

# Overview of Jmol Application

**Talk to a Teacher**

**<http://spoken-tutorial.org>**

**National Mission on Education through ICT**

**<http://sakshat.ac.in>**

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# Learning Objectives



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- ▶ **Important features of Jmol Application**



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- ▶ **Information regarding download Installation on various operating systems**



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- ▶ **Uses of Jmol Application**



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- ▶ 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



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- ▶ Knowledge of high school chemistry





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- ▶ Basic Organic Chemistry



# System Requirements



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- ▶ **Ubuntu OS version 12.10**



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- ▶ **Java(JRE) version 7**
- ▶ **Mozilla Firefox Browser 35.0**



# What is Jmol Application?



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- ▶ 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**



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- ▶ **Cross-platform application:**  
**Windows, Mac OS, Linux and**  
**Android Devices**



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# 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](http://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](http://www.jmol.sourceforge.net)



# Video Clippings



# Video Clippings

## Jmol Application Spoken-Tutorials



# Simulated $^1\text{H}$ NMR





# Simulated H NMR

**Simulated H 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](http://spoken-tutorial.org/What_is_a_Spoken_Tutorial)
- ▶ It summarises the Spoken Tutorial project



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- ▶ 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](mailto:contact@spoken-tutorial.org)





# Acknowledgements

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- ▶ 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>

