CHEM MAJOR NEWS

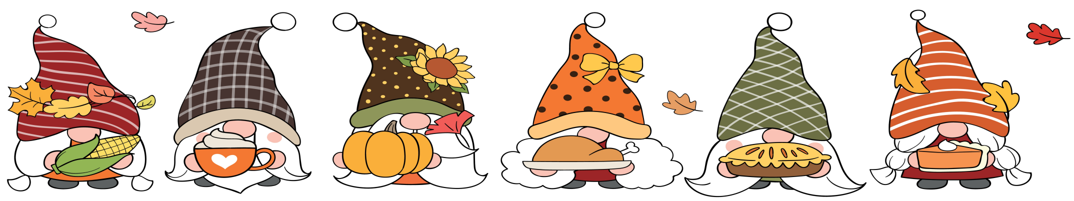
In Conjunction with the American Chemical Society
Student Affiliates at the University of Pittsburgh

Volume 29, Issue 3 **November 12, 2021**

Some Incredibly Important Dates to Know...

November 11 Deadline for undergraduates to apply for April 2021 graduation in 140 Thackeray Hall

November 21- November 28: Thanksgiving Recess-No Classes! Have a great Holiday!



December 10 Last day for undergraduate classes

December 13-17 Final Exams for 2221

December 19-January 9,2022 Winter Recess

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<u>Challenges and Obstacles of Teaching and Learning Chemistry</u>

Written by: Jack Levickas- *Newsletter Editor*

By the time a person is finished with their high school and college career most people will have taken at least one chemistry course, and many of them will describe that course as challenging, difficult, or even painful. Even those who choose to study chemistry as a major have undoubtedly found themselves frustrated and confused countless times. The difficulty of understanding chemistry comes from a variety of factors, with the most significant being its necessity of abstract thinking, the constant re-evaluation of understanding, and the language used.

Perhaps the most challenging part of understanding chemistry is that its core foundation, atomic theory, is not something that can be seen. In other fields, the most basic concepts can be visualized and understood by observation: the trajectory of a thrown object, the cell under a microscope, and addition or subtraction. In chemistry, the atom can only be visualized through models and pictures. While these models are understood by experienced chemists to only be estimates and their inaccuracies are known, a student seeing this for the first time will believe this to be an accurate representation of reality. This brings the issue of constantly needing to re-evaluate what has already been taught. In order to understand the most basic concepts of chemistry, many complicated factors need to be disregarded. This works well for teaching the basic concepts, but as material becomes more complex it becomes a hindrance. For example, using the octet rule to help early students understand the limits of bonding is an excellent way to begin, however when more complicated elements are used, the octet rule is no longer applicable and the concept of bonding must be reformed in the students mind. Reforming already known ideas is much more difficult than forming new ones, adding to the difficulty of learning chemistry. Another challenge that students are faced with is the vocabulary that is used in chemistry. Many of the words and descriptions used in chemistry are either entirely invented for the purpose of chemistry or do not match their formal definition. The most egregious example of this is the idea of the “orbital”. The concept of an orbit is that an object moves around another object in a circular pattern. This idea almost works for the s orbital, except for the quantum nature of electrons, but is entirely misleading for p, d, and f orbitals.

Solving the difficulties of teaching chemistry is a challenging task itself, but it does continue to improve. When a new idea is developed, it is examined by only those at the highest level of the discipline. As time goes on the idea is examined by more and more people, further improving the collective understanding of the subject until that idea is considered a basic concept. Chemistry is a rapidly expanding area becoming better understood with each generation. The idea that chemistry is being taught to all people would have been unimaginable a hundred years ago. Remember that there was a time when even basic arithmetic was only understood by a few people in the world.

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The Crown of Viruses

Written by: Michael Kosky

This is the 3rd installment of the series of articles dedicated to discuss the COVID-19 pandemic. Please look for future articles in upcoming editions of the Chem Major News.

The coronavirus name is simply the name for the family of viruses rather than being unique to the current strain COVID-19. The name was determined as under a microscope there are 2 unique sections visible: the round core and another round layer on top of it. This makes it appear to look like a solar corona as it mimics the shape of the sun during a solar eclipse with the light still emanating from behind. There are hundreds of different variations of coronaviruses spread out across many species. Coronaviruses were first identified in the 1960s but have a long history alongside their hosts for 1,000s of years.[5]

The family of coronaviruses are broken down into 4 genera: alpha, beta, gamma, and delta. The major difference between the categories is what kind of species that they can infect. Alpha coronaviruses prefer infecting most mammals and includes humans. One particular alpha strand is known for causing the common cold. Additionally, the alpha group is thought to have originated from the bat viral gene pool but has mutated to be able to infect most animals.[6] The beta category primarily infects small rodents and bats but has had several instances of mutating into affecting humans. COVID-19 is a member of the beta group, but this is not the first time that a beta coronavirus has mutated into being able to infect humans. In 2003, the SARS virus mutated into being able to infect humans, but it never reached the notoriety of COVID-19 as only 8,098 people became infected with SARS.[7] In 2012, the Middle East respiratory syndrome (MERS) started in Saudi Arabia and spread out to several countries. Gamma and Delta coronaviruses mainly affect birds. All forms of coronaviruses primarily target the host's respiratory system causing shortness in breath and cold symptoms. COVID-19 is a bit different from other coronaviruses due to 1 core feature.

What makes COVID-19 different from other coronaviruses is that it is a novel strain. A novel strain is when a virus mutates into affecting a different species rather than their normal targets. As mentioned above, COVID-19 mutated into being able to infect humans. Currently, it is still unknown which species the virus originally mutated from, but the 2 suspected sources are bats and pangolins. Overall, the virus is more infectious than other coronaviruses due to it being a novel strain. Our immune systems have not developed proper antibodies to counteract the virus and can experience a variety of severity based on the individual. The common cold is an obvious point of comparison as it has infected humans for a long time. Consequently, our immune systems have developed and passed down antibodies to counteract the virus so that we only experience a small cold that lasts for about a week. In comparison to the other outbreaks of novel coronavirus strains, COVID-19 is significantly more infectious with cases varying between asymptomatic to fatal cases. People infected with COVID-19 typically show symptoms after about 14 days, however, may be contagious 2 days before symptoms begin showing. The symptoms last for about 14 days depending on the severity of their infection. At the time of writing this article, the mortality rate of COVID-19 is about 2% with 3 million people having died since the start of the outbreak out of 139 million cases worldwide.[8] In contrast, the SARS virus from 2003 was more aggressive towards humans as the fatality rates were about 10%.[7] SARS was significantly deadlier than COVID-19 but was less infectious. Despite being less deadly, COVID-19 still has made its notoriety as it is far more infectious than any of the other novel strains that have appeared in recent times. The methods of treatment for coronaviruses and other viruses are the same. The symptoms can only be treated; however, vaccines are the primary method to preventing infection.

Please refer to 107 Chvrn for references regarding COVID-19 series.

Good Luck on Finals & Enjoy the winter break!!!

<u>Harvesting Green Chemistry</u>

Written by: Quincey Johnston, *Green Chemistry Contributor*

Fall break and the Thanksgiving holidays are approaching at a breakneck speed, and with harvest season now in full swing and a chill in the air as things are *finally* starting to feel like fall, I couldn't help but wonder if green chemistry had a seat at the metaphorical table. Considering that this article *exists* and you're reading it right now, I'm sure you've made the connection that it *does* indeed have a seat at said metaphorical table.

Probably one of the largest areas of impact that green chemistry has on the annual harvest season involves the crop protection industry and green pesticides that protect the world's agriculture. This crop protection industry uses commercial processes to manufacture active ingredients that are then later used to create products that protect farmer's crops and minimize food waste that results from pest damage.

Because the crop protection industry is all about minimizing food waste and protecting crops (as I'm sure you could gather from the name of the industry itself), perhaps the most important, and relevant, principle of green chemistry in the world of sustainable agriculture lies in the prevention of waste.

Effective minimization of waste results in a lower manufacturing cost and a reduction in the cost of waste treatment, and as such crop protection product producers are under pressure to develop these low-cost processes; farmers often operate within very small profit margins and fixed commodity prices, and it is because of this that the necessary compromise of finding a balance between sustainable greenness and a combination of both economic and societal value is needed.[1]

This efficiency is most commonly measured in E factor (kg of waste/kg of product) and the process mass intensity (PMI = kg raw materials/kg product). Though there aren't many reports documenting the waste generated from agrochemical processes, in fact there is only one published study that details the PMI analysis of an agrochemical manufacturing process, industrial producers do work internally to generate this data and work to improve efficiency within their own processes.[1]

One of the other major issues faced by the crop protection industry in particular is the use of pest control chemicals and other agricultural chemicals. Though their use has played an essential role in maximizing the efficiency and productivity of modern agriculture, the use of these agrochemicals (such as inorganic fertilizers and synthetic pesticides) has resulted in environmental problems due to a general misunderstanding of these chemical's environmental impact. In fact, agriculture has been identified as the largest nonpoint source of water pollution, and U.S. States have reported that 40% of the waters they have surveyed are impaired for recreational and wildlife uses[2] (think about it… would *you* want to go for a casual swim in *any* of the three rivers here in Pittsburgh?).

As a result of these impacts, the pressure on these industries to maintain and improve agricultural productivity and environmental quality is heavy, though the general potential seems to be largely unknown; in fact, the use of biotechnology in soil biological research suggests that we have yet to identify a vast majority of soil microorganisms, and as such the potential for bioengineering to manage soil biota and mediate soil processes is also unknown.[2]

It's also important to note that the increased use of these inorganic fertilizers and synthetic pesticides (in addition to other things like mechanization, increased use of irrigation, and on-farm processes like grain drying) has resulted in an increase in the total amount of fossil fuel used in agriculture. So, in addition to solar, wind, and biofuel usage needing to increased and further developed, management practices that better utilize the nutrients already present in manure (which is currently treated more like waste than it is as a fertilizer), crop residues (think about the waste management I mentioned a bit earlier), and cover crops *also* need to be further developed.

The race on sustainable practices is on, and with the agricultural industry being such an integral part of our daily lives, its impact is too great to be ignored.

References:

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Caf-fiends: How Caffeine Works

Written by: Jacob Kuzy

Though historically consumed in many parts of Eastern Africa, the coffee plant was first cultivated in the Oromia region of modern-day Ethiopia.[1] A hardy, self-pollinating plant, coffee was said to be taken by Arab merchants to neighboring Yemen. The port of Mocha in Yemen, famous in the coffee trade, is actually the origin of the word in mocha latte. From there, coffee spread throughout the Arab world in the 16th century as a beverage known for its stimulating effects. Today, coffee is the most consumed beverage in the world after water, with about 1.6 billion cups per day.[2] The principal chemical in coffee which imparts its stimulant activity is caffeine (also known as Guaranine); around sixty additional plants, including tea, also contain caffeine.[2] Understanding the chemical and physiological properties of coffee can yield important health implications for the many millions of coffee drinkers.

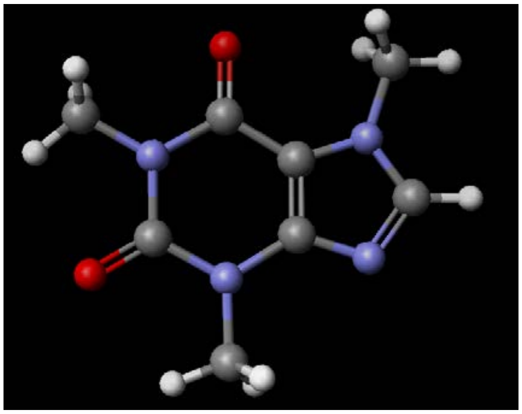

Figure 1: Caffeine structure ($C_8H_{10}N_4O_2$)

Chemical Properties:

The molecule of caffeine has an IUPAC name of **1,3,7-Trimethylxanthine**, placing it under a broader category of molecules called methylxanthines[3]. Other methylxanthines include theophylline which has historically been used to treat acute asthma as a bronchodilator.[10] This group bears a striking resemblance to purines found in the nitrogenous bases of nucleosides which make up DNA. The similarity in structure of trimethylxanthine and nucleosides play a crucial role in the action of caffeine on the central nervous system which will be later discussed.

Caffeine can also be classified as an alkaloid: a naturally occurring organic molecule containing a nitrogenous base.[4] The nitrogenous base in caffeine is its purine ring (xanthine) containing four nitrogen atoms and five carbon atoms. Since these atoms are all sp^2 hybridized and contain a total of ten pi electrons, according to Hückel's rule, caffeine can be considered aromatic. Like its purine cousin guanine, caffeine is capable of three hydrogen bonds, but unlike guanine, caffeine is only capable of accepting hydrogen bonds.[5] As Figure 1 shows, there are no hydrogen atoms directly attached to nitrogen atoms in the molecule. This makes hydrogen bond donation impossible, but the oxygen and nitrogen atoms are capable of accepting hydrogen bonds from other molecules.[5]

Caffeine is mildly basic, mainly due to the nitrogen atoms of the purine ring; the pKa of caffeine's conjugate acid is around 0.6.[5] When analyzing the basic properties of caffeine, it is important to treat the nitrogens of the pyrimidinedione ring (six-membered ring) as amides which are considerably less basic than amines.[4] This puts the most basic components of caffeine in the imidazole ring (five-membered ring) though caffeine is still generally uncharged at physiological pH.[3] Because of this, caffeine is only slightly soluble in water, but the solubility drastically increases when water is heated.[5] Additionally, the uncharged nature

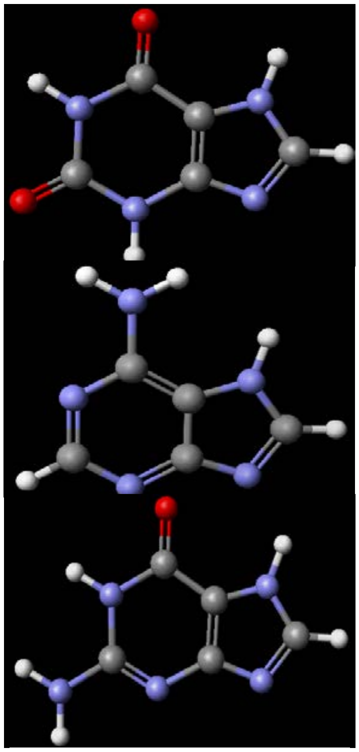

Figure 2: (top to bottom) Xanthine, Adenine, Guanine

and small size of caffeine are what allow it to readily pass through the blood-brain barrier to act on the brain and central nervous system.[3]

Physiological Mechanism:

Caffeine is technically toxic, but with normal human consumption there is very little chance of overdosing.[6] Typical caffeinated sodas contain anywhere from 35 to 55 mg. of caffeine in a twelve oz. can. Coffee concentrations can range from 80 to 150 mg of caffeine for a five oz. cup, and black tea would be less than 80 mg in the same volume.[6] Caffeine becomes fatal at around 10g. of caffeine per day, amounting to 50-100 cups of coffee. Additionally, though caffeine dependence occurs in caffeine users, the drug is not considered addictive by the American Psychiatric Association because caffeine users can typically control its use, unlike a drug such as nicotine.[4]

The source of caffeine's widely known stimulant properties lies in its structural similarities to the nucleoside adenosine.[3] A nucleoside is composed of a sugar covalently bonded to a nitrogenous base. In the case of adenosine, the sugar is ribose, and the nitrogenous base is adenine. Adenosine is an important molecule in the body in its own right, but in the central nervous system, there exist specific G-coupled protein receptors to which adenosine can bind.[10] When adenosine binds to these adenosine receptors, sleepiness is increased, and alertness is decreased. Caffeine is an adenosine receptor antagonist meaning that because caffeine shares the critical functional groups and similar size of adenosine, caffeine can bind within these adenosine receptors and prevent adenosine from binding. The result is a lack of sleepiness and increased alertness characteristic of caffeine. Additionally, caffeine has been shown to increase the physical performance of athletes, and it constricts blood vessels in the brain. For this reason, caffeine is typically included in headache medication.[4, 10]

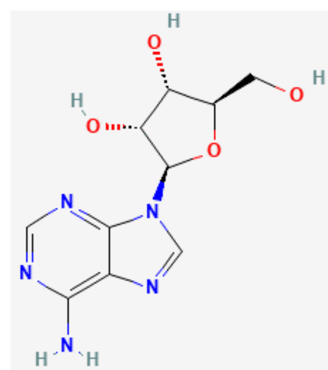

Figure 3: Adenosine nucleoside

Though research studies are difficult with caffeine due to it being metabolized differently in humans and animals, research into a more exact mechanism of action for caffeine is ongoing.[3, 7] For example, daily caffeine consumption has been shown to lower risk for developing certain neurodegenerative diseases such as Alzheimer's disease by preventing beta-amyloid plaque production.[2] Along with its effect as an adenosine receptor antagonist, caffeine was recently discovered to be involved in a dopamine pathway, acting similarly to amphetamine and methylphenidate in the brain.[9] Research by the Volkow group suggests that caffeine enhances dopamine signaling by increasing dopamine receptor levels rather than by increasing available dopamine which is the modus operandi of drugs like cocaine.[9] Caffeine also acts in the central nervous system to decrease inflammation due to inhibition of phosphodiesterases.[5] By continuing to examine these properties of caffeine, we can gain better insight into its effect on the health and functioning of the millions of coffee and tea drinkers around the world.

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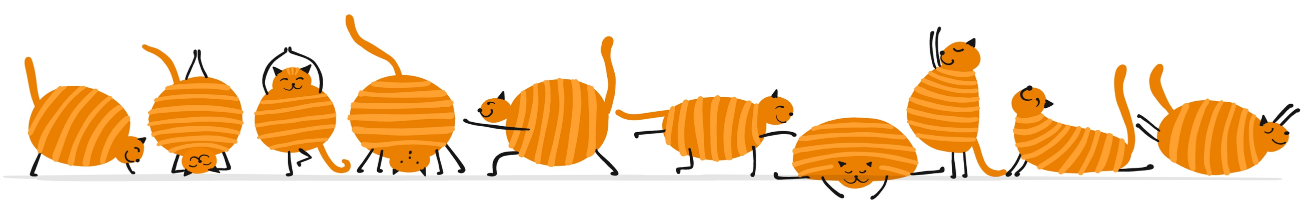

DEPARTMENT OF CHEMISTRY

2022
Undergraduate Summer Research Fellowship in Organic & Biological Chemistry

- We are pleased to offer an Undergraduate Summer Research Fellowship for Pitt students sponsored by *the Organic and Biological Chemistry Divisions*.
- This Fellowship is intended to support a 10-week full-time organic chemistry or chemical biology research project, including stipend & supplies, in the summer of 2022 at the Department of Chemistry in Pittsburgh.

Please submit applications consisting of a current resume, course records, and a letter of recommendation by a suitable Faculty Sponsor with details of the planned research project (not exceeding 1 page) electronically by

February 20, 2022 to Desirae Crocker, obc@pitt.edu.

- The Award will be presented at the Undergraduate Award Ceremony in April 2022.
- The Awardee and Faculty Sponsor(s) are strongly encouraged to present a poster on their research at Science 2022 in Pittsburgh in the fall of 2022, and/or actively participate in an equivalent departmental, regional or national scientific conference.

Our November Schedule

November

5 All About *Sherwin-Williams and the New Summer Internship*

12 All About Covestro with Mr. Ron Debiec

19 Green Chemistry Seminar with Dr. Nesta Bortey-Sam

Everyone is welcome to attend our weekly ACS-SA meetings. Every Friday at noon we get together in 150 Chevron Science Center to hear interesting talks, learn more about science and enjoy each other's company. Come join us for all of the above mentioned meetings.

Saturday Science Academy

Looking for something fun to do February 2021?

Try Saturday Science! It is an opportunity to help ambitious area high school students learn both general and organic chemistry in the lab. With your help, the students get to make crystal gardens, do a simple thin layer chromatography experiment, witness an acid base reaction with dry ice, measure the pH of some favorite soft drinks, and synthesize slime. Volunteers will play the role of the teacher: demonstrating the experiments, helping the students perform them, and finally, answering their questions. Saturday Science is a fun and rewarding volunteer experience in chemistry. So, are you still looking for something fun to this year?

More information to follow next term!

Happy Thanksgiving!