Organic Web: An interactive web-based approach to teaching and learning organic chemistry

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The Future of Chemistry Education

• Shaped by new technology
• Innovative use of the internet
• Engage students in interactive learning
Some Shortcomings of Textbooks

• Linear by design
• May promote memorization
• Not interactive, engaging
• Non-linear design, web-like
  – Layers of information
  – Big picture vs. details
• Highly visual, engaging
• New technological advances made every day
Organic Chemistry—A “Web-like” Subject

- Everything’s connected
- Major challenge for students: lose sight of the forest for the trees
- Why? Linear presentation of most textbooks
- Natural marriage: organic chemistry + internet
- Organic Web
  - Concept-map interface
  - Makes “big picture” more explicit; details accessible via layered links
Linear vs. Non-linear Presentation

- Alkanes
- Alkenes
- Alkynes
- Alkyl Halides
- Alcohols
- Ethers
- Epoxides
- Amines
- Aromatics
- Carbonyls
- Nomenclature
- Physical Properties
- Reactivity
- Stereochemistry
- Synthesis
- Spectroscopy
Organization

• **Structure**
  – Atomic structure
  – Bonding and Molecular Structure
  – Stereochemistry and Conformational Analysis
  – Relationship between Structure and Properties/Reactivity
  – Physical Properties
  – Nomenclature
  – Spectroscopy

• **Reactivity**
  – Thermodynamics and Kinetics
  – Acid-Base; Elimination; Addition; Substitution; Redox

• **Synthesis**
  – Big Picture
  – Connectivity
Welcome! Organic Web is an interactive website for teaching and learning organic chemistry through a concept-map interface that allows students to see the "big picture" while also exploring detailed information accessible through a series of "clicks." The web-like structure of the Internet allows for a much more logical presentation of the subject matter of organic chemistry (which is itself web-like) than is possible with traditional textbooks. Textbooks are linear in structure, by design, and promote memorization or surface learning of the material, which rarely leads to success.

Organic chemistry is the chemistry of carbon compounds, and Organic Web organizes the content of organic chemistry into three main categories: Structure, Reactivity, and Synthesis. A logical place to begin the study of organic chemistry is by examining structural features of organic compounds, beginning with atoms and molecular structure (in both two dimensions and three), bonding and how the structure of a molecule affects its properties and how it reacts. There are millions of organic compounds, and so learning how to classify and name them is important. Organic compounds are categorized by their structures and how they react. All of these topics are covered in the Structure module.

The Reactivity module reviews concepts related to chemical reactions (chemical changes) and the energy changes associated with them. General types of reactions that organic compounds undergo, and how to represent the mechanisms of those reactions are also covered in the Reactivity module.

One of the most interesting facets of organic chemistry is the synthetic schemes that allow for the inter-conversion of organic compounds and the construction of complex target compounds from simpler starting materials. You will learn that most types of organic compounds can be converted to other types, either in one step or through a series of steps, and this connectivity contributes to the "big picture" of organic chemistry, as a web-like scheme of reactions that is presented in the Synthesis module.

Welcome to the homepage of Organic Web, a website designed to help you learn about organic chemistry.
The Structure Module

Chemistry is the science of matter, energy, and change, and organic chemistry focuses on the chemistry of carbon-containing compounds. Carbon is interesting and unique because it forms strong bonds with itself, along with other atoms like hydrogen, oxygen, nitrogen and the halogens. All living things are made up of carbon compounds, and so organic chemistry is fundamental to biology and biochemistry, as well. We start by looking at the structure of a carbon atom and its place within the Periodic Table. This leads to a discussion of bonding and molecular structure, both in two dimensions, and three. The study of molecules in three dimensions constitutes stereochemistry, which is particularly important and relevant in organic chemistry. We will look at how structure affects physical properties and reactivity, and learn to classify of organic compounds based on their structure or functional groups. The figure shown below is interactive—you can click on words, boxes, and arrows to link to pages that describe the structure and classification of organic compounds, beginning with the structure of a carbon atom. Within each page you will also find self-assessment exercises and quizzes to complete before moving on to the next topic. You can also navigate the content from the breadcrumb drop-down menu above.
Chapter 3: Isomers, Stereochemistry, and Conformational Analysis

Contents:

3.1 Isomers
3.2 Stereochemistry
3.3 Conformational Analysis
3.4 Summary and Conclusions
Interactive Practice Problems
Written Problem Set
Quiz

So far we've discussed the structure of atoms and molecules, both in two and three dimensions. In this chapter we look at the structure of organic molecules in greater detail. Lewis dot structures were a useful model for beginning to think about the two-dimensional structure of molecules, and hybridization and VSEPR theories to consider the structure of molecules in three dimensions. We'll focus here on the structure of organic molecules, specifically with regard to how the atoms in organic molecules are connected or arranged, both in two and three dimensions. We'll also look at the three-dimensional structure of molecules with respect to rotation around single bonds of acyclic compounds and "flexing" of bonds of cyclic compounds. Upon successful completion of this chapter you will be able to:

- differentiate between types of isomers
- draw structures for all of the isomers (both constitutional and stereoisomers) that exist for a given molecular formula
- identify stereocenter(s) within a molecule
- determine the maximum number of stereoisomers that exist for a given constitution
- differentiate between enantiomers, diastereomers, and meso compounds
- determine the configuration (R or S) of a stereocenter in a molecule
- calculate the specific rotation of a pure enantiomer
- calculate the optical purity (ee) of a mixture of enantiomers
- perform a conformational analysis of an acyclic compound, using Newman projections to illustrate rotation around a given single bond
- perform a conformational analysis of a cyclic compound (especially 6-membered rings)

3.1 Isomers

Organic compounds are comprised mostly of carbon and hydrogen, as well as a few other heteroatoms, like nitrogen, oxygen and the halogens. Organic compounds, however, exist in all shapes and sizes, and how they're connected in two dimensions or arranged in three dimensions is of considerable importance—as we've mentioned previously and will look at in further detail later, molecular structure determines physical properties and chemical reactivity. In the previous chapter we learned about constructing Lewis structures for molecules of a given molecular formula (CH₄O was used as an example). For many (if not most) molecular formulas, however, it's possible to connect the atoms into more than one coherent, stable molecule. Different molecules with the same molecular formula are called
3.2.2 Configuration, R or S?

Thus far we have been talking about stereochemistry, stereocenters, chirality, optical activity and purity. A detail we have yet to discuss is the configuration of a stereocenter—the specific 3-dimensional arrangement in space of the four different atoms or groups of atoms bonded to an sp³ hybridized carbon (a stereocenter). Simply put, there are two possible configurations, and in keeping with the "handedness" analogy, one is the "right-handed" configuration (R), and the other is the left-handed configuration (S). The question is, how do you determine which is which? For example, refer back to Figure 2—the 2α enantiomer has the R configuration and the 2β has the S configuration. But, how is this determined? Click here for a tutorial on determining the configuration, R or S, of a stereocenter. Then, refer back to Figures 5 and 6 and assign the configuration of each stereocenter.

3.2.3 Chirality and Optical Activity

One unique physical property of chiral compounds is that they are optically active. Visible light propagates in all directions; plane-polarized light is light that has been "handedness" of chiral compounds, when plane-polarized light is passed through a video animation of this process using an instrument called a polarimeter, click here. The extent to which a chiral compound rotates plane-polarized light is quantified by calculating specific rotations.

An optically pure compound consists of 100% of one enantiomer, click here for any other information. A sample that contains an exactly equal combination of the two enantiomers is optically inactive; that is, they do not rotate light. A simplified explanation. In reality, one enantiomer rotates light in one direction, while the other rotates it in the opposite direction, and the net effect is no rotation. The optical purity of a compound can be calculated by comparing the rotation of the compound to the rotation of a standard sample of known purity. Click here for a tutorial on calculating ee and assessing optical purity.

3.3 Conformational Analysis

In addition to stereochemistry, another concept to consider when thinking about the 3-dimensional structure of organic molecules, is the relative energy associated with rotation around a single bond within an acyclic molecule, and the flexing/bending of bonds within a cyclic molecule. This is formally known as conformational analysis, and is intimately tied with stereochemistry in the consideration of a molecule’s 3-dimensional structure and chemical reactivity. Conformational analysis will be illustrated through three examples: ethane (C₂H₆), n-butane (C₄H₁₀), and cyclohexane (C₆H₁₂), and substituted cyclohexanes.
Sample Video Animation Link
3.4 Summary and Conclusions

All organic compounds are made up of carbon (C), and most also contain hydrogen (H). There are relatively few other types of atoms (heteroatoms) that are typically present in organic compounds. However, there are literally millions of different organic compounds, because there are many different ways the carbon and other atoms may be connected or arranged in space. In this chapter we learned:

- Isomers are different compounds with the same molecular formula
  - constitutional isomers are isomers that differ in how the atoms are connected together
  - stereoisomers are isomers in which the atoms have the same connectivity, but are arranged differently in space
    - stereoisomers contain one or more stereocenters—a tetrahedral, sp³ hybridized carbon atom with four different atoms or groups of atoms bonded to it; stereocenters have either the R or S configuration
    - one type of stereoisomers are enantiomers, which are non-superimposable mirror image compounds
    - all other stereoisomers are diastereomers
  - stereochemistry is important because subtle differences in the three-dimensional arrangement of atoms within a molecule can manifest as significantly different interactions with bio-molecules (like proteins)
    - compounds that are non-superimposable on their mirror images are said to be chiral or optically active—they rotate plane-polarized light
    - specific rotation is a measure of the extent to which a chiral compound rotates plane-polarized light; enantiomers rotate plane-polarized light by the same extent, but in opposite directions
    - a 50:50 (exact) mixture of enantiomers is called a racemic mixture and is optically inactive; a mixture of enantiomers in any other proportion is optically active, and the enantiomeric excess (ee) is a measure of optical purity
  - another factor to consider when thinking about the 3-dimensional structure of a molecule is orientation or conformation of the molecule with respect to rotation around s bonds in acyclic molecules, or flexing/bending of cyclic molecules
    - different conformations have different energies (stabilities) due to different forms of strain: torsional, stereo, or angling strain
    - molecules minimize strain by rotating around s bonds in acyclic compounds or flexing/bending in cyclic compounds

Interactive Practice Problems

Written Problem Set

Quiz
The Reactivity and Synthesis Modules
Organic Web: The Concept Map
Sample Link: Alcohols

**Alcohols**

**General Structure:**

```
\[ \text{R} - \text{OH} \]
```

**Nomenclature:** IUPAC rules apply:
1. Find the longest continuous chain that contains the -OH group
2. Name the parent chain, drop the final "e" of the corresponding alkane name and replace with "-ol"
3. Number the parent chain; assure the -OH group gets the lowest possible number

```
2-methyl-2-butanol  
cyclopentanol  
(3S)-8-methyl-4-nonanol
```

**Classification:**

- **1°**
- **2°**
- **3°**
- **vinyl**
- **benzylic**

- undergo substitution and elimination reactions
- do not undergo substitution or elimination reactions

**General Features:**

- polar covalent bond
- acidic proton: Lewis/boron acid 
- electrophile at C1

**General Reactivity:**

```
\[ \text{R} - \text{OH} + \text{H}_2\text{O} \rightarrow \text{R} - \text{OH} + \text{H}^+ \text{ and } \text{OH}^- \]
```

Elimination, several methods

```
\[ \text{R} - \text{OH} + \text{H}_2\text{O} \rightarrow \text{R} + \text{OH}^- \]
```

Substitution, several methods

```
\[ \text{R} - \text{OH} + \text{H}_2\text{O} \rightarrow \text{R} + \text{OH}^- \]
```

- Alcohols are organic compounds that contain a hydroxyl group (-OH) bonded to an sp³-hybridized carbon atom

- Physical properties:
  - Both the C-O and O-H bonds are polar, giving these compounds a net dipole in the direction of the oxygen atom and making them polar.
  - The hydroxy proton forms hydrogen bonds with the oxygen lone pair electrons of neighboring alcohol molecules, increasing the boiling points of these compounds relative to compounds of similar size that lack the hydroxyl group.
  - The hydroxy group proton is also considerably acidic (pK₆ ~ 16)

- Classification:
  - Alcohols are classified as 1°, 2°, or 3° based on the degree of substitution or the carbon atom to which the hydroxyl group is bonded.
  - Alcohols can also be classified as allylic or benzylic (see figure).
  - A compound that bears a hydroxyl group that is directly bonded to the sp3 hybridized carbon of an alkane is called an enol.
  - A compound that bears a hydroxyl group that is directly bonded to one of the carbon atoms of a benzene ring is called a phenol.

- Nomenclature: alcohols are named by applying the IUPAC rules:
  - Find the longest chain that contains the hydroxyl group; this is the parent chain.
  - Number the parent chain such that the hydroxyl group gets the lowest possible number.
  - Find and name all other substituents/alkyl groups.
  - Alphabetize the substituents/alkyl groups and assemble the name.
Future Development

• Finish content
• Include more interactive problems and links
• Incorporate more visual components
  – Molecular Modeling
  – Video animations
  – Short video lecture presentations
• Allow for more problem-based learning during class meetings; less lecture, more interaction
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