

SOLUBILITY OF ORGANIC COMPOUNDS

OTHER DOCUMENTS:

[Experimental procedure](#), [Extraction](#) (technique), [Report template](#), [Report QU 4](#)

INTRODUCTION

The objective of this experiment is to investigate the solubility characteristics of some simple organic molecules and to look at relationships between the solubility properties of an organic molecule and its structure, and *vice versa*. This leads to the important idea that **structure dictates function** which means that by knowing the structure of a molecule, we should be able to predict its “function” such as its solubility, acidity or basicity, stability, reactivity towards a particular species such as H⁺ *etc.* Predicting the solubility of an organic molecule is a very useful skill. For example, most reactions are carried out in solution where a solvent needs to dissolve the reactants to allow the molecules to be in the same phase so that they can collide with each other and then react (the solvent also helps absorb and dissipate the heat released). Solubility can be useful when trying to purify samples (*e.g.* recrystallisation: picking a suitable recrystallisation solvent) or isolate products from a multi-component reaction mixture (*e.g.* via extraction), or when extracting a molecule from a natural source such as a plant, or designing a new pharmaceutical that needs to be soluble in the blood stream (aqueous and alkaline), the stomach (aqueous and acidic) or enter the central nervous system (“fatty”). You will learn more about some of these topics and experimental techniques later this semester. For example, you will extract and then isolate caffeine from tea leaves - an “experiment” that you may perform several times per day while making tea (or similarly for coffee from ground coffee)! Solubility is also an important consideration when performing reactions to synthesise molecules; usually, reagents and starting materials are mixed together in a solution. The partitioning of drug molecules within the body between the blood and various tissues is also related to solubility properties.

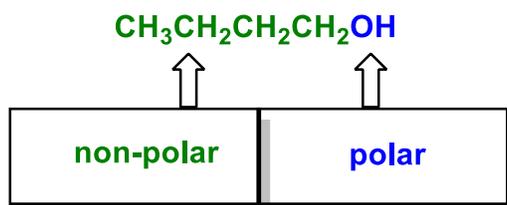
Key practical things to make about solubility:

- Remember that the important phrase “like dissolves like” is referring to the polarity of the materials involved. (polarity controls solubility)
- Solubility of solids in liquids tends to increase with increasing temperature
- Mixing solvents can help modify polarity (*e.g.* adding water to ethanol makes the ethanol more polar)

Solubility

At the molecular level, solubility is controlled by the energy balance of intermolecular forces between solute-solute, solvent-solvent and solute-solvent molecules. Recall from general chemistry that intermolecular forces come in different strengths ranging from very weak induced dipole – induced dipole

interactions to much stronger dipole-dipole forces (including the important special case, hydrogen bonding). However there is a simple, very useful and practical empirical rule that is quite reliable. That simple rule is “**like dissolves like**” and that is based on the **polarity** of the systems *i.e.* polar molecules tend to dissolve in polar solvents (*e.g.* water, alcohols) and non-polar molecules in non-polar solvents (*e.g.* the hydrocarbon hexane). This is why ionic compounds like table salt (sodium chloride) or compounds like sugar, dissolve in water but do not dissolve to any great extent in most organic solvents. It also applies to the separation of oil and water (*i.e.* they are immiscible, *e.g.* think of a salad dressing). The polarity of organic molecules is determined by the presence of polar bonds¹ due to the presence of electronegative atoms (*e.g.* N, O) in polar functional groups such as amines (-NH₂) and alcohols (-OH). Overall, polarity is a balance of the non-polar parts and polar parts of a molecule and it can be convenient to mentally break a molecule into its polar and non-polar components. A larger non-polar “organic” hydrocarbon part will tend to make the molecule less soluble in polar solvents while more polar parts will tend to make it more water soluble (polar solvent) and vice versa for non-polar solvents.



For example, look at the following solubilities in water (g / L) of the straight chain alcohol series :

Methanol and ethanol : infinitely soluble

1-propanol 1000

1-butanol 73

1-pentanol 22

1-hexanol 5.9

1-octanol 0.3

1-nonanol 0.13

1-decanol 0.037

1-dodecanol 0.004

The polar hydroxyl group (-OH) can interact favourably with the structurally similar water molecules (via hydrogen bonding). Therefore, short chain alcohols are water soluble, but as the organic part gets larger (*i.e.* has more C atoms = a longer chain in this series) then this interaction is less effective and so the water solubility decreases. This trend is quite general and applies to other functional groups.

Solubility Classification

Since the polarity of an organic molecule is related to the presence of polar bonds that are found within functional groups, the solubility characteristics of an organic compound can provide experimental evidence for the presence (or absence) of several important organic functional groups*, as indicated in the chart below.

***Review the structure of common organic functional groups BEFORE you come to class - note that [functional groups](#)¹ are covered by CAL351.1**

Most organic molecules are typically relatively non-polar and are usually soluble in less polar solvents. Organic solvents come in a range of polarity depending on the functional groups that they have present within the molecules. For example, methanol, CH₃OH is quite polar (note the structural similarity to water) and ethanol, CH₃CH₂OH, a little bit less so. Acetone (also known as propan-2-one), (CH₃)₂C=O is a moderately polar organic solvent while petroleum ether (a mixture of alkanes) and hexanes are non-polar.

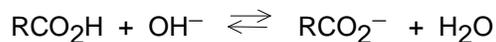
<u>Solvent</u>	<u>Some solubility or complete miscibility</u>
Water	alcohols, amines, acids, esters, ketones, aldehydes (typically only those with <u>4 carbons or fewer</u>)
5% NaHCO ₃	carboxylic acids
5% NaOH	carboxylic acids and phenols
5% HCl	amines
diethyl ether	most organic molecules

Thus, most organic molecules are typically relatively non-polar and are usually soluble in organic solvents (e.g. ethyl acetate, diethyl ether, dichloromethane, chloroform, petroleum ether, hexanes *etc.*) but less soluble or insoluble in polar solvents like water. However, some organic molecules are more polar and therefore, more soluble in water. This denotes a rather high ratio of polar group(s) to the non-polar hydrocarbon chain, *i.e.*, a low molecular weight compound containing an -OH, -NH₂ or -CO₂H group, or a larger molecule containing multiple polar groups (e.g. a molecule of sucrose (sugar) C₁₂H₂₂O₁₁ with 8 hydroxyl groups (-OH) where at 20C, over 200g can be dissolved in just 100 mL of water !)

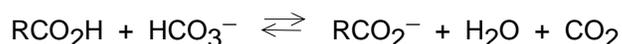
The presence of an acidic -CO₂H or basic -NH₂ functional groups² in a water-soluble compound can be detected by measuring the pH of the solution (low (acidic) or high pH (basic) respectively).

Compounds that contain acidic functional groups that are insoluble in water can become soluble in an aqueous environment if they form an ionic species when treated with a base. This is because the ionic form is much more polar. Similarly, compounds that contain basic functional groups that are insoluble in water can become soluble in an aqueous environment if they form an ionic species when treated with an acid. This is because the ionic form is much more polar.

The solubility of carboxylic acids (typical pKa = 3 to 5) and phenols (pKa = 9 to 10) in aqueous sodium hydroxide (a base) is due to the formation of the polar (ionic) carboxylate or phenoxide groups, since acids and phenols are much stronger acids than water (pKa about 15), and therefore the acid-base equilibria lie far to the right (products), which is the **more polar** side:



Carboxylic acids, but not phenols, are also stronger than carbonic acid, H_2CO_3 , (pKa = 7), and are therefore also soluble in aqueous NaHCO_3 solution:



The solubility of amines in dilute aqueous acid similarly reflects the fact that they are stronger bases than water, and are converted by protonation (*i.e.* reaction with a proton) to the polar ammonium ion:



Amines are the only common class of organic compounds which are protonated in dilute aqueous acid.

In this experiment you will test the solubility of a series of organic compounds containing a variety of common functional groups in the series of five solvent systems. Each test will allow you to classify the organic compound as either **soluble** or **insoluble** in each of the test solvents.

REFERENCES

1. Functional groups
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2. Acidity and basicity
<https://www.chem.ucalgary.ca/courses/351/Carey5th/useful/acidbase.html>