Lesson Plan: Structural Isomers

FOR THE TEACHER

Summary
In this lesson, students will use models to explore structural isomers, and create explanations for the impact of structure on intermolecular forces (London dispersion) and physical properties (boiling point).

Grade Level
High School

NGSS Alignment
This lesson will help prepare your students to meet the performance expectations in the following standards:

- **HS-PS1-1**: Use the periodic table as a model to predict the relative properties of elements based on the patterns of electrons in the outermost energy level of atoms.
- **HS-PS1-3**: Plan and conduct an investigation to gather evidence to compare the structure of substances at the bulk scale to infer the strength of electrical forces between particles.
- **HS-PS2-6**: Communicate scientific and technical information about why the molecular-level structure is important in the functioning of designed materials.

- **Scientific and Engineering Practices**:
  - Developing and Using Models
  - Analyzing and Interpreting Data

AP Chemistry Curriculum Framework
This lesson supports the following learning objectives:

- **Unit 3: Intermolecular Forces and Properties**
  - **Topic 3.1**: Intermolecular Forces
    - **SAP-5.A**: Explain the relationship between the chemical structures of molecules and the relative strength of their intermolecular forces when:
      - a. The molecules are of the same chemical species.
      - b. The molecules are of two different chemical species.
  - **Topic 3.2**: Properties of Solids
    - **SAP-5.B**: Explain the relationship among the macroscopic properties of a substance, the particulate-level structure of the substance, and the interactions between these particles.
  - **Topic 3.9**: Separation of Solutions and Mixtures Chromatography
    - **SPQ-3.C**: Explain the relationship between the solubility of ionic and molecular compounds in aqueous and nonaqueous solvents, and the intermolecular interactions between particles.

Objectives
By the end of this lesson, students should be able to

- Draw structural isomers for a specified molecular formula.
- Relate physical structure to intermolecular forces and boiling points.

Chemistry Topics
This lesson supports students’ understanding of
- Molecules & Bonding
- Structural isomers
- Intermolecular forces (IMF), particularly London dispersion forces
- Physical properties, particularly boiling points
- Organic Chemistry
- Chemical information literacy

**Time**

**Teacher Preparation:** <30 minutes  
**Lesson:** 1-2 class periods (80 to 130 minutes)
- Engage: 10 minutes  
- Explore: 30-40 minutes (Part 1), 40-60 minutes (Part 2)  
- Explain: 20 minutes  
- Elaborate: 30 minutes  
- Evaluate: 1 hour (approximately, per class)

**Materials**
- Molecular model Kits, recommended:
  - Darling Models (http://www.darlingmodels.com)
- Molecular Structure references/databases, such as:
  - The Sigma-Aldrich catalog (http://www.sigmaaldrich.com)
  - The CRC handbook
  - PubChem Database (pubchem.ncbi.nlm.nih.gov/search/)
  - ChemSpider Chemical Structure Database (www.chemspider.com)

**Safety**
- No specific safety precautions need to be observed for this activity.

**Teacher Notes**
- This lesson can be included within units on bonding and molecular structure, states of matter, intermolecular forces, organic chemistry, or structural isomers. This is appropriate for Honors and AP Chemistry students.

- This can be used as a standalone lesson to introduce isomers, the effect of structure on physical properties, and organic chemistry. In addition, it can be used in connection with another Chemistry of Cars resource, “Lab: Fractional Distillation of Crude Oil” which is a laboratory experiment, that uses fractional distillation to separate a mixture of organic molecules.

- London dispersion forces or induced dipole intermolecular forces are a common source of misconceptions for students. As necessary, review the different types of IMFs. This is a useful background video for London dispersion forces (Bozeman Science)

- **Engage:** Ask students about a recent trip to the gas station and the different grades of gasoline to introduce the concept of octane number, isoctane, and octane isomers. The teacher may want to to have a picture of a gas pump showing octane numbers.

Use the podcasts below as an introduction (some students may be distracted by the British pronunciations of methyl, garage, petrol in the second podcast):
- http://indianapublicmedia.org/amomentofscience/octane-numbers/ or
Leading Question: Why might octane and isooctane—compounds with the same chemical formula (C₈H₁₈)—have different combustion properties in an engine?

**Explore:**
- Part 1: Students will begin by drawing different isomers. The isomer drawing activity can be assigned as homework before the in-class modeling exercises (Part 2).
- Part 2: Students explore differences in physical interactions through examination of molecular models of octane isomers. The modeling exercise can be adapted for group jigsaw by assigning one molecule per group, then re-forming groups to share information.

**Part 1:** This activity can be adapted to the skill and experience of the students in your class. For example, use the following suggested variations in student handouts provided:
  - Octanes for “experts”
  - Hexanes for “intermediates”
  - Pentanes for “novices”

Students may find it useful to share ideas for systematically drawing structural isomers. In addition, it may be beneficial to provide a short period of time for all students to pool their structures. For example, students could be called upon to contribute structures to the board.

The Compound Interest resource A Brief Guide to Types of Organic Chemistry Formulae is a useful introduction to different representations for organic molecules.

**Answers for each of the isomer variations in Part 1 are as follows:**
- Novices: There are 3 isomers of C₅H₁₂: pentane, 2,2-dimethylpropane, and 2-methylbutane.
- Intermediates: There are 5 isomers of C₆H₁₄: hexane, 2,2-dimethylbutane, 2,3-dimethylbutane, 3-methylpentane, and 2-methylpentane.
- Experts: Some students may have difficulty independently drawing all 18 isomers of C₈H₁₈, especially some of the ethyl isomers. It is not necessary to draw all 18 isomers before proceeding, but a complete list of all isomers can be provided to students.
  - Octane
  - 2-Methylheptane
  - 3-Methylheptane
  - 4-Methylheptane
  - 2,2-Dimethylhexane
  - 2,3-Dimethylhexane
  - 2,4-Dimethylhexane
  - 2,5-Dimethylhexane
  - 3,3-Dimethylhexane
  - 3,4-Dimethylhexane
  - 3-Ethylhexane
  - 2,2,3-Trimethylpentane
  - 2,2,4-Trimethylpentane
  - 2,3,3-Trimethylpentane
  - 2,3,4-Trimethylpentane
  - 2-Methyl-3-ethylpentane
  - 3-Methyl-3-ethylpentane
  - Tetramethylbutane

**Part 2:** The skeletal formulas below are a simplistic way to show preferred orientations for each set of octane isomers. A space-filling 3-D image is provided for reference (3-D images can be modeled and rotated on www.chemspider.org). Student answers for the modeling exercise should be similar to the following, though the level of detail and 3-dimensionality may vary. If appropriate, students may prefer to take photos of the models.

**Answers for Part 2 are as follows:**
Boiling point: 125°C
Melting point: -57 °C

For 2,5-dimethylhexane, maximum surface area contact is possible if oriented as shown on the left. The surface area contact is minimized in other configurations.
Boiling point: 107-108 °C
Melting point: -91 °C
Though London dispersion forces are typically characterized as weak in most textbooks, they are not inconsequential as we can see in the \( \sim 25^\circ \text{C} \) spread in boiling points for the isomers. More surface area = increased IMF = higher boiling points.

Conceptual Questions:
- How many different ways can carbon atoms and hydrogen atoms be arranged to form an alkane (how many structural isomers of octane or hexane or pentane are there)?
- Do you expect the different isomers to have the same physical properties (such as solubility, boiling point)?
- How might different isomers be separated from each other using only physical properties (physical separation methods include distillation)?

- **Explain**: There is a characteristic odor associated with gasoline that can be connected to the physical properties of the hydrocarbon molecules. Many of the hydrocarbons in gasoline are small and have relatively weak London dispersion forces (thus low-boiling) and present in vapor phase near gasoline pumps; we can inhale and smell them.

Focus questions:
- What is the smell when you pump gas? Why does gasoline—a liquid—smell so strongly? Does the smell seem stronger on hot days?
- What keeps molecules together to form liquids?
- What happens to molecules during boiling/evaporation (liquid to gas transition)?
- Would a low boiling liquid have strong intermolecular forces?
From the activity, students should observe that the linearity of n-octane maximizes contact of adjacent molecule’s surface area. In contrast, the branching in 2,4-dimethylhexane and 2,2,4-trimethylpentane reduces surface area and potential interaction.

- **Elaborate:** Analysis questions are provided in Part 2 for students to connect structure to physical properties (both intermolecular forces and boiling point). Students will consider how physical properties such as a boiling point can be used to separate chemical compounds, and learn about the technique of fractional distillation in the laboratory and industry through this video.

- **Evaluate:** Students will draw structural isomers and answer analysis questions to demonstrate understanding of the key concepts. Students will create a brief procedure for fractional distillation to demonstrate the use of physical properties as a means to separate chemical compounds.

  Student explanations should relate the greater surface area of n-octane to the greater intermolecular forces between molecules of n-octane and thus a higher boiling point when compared to either 2,5-dimethylhexane or 2,2,4-trimethylpentane. Similarly, 2,5-dimethylhexane has a greater surface area and IMF than 2,2,4-trimethylpentane. In a fractional distillation, the lowest boiling component (2,2,4-trimethylpentane) is collected first.
Lesson

Part 1: Structural Isomers of Octane

Background

We encounter a variety of hydrocarbons, compounds that consist only of carbon and hydrogen, in our daily life. These compounds may have only single bonds (alkanes), at least one double bond (alkenes), or at least one triple bond (alkynes).

Alkanes have the general molecular formula $C_nH_{2n+2}$. In these molecules, each carbon atom can bond to 4 different atoms (either carbon or hydrogen) and each hydrogen can only bond to 1 other atom (which must be carbon). Alkanes are commonly referred to as saturated compounds because the molecule has the maximum possible number of hydrogen atoms relative to number of carbons present.

Gasoline is a complex mixture of hydrocarbons of all types, and is often characterized by its octane number. The octane number is a means to relate the combustion properties of the fuel to a standard, isooctane, $C_8H_{18}$, with an octane number of 100. The octane number you see at the pump doesn’t actually represent the amount of octane in the fuel, but rather the combustion behavior of the fuel in an engine as compared to isooctane.

Isooctane is the common name; the systematic IUPAC name for this molecule is 2,2,4-trimethylpentane, and it can be represented symbolically in several ways as shown below:

<table>
<thead>
<tr>
<th>Displayed Formula</th>
<th>Structural Formula</th>
<th>Skeletal (line-angle) Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image1" alt="Displayed Formula" /></td>
<td><img src="image2" alt="Structural Formula" /></td>
<td><img src="image3" alt="Skeletal Formula" /></td>
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As all bonds and atoms are shown in the displayed formula, it looks cluttered. For clarity, chemists use either the structural formula (which shows all atoms but simplifies the representation of carbon-hydrogen bonds) or the skeletal formula. The skeletal formula does not explicitly show each C and H atoms; it is understood that each vertex or line terminus represents a carbon atom. The number of hydrogen atoms attached to each carbon atom is equal to 4 - # of lines shown (because each carbon atom can only make a total of 4 bonds).

Iooctane is a branched alkane; that is, it is not linear. The same 8 carbon and 18 hydrogen atoms can be arranged in a straight line to make n-octane:
Isooctane and n-octane have the same atoms and molecular formula but differ in the arrangement of these atoms; they are structural or constitutional isomers, and are different chemical compounds with different chemical properties.

**Problem**
How many different ways can 8 carbon atoms and 18 hydrogen atoms be arranged to form an alkane (how many structural isomers of octane are there)? Do the different isomers have the same physical properties? How might different isomers be separated from each other?

There are nearly 20 different structural isomers for C₈H₁₈. Draw as many as you can. You may find it most convenient to use the structural or skeletal formula.
# FOR THE STUDENT

Lesson

## Part 1: Structural Isomers of Pentane

### Background

We encounter a variety of hydrocarbons, compounds that consist only of carbon and hydrogen, in our daily life. These compounds may have only single bonds (alkanes), at least one double bond (alkenes), or at least one triple bond (alkynes).

Alkanes have the general molecular formula \( C_nH_{2n+2} \). In these molecules, each carbon atom can bond to 4 different atoms (either carbon or hydrogen) and each hydrogen can only bond to 1 other atom (which must be carbon). Alkanes are commonly referred to as saturated compounds because the molecule has the maximum possible number of hydrogen atoms relative to number of carbons present.

Gasoline is a complex mixture of hydrocarbons of all types, and is often characterized by its octane number. The octane number is a means to relate the combustion properties of the fuel to a standard, isooctane, \( C_8H_{18} \), with an octane number of 100. The octane number you see at the pump doesn't actually represent the amount of octane in the fuel, but rather the combustion behavior of the fuel in an engine as compared to isooctane.

Isooctane is the common name; the systematic IUPAC name for this molecule is 2,2,4-trimethylpentane, and it can be represented symbolically in several ways as shown below:

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Isooctane is a branched alkane; that is, it is not linear. The same 8 carbon and 18 hydrogen atoms can be arranged in a straight line to make n-octane:
Isooctane and n-octane have the same atoms and molecular formula but differ in the arrangement of these atoms; they are structural or constitutional isomers, and are different chemical compounds with different chemical properties.

**Problem**

How many different ways can 5 carbon atoms and 12 hydrogen atoms be arranged to form an alkane (how many structural isomers of pentane are there)? Do the different isomers have the same physical properties? How might different isomers be separated from each other?

There are 3 different structural isomers for C₅H₁₂. Draw them. You may find it most convenient to use the structural or skeletal formula.
FOR THE STUDENT
Lesson

Part 1: Structural Isomers of Hexane

Background

We encounter a variety of hydrocarbons, compounds that consist only of carbon and hydrogen, in our daily life. These compounds may have only single bonds (alkanes), at least one double bond (alkenes), or at least one triple bond (alkynes).

Alkanes have the general molecular formula $C_nH_{2n+2}$. In these molecules, each carbon atom can bond to 4 different atoms (either carbon or hydrogen) and each hydrogen can only bond to 1 other atom (which must be carbon). Alkanes are commonly referred to as saturated compounds because the molecule has the maximum possible number of hydrogen atoms relative to number of carbons present.

Gasoline is a complex mixture of hydrocarbons of all types, and is often characterized by its octane number. The octane number is a means to relate the combustion properties of the fuel to a standard, isooctane, $C_8H_{18}$, with an octane number of 100. The octane number you see at the pump doesn’t actually represent the amount of octane in the fuel, but rather the combustion behavior of the fuel in an engine as compared to isooctane.

Isooctane is the common name; the systematic IUPAC name for this molecule is 2,2,4-trimethylpentane, and it can be represented symbolically in several ways as shown below:

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Isooctane is a branched alkane; that is, it is not linear. The same 8 carbon and 18 hydrogen atoms can be arranged in a straight line to make n-octane:
Isooctane and n-octane have the same atoms and molecular formula but differ in the arrangement of these atoms; they are structural or constitutional isomers, and are different chemical compounds with different chemical properties.

**Problem**
How many different ways can 6 carbon atoms and 14 hydrogen atoms be arranged to form an alkane (how many structural isomers of hexane are there)? Do the different isomers have the same physical properties? How might different isomers be separated from each other?

There are 5 different structural isomers for C₆H₁₄. Draw them. You may find it most convenient to use the structural or skeletal formula.
FOR THE STUDENT
Lesson

Part 2: Molecular Modeling of Octane Isomers

Part A: Getting started with the molecular modeling kit

1. Assemble 8 sp³-hybridized carbon atoms from a molecular model kit. You do not need to add anything to represent the hydrogen atoms since the molecular model is similar to a skeletal formula—the hydrogens are not shown but we understand that they are present.

2. Look at the carbon atoms you have built; they should be tetrahedral with the four arms (or bonds) at angles of 109.5º.

3. Connect 2 carbons to each other. The two atoms should spin freely around the connecting bond so that the 3 hydrogens on each carbon can either line up (“eclipsed conformation”) or alternate (“staggered conformation”). The lowest energy conformation is the staggered conformation where the atoms in the molecule are as far apart as possible.

4. Connect 4 carbons to each other. The atoms should spin freely so that the 3 hydrogens on any two adjacent carbons can either line up or alternate. In addition, the molecule can be bent to bring the ends close together or the molecule can be stretched out (see picture). Again, the lowest energy conformation is the one where the atoms in the molecule are as far apart as possible. Notice how the zigzag line-angle skeletal formula resembles the lowest energy conformation.

5. Lay the model on a sheet of paper and draw a zigzag line to represent the molecule’s surface area. An atom for each molecule can touch the line, but none can cross over; this is the closest any two molecules can approach each other.
Part B: Build the octane isomers

1. Begin attaching additional carbons until you have a straight chain of 8 carbons. This is the n-octane isomer. Position the atoms in your octane molecule so that they are as far away from each other as possible. Draw a 3-D sketch of this conformation of octane in the box below.

2. Place the model of octane on your sheet of paper with the zigzag line. Place a second model of octane (in the same low energy conformation) next to the first. Line-up the two molecules to maximize surface area contact.

3. In the box below, use a different color to show how the second octane molecule aligns with the first. Use a third color to show how a third octane molecule might align with the first two.

4. Remove two carbons from the end of your octane molecule and build the 3,5-dimethylhexane isomer. Position the atoms in your molecule so that they are as far away from each other as possible. Draw a 3-D sketch of this conformation in the box below.

5. Place the model on your sheet of paper with the zigzag line. Place a second model this molecule (in the same low energy conformation) next to the first. Line-up the two molecules to maximize surface area contact.

6. In the box below, use a different color to show how the second molecule aligns with the first. Use a third color to show how a third molecule might align with the first two.
7. Remove a carbon from the end of your molecule and build 2,2,4-trimethylpentane molecule isomer (this is also called isoctane). Position the atoms in your molecule so that they are as far away from each other as possible. Draw a 3-D sketch of this conformation in the box below.
8. Place the model on your sheet of paper with the zigzag line. Place a second model of this molecule (in the same low energy conformation) next to the first. Line-up the two molecules to maximize surface area contact.
9. In the box below, use a different color to show how the second molecule aligns with the first. Use a third color to show how a third octane molecule might align with the first two.

**Observations**

1. Based on the molecular modeling and your figures above, which isomer has the greatest surface area?

2. Predict the boiling points of the three octane isomers (1 = highest boiling point, 3 = lowest boiling point) and record in the table below.

<table>
<thead>
<tr>
<th>Octane</th>
<th>Predicted BP rank</th>
<th>BP (actual)</th>
</tr>
</thead>
<tbody>
<tr>
<td>3,5-Dimethylhexane</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2,2,4-Trimethylpentane</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

3. Look up literature values for the boiling points and report each in the data table. You may not use Wikipedia, but can use the following databases:
   - pubchem.ncbi.nlm.nih.gov/search/
   - www.chemspider.com/
   - reference book or chemical catalog in the classroom
**Analysis**

1. What types of intermolecular forces (IMFs) are present in alkanes?

2. Which of the three molecules has the highest boiling point? The lowest?

3. Which of the three molecules has the strongest IMFs? The weakest? Explain your choices.

4. Predict the *melting points* of the three octane isomers (1 = highest melting point, 3 = lowest melting point)

**Conclusion**

Fractional distillation is a physical separation process that is commonly used in the chemical lab and industry. Watch [this video](#) to see how this is used in petroleum refining.

Write a paragraph that explains how fractional distillation could be used to separate the three isomers of octane you modeled. You must explain how surface area and intermolecular forces affect the physical properties of the molecules and allow this separation. Your explanation must indicate what compound would be the first fraction, the second fraction, and the third fraction.