### The Spoken Tutorial Project

- Self-explanatory: uses simple language
- Audio-video: uses multisensory approach
- Small duration: has better retention
- Learner-centered: learn at your own pace
- Learning by doing: learn and practise simultaneously
- Empowerment: learn a new FLOSS (Free/Libre and Open Source Software)

### Target Audience

- School students
- Undergraduates / Postgraduates
- Research scholars
- Teachers

# Workshops

The Spoken Tutorial Project Team conducts workshops on Jmol Application and other FLOSS using spoken tutorials and gives certificates to those who pass an online test.

For more details, please visit https://spoken-tutorial.org

### Forum

We have developed a beginner friendly Forum to answer specific questions pertaining to any part of a particular tutorial.

For more details, please visit https://forums.spoken-tutorial.org.



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Government of India.

### Contact us

Email: contact@spoken-tutorial.org Website: https://spoken-tutorial.org



Content available in 22 Indian languages



IIT Bombay

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visit Spoken Tutorial website

# **Jmol Application**



National Mission on Education through Information and Communication Technology (NMEICT)

www.sakshat.ac.in

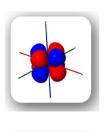
Funded by MHRD, Government of India.

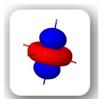
#### Introduction

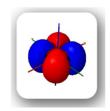
Jmol Application is a three-dimensional viewer for chemical structures and macromolecules. It is a Free Open Source Software (FOSS) developed in Java. We can create and edit 3D models of Structures. Runs on Windows, macOS, Linux and Android Systems. Useful for students, educators and researchers in chemistry and biochemistry. For download and installation visit: www.jmol.sourceforge.net.

### **Jmol Application for Biomolecules**

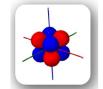
- 3D Interactive images of biological molecules can be viewed.
- Secondary structures of proteins can be rendered using pdb files.
- Display of secondary structural patterns such as alpha-helix, beta-sheets, loops, random-coils in cartoon format.
- Active-sites, hydrogen bonds and disulfide bonds can be highlighted.



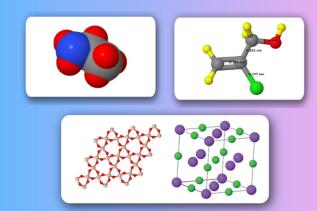












# Features of Jmol Application

- Energy minimization to get the most stable conformation.
- High-quality 3D image rendering can be done with no special hardware requirements.
- It can read various file formats for example pdb, cif, mol and cml.
- We can export images to jpg, png, gif, pdf, POV- Ray and Gaussian file formats.
- We can view plane of symmetry and point groups for molecules.
- It provides simulated Proton and Carbon NMR for organic compounds.
- It loads models directly from databases (Pubchem and PDB).
- For more information visit
   http://wiki.jmol.org/index.php/Main Page

### Uses of Jmol Application

- To create and visualize chemical structures in 3D.
- To render secondary structures of proteins and nucleic acids.
- View crystal structure and unit cell parameters.
- It displays structures in various display formats such as ball-and-stick, CPK, sticks etc.
- We can change the thickness of bonds, color of atoms and bonds.
- Rotate and view the molecule from various angles.
- Displays interatomic distances, bond-angles, dihedral-angles, dipoles, charges and symbols.
- Surfaces, atomic and molecular orbitals can be displayed.
- We can produce animations and create GIF files.
- Images can be used in print media-journals/ publications/books.
- Useful for presentations in classrooms and lectures.

