The Chemistry of Coffee

The Chemistry of Coffee Project consists of learning about the chemistry behind coffee. This includes the chemistry of solutions, acids / bases and pH, the chemical compounds in coffee beans, the roasting process, and coffee tasting.

The Chemistry of Coffee Sequence:

Lesson 1) How Stuff Works Video - Coffee and Coffee Facts Written in Lab Notebook

Video is found online here: Introduction to Coffee

Be sure to write down facts from the video and answer all the questions during the video

Lesson 2) Introduction to Acids and Coffee Flavor - Videos - Open pdf below

Lesson 3) Lab: Discovering Acids, Bases, and pH - Open pdf below

Lesson 4) Lab: Roasting Stages of Coffee

Lesson 5) Chemicals in Coffee

Lesson 6) Lab: First Roast - Full City Roast

Lesson 7) Lab: Brewing and Cupping First Roast

Lesson 8) Lab: Master Roaster

Lesson 9) Lab: Brewing and Cupping your Master Roast

Lesson 10) Lab: Coffee pH and Color (Absorbance)

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Lesson 2

Chemistry and Coffee– Introduction to Acids and Coffee Flavor

Acidity is a desirable characteristic in coffee. It is the sensation of dryness that the coffee produces under the edges of your tongue and on the back of your palate. It provides a sharp, bright, vibrant quality. Without sufficient acidity, the coffee will tend to taste flat. Acidity should not be confused with sour, which is an unpleasant, negative flavor characteristic.

Watch the video "Acids Bases and pH" by Bozeman High School teacher Mr. Andersen https://youtu.be/V4S1KlJdMbE

1. Draw a Hydroxide Ion molecule
2. Draw a Hydronium Ion molecule
3. What is the pH of water?
4. Describe acids?
5. What is the pH of coffee @ 5:05?
6. Describe bases?
7. Describe strong acids
8. Describe strong bases
9. Look at the chart at http://www.coffeeresearch.org/science/sourmain.htm , how many acid types are found in coffee?

Extra credit videos

Watch the video "Introduction to pH, pOH, and pKw" from KhanAcademy https://youtu.be/2q4vSKwaBtw

1. Draw a Hydroxide Ion molecule
2. Draw a Hydronium Ion molecule
3. What is autoionization?
4. What is the concentration of H+ ions in water? (this is expressed in Molarity "M")
5. What is the concentration of OH- ions in water? (this is expressed in Molarity "M")

You may stop watching at 9:24, but feel free to continue watching if you are interested, or if you would like to learn more about calculating pH.

Watch the video "Acid Base Introduction" from KhanAcademy https://youtu.be/vShCnTY1-T0

1. What is the pH of water at 25deg C?
2. Describe an acid (according to the Arrhenius definition).
3. Describe a base (according to the Arrhenius definition).
4. Why is HCl acidic?
5. Why is LiOH a strong base?

You may stop watching at 11:30, but feel free to continue watching if you are interested or if you'd like to learn about the Bronsted-Lowry definition of an Acid.

Lesson 3

Lab: Discovering Acids, Bases, and pH

Objective: Discover differences in pH of common solutions

Introduction: Universal Indicator is a solution of several compounds that change color depending on the pH of the solution it is added to. Each of the compounds in Universal Indicator reacts with different levels of Hydrogen Ions and Hydroxide Ions, as the compounds bond to these ions, their molecular shape changes slightly; When the molecular shape changes, different wavelengths of light are reflected from the surface, giving us a different color for each level of pH.

Background: Lab goggles, lab shoes, aprons must be worn at all times. If a solution gets on your skin, immediately wash your hands with water in the sink. All solutions can be rinsed down the sink with excess water.

Supplies:

- Universal Indicator
- spot plate
- Several different solutions of varying pH

Procedure:

1. Place one dropper-full of solution into a well
2. Drip 4 drops of Universal Indicator into the well
3. Record the color
4. Record the pH
5. Repeat for all solutions

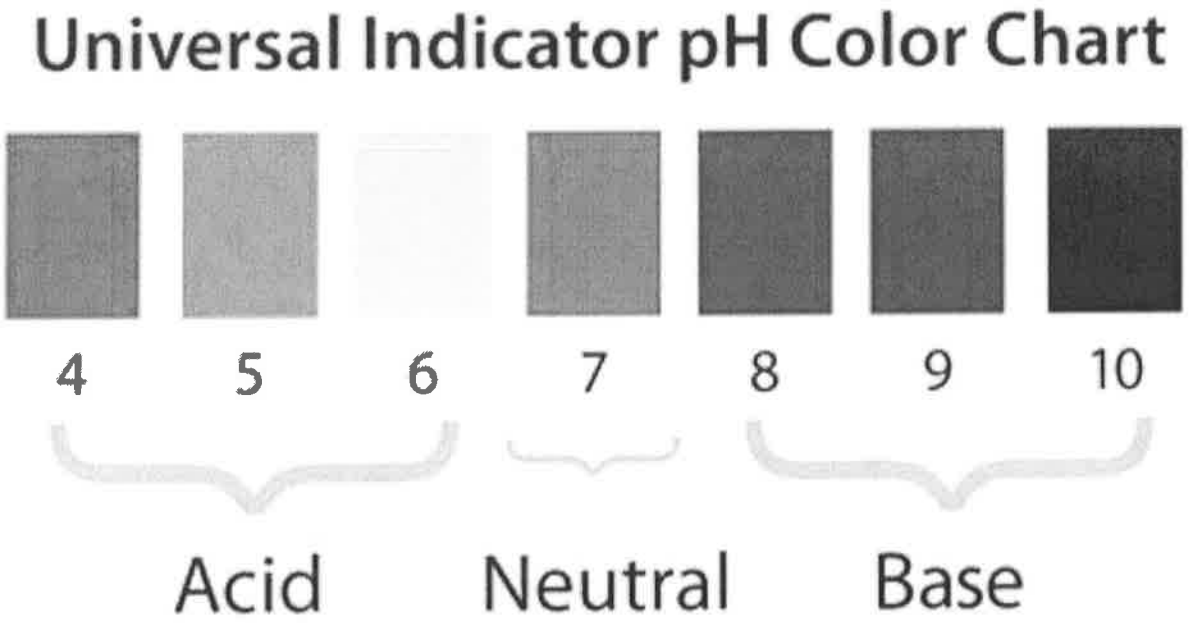
Data / Observations: Draw a data table similar to the one below for 15 solutions

Solution #	Solution name	Universal Indicator Color	pH	Acid or base?
1				
2				
3				
4				
5 – 15 ...				

Post lab questions:

1. Which solution was the most acidic?
2. Which solution has the greatest amount of free hydrogen Ions?
3. Which solution was the most basic?
4. Which solution has the greatest amount of hydroxide Ions?

5. Which solution is the most neutral?
6. What was the pH of Coffee A? Coffee B?
7. Coffee B was ½ Coffee A and ½ distilled water, which means it was diluted by 50%. What affect does diluting a solution have on the acidity level of the coffee?
8. When you begin roasting coffee, why will it be important for all groups to use the same amount of ground coffee and water for each cup?



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Lesson 4

Post Lab Questions:

1. The different type of "official" roasts that coffee roasters make are the same that you have done for #9-14. Compare your coffee bean card with the one at the following link: https://www.sweetmarias.com/library/content/using-sight-determine-degree-roast
    - How does yours compare with #9, #10, #11, #12, #13, #14 on the chart from "Sweet Maria's" website.
2. After comparing your beans for #9-14 (the different types of official coffee roasts), which roast would you prefer to make to sample in class?
3. Write a conclusion for this lab
    - Your conclusion should be a short synopsis of what you learned. This will be different for everybody. There is no length limit but I would assume that it should take at least a short paragraph to communicate what you have learned.
    - See me if you are confused.

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Lesson 5

Chemicals in Coffee

Basic Chemical Reactions Occurring in the Roasting Process

by Carl Staub

(sourced from the SCAA Roast Color Classification System developed by Agtron - SCAA in 1995)

Many thermal and chemical reactions occur during the roasting process:

Sucrose: Disaccharide of d-Glucosyl and d-Fructosyl Moieties

Sucrose is the principle sugar in coffee. The melting point of pure crystalline sucrose is in the 320-392 degrees F with 370 degrees F most commonly accepted. Between 338 and 392 degrees F, carmelization begins. It is at this point that water and carbon dioxide fracture and out-gassing begins causing the first **crack**. These are the chemical reactions, occurring at approximately 356 degrees F, that are exothermic. Once carmelization begins, it is very important that the coffee mass does not exotherm (lose heat) or the coffee will taste "baked" in the cup. Dark roasts represent a higher degree of sugar carmelization than light roasts. The degree of carmelization is an excellent and high resolution method for classifying roasts.

Cellulose: A Long Linear Polymer of Anhydroglucose Units

Cellulose is the principle fiber of the cell wall of coffee. The second crack, associated with darker roasts, is the fracturing of this cell wall of fiber. Under controlled roasting conditions, the bean environment temperature should never exceed 536 degrees F. These temperature limits minimize damage to the cell matrix and enhances cup complexity, roasting yield, and product shelf life.

Trigonelline: A Nitrogenous Base Found in Coffee

Trigonelline is 100% soluble in water and therefore will end up in the cup. Trigonelline is probably the most significant constituent contributing to excessive bitterness. At bean temperatures of 445 degrees F, approximately 85% of the trigonelline will be degraded. This bean temperature represents a moderately dark roast. For lighter roasts there will be more trigonelline, hence bitterness, but also less sugar carmelization. Caramelized sugar is less sweet in the cup than noncaramelized sugar, so when properly roasted these two constituents form an interesting compliment to each other.

Quinic Acid: Member of the Carboxylic Acids Group

Quinic Acid melts in pure crystalline form at 325 degrees E, well below the temperatures associated with the roasting environment. Quinic Acid is water soluble and imparts a slightly sour and sharp quality, which adds to the character and complexity of the cup. Surprisingly, it adds cleanness to the finish of the cup as well.

Nicotinic Acid: Member of the Carboxylic Acid Group

Nicotinic Acid melts in pure crystalline form at 457 degrees F. Higher levels of Nicotinic Acid for any given degree of roast are associated with better cup quality. Nicotinic Acid contributes to favorable acidity and clean finish.

Environment Temperature

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Lesson 5

The temperature of the roasting environment determines the specific types of chemical reactions that occur. There is a small range of temperatures (between 350-400F for our supplies in this class) that produce favorable reactions for the ideal cup characteristics. Temperature values outside of this range have a negative effect on the coffee flavor quality. Even within the window values, different temperatures will change the character of the cup, giving the roaster the latitude to develop a personality or style desired, or to tame the rough signature of certain coffees while still optimizing relative quality. System Energy: At any given environment temperature, the amount of energy (BTU) and the roasting system's transfer efficiency will determine the rate at which the specific chemistry will occur.

Complete the following in your lab notebook:

http://archive.wired.com/science/discoveries/magazine/17-10/st_coffee

1. How many pounds of coffee are produced worldwide each year?

In one sentence, describe the following chemical compounds found in coffee.

2. Caffeine
    a. What is a diuretic (read about water below)?
3. Water
4. 2-Ethylphenol
5. Quinic Acid
    a. What is Tamiflu?
6. 3,5 Dicaffeoylquinic Acid
    a. What is an antioxidant? Is it good for you?
    http://www.nlm.nih.gov/medlineplus/antioxidants.html
7. Dimethyl Disulfide
    a. Write the chemical formula for Dimethyl Disulfide
8. Acetylmethylcarbinol
9. Putrescine
10. Trigonelline
11. Niacin
    http://www.nlm.nih.gov/medlineplus/druginfo/natural/924.html

    What is niacin? Is it good for you?

    https://youtu.be/Xl1XBJLflDU

12. Redraw the caffeine molecule below
13. What does the caffeine molecule do to the brain?
14. How many mg of caffeine would a person have to consume before it would "harmful?
15. How many cups of coffee is this (from above)?

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Lesson 7

Brewing and Cupping Your First Roast

We will be tasting your "First Roast" and determining which type of roast you would like to achieve in a larger batch which will be used to "judge" your skills against other groups.

Each cup requires ~ 10.6 g or .38 oz – You are making 2 cups today → ~ 21.2 g with 12 oz of water

1. *DO NOT OPEN YOUR BAG YET.* Mass of Beans in Bag_____
2. Open bag, smell, describe what you smell (ex. smoky fruit, buttery popcorn, etc)
3. Mass of Beans in bag (after opened) _____
4. Was there any difference in the mass before opened and after opened? If so, what was the difference in mass. What does this difference tell us? (think about the beans "degassing" CO_2 after they roast)
5. Place your beans in grinder, hold down button until it stops grinding.
6. Smell, describe.
7. Remove top of grinder and pour contents into Coffee Press
8. Wipe out grinder with dry paper towel, return to grinder base
9. Add 12 oz of *hot* water (enough for two cups, coffee measurements are 6 oz = 1 cup), a line has been marked on the Coffee Press to mark 12 oz.
10. Place lid on Press with plunger in the UPRIGHT position.
11. Let coffee *steep* for 3.5 minutes, observe changes in the liquid
12. **While waiting:** Put your name on a cup, you will use this cup throughout the next few days. DO NOT THROW AWAY. RINSE AND STORE IN YOUR LAB DRAWER AT THE END OF THE DAY
13. **While waiting:** Get one larger Styrofoam cup and put your group's name on it (save this cup for future activities)
14. **While waiting:** Read "Coffee Cupping" handout to learn what to look for, smell and taste in your coffee.
15. Gently press plunger down to bottom.
16. Turn lid gently so that the slots in the lid are open to the pour nozzle and pour a small amount into your cup.
17. **Taste according to the "Coffee Cupping"** parameters on the handout. **Record** "coffee cupping" information about your roast.
18. Try other group's coffee if they are willing to share, and compare.

    -Why does each group have a different flavor?

When Finished:

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Lesson 7

Begin preparing your roast for tomorrow – you need to decide which roast you would like to achieve and write a procedure for YOUR roast in your lab notebook (include temperature, time, reasons for roast, etc)

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Lesson 8

Master Roaster – Roasting With Your Own Vision

Day 1:

1. As a group, determine which type of roast you would like to achieve for your next larger batch roast (visit https://www.sweetmarias.com/library/content/using-sight-determine-degree-roast)
2. You will be roasting a larger batch of 64 g
3. Write a procedure for YOUR roast in your lab notebook (include temperature, time, reasons for roast, etc)
4. Have instructor APPROVE your roast plan before roasting.
5. Roast Beans CAREFULLY!
6. When roasted, shake, in colander, over trash bin.
7. Allow to cool
8. Place your roasted beans in a Ziploc bag and measure the mass of the beans
9. Write roast type , country of origin, and group members names on Ziploc bag and place in lab locker to de-gas overnight.

Day 2:

Brewing

10. Follow Brewing/Cupping instructions from the last handout.
11. Pour one inch of coffee in a small beaker, allow to cool (do not drink from this cup)
12. When cooled, use pH probe to determine the pH of your coffee

Cupping

13. Pour remaining coffee (from above) into your group's large Styrofoam cup.
14. Place cup on "Tasting Table" in appropriate spot (according to instructor)
15. Perform "Coffee Cupping" using the handout provided.
16. Turn in "Cupping Card" to instructor when completed

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Lesson 9

Brewing and Cupping your Master Roast

Brewing

1. Follow Brewing/Cupping instructions from the last handout :
    a. Place 21 g of your roasted beans in grinder, hold down button until it stops grinding.
    b. Smell, describe.
    c. Remove top of grinder and pour contents into Coffee Press
    d. Wipe out grinder with dry paper towel, return to grinder base
    e. Add 12oz of *hot* water (enough for two cups, coffee measurements are 6oz = 1 cup), a line has been marked on the Coffee Press to mark 12oz.
    f. Place lid on Press with plunger in the UPRIGHT position.
    g. Let coffee *steep* for 3.5 minutes, observe changes in the liquid
    h. Gently press plunger down to bottom.
    i. Turn lid gently so that the slots in the lid are open to the pour nozzle and pour into your community cup.
2. Pour half an inch of coffee in a small beaker and label it with your name, allow to cool
3. Bring your remaining coffee to your instructor to be placed on the "Tasting Table"
4. When cooled, use pH probe to determine the pH of your coffee

Cupping

5. Perform "Coffee Cupping" using the handout provided
6. Turn in "Cupping Card" to instructor when completed

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Lesson 10

Coffee pH and Color (Absorbance)

Questions to Ponder:

- Did you notice the color differences of your roasted coffees?
- What did you decide to roast for your master roast?
- Why did you decide to roast that type of coffee for your master roast?
- What did you notice when tasting everyone's master roast brew?
- How did your coffee compare to everyone else's?
- How did your group's coffee compare to the two commercial brews?
- Is there a relationship between your coffee's acidity and your group's cupping score?

Experimental Question:

Is there a relationship between the pH of your coffee and its color (absorbance) when brewed?

Pre-lab Questions:

1. What does a colorimeter measure?
2. The Vernier colorimeter can be adjusted to measure at wavelengths of 430 nm, 470 nm, 565 nm, and 635 nm. What wavelength are you going to select? Why?
3. Why must a piece of lens paper (goggle cleaning paper) be used to wipe the cuvettes instead of a paper towel?
4. What is a serial dilution?
5. If you perform a serial dilution by using 50% of your coffee and diluting with 50% water, what will the concentration be after four dilutions if the coffee concentration starts at 2.00 mol/L?

Procedure:

- Design an experiment to test your coffee's pH and absorbance values as you dilute the brew
  - Reminder – When we brewed coffee, we used 21 g of roasted beans with 12 oz of water
  - You need to brew 50 ml of coffee for this experiment (1 fluid oz = 29.57 ml)
- You must use - Vernier LabQuest or LoggerPro, Vernier pH probe, Vernier Colorimeter
- One hint – You must change the settings on the LabQuest to record points as you wish to keep them – this is called "Selected Events" mode and is accessed by clicking on the mode button in the top right corner of the live readout screen. When you want to keep your data points, you click "Keep" at the bottom of the screen and it will record your data points
- When complete, you need to print a graph showing pH and absorbance for your coffee dilutions

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Coffee Cupping

Tasting a selection of coffees so that they can be inter-compared is called cupping. Each coffee is rated according to whatever evaluation guidelines you have, and the scores recorded on a form.

The criteria we have used are:

1. **Aroma**: Describe the smell of the coffee before tasting, and rate the intensity of the aroma.

2. **Acidity**: The pleasing brightness or sharpness in the coffee. Acidity can be intense or mild, round or edgy, elegant or wild, and everything in between. It is the high, thin notes, the dryness the coffee leaves at the back of your palate and under the edges of your tongue. It's the pleasant tartness, snap, or twist, combined with an underlying sweetness; it is bright, dry, sharp, brisk, vibrant. A coffee that lacks acidity tastes flat. Acidity should be distinguished from sour or astringent.

3. **Body/Mouthfeel**: The sense of weight, tactile richness, thickness or heaviness that the coffee exerts in the mouth when you swish it around; how it coats the palate; its balance. Can be very difficult for beginning cuppers to identify – it is useful to think about the viscosity or thickness of the coffee, and concentrate on the degree to which the coffee has a physical presence. It also describes texture: oily, buttery, thin, etc.

4. **Sweetness Balance**: The extent to which the sweetness provides balance and eases the finish. The degree of harmony between the acidic and sweet flavors.

5. **Aftertaste/Finish**: Describes the immediate sensation after the coffee is swallowed; the coffee's finish in your mouth. Some coffees develop in the finish; they change in pleasurable ways. The ideal finish has enough endurance to carry the flavor for 10 seconds after swallowing, affirming with great clarity the principal flavor of the coffee, leaving a lingering, pleasant, non-bitter and non-sour aftertaste.

6. **Overall Taste**: The catch-all for all the actual "tastes" the coffee gives. What does it taste like? Describe any directly identifiable fleeting flavor notes you may taste.

7. **Personal Preference**: Do I like it? Does it taste nice?

These parameters were borrowed from psychohistorian.org

Senior High Chemistry - The Chemistry of Coffee - Cupping Card

Cupper Name_____Date_____Class Period_____

lacking	very low	lower	below avg	average	above avg	high	very high	striking
1	2	3	4	5	6	7	8	9
yack!	bad	odd	unpleasant	normal	nice	pleasant	lovely	wonderful

Coffee Code				
A	1. Aroma	2. Acidity	3. Finish	4. Body/Mouthfeel
Total score				
	5. Sweetness/Balance	6. Aftertaste/Finish	7. Overall Taste	8. How much do I like it

Coffee Code				
B	1. Aroma	2. Acidity	3. Finish	4. Body/Mouthfeel
Total score				
	5. Sweetness/Balance	6. Aftertaste/Finish	7. Overall Taste	8. How much do I like it

Coffee Code				
C	1. Aroma	2. Acidity	3. Finish	4. Body/Mouthfeel
Total score				
	5. Sweetness/Balance	6. Aftertaste/Finish	7. Overall Taste	8. How much do I like it

Coffee Code				
D	1. Aroma	2. Acidity	3. Finish	4. Body/Mouthfeel
Total score				
	5. Sweetness/Balance	6. Aftertaste/Finish	7. Overall Taste	8. How much do I like it

Coffee Code				
E	1. Aroma	2. Acidity	3. Finish	4. Body/Mouthfeel
Total score				
	5. Sweetness/Balance	6. Aftertaste/Finish	7. Overall Taste	8. How much do I like it

Coffee Code				
F	1. Aroma	2. Acidity	3. Finish	4. Body/Mouthfeel
Total score				
	5. Sweetness/Balance	6. Aftertaste/Finish	7. Overall Taste	8. How much do I like it

Coffee Chemistry Lab

Nathan Tallafuse Billing Senior HS Chemistry Website

https://sites.google.com/a/billingsschools.org/talafuse/chemistry-of-coffee