



# CHED Committee on Computers in Chemical Education

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## The Jmol Virtual Molecular Model Kit: A Resource for Teaching and Learning Chemistry

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### The Jmol Virtual Molecular Model Kit: A Resource for Teaching and Learning Chemistry

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#### Background

Until 2009, the Jmol applet was used primarily as a model display and animation tool. During the 2009 calendar year, a group of Jmol users and developers added a molecular editor to the Jmol applet capability (1). The authors of this report worked as part of that team, creating a Web-based small molecule model kit and providing enhanced applet development. The model kit served as a source of ideas as well as a testing platform for the overall project. It also provided a Web application, the Jmol Virtual Molecular Model Kit (VMK) that was released simultaneously with Jmol v.12.0.RC15 in 2010: [chemagic.com/vmk](http://chemagic.com/vmk) or [chemistry.illinoisstate.edu/osrothen/vmk](http://chemistry.illinoisstate.edu/osrothen/vmk).

#### VMK Overview

The VMK is designed to provide easy control panel access to Jmol's model editing ability. This means that users can build models directly in the kit's Jmol window. Users can add or delete atoms or groups at will. With the click of a mouse, they can convert, for example, (2R)-2-chlorobutane to its (2S) enantiomer. Changing (Z)-but-2-ene to the E stereoisomer is almost as easy. The kit's MultiUser function allows two or more people to work with the same model at the same time, a feature that enables collaboration between teachers and students.

While the VMK allows users to create models "from scratch", it also offers a rich source of starter models via links to PubChem (2) and the NIH/NCI Chemical Identifier Resolver (3,4), a Web application that translates one chemical identifier, such as an IUPAC name, into another, e.g. a SMILES, InChI, or SDF, thereby enabling the VMK to display models of, and to find information about, more than 30 million compounds! The link to PubChem provides a large library of stored SDF data, while that to Resolver generates SDF data by calculation. Using the embedded JME structure drawing applet (5,6), VMK also allows users to draw 2D structures that can be rendered as 3D models.

As the development of the VMK progressed, a new browser application called AKA that interfaces with PubChem and ChemSpider to construct compound-specific queries used in chemical database searches was created. Figure 1 identifies the principle data connections that VMK and AKA utilize.

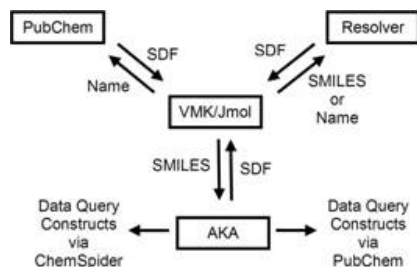


Figure 1-A flow diagram illustrating the communication pathways between the components of the VMK and AKA

The identifiers in these queries, SMILES, InChI, InChIKey, etc., allow rapid transfer of information from PubChem, ChemSpider, NIST, ChEBI, Wikipedia, and other data sources. AKA sends an initial query to PubChem that returns the structure, formula, and missing identifiers for the

identifier that was sent in the initial query. A search algorithm then constructs several identifier-specialized queries that return links to specific chemical database information: [chemagic.com/aka](http://chemagic.com/aka).

The Control Panels of the VMK

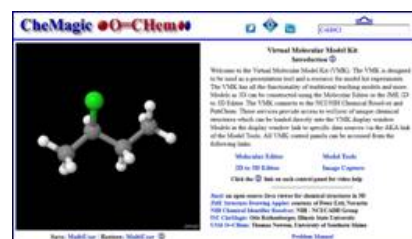
In addition to the Jmol display window, the VMK consists of five control panels. A brief description of the features of each control panel follows. Clicking the name of a control panel will load a YouTube video demonstrating that panel's functionality.

## Introduction

**provides an introduction to VMK and identifies important contributors**

**provides access to the other control panels**

**provides a link to the Problem Manual**



## Molecular Editor

**create, edit, and optimize models**

**work with multiple models**

**make structural comparisons of two models**

**find chemical identifiers such as compound names and SMILES**



## Model Tools

**load pre-assembled models from two local databases allowing display of MEPs, MOs, and partial charges**

**link models to external searches**

**display animations and vdW surfaces**

**load templates for making models of inorganic compounds**



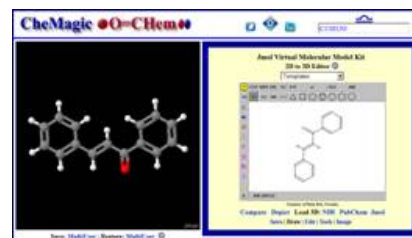
## 2D to 3D Editor

**convert a 2D drawing into a 3D model**

**depict 3D model as 2D JME drawing**

**compare two drawings to determine their structural relationship**

**select 2D to 3D optimization method: Jmol (UFF), PubChem (MMFF94), Resolver (CORINA)**

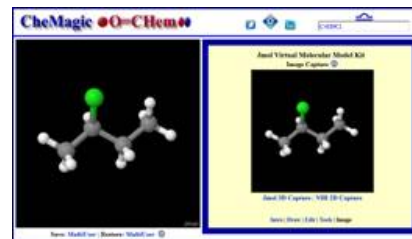


## Image Capture

**copy and save an image of a line drawing of the model that is in the Jmol window**

**copy and save an image of the model that's in the Jmol window.**

**determine R/S stereochemistry of model**



The ability to translate 2D structures drawn in JME into fully editable 3D models makes the VMK ideally suited for classroom use. The kit's multi-user feature allows for interaction/collaboration between teachers and students alike.

## Additional Information

### Data Bases

In addition to PubChem, VMK is connected to a local database of 2000 compounds. This local database will continue to grow. Models loaded from PubChem contain partial atomic charge data, allowing display of partial charges and MEP surfaces

### Jmol SMILES

Jmol can create a SMILES for any displayed model. Jmol also uses an approach to SMILES comparison that eliminates the need for canonical SMILES algorithms (7).

### Help Files

The Introduction control panel contains a link to a Problem Manual, which at the present time has 12 problems, each of which provides step-by-step instructions about a specific feature of the VMK. Each VMK control panel also has an information help link to YouTube video help.

## References

Jmol: an open-source Java viewer for chemical structures in 3D - <http://jmol.sourceforge.net/>

PubChem SD File Formatted Data - [ftp://ftp.ncbi.nih.gov/pubchem/specifications/pubchem\\_sdtags.pdf](ftp://ftp.ncbi.nih.gov/pubchem/specifications/pubchem_sdtags.pdf)

The NIH - NCI/CADD Chemical Identifier Resolver - <http://cactus.nci.nih.gov/chemical/structure>

NCI/CADD Chemical Identifier Resolver: Indexing and Analysis of Available Chemistry Space, Markus Sitzmann, National Cancer Institute (NCI) - [http://www.int-conf-chem-structures.org/fileadmin/user\\_upload/lectures/ICCS2011\\_D8\\_Sitzmann.pdf](http://www.int-conf-chem-structures.org/fileadmin/user_upload/lectures/ICCS2011_D8_Sitzmann.pdf)

JME Molecule Editor - <http://www.molinspiration.com/jme/index.html>

P. Ertl, Molecular structure input on the web, J. Cheminformatics 2010, 2:1 - <http://www.jcheminf.com/content/2/1/1>

A Universal SMILES String Comparator: Robert M. Hanson, St. Olaf College - <http://chemapps.stolaf.edu/jmol/docs/examples-12/JmolSmilesTest.htm>

Attachment	Size
<a href="#">fig1p3fall2011cccenl.jpg</a>	8.25 KB
<a href="#">fig2p3fall2011cccenl.jpg</a>	9.53 KB
<a href="#">fig3p3fall2011cccenl.jpg</a>	8.91 KB
<a href="#">fig4p3fall2011cccenl.jpg</a>	9.9 KB
<a href="#">fig5p3fall2011cccenl.jpg</a>	8.39 KB
<a href="#">fig6p3fall2011cccenl.jpg</a>	8 KB

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