent, buffers the structure of ions in solution.

Describe an instance of bioselectivity resulting from the structure and bonding of carbon.

Describe the results of the hydrophobic effect, which is the interaction of hydrophobic molecules to the exclusion of water.

Molecular Bonding

Three major types of chemical bonding have been described thus far: [covalent bonding](#), and two forms of non-covalent bonding, [ionic](#) and [hydrogen](#). These bonds are all important in the functioning of a cell.

Covalent Bonds

Covalent bonds are the strongest. One atom fully shares one, two or three electrons with another atom., forming a single, double, or triple bond, respectively. The bonds can be between the same element (e.g., C-C bonds) or between different elements (e.g., C-O, C-N, H-O). The nature of the covalent bond is determined by the number of electrons shared and the nature of the two elements attached.

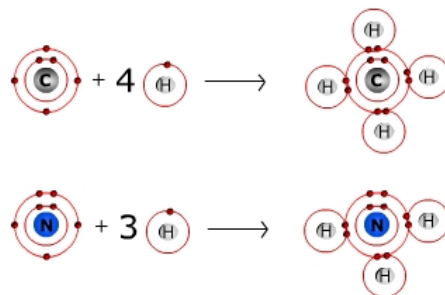
Single bonds: Two atoms attached by a single covalent bond have free rotation about the bond.

Double bonds: Two carbons attached by a double covalent bond can only undergo 180 degree rotations and the atoms bound to these carbons are constrained to lie in the same plane as the carbon atom.. Rotation about the carbon-carbon bond has structural implications for molecules in which they are found. For example, the type of bond can influence the fluidity of biological membranes and restrict the folding of proteins.

Triple bonds. Although carbon can form triple bonds, such as in the compound acetylene (HCCH), triple bonds are not found in biological systems.

Aromatic Compounds: Involve the sharing of electrons between atoms that form a ring. The shared electrons form a partial (1/2) double bond between each atom in the ring structure. Aromatic compounds have unique geometrical properties and absorb ultraviolet light .

FORMATION OF A COVALENT BOND



A covalent bond is formed between two hydrogen atoms.

Covalent bonds involving electronegative atoms often result in polar molecules. As discussed earlier, the bonds between the hydrogen and oxygen atoms of water are polar, due to the fact that oxygen is electron withdrawing and hydrogen is willing to give up its lone electron. The double bond between carbon and oxygen atoms in a carbonyl group is polar, for the same reason that the oxygen attracts the electrons to itself.

Geometry

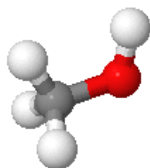
The overall shape of molecules depends on the geometry of the bonds that are formed between atoms. The shape of a molecule can have a large effect on its biological activity, often small changes in the shape of a molecule will make it biologically inactive.

We saw with water that the orientation of atoms around the oxygen was tetrahedral with the angle between the two hydrogen atoms close what would be expected for a tetrahedral shape. Both carbon and nitrogen also form tetrahedral shapes. In the case of methane the four hydrogen atoms are at the corners of a tetrahedron. In ammonia, the three attached hydrogens form the base of a tetrahedron. In the ammonium ion, the addition of a fourth hydrogen, to form NH_4^+ , places the fourth hydrogen at the last unoccupied corner of the tetrahedron.

Carbon and nitrogen can also form planer geometries, where all of the atoms that are bound to the carbon (or nitrogen) are in the same plane as the carbon or nitrogen. In the case of carbon, a planer geometry is usually observed if the carbon is involved in a double bond, while the tetrahedral geometry is found if the carbon is forming single bonds. Compare the structure of methanol to formaldehyde in the Jmol below. In methanol, carbon forms four single bonds while in formaldehyde there is a double bond between the carbon and the oxygen. The carbon atom in methanol shows tetrahedral geometry, while the carbon atom in formaldehyde is planer; the two hydrogens and oxygen lie in the same plane as the carbon..

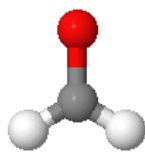
Instructions: Compare the geometries of carbon atom in methanol and formaldehyde and then answer the questions below.

Methanol



JSmol

Formaldehyde



JSmol

Cyclohexane is a ring structure formed with 6 carbons, each carbon forms one bond with the carbon adjacent to it. It has the formula C_6H_{12} . The carbons in this molecule are involved in:

Based on your answer to the first question - do you expect cyclohexane to be planer? You can use the Hint to view the 3D structure of cyclohexane.



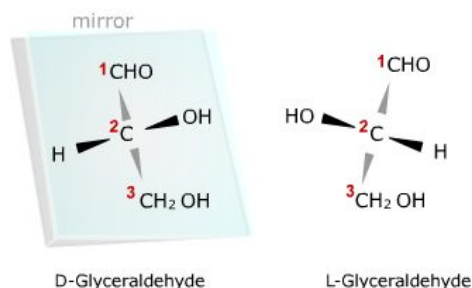
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Chirality

An important aspect of carbon bonding is the fact that carbon can covalently bond to four groups and that the bonding geometry of the carbon atom is tetrahedral. Therefore, if the four groups attached to the carbon are different, then two unique arrangements of the groups around the carbon atom are possible and this carbon is said to be an **asymmetric center** or a **chiral center**. The two arrangements of groups about the carbon are mirror images of each other and these two structures are referred to as **enantiomers**. It is impossible to superimpose these two mirror images, consequently they are distinct molecules.

Because the enantiomers have identical functional groups attached to the chiral center they have identical physical and chemical properties - except for the direction they rotate plane polarized light. Experimentally, the enantiomers are distinguished by the direction of rotation of plane polarized light. The enantiomer that rotates light to the right is designated as D (dextro) form of the compound. The other enantiomer will rotate light in the opposite direction, and is designated as the L (levulo) form of the compound.

The example shown below is the three carbon carbohydrate, glyceraldehyde. This compound contains a chiral center at the middle, or second carbon, because that carbon has four different groups attached to it. The configuration of atoms in the left-hand structure causes polarized light to be rotated to the right and is therefore the D form. Its mirror image shown on the right, rotates polarized light in the opposite direction, and is therefore the L form. Note that in both compounds the H and OH groups project out of the page towards you, but in the D form the -OH group is to the right of carbon two while in the L-form it points to the left.



The two arrangements of atoms around a chiral center are mirror images much as the right hand is a mirror image of the left. The dark black arrows indicate that atoms are above the page and the gray arrows indicate the atoms are below the page.

While enantiomers usually undergo chemical reactions in an identical fashion, biological systems are capable of discriminating between these structurally different molecules because biological systems themselves contain chiral centers, such as in amino acids. The ability to discriminate between the enantiomers is an

example of **biological selectivity**. The chemical world has been narrowed by the selective use of specific enantiomers

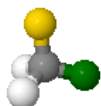
example of bioselectivity. The chemical world has been narrowed by the selective use of specific enantiomers (in this case only D-glyceraldehyde) by biological systems.

chirality

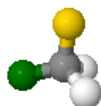
(definition) When identical groups attached to a carbon are arranged in multiple ways such that two of the resulting structures are non-superimposable, they are mirror images of each other.

Chirality of Chloro-Fluoro Methane

Instructions: Chloro-fluoro methane and its mirror image are shown below. Please answer the question using these two structures.



JSmol



JSmol

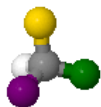
How many different groups are attached to the central carbon atom?



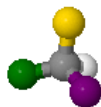
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Chirality of Chloro-Fluoro-Bromo Methane

Instructions: One additional hydrogen has been replaced by bromine (colored purple). One form of the molecule is shown on the left and its mirror image is on the right. Use these two structures to answer the question on the right.



JSmol



JSmol

Is it possible to superimpose one molecule on to its mirror image?

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Chirality of Glyceraldehyde

Instructions: Try to determine the chirality of glyceraldehyde, one of the simplest organic molecules found in biology. A static image of L-glyceraldehyde is shown on the left. Is the right 3D structure the D form or the L form of glyceraldehyde?

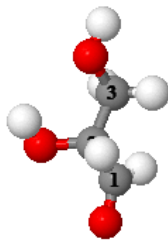
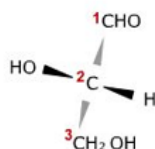
The Jmol model below is of the carbohydrate glyceraldehyde.

What is the chirality of carbon 2 in this molecule?

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L-Glyceraldheyde

Glyceraldheyde



JSmol

Chirality of Threonine

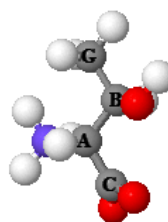
Instructions: Try to identify the chiral center(s) of a more complicated molecule - the amino acid threonine, one of the building blocks of proteins.

This Jmol model is of the amino acid Threonine. This amino acid contains four carbons, labeled A, B, C, G. Which of the following carbons are chiral?

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L-Threonine



JSmol

Non-Covalent Bonds

Ionic Bonds

Ionic bonds form between oppositely charged atoms. No electron sharing or transfer occurs. The atoms are attracted to each other due to their opposite charges. For example, the positive Na ion, and negatively charged Cl ion, are attracted to each other and form table salt. In an aqueous solution, these ions are completely dissociated and are defined as strong electrolytes. In water molecules surround the ions to form polar interactions to satisfy the charges on the ions. Thus the ions become encapsulated by water spheres, which are called **spheres of hydration**. The biological world is very ionic and the spheres of hydration are important in a cell because they maintain the separation of the many ions of the cell from each other. The sphere of hydration must be broken in order for binding to take place with a specific binding partner.

Previously, water was described as having a high dielectric constant. This property that is a measure of the polarity of the covalent bond within the molecule accounts for the separation of ions by polar molecules such as water. The force of attraction between two oppositely charged ions is inversely proportional to the dielectric constant. Thus water with a high dielectric constant decreases the attraction between opposite charges. This is physically explained by the ability of polar solvents to form ordered hydration layers around ions.

Hydrogen Bonding

Hydrogen bonding was covered in Water - Hydrogen Bonding (go there now) Remember that hydrogen

Hydrogen bonding was covered in water -- hydrogen bonding ([go there now.](#)) Remember that hydrogen bonding occurs between partially negatively charged electronegative atoms, and partially positively charged hydrogen atoms that are attached to electronegative atoms such as oxygen, nitrogen or sulfur. Hydrogen bonding is a critical bonding in the cell. It is the principal bonding that holds the tertiary structure of proteins, carbohydrates and nucleic acids together and the overall stability of these molecules is due in part to the cumulative effect of the large number of hydrogen bonds found in the functional structures. Hydrogen bonds are found in and between a variety of molecules. For example, the enormous number of hydrogen bonds between strands of cellulose provide the strength and structure of the plant cell wall.

Hydrophilic Interaction

The nature of polar molecules is that they contain electronegative atoms, consequently they are capable of [hydrogen bonding](#) with aqueous or polar solvents. Because polar molecules are generally water soluble, they are referred to as being **hydrophilic**, or water-loving. The one-carbon alcohol, methanol, is an example of a polar molecule.

Hydrophobic Interaction

The final type of interaction occurs between neutral, **hydrophobic**, or water-fearing, molecules. These molecules do not interact with water and are characterized by a complete lack of electronegative atoms. In aqueous solutions the hydrophobic molecules are driven together to the exclusion of water. For example, shaking a bottle of oil and vinegar (acetic acid in water), such as in a salad dressing, results in the oil being dispersed as tiny droplets in the vinegar. As the mixture settles, the oil collects in larger and larger drops until it only exists as a layer, or phase, above the vinegar.

A similar effect occurs in biological systems. As a protein folds to its final three-dimensional structure, the hydrophobic parts of the protein are forced together and away from the aqueous environment of the cell. Similarly, biological membranes are stabilized by the exclusion of water between layers of lipids as we will see later.

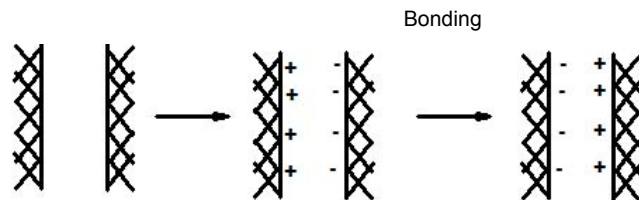
The hydrophobic effect does not involve direct bonding between the non-polar molecules, it is an entropy driven process. You may recall that processes that increase the disorder of a system are more favorable. When a hydrophobic molecule is truly dissolved in water, the water forms a highly ordered ice-like shell around the compound. When the hydrophobic molecules contact each other during separation of the aqueous and non-polar phases, the ordered water is released and become highly disordered. The increase in disorder of the released water molecules is responsible for the spontaneous assembly of many biological systems, such as proteins and membranes.

Mixed Non-polar/polar molecules: Of course, there are instances where even molecules with electronegative atoms will not be water soluble. Computer algorithms are currently used to predict water solubility based on structure. For our purposes, we will balance the ratio of polar and non-polar elements in a structure to estimate the chemical nature of any compound we are going to study.

Amphipathic molecules are molecules that have a distinct non-polar, or hydrophobic region, and a distinct polar region. These molecules do not form true solution in water. Rather, the non-polar parts are forced together into a non-polar aggregate, leaving the polar part of the molecule to interact with the aqueous phase. Detergents and long-chain carboxylic acids are examples of amphipathic molecules.

van der Waals Interactions

An important force in biochemistry is due to **van der Waals** interactions. This interaction occurs between any two surfaces that are in contact. The force is actually an electrostatic one that occurs as a result of a momentary fluctuation in the charge on one surface.. This charge causes the other surface to momentarily assume the opposite charge, leading to a net attractive force. If one of the surfaces has a permanent dipole, due to the presence of electronegative or electropositive atoms, then the attraction is stronger. The strength of van der Waals forces depend on the contact surface area; the larger the area the larger the interaction. At the molecular level, van der Waals interactions can contribute 10s of kJ/mol of energy. At the macroscopic level van der Waals forces can become quite large. For example, the common gecko generates sufficient van der Waals forces due to the large surface area of its foot pads to walk on the ceiling!



Origin of van der Waals effects. Two neutral surfaces (left) have no net attraction. One surface becomes charged for a short period of time. The charge on one surface generates a charge of the opposite sign on the other surface, leading to an attractive force between the two surfaces. A short time later the charges reverse in sign, again generating an attractive force between the two surfaces.

Energy Associated with the Bonds

Each of the bond types represents a measurable amount of energy. To break a bond, the equivalent amount of energy must be expended. In metabolism, bonds are broken in molecules, such as glucose, to "release" the energy. The cell utilizes this energy to drive other energy consuming reactions. The covalent bond has the most energy associated with it, on average approximately 100 kilocalories/mole (kcal/mol). The non-covalent bonds, ionic and hydrogen, and hydrophobic interactions, have approximately 5 kcals/mol associated with each of them.

It should be noted here that throughout the presentation of this course approximations will be used for certain values so that estimations can be made as we move to more complex systems. It is to be acknowledged that very precise values for each of the measurements are not available.

Thus the non-covalent bonds that have been introduced have approximately 20 times less energy associated with them and, thus, are more easily broken individually. However, hydrogen bonds generally form extensive networks, and the total energy associated with the network is the sum of the individual interactions. As anyone who has done a "belly buster" knows, breaking a large surface area of water is extremely difficult (and painful!).

Energy Associated with the Different Bonds

Bond	Energy, kcal/mol
Covalent	100
Ionic	5
Hydrogen	5
Hydrophobic interactions	5
van der Waals	5 (depends on surface area)

When NaCl dissolves in water, each atom becomes surrounded by at least 20 water molecules. As NaCl there is 5 kcal/mol of energy associated with the ionic attraction of the cation and anion, but when a Na ion is surrounded by 20 water molecules, there is 100 kcal/mol of energy associated with just the Na ion. Thus, NaCl in an aqueous solution is energetically more favored than NaCl as the ionically bonded molecule due to the resulting hydrated state. You will explore what happens to molecules that only partially dissociate, or weak electrolytes, in water in the next module.

Practice

did I get this

How would you explain what happens to a salt crystal that remains in a non-polar solvent or a protein that finds itself buried in a sea of lipid?

Submit and Compare

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did I get this

Hydrophobic interactions

- are stronger than covalent bonds.
- can hold two ions together.
- are responsible for the surface tension of water.
- are the major force forming lipid bilayers.



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