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## Introduction to CAChe

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CAChe computer-aided chemistry enables you to apply mathematical models from classical and quantum mechanics to calculate experimental results.

This introduction to CAChe includes:

- an outline of the benefits of using CAChe, including a short description of the experimental capabilities of CAChe
- tips on calibrating CAChe
- an overview of experimental properties and property classes in CAChe
- a comparison of the CAChe workspace and ProjectLeader
- an introduction to CAChe computational applications

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## Overview of CAChe

CAChe is a computer-aided molecular design (CAMD) modeling tool for the Apple® Mac OS X, Microsoft® Windows® XP, Windows 2000, Windows ME, and Windows 98 operating systems.



Release Notes found in the CAChe application folder provide up-to-date operating system requirements and other important details.

CAChe enables you create a chemical sample model and perform calculations to discover molecular properties and energy values using computational applications which apply equations from classical mechanics and quantum mechanics.

CAChe enables you to:

- draw the atoms and bonds of a molecule
- copy a molecular structure from a built-in Fragment Library of samples
- copy and paste a sample structure from another application such as ChemDraw or Isis/Draw

To discover molecular properties and energy values, you can manipulate and examine your chemical sample as well as perform experiments on it.

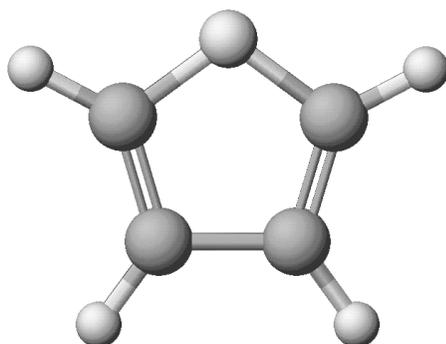
Experimental results are provided in a variety of ways, including:

- adjusting the positions of atoms and bonds to produce an optimized or low-energy structure
- displaying electronic properties as surfaces superimposed on a molecule
- providing three-dimensional energy graphs viewed alongside a series of low-energy conformations
- saving experimental data as a range of values contained in the log file and output file automatically generated by each experiment

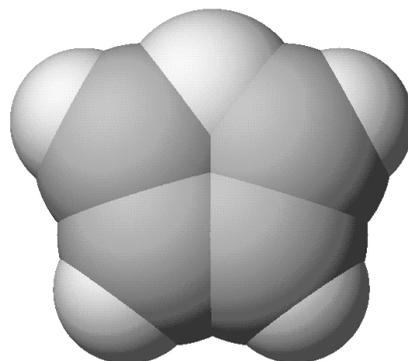
CAChe provides the following tools:

- drawing tools to create your molecule's atoms and bonds
- manipulation tools to rotate, scale, and move a chemical sample in three dimensions
- selection tools to modify all or part of a structure once it is built

You can apply a selection of modeling styles to your sample to view its structure in many different ways. The following example shows two different ways that you can view the same molecule in CAChe.



Ball &amp; cylinder model



Space filling model

You can rotate, enlarge, and move a chemical sample around the screen's 3D structure workspace to view a molecule more closely both before and after experimenting because CAChe shows most experimental results graphically.

CAChe can also quickly and easily correct the geometry, valency, and hybridization of your chemical sample.

The following illustrates a molecule before and after a CAChe optimization experiment designed to lower the steric energy of the molecule using calculations from classical mechanics.

