OCHEM REAX

TECHNICAL DOCUMENTATION

2018

Produced and Designed by Megan Lim

Written by Megan Lim

TABLE OF CONTENTS

I. PRODUCT

ochemreax.com is a website designed to help users better visualize Organic Chemical structure and reactivity. This website is largely inspired by Phillip Guo's Python Tutor tool that aids in the visualization of environment diagrams within computer science. Its two main features include interactive user input and Dictionary of Common Mechanisms.

Upon user entry of reactant(s) and reagent/catalyst(s) and selection of either acidic or basic conditions, the chemical reaction is then computed. Controlling the forward and backward buttons, the user is walked through each step of the chemical reaction through annotated images drawn by ChemAxon software.

The Dictionary of Common Mechanisms has the same display process except it doesn't involve user input. Instead, certain mechanisms designated of importance within Organic Chemistry, are already computed and programmed within the website. The dictionary is organized in terms of categorization by topic and intended to represent the chronological progress of an Organic Chemistry class.

II. PURPOSE

This website was designed with the intent to help Organic Chemistry learners become more flexible with the material through visualization and interpretation of chemical reaction patterns. What makes Organic Chemistry such a rigorous and intimidating subject is the natural tendency of its learners to merely memorize rather than step back and process the flow of the reactions. This enables them to solve simple, linear situations but severely limits their foresight when dealing with larger and more complex problems.

The show-hide toggle nature of the forward and backward buttons of each step is crucial to the learner's development of chemical intuition. Analogous to the flashcard construct, hiding and displaying content allows the learner to predict then check what should appear next in the chemical reaction.

This website's great contribution to the field of academic learning is its ability to resolve any question a student may have in terms of chemical reaction. Instead of remaining in doubt until help or assistance can be reached, ochemreax brings efficiency and convenience to the user.

Once being an Organic Chemistry student myself, I understand the struggles and demands of learning this subject. However, when conquered, Organic Chemistry unlocks a limitless field of applications and chemical possibilities. I hope that, through this product, all can experience the beauty of this subject.

III. RELATED PRODUCTS

Interestingly, there are not many available resources to help Organic Chemistry learners. Even more so, it is very rare of any to include interactive/dynamic chemical display of reactions. This may be because there simply aren't as many pursuing study of this field or possibly because the unity of design, programming, and organic chemistry is a unique combination.

However, there are a substantial amount of Organic Chemistry videos, available on YouTube by great providers including Khan Academy and AK Lectures. There are also very useful chemical design/drawing toolkits such as Marvin JS by ChemAxon, ChemDoodle, and ACD/ChemSketch.

There have been a plethora of inquiries and investigations on what exactly are the best ways to learn Organic Chemistry. The answers have varied but the most popular are: YouTube videos and the skill of mastering the basics rather than memorizing.

IV. PRIMARY AUDIENCE

The intended audience for this website include Organic Chemistry students or learners that do already have a baseline of understanding for the subject. However, they have not yet achieved mastery of the material. They understand what they should know but have not yet developed maximum flexibility with certain mechanisms or reactions under a different set of conditions. This website could also be targeted for instructors or tutors needing a simplified and visual mechanism for detailing reactions. In addition, this product could be helpful for those in the process of synthesizing chemical compounds and searching for the correct reagents/materials to yield their desired product.

Prerequesites:

- Understands the general flow of a chemical reaction
- Familiar with common mechanisms
- Aware different sets of conditions, reactants, and catalysts/reagents are possible for a chemical reaction
- Understands charges of atoms change between steps, but may still not yet be entirely comfortable with keeping track of them.
- Understands IUPAC nomenclature to some extent in order to complete the user inputs

V. SECONDARY AUDIENCE

The secondary or resultant audience may be those possibly enrolled in general Chemistry course or simply just curious learners. While they may not be existing clients, they are possibly future users of the product. They are also crucial to offering perspective of its design and clarity from an indirect Organic Chemistry outlook.

Attributes:

- Has a baseline of understanding for General Chemistry, possibly not Organic Chemistry
- Familiar with molecular orbitals and hybridization
- Understands the flexibility of reactions possible (past experience of balancing chemical equations)

VI. TRANSFORMED AUDIENCE

Most exciting is seeing how the users have transformed after utilizing the product. Progression of comfort with the material is measurement of the website's effectiveness. Mastery and ability to adapt to any reaction presented is the ultimate goal.

Goals:

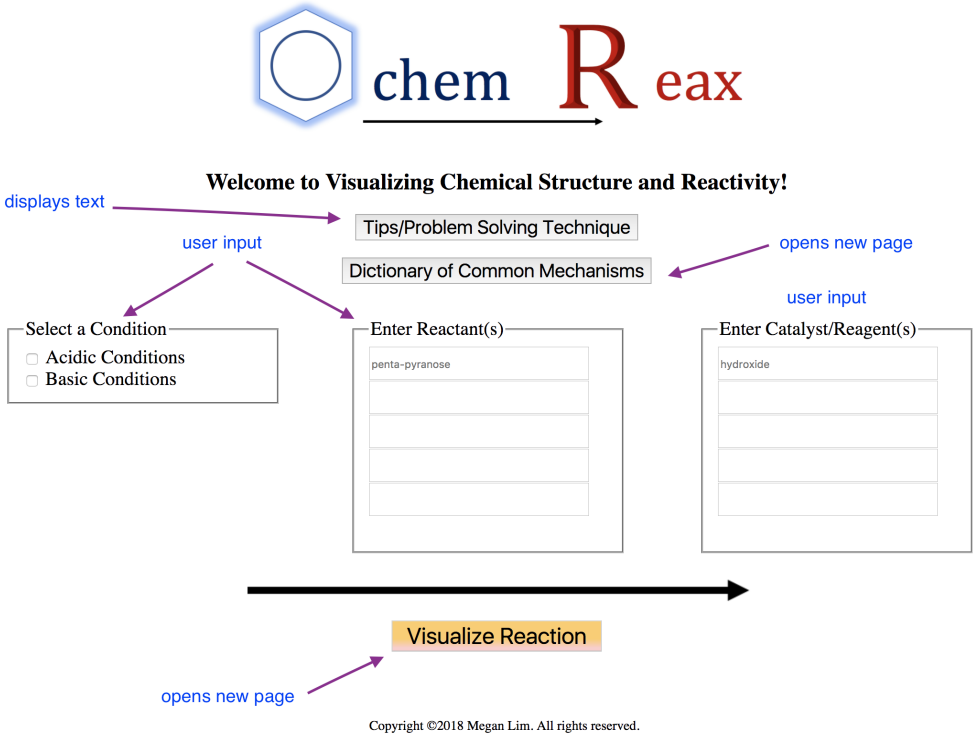
- Deeply understands the flow of electrons and arrow pushing
- Walks away with a strong understanding of resulting charges before and after arrow pushing
- Can independently perform reactions that are most nearly or perfectly correct
- Has initiative and flexibility when presented with either acidic or basic conditions
- Does not violate the rules of acidic and basic conditions
- Has not memorized and can recognize patterns
- Maintains a strong grasp of all those listed and displayed within the Dictionary of Common Mechanisms
- Mastered the ability to troubleshoot

VII. USER INSTRUCTION

The home page includes two centered gray buttons. The first, "Tips/Problem Solving Technique Involves" reveals a quick statement on how to approach learning Organic Chemistry and certain principles to keep in mind. The second, "Dictionary of Common Mechanisms", takes the user to a separate page with a comprehensive list of core mechanisms. Each already contains programmed display that do not require further user input.

The interactive section of the program is comprised within the home page. The first fieldset involves the user selection of either acidic or basic conditions. This specifies the set of guidelines, which is displayed on click, the following reaction cannot break. The second fieldset allows the user to enter the reactants in IUPAC form. This may be only one if it is a transformative process, e.g: penta-pyranose to penta-furanose. Or this may be several that interact in the order of user input. The third fieldset is for reagent/catalyst entry, the materials usually displayed directly above the arrow of a chemical reaction.

The Visualize button will take the user to a separate page in which they can finally view the reaction. On that separate page there will be another Visualize button that reveals the entirety of the reaction, from reactants to products. The Next button directly below enables the user to walk through each step at their own pace.



Dictionary of Common Mechanisms

Things to keep in Mind

Resonance: the backbone of Organic Chemistry

Diels Alder: a Cycloaddition

Electrophilic Aromatic Substitution (EAS)

Diazotization of Aniline

Nucleophilic Aromatic Substitution (SnAR)

Ylide: Wittig Reaction

Formation of Acetals

Reduction of Hemi-Acetals

Ene-diol Rearrangement

Conversion of Penta-pyranose to Penta-furanose

Amines as Nucleophiles

Reductive Amination

Chem of Enol(ate)s

Halogenation at Carbonyl Alpha Position

Aldol Addition

Aldol Condensation

Michael Addition

Robinson Annulation

each take user to separate page

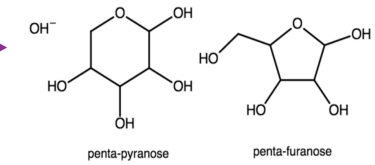
separate page does not involve further user input

Conversion of penta-pyranose to penta-furanose under basic conditions.

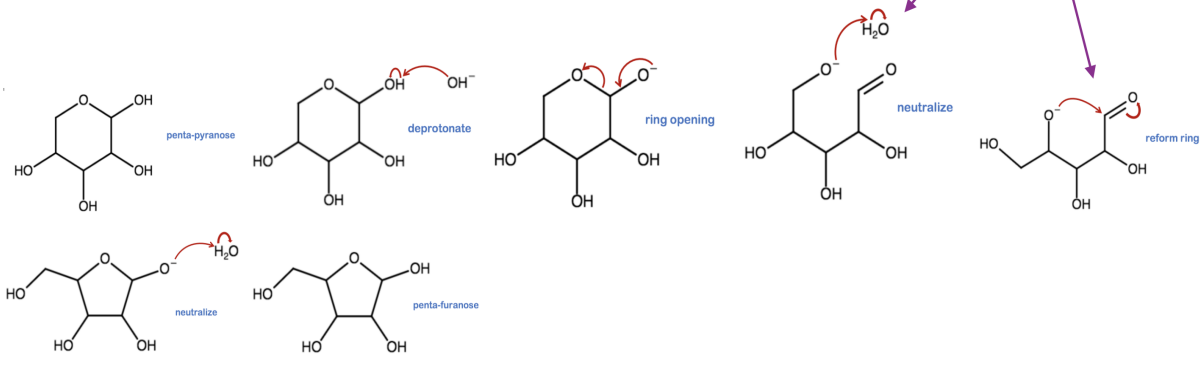
Visualize

Next Step 7 of 7

overall reaction displayed onclick Visualize



each image is displayed onclick Next



VIII. PRODUCTION

This website was originally inspired by Philip Guo's Python Tutor that visualizes code through a step by step display of environment diagrams. The making of the site involves a main set of HTML, JS, CSS files. Each reaction within the Dictionary of Common Mechanisms is embedded with their own sources of HTML, JS, CSS files. Because there existed a common overlap of code in these 3 files between the reactions, it was thought that a universal set to all reactions could be produced. However, preference in design and style of teaching for specific reactions let to the decision that each will maintain their own files.

It was important to keep a small list of crucial concepts to remember at the top of the page of each mechanism. This was intended for the user to practice associating mechanisms with their core principles and start establishing the basic foundations of Organic Chemistry. The smaller details were left to be included in the brief annotations of images for each step of the chemical reaction. Each image was hand-drawn by Marvin JS ChemAxon software. This particular chemical molecule drawing kit was selected for this purpose partly because its downloadable version was easily compatible with Mac computers but also because the electron movement arrows were elegantly displayed.

The Visualize button was selected to be of a specified gradient of color from orange to pink (analogous to an acid/base color change). It was intended to be a clear visual for the user and to display the overall reaction on click. This is important in preparing the user for what they should predict out of the mechanism.

Embedded in the Next button is an Event Listener that also acts on click. Links to each image of the chemical reaction are stored in a list personalized to each mechanism. Each user click on the Next button walks down the list through each image while simultaneously incrementing the step counter. The step counter serves to inform the user how many times to click through the reaction. Without it, they would be unable to determine their position in the reaction.

The home page consists of three fieldsets designed to receive user input. The first requires the user to select a condition through a checkbox form. The text displayed upon selection of a particular checkbox reminds the user of specific principles to not violate. The second fieldset allows the user up to 5 text boxes for reactant input. The third does the same but for catalyst/reagent reception of data.

Key Components in Design:

- Crucial concepts stated clearly at top of page of each mechanism
- Selection of ChemAxon software for ease and elegance of electron pushing arrows
- Clear and obvious visualization button
- Incremental counter of each step until completion
- Display of rules upon selection of condition checkbox

IX. SCOPE

The material that this website encompasses is that of a first year organic chemistry course. More specifically, it adheres to the UC Berkeley series: Chem 3A and Chem 3B. Some reactions, such as the Suzuki reaction, from the corresponding laboratory sections are included.

There is a large emphasis on recognizing patterns, such as activate, attack, and neutralize, within this website. This was intended to train the user how to troubleshoot and independently reason when presented with an unseen reaction. Annotations of images focused on drawing attention to these trends and conditioning the user to think several steps ahead. By picturing a future desired molecule, they can better strategize what steps to take in order to achieve it.

Emphasis in Material:

- First year introductory level Organic Chemistry
- Recognizing patterns (e.g: activate, attack, neutralize)
- Strategy and foresight several steps ahead
- Resonance and its stability contribution
- Maintain control of charges
- Recognizing functional groups and how to act on them

X. PRODUCT USABILITY

Scan:

Upon first sight of the home page, the most striking images to the eyes of the user are the OchemReax logo and three empty fieldsets. This is important in guiding the user to the role their input plays and how the website will respond. The Visualize button was designed to be a gradient of orange, contrary to the gray Technique and Dictionary buttons, in order to emphasize the core functionality of the website. The page of each reaction also contains a more obvious Visualize button compared to the Next button. The Dictionary of Common Mechanisms page contains a list of onclick links that are each equal in design and visual appearance.

Clarity:

The design of the website is to be minimal as possible. Extraneous decorations or designs are omitted as to not distract the user's attention away from core concepts or images of the reaction. Labeled fieldsets are provided to clearly inform the user what inputs are required. Lightly stated examples are provided in the reactant and catalyst/reagent fieldsets as to demonstrate the IUPAC molecular nomenclature required.

Simplicity:

The product is intended to display chemical reactions through clear images of each step. After user input, their only role remaining is to walk themselves through the reaction upon each Next click.

XI. FUTURE GOALS

There are many ways this product can be improved and additional features that can be included. So far it has satisfied its original purpose but is always looking for ways to improve.

Product Expansion:

- Expand scope of Organic Chemistry material to include more complex reactions
- Include and detail more reactions under each category within Dictionary of Common Mechanisms
- Connect product to classes/courses in order to reach more learners
- Simplification and readability of code- currently occupies lots of unneeded space and repetition of code
- Improve run time
- Remove need to store images in online source: Imgur
- Be able to construct molecules through code rather than walking through list of pre-drawn images by ChemAxon software

XII. REFERENCES

Vollhardt Chem 3A UC Berkeley lecture material

Peter Marsden Chem 3B UC Berkeley lecture material

ChemAxon Marvin JS- molecule drawing purposes

Imgur- online storage of photos for drawn molecules

Philip Guo's Python Tutor- model inspiration