



Molecular models

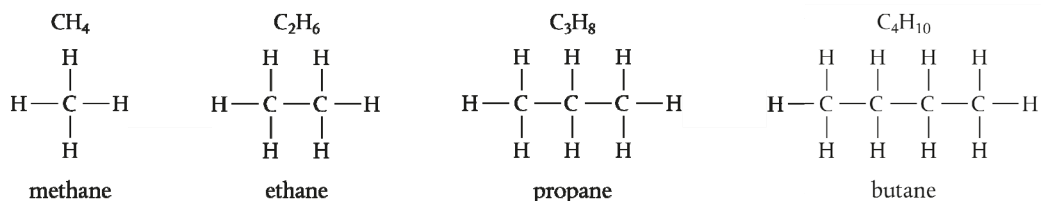
Reference: Chapter 10, Section 10.1, pages 464–473, and Section 20.3, pages 514–521

Aim

To explore both real and virtual molecular models of organic molecules.

Introduction

In organic chemistry we commonly represent structural formulas in two dimensions on paper for convenience. For example:



But in order to understand several aspects of organic structure and reactions, we need to consider the three-dimensional shape. This can be visualized by building real molecular models, and also virtually using molecular software programs. In this experiment you will have the chance to explore some of these ways of representing the three-dimensional shapes of organic molecules.

Pre-lab questions

- 1 Consider the ways in which two-dimensional structural formulas of the type shown on page 468 can provide misleading or incomplete information about the geometry of molecules.

Method

Molecular models can be built using toothpicks to represent bonds and spherical materials to represent atoms, such as Plasticine or polystyrene balls. Several scientific kits are also available commercially. (The models photographed in Chapter 10, for example on pages 476 and 477, are built using Molymod kits.)

There are many software programs available to build and explore molecular models. Some free ones include:

- [Chemsketch](#) (not for Mac users)
- [Avogadro](#)
- [Phet Colorado](#)

Reference to Chapter 10, especially pages 472 and pages 519–521 will be helpful in the following exercise.

Using both real and virtual models, build the following molecules:

- the first 6 members of the alkanes
- all straight-chain isomers of C_6H_{12}



- four different alcohols which are all isomers of C_4H_9OH
- models to show the relationship between an ether and an alcohol
- models to show the relationship between a carboxylic acid, an amide, and an ester
- models to show the relationship between ammonia and primary, secondary, and tertiary amines
- models to show the relationship between butanal and butanone
- models to show the differences in the following pairs of stereoisomers:
 - *cis*-1,3-dichlorocyclobutane and *trans*-1,3-dichlorocyclobutane
 - *cis*-butenedioic acid and *trans*-butenedioic acid
 - (*Z*)-3-methylpent-2-ene and (*E*)-3-methylpent-2-ene
 - optical isomers of butan-2-ol
 - optical isomers of 2-chlorobutane

Build molecules containing up to six carbon atoms and one of the functional groups listed on page 470. Pass your models to a classmate and ask them to give the IUPAC name for your model.

For consideration:

- 1 Discuss the advantages and disadvantages of real versus virtual models as tools to help understand the three-dimensional structure of organic molecules.
- 2 The pharmaceutical industry often uses a process called 'computer-aided design' as part of the research and development of new drugs. Consider how the use of computers may be useful in this way. What aspects of drug design may not be usefully investigated using computers?



Equipment list

polystyrene / Plasticine balls and toothpicks
or
model kits such as [Molymod](#)
access to computer software