2.6: Intermolecular Force and Physical Properties of Organic Compounds

2.6.1 Intermolecular Forces

In Organic Chemistry, the understanding of physical properties of organic compounds, for instance boiling point (b.p.), molecular polarity and solubility, is very important. It provides us with helpful information about dealing with a substance in the proper way. Those physical properties are essentially determined by the intermolecular forces involved. **Intermolecular forces** are the attractive force ***between*** molecules and that hold the molecules together; it is an electrical force in nature. We will focus on three types of intermolecular forces: dispersion forces, dipole-dipole forces and hydrogen bonds.

Dispersion Forces

Dispersion Forces (also called London Forces) result from the instantaneous dipole and induced dipole of the molecules. For nonpolar molecules, the constant shifting and distortion of electron density leads to a weak short-lived dipole at a given moment, which is called an instantaneous dipole. Such temporary dipoles will induce the electrons in a neighbouring molecule to get distorted as well, and to develop a corresponding transient dipole of its own, which is the induced dipole. At the end, all nonpolar molecules are attracted together via the two types of temporary dipoles as shown in **Fig. 2.6a**. The dispersion force is weak in nature, and is the weakest intermolecular force. However, since it applies to all types of molecules (it is the only intermolecular force for nonpolar molecules), dispersion forces are also the most fundamental intermolecular force.

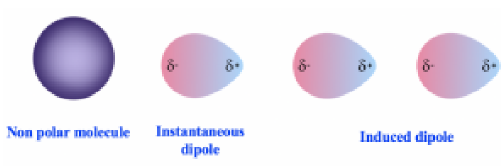

Figure 2.6a Instantaneous Dipole and Induced Dipole

The magnitude of dispersion forces depends on two factors:

- The relative ***polarizability*** of electrons. The simple understanding of polarizability is how easily the electrons get distorted. For larger atoms, there are more electrons in a larger space, therefore the electrons are more loosely held and more easily polarized, so the dispersion force is stronger. Generally, the larger the molar mass of the molecule, the stronger the dispersion force.
- The relative ***surface area*** of the molecule. Molecules with longer, flatter or cylindrical shapes have a greater surface area compared to the bulky, branched molecules, and therefore have a stronger dispersion force. Taking the two constitutional isomers of C_4H_{10} (**section 2.1.2**), butane and isobutane as an example, the dispersion force of butane is stronger than that of isobutane.
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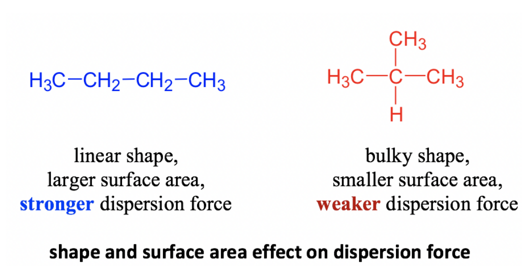
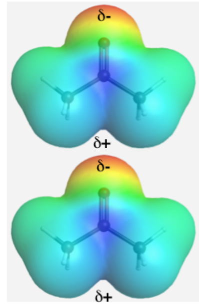


Figure 2.6b Shape and surface area effect on dispersion force

Dipole-Dipole Force

For polar molecules, molecules are attracted to each other because of a permanent dipole, and this type of attractive force is called a dipole-dipole force. As shown below in the electrostatic potential map of acetone, one end of acetone has a partial negative charge (red) and the other end has a partial positive charge (blue). The dipole-dipole force is an attraction force between the positive end of one molecule and the negative end of the neighbouring molecule.



electrostatic potential map of acetone

Figure 2.6c Electrostatic potential map of acetone

Hydrogen Bonds

First of all, do not let the name mislead you! Although it is called a “bond”, a hydrogen bond is not a covalent bond, it is a type of intermolecular force. The hydrogen bond is the force between a H atom that is bonded to O, N or F (atoms with high electronegativity) and the neighbouring electronegative atom,. It can be shown in a general way as:

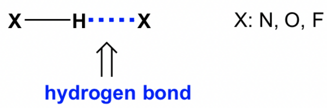


Figure 2.6d Hydrogen bond

The most common example of hydrogen bonding is for water molecules. Water has two O-H bonds, and both are available as hydrogen bond donors for neighbouring molecules. This explains the extraordinarily high b.p. of water (100 °C), considering the rather small molar mass of 18.0 g/mol. As a comparison, the methane molecule CH_4 with a similar size has a b.p. of -167.7 °C.

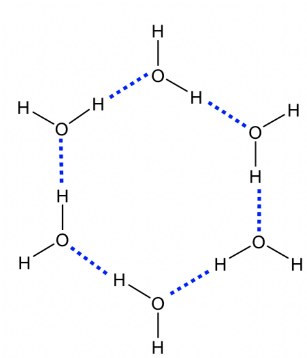


Figure 2.6e Simplified Diagram of Hydrogen Bonds between Water Molecules

For organic compounds, hydrogen bonds play important roles in determining the properties of compounds with OH or NH bonds, for example alcohol (R-OH), carboxylic acid (R-COOH), amine ($R\text{-}NH_2$) and amide $RCONH_2$.

The three major types of intermolecular forces are summarized and compared in **Table 2.6**.

Type of Force	Applied to	Strength
Dispersion Forces	All molecules	0.1 – 5 kJ/mol
Dipolar Forces	Polar molecules	5 – 20 kJ/mol
Hydrogen Bonding	Polar molecules with N – H, O – H or F – H bond	5 – 50 kJ/mol

Increasing

Table 2.6 Summary of the Three Major Intermolecular Forces

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Polar vs Non-Polar molecules

As indicated in **Table 2.6**, the nature of molecular polarity determines the types of force(s) applied to a certain substance. So here we will have discussions about how to tell whether a molecule is polar or non-polar.

The polarity of the compound can be determined by its formula and shape.

For **diatomic molecules**, the molecular polarity is the same as the bonding polarity. That means all homonuclear molecules, like H_2, N_2, O_2, F_2, are non-polar because of their non-polar bond, while all heteronuclear molecules, like HF, HCl, are polar.

For **polyatomic molecules**, the molecular polarity depends on the shape (refer to VSEPR in **Section 1.5**) of the molecule as well. Let's see the examples of H_2O and CO_2.

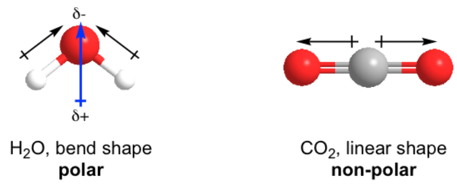


Figure 2.6f Polar and non-polar

Both H_2O and CO_2 have two polar bonds. H_2O is in the bent shape, so the bond polarities of the two O-H bonds add up to give the molecular polarity of the whole molecule (shown above), therefore H_2O is polar molecule. On the other hand, the shape of CO_2 is linear, and the bond polarities of the two C=O bonds cancel out, so the whole CO_2 molecule is non-polar.

There are other examples of non-polar molecules where the bond polarity cancels out, such as BF_3, CCl_4, PCl_5, XeO_4 etc.

For organic compounds, the hydrocarbons (C_xH_y) are always non-polar. This is mainly because of the small electronegativity difference between carbon atoms and hydrogen atoms, making C-H bonds technically non-polar bonds.

For other organic compounds that contain functional groups with heteroatoms, like R-O-R, C=O, OH, NH, they are all polar molecules.

The diagram here (**Fig. 2.6g**) provides a summary of all the discussions about molecular polarities.

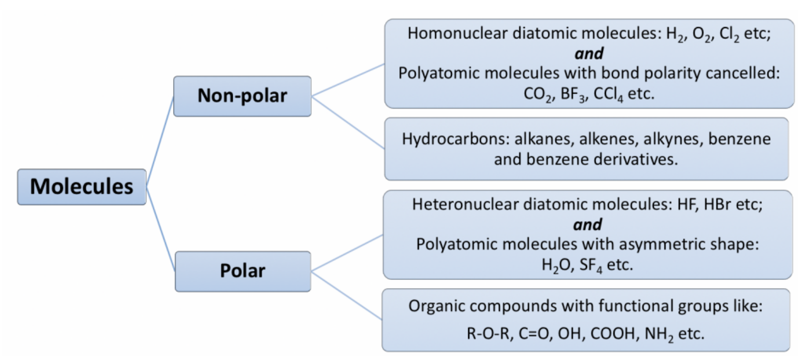


Figure 2.6g Summary of Molecular Polarities

Other than the three types of intermolecular forces, there is another interaction that is very important for understanding the physical property of a compound, which is the ion-dipole force.

Ion-Dipole Force

Ion-dipole force is not categorized as an intermolecular force, however it is a type of important non-covalent force that is responsible for the interaction between ions and other polar substance. A simple example is the dissolving of an ionic solid, or salt, in water. When table salt (NaCl) is dissolved in water, the interactions between the ions and water molecules are strong enough to overcome the ionic bond that holds the ions in the crystal lattice. As a result, the cations and anions are separated apart completely, and each ion is surrounded by a cluster of water molecules. This is called a **solvation** process. The solvation occurs through the strong ion-dipole force. Lots salts, or ionic compounds, are soluble in water because of such interactions.

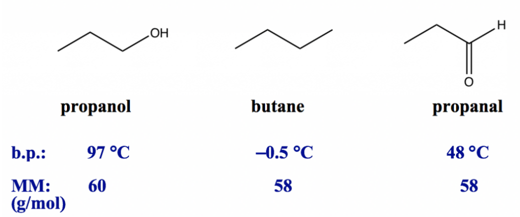
2.6.2 Physical Properties and Intermolecular Forces

The comprehension of intermolecular forces helps us to understand and explain the physical properties of substances, since it is intermolecular forces that account for physical properties such as phases, boiling points, melting points, viscosities, etc. For organic chemistry purposes, we will focus on boiling point (b.p.) and solubility.

Boiling point (b.p):

The boiling point trend of different substance directly correlates with the total intermolecular forces. Generally speaking, the stronger the overall intermolecular force applied to a certain substance, the higher the boiling point of the substance. Boiling point is the temperature at which the liquid phase of the substance vaporizes to become a gas. In order to vaporize a liquid, the intermolecular forces that hold the molecules together must be overcome. The stronger the forces, the more energy is needed to overcome the forces, and a higher temperature is required, thus leading to a higher boiling point.

Example:



All three compounds here have similar Molar Masses, so the dispersion forces are at a similar level. However, the three compounds have different molecular polarities. Butane is a non-polar substance that only has dispersion forces, propanal is a polar molecule with both dispersion forces and dipole-dipole forces, and propanol is a polar molecule with an OH bond, so all three types of forces apply to. Therefore, the overall amount of intermolecular forces is strongest for propanol, and weakest for butane, which is in the same order as their boiling points.

Solubility:

A general rule for solubility is summarized by the expression "like dissolves like". This means that one substance can dissolve in another with similar polarity, and as a result, with similar intermolecular forces. More specifically:

- Nonpolar substances are usually soluble in nonpolar solvents.
- Polar and ionic substances are usually soluble in polar solvents.
- Polar and nonpolar substances are insoluble to each other.

Determining the polarity of a substance has already been summarized in an earlier part of this section (**Fig. 2.6g**). Water, methanol and ethanol are examples of very polar solvents that can form Hydrogen bonds. Ether, ketone, halide and esters are polar solvents as well, but not as polar as water or methanol. Non-polar solvents include hydrocarbons like hexane, benzene, toluene etc.

For some organic compounds, however, it may not be that easy to simply call it polar or non-polar, because part of the compound may be polar, and the another part may be nonpolar. This is often described as hydrophilic or hydrophobic.

- **Hydrophobic** (*hydro*, water; *phobic*: fearing or avoiding) meaning it does not like water, or is insoluble in water;
- **Hydrophilic** (*hydro*, water; *philic*: loving or seeking) meaning it likes water, or is soluble in water.

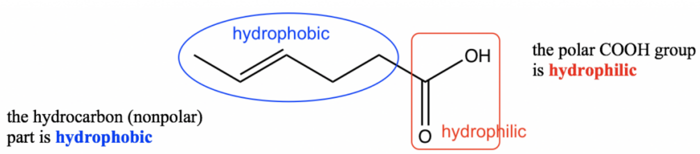


Figure 2.6h Hydrophobic and Hydrophillic

The hydrocarbon part of the organic compound is *hydrophobic*, because it is nonpolar and therefore does not dissolve in polar water. The functional group of OH, COOH, NH_2etc is polar and is therefore *hydrophilic*. With both hydrophobic and hydrophilic parts present in an organic compound, the overall polarity depends on whichever part is the major one. If the carbon chain is short (1~3 carbons), the hydrophilic effect of the polar group is the major one, so the whole compound is soluble in water; with carbon chains of 4~5 carbons, the hydrophobic effect begins to overcome the hydrophilic effect, and water solubility is lost.

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The solubility differences of different alcohols demonstrates this trend clearly; as the length of the carbon chain increases, the solubility of alcohol in water decreases dramatically (**Table 2.7**):

Alcohol	Solubility in water (g/100mL)
methanol, ethanol, propanol (CH_3OH, CH_3CH_2OH, $CH_3CH_2CH_2OH$)	miscible (dissolve in all proportions)
1-butanol ($CH_3CH_2CH_2CH_2OH$)	9
1-pentanol ($CH_3CH_2CH_2CH_2CH_2OH$)	2.7
1-octanol ($CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2OH$)	0.06

Table 2.7 Solubility of different alcohols in water

For organic compounds that are water *insoluble*, they can sometimes be converted to the "salt derivative" via a proper reaction, and thus can become water soluble. This method is used commonly in labs for the separation of organic compounds.

Example:

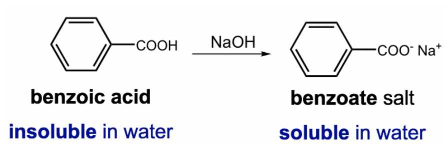

Figure 2.6i Convert insoluble organic compound to the soluble salt derivative

Applying acid-base reactions is the most common way to achieve such purposes. As shown in the above example, by adding a strong base to the benzoic acid, an acid-base reaction occurs and benzoic acid is converted to its salt, sodium benzoate, which is water soluble (because of the ion-dipole force as we learned earlier). The benzoic acid can therefore be brought into water (aqueous) phase, and separated from other organic compounds that do not have similar properties.

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