

Script console and Script commands

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

- ▶ **About script commands**



Learning Objectives

- ▶ **About script commands**
- ▶ Script console **window**



Learning Objectives

- ▶ **About script commands**
- ▶ Script console **window**
- ▶ **Change display of the model by using script commands**



Learning Objectives

- ▶ **About script commands**
- ▶ **Script console window**
- ▶ **Change display of the model by using script commands**
- ▶ **Display lines of text on the panel**



Pre-requisites



Pre-requisites

- Know to create and edit molecular models in Jmol Application



Pre-requisites

- ▶ Know to create and edit molecular models in Jmol Application
- ▶ If not, watch the videos available at <http://spoken-tutorial.org>



System Requirements



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- ▶ **Ubuntu OS version 12.04**



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- ▶ **Jmol version 12.2.2**



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- ▶ **Ubuntu OS version 12.04**
- ▶ **Jmol version 12.2.2**
- ▶ **Java (JRE) version 7
(Sun Microsystems)**



Modify Display in Jmol Application



Modify Display in Jmol Application

Display on Jmol panel can be modified using



Modify Display in Jmol Application

Display on Jmol panel can be modified using

- ▶ **Options in menu bar**



Modify Display in Jmol Application

Display on Jmol panel can be modified using

- ▶ Options in menu bar
- ▶ Options in the Pop-up menu



Modify Display in Jmol Application

Display on Jmol panel can be modified using

- ▶ Options in menu bar
- ▶ Options in the Pop-up menu
- ▶ Scripting commands on the script console



Script Commands



Script Commands

- ▶ **A set of commands is called a script command**



Script Commands

- ▶ **A set of commands is called a script command**
- ▶ **Script commands control the display of the model on screen**



Script Commands

- ▶ **A set of commands is called a script command**
- ▶ **Script commands control the display of the model on screen**
- ▶ **Jmol uses a command language based on Rasmol program**



Script Commands



Script Commands

- ▶ Writing such commands is called scripting



Script Commands

- ▶ Writing such commands is called scripting
- ▶ Documentation of Jmol's scripting language and list of script commands is available at this link
<http://chemapps.stolaf.edu/jmol/docs/>



Using Commands



Using Commands

- ▶ **Script commands are typed on script console window**



Using Commands

- ▶ **Script commands are typed on script console window**
- ▶ **Script console is Jmol's command line interface**



Using Commands

- ▶ **Script commands are typed on script console window**
- ▶ **Script console is Jmol's command line interface**
- ▶ **It is available in the menu bar, under File and Console option**



How to write Commands



How to write Commands

- ▶ Type the command at the \$ prompt on the script console window



How to write Commands

- ▶ **Type the command at the \$ prompt on the script console window**
- ▶ **Script command starts with a command word**



How to write Commands



How to write Commands

- ▶ **Continues with a set of parameters, separated by spaces**



How to write Commands

- ▶ **Continues with a set of parameters, separated by spaces**
- ▶ **Is terminated by the end of line character or semicolon (;)**



How to write Commands



How to write Commands

- ▶ The command will appear red, until you have completed typing the command



How to write Commands

- ▶ The command will appear red, until you have completed typing the command
- ▶ Press Enter key on the keyboard, to activate the command



Summary

- ▶ **Script commands**
- ▶ **Script console window**
- ▶ **Change the display of the model using script commands**
- ▶ **Display lines of text on the panel**



Assignment

1. Create a model of 3-methylpentane

2. Use script commands to do the following

- ▶ Change the color of all hydrogens to **blue**
- ▶ Change the color of all the bonds to **red**
- ▶ Set the molecule to spin



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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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



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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>

