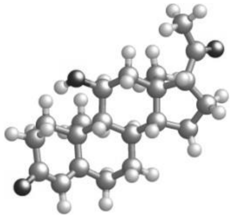

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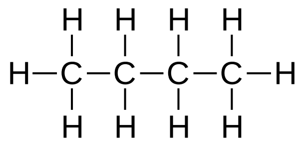
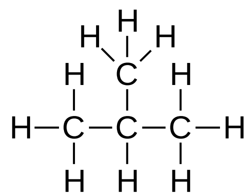
<u>Structural and Geometric Isomerism – Macroconcept: Models</u>

• Study the structures of the two molecules shown in **Figure 1** and consider the answers to the following questions. In what way are the two molecules the same? In what way are the two molecules different?

Figure 1.
The same, but different?



butane



2-methylpropane

• *Isomers* are compounds that share the *same molecular formula*, but have *different structural formulae*, *i.e.* have a different arrangement of atoms.

• The simplest type of isomerism is *structural isomerism*. For example, the two structural isomers of C_4H_{10}, butane and 2-methylpropane, are shown in **Figure 1**.

These isomers have similar chemical properties, for example, the complete combustion of both isomers results in the formation of carbon dioxide and water according to the balanced chemical equation:

$$2C_4H_{10(g)} + 13O_{2(g)} \rightarrow 8CO_{2(g)} + 10H_2O_{(l)}$$

In addition, both isomers will undergo a free radical substitution reaction with chlorine in the presence of ultra-violet radiation to form a halogenoalkane according to the balanced chemical equation:

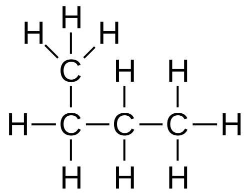
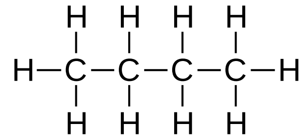
$$C_4H_{10(g)} + Cl_{2(g)} \rightarrow C_4H_9Cl_{(l)} + HCl_{(g)}$$

However, the physical properties of these isomers are different:

boiling point of butane = 0°C

boiling point of 2-methylpropane = –11°C

Question 1.

Explain why  is *not* an isomer of 

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Question 2.

Explain why the boiling point of butane is higher than that of its isomer 2-methylpropane:

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Question 3.

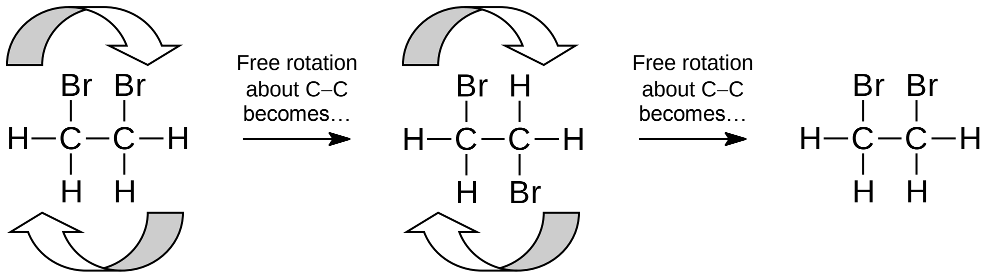
There are *five* structural isomers of C_6H_{14}. Give the full structural formula and name of each isomer in the space provided below:

Question 4.

There are *four* structural isomers of C_4H_9Br. Give the full structural formula and name of each isomer in the space provided below:

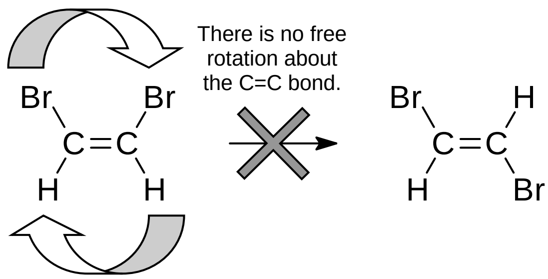
• In *saturated* organic compounds there is *free rotation* about the carbon-to-carbon single covalent bond:

Figure 2.
Free rotation about the C–C bond.



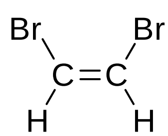
• In *unsaturated* organic compounds there is *no free rotation* about the carbon-to-carbon double covalent bond. Because of this limited rotation, atoms that are attached to each carbon atom of the carbon-to-carbon double covalent bond are fixed, either on the *same side* of the molecule, or on *opposite sides* of the molecule:

Figure 3.
No free rotation about the C=C bond.

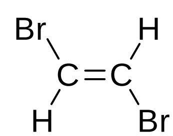


This leads to *geometric isomerism* in unsaturated organic compounds. The isomer in which both atoms are arranged on the *same side* of the molecule is known as the *cis*– isomer, while the isomer in which the atoms are arranged on *opposite sides* of the molecule is known as the *trans*– isomer:

Figure 4.
Geometric isomers of 1,2-dibromoethene



cis-1,2-dibromoethene



trans-1,2-dibromoethene

Question 5.

a) What do you understand by the term *saturated organic compound*?

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b) What do you understand by the term *unsaturated organic compound?*

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Question 6.

Draw and name *all* possible isomers of C_4H_8 in the space provided below:

Question 7.

● Molecular modelling kits are very useful tools for studying the structures of organic compounds, including isomers. For example, James Watson's and Francis Crick's insight into the structure of the DNA double helix involved the construction and analysis of a three-dimensional *model*.

● Chemists use both physical and virtual (using computers) *models* to help them understand the structures of organic compounds as well as the interactions that take place between one molecule and another.

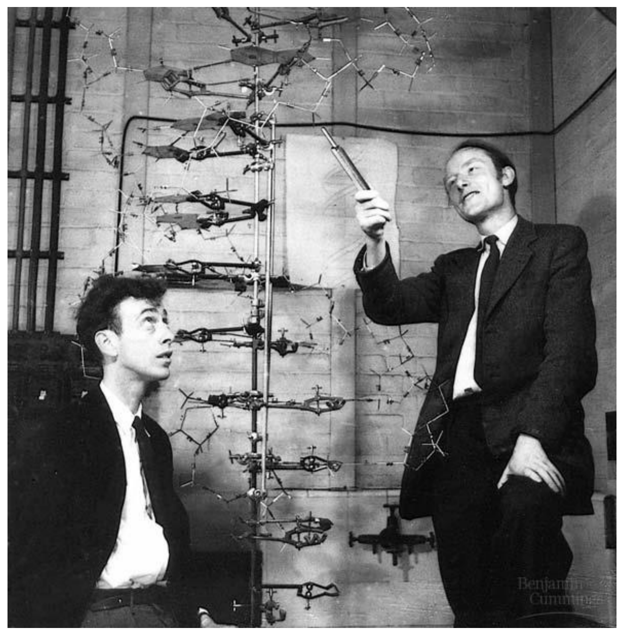

Figure 5. Watson and Crick studying their molecular *model* of the DNA double helix.

● List the possible advantages and disadvantages of using a molecular modelling kit to study the structure and predict the chemistry of a complex biologically active molecule.

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● What are the possible advantages and the disadvantages of using a physical molecular modelling kit compared to a virtual modelling kit run on a computer?

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Question 8.

a) Draw and name the two geometric isomers of butenedioic acid in the space provided below:

b) When *cis*-butenedioic acid is heated to 160°C, it undergoes thermal decomposition forming compound **X** and water. Give the full structural formula of compound **X** and explain why there is no observed reaction when *trans*-butenedioic acid is heated to 160°C:

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You may find the following information useful when answering questions **7 c)** and **7d)**:

electronegativity values (Pauling Scale): C = 2.5 H = 2.1 O = 3.5

c) Explain why the melting point of *trans*-butenedioic acid (287°C) is much higher than the melting point of *cis*-butenedioic acid (135°C):

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d) Explain why *trans*-butenedioic acid is 100 times more soluble in water than that *cis*-butenedioic acid:

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- Scan the QR code given below to view the answers to this assignment.

http://www.chemist.sg/organic_chem/worksheets/isomerism/isomerism_ans.pdf