



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.

The angle not always the same as in the given structural formulas. It does not give the real proportion of the lengths of the bonds and sizes of the atoms.

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](#)

Conclusion For Molecular Models Lab In Chemistry

Clifford Lane

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Exploring General Chemistry in the Laboratory Colleen F. Craig, Kim N. Gunnerson, 2017-02-01 This laboratory manual is intended for a two semester general chemistry course. The procedures are written with the goal of simplifying a complicated and often challenging subject for students by applying concepts to everyday life. This lab manual covers topics such as composition of compounds, reactivity, stoichiometry, limiting reactants, gas laws, calorimetry, periodic trends, molecular structure, spectroscopy, kinetics, equilibria, thermodynamics, electrochemistry, intermolecular forces, solutions, and coordination complexes. By the end of this course you should have a solid understanding of the basic concepts of chemistry which will give you confidence as you embark on your career in science.

Computational Modelling and Simulations for Designing of Corrosion Inhibitors Daksheshwar Kumar Verma, Chandrabhan Verma, Jeenat Aslam, 2023-04-19 Computational Modeling and

Simulations for Designing of Corrosion Inhibitors Fundamentals and Realistic Applications offers a collection of major advancements in the field of computational modeling for the design and testing of corrosion inhibition effectiveness of organic corrosion inhibitors. This guide presents the latest developments in molecular modeling of organic compounds using computational software which has emerged as a powerful approach for theoretical determination of corrosion inhibition potentials of organic compounds. The book covers common techniques involved in theoretical studies of corrosion inhibition potentials and mechanisms such as density functional theory, molecular dynamics, Monte Carlo simulations, artificial neural networks, and quantitative structure activity relationship. Covers basic fundamental principles, advantages, parameters, and applications of computational and molecular modeling for designing potential corrosion inhibitors for metals and alloys. Describes advancements of computational modeling for the design of organic corrosion inhibitors and applications in electrochemical engineering and materials science. Focuses on the most advanced applications in industry oriented fields including current challenges. Includes websites of interest and information about the latest research.

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