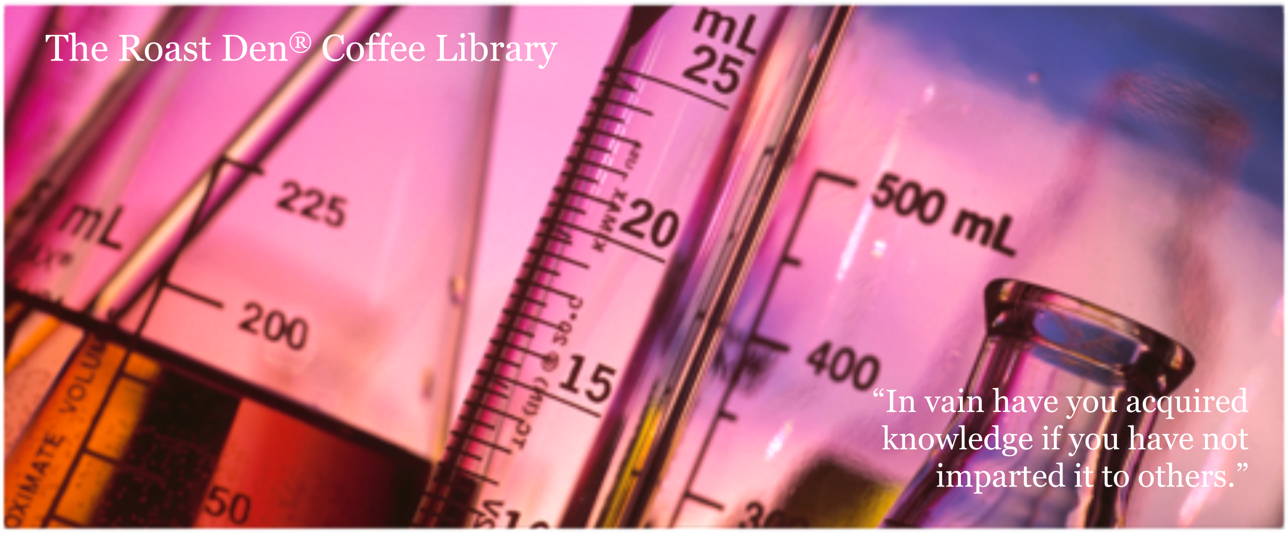


Coffee Chemistry

Coffee is all about the chemistry, on both a scientific level and a psychological level.

Psychological Chemistry

Psychological chemistry occurs when we find a great match. When we find a coffee that we really like, we have definitely found chemistry and this is, of course, a very subjective matter but it is also one of the most alluring qualities of coffee… what I like might not be what you like and vice versa. So we can each embark on a quest for the perfect coffee match for our unique self, a flavour and acidity balance that suits the specific likes and dislikes of our individual palate.

Traditionally, bespoke coffee blends have been the domain of large companies with sufficient purchasing power to buy enough coffee to justify a new blend from a coffee roasting company but The Roast Den®

do not impose such restrictions, at The Roast Den® anyone can create a custom mix bespoke blend from as little as 200g of coffee. With the financial and volume restrictions lifted, the world of the perfect coffee is open to everyone. Don't delay, begin today and pretty soon you will marvel at what you have been missing in psychological coffee chemistry.

Scientific Chemistry

The scientific chemistry is more straightforward. The subjective element can be put aside for a moment and we can concentrate on scientific facts. It will not necessarily guarantee we find the perfect coffee but knowing the chemistry behind the process will certainly assist us to go in the right direction when we begin our quest for perfection.

We could delve into the science of the soils where the coffee plants grow, the plant genus, the climate, the biodiversity of the area where the coffee originates from or the farming techniques but for this short paper we are going to keep it simple, concentrate on post-harvest and, short of noting the basic rule of thumb that the higher the site, the slower the growth, the more concentrated the flavours and the more acidic the coffee bean, we are going to jump to the basic chemistry of the roast process.

In it's simplest form we can consider the roast process to have 5 stages...

Endothermic → Exothermic → Endothermic → Exothermic → Cool Down

During the **Endothermic** stages, we add heat to change the state of the bean.

The **Exothermic** stages occur where a physical change takes place and energy is released from the bean creating it's own heat.

The **Cool Down** stage is used to halt the roasting process.

In the primary stage we introduce a heat source and that heat source is transferred to the bean either through conduction, convection or a combination depending on the roast method we are employing. There can be many arguments about which is the best method but from a scientific chemistry perspective let's consider, at this point, the processes to have equal merit.

As the bean absorbs heat in the primary endothermic stage it will begin to change colour from a green to a golden colour, the bean will expand and the outer silver skin (testa epidermis or chaff) comes off the bean. The bean undergoes an irreversible physical and chemical change known as Pyrolisis. This is a common thermochemical decomposition that combines a change in the beans physical and chemical structure. It is a normal chemical reaction in baking. During this process carbohydrates and proteins in the bean undergo Pyrolisis and a special chemical reaction occurs (quite quickly at around 140^{o}C and 165^{o}C) between the reducing sugars and amino acids, this reaction is typically known as the Maillard reaction and causes the bean to turn a brown colour and develop a desirable roasted flavour (nonenzymatic browning). During the process hundreds of different flavour compounds are created which, in turn, break down further into more flavour compounds, creating a complex flavour structure. As the bean continues to absorb heat, the caramelisation of the sugars becomes more pronounced.

As heat is absorbed by the bean, the moisture in the bean evaporates. At about 175^{o}C the bean moves to the second phase of roasting and becomes exothermic (it begins to give off it’s own heat) and by the time the temperature reaches 196^{o}C all of the moisture will have gone and the bean will have expanded to a point were it will give off a “crack”. We have reached a “light roast” and can stop the roasting at any point from here forward. The bean has completed it’s first exothermic stage and continues its endothermic recovery until the bean temperature reaches approximately 225^{o}C where it emits a second “crack”, this signals the start of the structure of the bean collapsing and a second exothermic reaction. From this point the bean will carbonise until eventually, if left, it will combust.

The time from a great roasted coffee to a terribly roasted coffee can be just a few seconds, so the roaster must maintain a vigilance throughout the process utilising the senses of sight, sound and smell.

When the coffee has been roasted to the desired level, it is necessary to quickly stop the process. This is the Cool Down and can be either dry or wet cooled. In dry cooling, air is forced over the beans to extract the heat and in wet cooling the beans are water drenched to allow the heat to transfer out of the beans. Whatever method is applied, the important aspect is to stop the beans from continuing to roast beyond the final desired point. The skill of the roaster plays an important part in knowing when to stop the heat input and allow the residual heat to complete the process during the cool down.

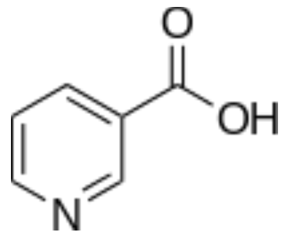
At first crack, all of the desirable flavours have been created so further roasting will only reduce those flavours and draw bitter oils from the bean so one might be forgiven for thinking it best to roast all coffee to 196^{o}C but the chemical process is much more complicated than just flavour complexes, as the roast develops, the carbohydrate breakdown determines the body of the coffee so a longer roast will typically give more body to the end cup. In simple terms we are trading flavour for body when we decide how long we should roast. We can, to an extent, increase the body of the end cup by stretching the roast time, which is a terribly important fact because this gives us the clue that time plays a critical element, alongside temperature, in maximising flavour balance during the roasting process.

If we look more closely at the time-temperature profile in roasting, and study what creates the best cup characteristics, we note that when the ratio of the degradation of Trigonelline to the derivation of Nicotinic acid remains linear we achieve "typically best results".

Let's look at three important chemical compounds…

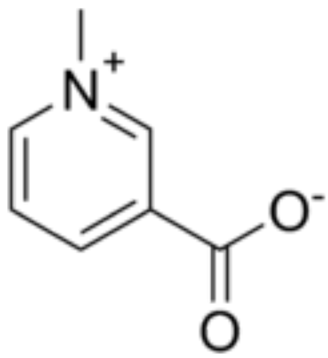
Nicotinic Acid (also known as Vitamin B_3)

Nicotinic acid, sometimes called Niacin or vitamin B_3, is an organic compound with formula $C_6H_5NO_2$ and is one of the essential human nutrients.



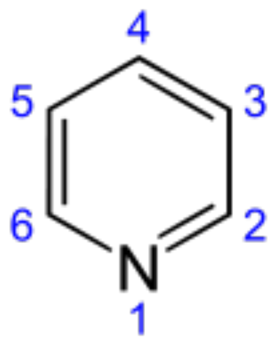
Trigonelline (also known as coffearine)

Trigonelline is a bitter alkaloid ($C_7H_7NO_2$), it is a zwitterion (amino acid) formed by the methylation of the nitrogen atom of Niacin (Vitamin B_3). It is found in many plants including coffee and has a higher concentration in Arabica than Robusta.



Pyridine

Pyridine is a basic heterocyclic organic compound (C_5H_5N). It is a colourless, highly flammable, weakly alkaline water-soluble liquid with a distinctive, unpleasant odour.



So, as we roast the coffee we degrade the Trigonelline and create Vitamin B3 plus generate trace amounts of Pyridine. Pyridine is dominant in the mass spectrum analysis of coffee vapour and Vitamin B_3 increases by as much as 10 times the green bean levels. During the process Trigonelline degrades by 85% or more. So what we are doing is manipulating the aroma and thereby triggering the psychological chemistry that causes us to consider a coffee “typically better” or “typically worse”.

Acidity

In addition to flavour and aroma, the coffee drinker can be acutely aware of acidity. Especially in what is often considered the “better” coffee from high grounds where the beans have matured more slowly and developed more flavours there is also typically an increase in acidity.

In scientific terms, we measure acidity by pH level, with a pH of 7.0 being neutral and the pH number reducing with increased acidity and the pH number increasing with increased alkalinity.

For coffee drinkers we are interested in the pH of the coffee which would be expected in the range of pH 4.0-5.0 (as a benchmark some typical pH measures: lemon juice pH 2.0; milk pH 6.5; Baking Soda pH 9.0; Soapy Water pH 12.0).

Coffee green beans begin with a higher acidity than the roasted beans and as we roast, the acidity level reduces, so a light roast may have pH 4.0 and a dark roast pH 5.0. In determining our ideal coffee we may wish to roast out acidity or minimise the roast to retain acidity.

Many coffee drinkers have the perception that acidity on completion of the roast is not important as they take milk in their coffee and can use that to balance the acidity. It is often considered that if the coffee has pH 4.3 and milk pH 6.5 then combining equal parts will result in a drink with pH 5.4 but this is not the case. We could do an approximation by using the formula pH = -log [h+]

$$pH = -\log [0.5(10^{-4.3}) + 0.5(10^{-6.5})]$$

$$-pH = \log[2.52174^{-6}]$$

$$pH = 4.598 \approxeq pH\ 4.6$$

But we have critically not accounted for buffers. pH is a measure of the concentration of free H+ ions in a solution. Acids release H+ ions and bases trap H+ ions. Buffers resist change to pH because they can take up or release H+ ions to create a pH balance. Both milk and coffee have a number of buffers in them so unless we know the dynamic ranges of the buffers and what buffers are in the solutions, it is impossible to say what will happen. Most probably the buffers would tend the pH towards the pH level of the milk but only if sufficient buffers existed to trap the H+ ions or the acids had sufficiently few buffers to release more H+ ions. The only way we would be able to tell is to measure the coffee/milk mixture but by that time the coffee would already have been roasted.

So we need to be very careful when looking for our perfect coffee and ensure that we understand how we are going to brew the coffee and what we plan to add to it (if anything).

Summary

We will roast out flavour and acidity, we will roast in body, we will generate Vitamin B3 and the rate of roast will manipulate the aroma to engage our psychological senses from where we will establish a subjective "better" or "worse" coffee. We must consider how we plan to drink the coffee and manage acidity levels with our knowledge and experience - not very scientific really.

So there you have it, the Chemistry of Coffee. It all comes down to the skills of the roaster, knowledge of the beans and the subjective taste of the drinker.