Overview of Jmol Application

Spoken Tutorial Project
https://spoken-tutorial.org
National Mission on Education through ICT
http://sakshat.ac.in

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30 April 2019

Learning Objectives

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- **About Jmol Application**

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- **Download and run Jmol Application on Linux OS**

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- Uses and Advantages

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- Play video clippings of Jmol tutorials available on our website

System Requirements

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- **Mozilla Firefox Browser 54.0**
- **Working internet connection**

Pre-requisites

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Knowledge of high school chemistry

About Jmol Application

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- **Jmol is an open-source 3D viewer for chemical structures, biomolecules, crystal structures and materials**
- **Runs on Windows, Mac OSX , Linux Operating Systems and Android devices**

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- **Used to create and edit 3D models of chemical structures**

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- **Used to create and edit 3D models of chemical structures**
- **Used by students, educators and researchers in the fields of chemistry and biochemistry**

Jmol Website

http://jmol.sourceforge.net

Installation on Linux OS

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

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- www.spoken-tutorial.org

Advantages of Jmol Application

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- **No special hardware is required for high quality 3D rendering**

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- **Load structures from PubChem and PDB database**

Uses of Jmol Application

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Teaching tool

- **Structure and functional groups**

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- **Atomic and Molecular orbitals**

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- **Atomic and Molecular orbitals**
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- **Crystal structure and Unit cell**

Uses of Jmol Application

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- **High quality 3D images for publications and presentations**

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- **View simulated 1H and 13C NMR spectra for molecules (Jmol version 14.0 and above)**

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- **Structure Activity Relationship**

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- **Molecular modelling**

Uses of Jmol Application

- **Structure Activity Relationship**
- **Molecular modelling**
- **Animation of molecules**

Video Clippings

Video Clippings

Jmol Application Spoken Tutorials

Spoken Tutorial: Introduction to Jmol Application

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- **Various features available on Jmol window**
- **Create models of simple organic molecules**
- **Energy minimization**
- **Save image**

Spoken Tutorial: Create and Edit Molecular Models

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- **Add functional group**
- **Add and delete atoms and bonds**
- **Pop-up-menu**

Spoken Tutorial: Modify Display and View

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- **Modify the view**
- **Change the style of the display**
- **Save the image in various file formats**

Spoken Tutorial: Measurements and Labeling

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- **How to measure bond lengths, bond angles and dihedral angles for a model**
- **Label atoms with symbol and number**

Spoken Tutorial: Script Console and Script Commands

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How to use script console and write script commands

Spoken Tutorial: Surfaces and Orbitals

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Show surfaces, create models of aromatic molecules, atomic orbitals and molecular orbitals

Spoken Tutorial: Structures from Database

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- **How to load structures directly from chemical structure database such as PubChem**
- **Convert 2D structures drawn in GChemPaint to 3D models in Jmol**

Spoken Tutorial: Crystal structure and Unit Cell

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- **Download and open CIF files in Jmol**
- **Display unit cell and unit cell parameters**
- **Display crystal structures of different crystal systems**

Spoken Tutorial: Proteins and Macromolecules

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- **Download pdb files from database**
- **View and modify secondary structure of protein**

Spoken Tutorial: 3D Models of Enzymes

Spoken Tutorial: 3D Models of Enzymes

- **Modify the display of secondary structure**
- **Highlight amino acid residues and substrate**
- **View Ramachandran plot for proteins**

Spoken Tutorial: Symmetry and Point Groups

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C2 and C3 rotational axes, reflection planes and point group classification

Spoken Tutorial: Animation using Script Commands

Spoken Tutorial: Animation using Script Commands

- **Animation using script commands**
- **Save the animation as GIF file**

Summary

- About Jmol Application
- Download and run Jmol Application on Linux Operating System
- Uses and Advantages
- Played video clippings of Jmol tutorials available on our website

Assignment

1. **Explore Jmol Application interface**
2. **On the Jmol Wiki main page, explore Jmol Documentation page**

About the Spoken Tutorial Project

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- **It summarises the Spoken Tutorial project**

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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**

Forum for specific questions

- **Do you have questions in THIS Spoken Tutorial?**
- **Please visit**

  http://forums.spoken-tutorial.org
- **Choose the minute and second where you have the question**
- **Explain your question briefly**
- **Someone from our team will answer them**

Forum for specific questions

- **The Spoken Tutorial forum is for specific questions on this tutorial**
- **Please do not post unrelated and general questions on them**
- **This will help reduce the clutter**
- **With less clutter, we can use this discussion as intructional material**

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