

SOLUBILITY OF ORGANIC COMPOUNDS

OTHER DOCUMENTS:

[Experimental procedure](#), [Report template](#)

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 *etc.* Predicting the solubility of an organic molecule is a useful skill. For example, it can be useful when trying to purify (*e.g.* recrystallisation: picking a suitable solvent) or isolate it 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 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)! 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.

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 it is based on the **polarity** of the systems *i.e.* polar molecules 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 (*e.g.* in salad dressings). The polarity of organic molecules is determined by the presence of polar bonds¹ due to electronegative atoms (*e.g.* N, O) in polar functional groups such as amines (-NH₂) and alcohols (-OH).

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

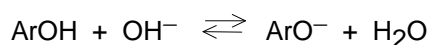
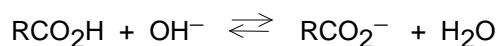
<u>Solvent</u>	<u>Some solubility or complete miscibility</u>
Water	alcohols, amines, acids, esters, ketones, aldehydes (typically only those with <u>4 carbons or fewer</u>)
5% NaHCO ₃	carboxylic acids
5% NaOH	carboxylic acids and phenols
5% HCl	amines
diethyl ether	most organic molecules

Most organic molecules are typically relatively non-polar and are usually soluble in organic solvents (e.g. diethyl ether, dichloromethane, chloroform, petroleum ether, hexanes etc.) but not 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 several polar groups.

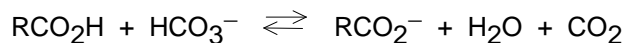
The presence of an acidic -CO₂H or basic -NH₂ functional groups² in a water-soluble compound can be detected by low or high pH, respectively, of the solution.

Compounds that contain acidic or 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 or a base. This is because the ionic form is much more polar.

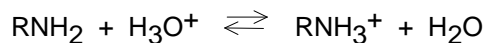
The solubility of carboxylic acids (pK_a = 3 to 5) and phenols (pK_a = 9 to 10) in aqueous hydroxide is due to the formation of the polar (ionic) carboxylate or phenoxide groups, since they are much stronger acids than water (pK_a about 15), and therefore the acid-base equilibria lie far to the right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



Carboxylic acids, but not phenols, are also stronger than carbonic acid, H_2CO_3 , ($\text{pK}_a = 7$), 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
<http://www.chem.ucalgary.ca/courses/351/WebContent/orgnom/functional/func.html>
2. Acidity and basicity
<http://www.chem.ucalgary.ca/courses/351/Carey5th/useful/acidbase.html>