

Overview of Jmol Application

Talk to a Teacher

<http://spoken-tutorial.org>

National Mission on Education through ICT

<http://sakshat.ac.in>

Snehalatha Kaliappan

IIT Bombay

21 October 2015



Learning Objectives



Learning Objectives

- ▶ **Important features of Jmol Application**



Learning Objectives

- ▶ **Important features of Jmol Application**
- ▶ **Information regarding download Installation on various operating systems**



Learning Objectives

- ▶ **Important features of Jmol Application**
- ▶ **Information regarding download Installation on various operating systems**
- ▶ **Uses of Jmol Application**



Learning Objectives

- ▶ **Important features of Jmol Application**
- ▶ **Information regarding download Installation on various operating systems**
- ▶ **Uses of Jmol Application**
- ▶ **Clippings of video tutorials available in Jmol Application series**



Pre-requisites



Pre-requisites

- ▶ **Knowledge of high school chemistry**



Pre-requisites

- ▶ Knowledge of high school chemistry
- ▶ Basic Organic Chemistry



System Requirements



System Requirements

- ▶ **Ubuntu OS version 12.10**



System Requirements

- ▶ **Ubuntu OS version 12.10**
- ▶ **Jmol version 14.1.11**



System Requirements

- ▶ **Ubuntu OS version 12.10**
- ▶ **Jmol version 14.1.11**
- ▶ **Java(JRE) version 7**



System Requirements

- ▶ **Ubuntu OS version 12.10**
- ▶ **Jmol version 14.1.11**
- ▶ **Java(JRE) version 7**
- ▶ **Mozilla Firefox Browser 35.0**



What is Jmol Application?



What is Jmol Application?

- ▶ Jmol is a molecular viewer for three-dimensional chemical structures and macromolecules



What is Jmol Application?

- ▶ **Jmol is a molecular viewer for three-dimensional chemical structures and macromolecules**
- ▶ **Create and edit 3D models of chemical structures**



What is Jmol Application?

- ▶ Jmol is a molecular viewer for three-dimensional chemical structures and macromolecules
- ▶ Create and edit 3D models of chemical structures
- ▶ For students, educators and researchers in chemistry and biochemistry



Important Features



Important Features

- ▶ **A free and open source software**



Important Features

- ▶ **A free and open source software**
- ▶ **Cross-platform application:**
Windows, Mac OS, Linux and
Android Devices



Important Features

- ▶ **A free and open source software**
- ▶ **Cross-platform application:**
Windows, Mac OS, Linux and
Android Devices
- ▶ **Supports all major web browsers**



Important Features

- ▶ **A free and open source software**
- ▶ **Cross-platform application:**
Windows, Mac OS, Linux and Android Devices
- ▶ **Supports all major web browsers**
- ▶ **High-quality 3D rendering with no special hardware requirements**



Important Features

- ▶ Images can be exported to various file formats:
jpg, png, gif, pdf etc
- ▶ Reads various file formats: **pdb, cif, mol, cml, xyz** etc
- ▶ Loads models directly from databases: **pubchem** and **PDB**



Important Links

<http://jmol.sourceforge.net/>
<http://www.jmol.org/>



Uses of Jmol

- ▶ Teaching tool to explain concepts in chemistry
- ▶ For producing high quality 3D images that can be used in print media:
journals, publications and books
- ▶ Presentations in classrooms and lectures



Uses of Jmol

- ▶ **Molecular Modelling**
- ▶ **Animation movies**



Teaching Chemistry using Jmol

Basic Level

- ▶ **Structure and functional groups.**
- ▶ **Atomic and Molecular orbitals**



Teaching Chemistry using Jmol

Advanced Level

- ▶ Stereochemistry
- ▶ Symmetry and Point-groups
- ▶ Crystal Structure and Unit cell
- ▶ Simulated H NMR (Jmol Version 14.0 and above)
- ▶ Structure Activity Relationship (SAR)



Download and Installation



Download and Installation

- ▶ Jmol can be installed on **Windows, Mac OS** and **Linux OS**
- ▶ A special version of Jmol for **Android devices** is available at the following link

<http://wiki.jmol.org/index.php/Support/Android>



Download and Installation



Download and Installation

- ▶ **For Linux OS: Download using Ubuntu Software Center or Synaptic Package Manager**



Download and Installation

- ▶ **For Linux OS: Download using Ubuntu Software Center or Synaptic Package Manager**
- ▶ **Follow this tutorial in the Linux series**

www.spoken-tutorial.org



Download and Installation



Download and Installation

- ▶ For Windows and Mac OS



Download and Installation

- ▶ For Windows and Mac OS
- ▶ www.jmol.sourceforge.net



Video Clippings



Video Clippings

Jmol Application Spoken-Tutorials



Simulated ^1H NMR



Simulated ^1H NMR

Simulated ^1H NMR can be displayed starting from **Jmol version 14.0**



Animating Vibrations



Animating Vibrations

GAMESS .log files and **Spartan output files** include information about molecular vibrations



Summary

- ▶ **Important features of Jmol Application**
- ▶ **Information regarding Installation on various operating systems**
- ▶ **Uses of Jmol Application**



Summary

- ▶ **Clippings of video tutorials in Jmol Application series**
- ▶ **Animation videos showing vibrations and conformations of cyclohexane**



About the Spoken Tutorial Project

- ▶ Watch the video available at http://spoken-tutorial.org/What_is_a_Spoken_Tutorial
- ▶ It summarises the Spoken Tutorial project



About the Spoken Tutorial Project

- ▶ Watch the video available at http://spoken-tutorial.org/What_is_a_Spoken_Tutorial
- ▶ It summarises the Spoken Tutorial project
- ▶ If you do not have good bandwidth, you can download and watch it



Spoken Tutorial Workshops

The Spoken Tutorial Project Team

- ▶ Conducts workshops using spoken tutorials
- ▶ Gives certificates to those who pass an online test
- ▶ For more details, please write to contact@spoken-tutorial.org



Acknowledgements

- ▶ **Spoken Tutorial Project is a part of the Talk to a Teacher project**
- ▶ **It is supported by the National Mission on Education through ICT, MHRD, Government of India**
- ▶ **More information on this Mission is available at**

<http://spoken-tutorial.org/NMEICT-Intro>

