

4.2: Solvent Concepts

According to GC Principle No. 5, “The use of auxiliary substances (solvents, separation agents, etc.) should be made unnecessary wherever possible, and innocuous when used.” This statement signifies or upholds the dogma in GC that simplification to execute a specific transformation should be observed. In other words, if we can find a way to not use a solvent, let’s not use it! Although in our modern society such a stance is almost untenable, the ideal nevertheless is what we as a society should contend to achieve. For example, as shown in Figure 4.2.1, we have an overwhelming influx of medicines, drugs, etc., within our society to promote our health. We typically take these concoctions with water, in emulsions, in solutions, in suspensions, etc.



Figure 4.2.1: The gamut of medicines and its varieties in our culture and life is staggering. pixabay.com/en/health-medicine-tablets-846862/

Of course, taking a medicine without solution is a difficult proposition, but there are a number of ways to do it:

- Dry swallowing or sublingually (e.g., nitroglycerin tablets for angina);
- Patch application (microneedles or high concentration, usually done dermally);
- Inhaled by a mist/spray (e.g., gaseous phase);
- Via a tube (e.g., stomach tube or intravenous).

Nevertheless, the use of solvents and solvent-based systems are deeply ingrained in our culture and society. The reasons are many, but they tend to be tradition, ease of use, reduced cost, and convenience. Doing without solvents tends to require much more creativity and overall planning.

Reaction Energy Coordinate

Typically, a reaction profile or surface (where and how a reaction proceeds according to an energy perspective) provides sufficient information to understand the pathways (independent of final energy states) necessary to achieve a forward reaction. For example, the coordinate shown below illustrates the S_N2 reaction between *t*-butyl chloride and hydroxide. Note that most of the variables shown relate to the energy constraints or parameters associated with the reaction. The reaction has an inherent activation barrier for the forward direction. This barrier characterized by an energy differential input (DE_1^1), relates to the difficulty to accessing a transition state (1) that must be accessed for the forward reaction.

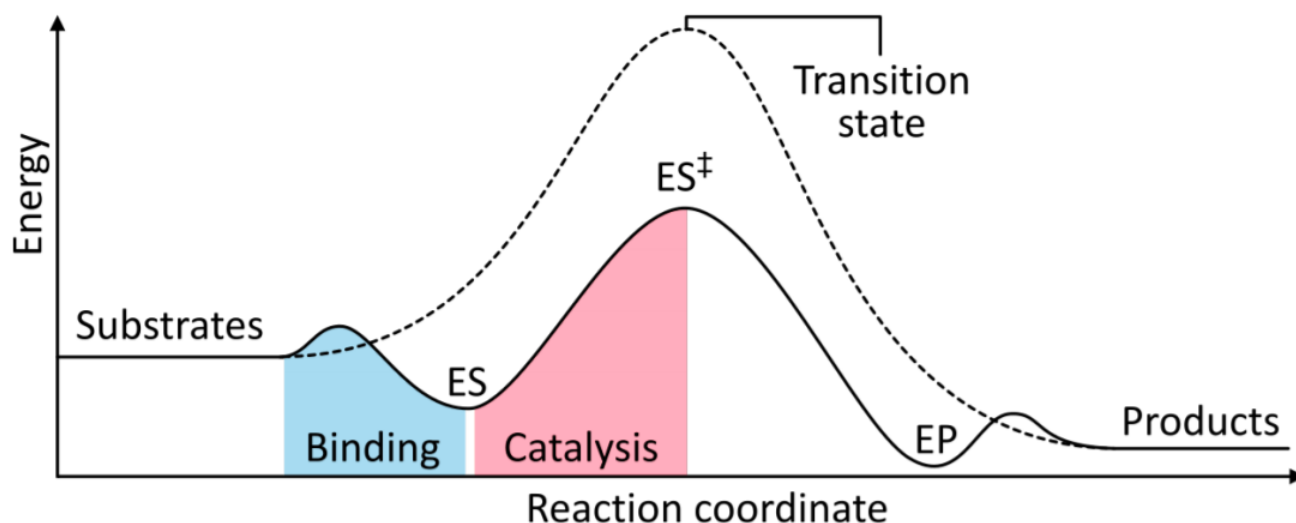


Figure 4.2.2 A typical representation of the energy surfaces obtained during the transformation of an organic halide in a classic S_N2 (bimolecular nucleophilic substitution) reaction. https://commons.wikimedia.org/wiki/File:Enzyme_catalysis_energy_levels_2.svg

Such an energy input, however, can be accommodated or lessened by a number of factors, viz., the use of a catalyst which in general has shown the ability to reduce the energetic considerations to access that state by virtue of its capacity to engage in structural or energetic interactions with the starting material and strongly encourage the formation of the transition state. The downhill nature of the coordinate surface is akin to rolling a ball whose potential energy conversion to kinetic energy is extremely facile. Thus, an intermediate is achieved (the trialkyl carbocation in Figure 4.2.2) that has a measurable lifetime and properties. Although it is by its fundamental character unstable, it nevertheless exists to then engage in further reactions. Notice that it still at an energy surface that is much higher to the starting energy state. Such a phenomenon is then predictive of its future course. In fact, as you move closer to the product along the abscissa of the reaction coordinate surface, the intermediate resembles in a number of properties the nature of the final product. In this case, the intermediate has to a great extent a number of the features of both the starting materials and the product. Indeed, the next activation barrier that must be crossed to access the final product is much lower in height than the normal activation barrier indicating the gradual easing of the transition of starting material(s) to product(s).

Solvent Categories

There are a number of solvents that from a green chemistry perspective must be dealt with judiciously. The following are representative solvent classes:

- Hydrocarbons
- Halogenated hydrocarbons
- Aromatic hydrocarbons
- Alcohols
- Ethers
- Aprotic solvents

Each of the above have their pros & cons in terms of environmental benefit/issue, economics, and social justice. Each may do different things; for example, the aprotic solvent class is one where there is no chance for the solvent to provide a proton to a reaction it is hosting. Alcohols, on the other hand, can easily do that and should not be used in reactions where water/protons could quench a reaction or trigger a violent reaction.

Methyl Soyate

Methyl soyate is a biobased solvent that is a mixture of long-chain fatty acid methyl esters. More information on its specific properties and potential uses can be found in the following tract:

<https://www.yumpu.com/en/document/view/10362159/the-formulary-guide-for-methyl-soyate-soy-new-uses>

In general, it can be used to clean countertops, pretreat fabric stains, clean concrete, degreaser, graffiti remover (with ethyl lactate and surfactants), paint stripper, mastic remover, varnish remover, deinker, asphalt remover, and waterless hand cleaner. In addition to the soyate, there are a number of other emerging biobased cleaners/solvents such as shown below:

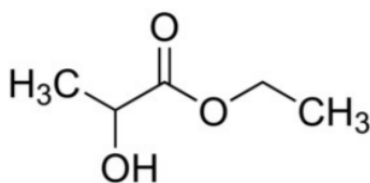


Figure 4.2.3: A representation of ethyl lactate, also known as lactic acid ester, which is a monobasic ester formed from lactic acid and ethanol, that can be used as a solvent. It is considered biodegradable and can be used as a water-rinseable degreaser.
https://www.wikiwand.com/en/Ethyl_lactate

Please see <http://pubs.rsc.org/en/Content/ArticleLanding/2011/GC/c1gc15523g#!divAbstract> for more information on this marvelous solvent.

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