

Introduction To 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



Learning Objectives

Jmol Application window and some basic operations



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Jmol Application window and some basic operations

- ▶ Menu bar, Tool bar and Jmol panel



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Jmol Application window and some basic operations

- ▶ Menu bar, Tool bar and Jmol panel
- ▶ Modify the size of the Jmol panel



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Jmol Application window and some basic operations

- ▶ Menu bar, Tool bar and Jmol panel
- ▶ Modify the size of the Jmol panel
- ▶ Create models of simple organic molecules



Learning Objectives

Jmol Application window and some basic operations

- ▶ Menu bar, Tool bar and Jmol panel
- ▶ Modify the size of the Jmol panel
- ▶ Create models of simple organic molecules
- ▶ Build molecules by substituting hydrogen with Methyl group



Learning Objectives



Learning Objectives

- ▶ **Energy minimization to get a stable conformation**



Learning Objectives

- ▶ Energy minimization to get a stable conformation
- ▶ Save the image as .mol file



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 12.04**



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- ▶ **Jmol Version 12.2.2**
- ▶ **Java(JRE) Version 7
(Sun Microsystems)**



About Jmol Application



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- ▶ A free and open source Molecular Viewer



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- ▶ **Used to create and view 3 dimensional models of Chemical Structures**



About Jmol Application

- ▶ A free and open source Molecular Viewer
- ▶ Used to create and view 3 dimensional models of Chemical Structures
- ▶ Used to view secondary structures of Proteins and Macromolecules



Download and Installation



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► Ubuntu Software Centre



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- ▶ **Follow this tutorial in the Linux series on www.spoken-tutorial.org**



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- ▶ **For Windows, Mac OS and Android devices, visit www.jmol.sourceforge.net**



Summary

- ▶ **About Jmol Application Window**
- ▶ **Resize the Jmol Panel**
- ▶ **Use the "Modelkit" function in the tool bar to create 3D models of simple organic molecules like Methane, Ethane and Propane**



Summary

- ▶ Build molecules by substitution of hydrogen with Methyl group
- ▶ Energy minimization to get a stable conformation
- ▶ Save the image as .mol file



Assignment



Assignment

- ▶ 2,4-dimethylpentane
- ▶ 3-ethyl-5-methylheptane
- ▶ Minimize energy to get the most stable conformation
- ▶ Save the image as .mol file
- ▶ Rotate the model using the “rotate molecule” in tool bar



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



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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

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- ▶ More information on this Mission is available at

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

