

Creating a Basic JSmol Integrated Web Page

Spoken Tutorial Project

<https://spoken-tutorial.org>

National Mission on Education through ICT

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Learning Objectives



Learning Objectives

We will learn to,



Learning Objectives

We will learn to,

- ▶ **Create a JSmol integrated HTML text document**



Learning Objectives

We will learn to,

- ▶ Create a **JSmol** integrated **HTML** text document
- ▶ Download **Jmol** binary zip file



Learning Objectives

We will learn to,

- ▶ Create a **JSmol** integrated **HTML** text document
- ▶ Download **Jmol** binary zip file
- ▶ Install **Apache** software



Learning Objectives

We will learn to,

- ▶ Create a **JSmol** integrated **HTML** text document
- ▶ Download **Jmol** binary zip file
- ▶ Install **Apache** software
- ▶ Run the **HTML** page locally using **HTTP** server, localhost 80



System Requirements

Here I am using,



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Here I am using,

- ▶ **Ubuntu Linux OS version 20.04**



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- ▶ **Ubuntu Linux OS version 20.04**
- ▶ **Firefox web browser version 100.0**



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- ▶ **Jmol version 14.32.83**



System Requirements

Here I am using,

- ▶ **Ubuntu Linux OS version 20.04**
- ▶ **Firefox web browser version 100.0**
- ▶ **Apache version 2.4.41**
- ▶ **Jmol version 14.32.83**
- ▶ **Working internet connection**



Pre-requisites



Pre-requisites

To follow this tutorial learner should be familiar with,



Pre-requisites

To follow this tutorial learner should be familiar with,

- ▶ **undergraduate chemistry**



Pre-requisites

To follow this tutorial learner should be familiar with,

- ▶ undergraduate chemistry
- ▶ basic skills in using a computer



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- ▶ using a computer terminal for typing commands



Pre-requisites

To follow this tutorial learner should be familiar with,

- ▶ undergraduate chemistry
- ▶ basic skills in using a computer
- ▶ using a computer terminal for typing commands
- ▶ basic operations of Jmol



Pre-requisites



Pre-requisites

- ▶ Please use the link given here for Spoken Tutorials in Jmol Application series

https://spoken-tutorial.org/tutorial-search/?search_foss=Jmol+Application&search_language=English



Code Files

- ▶ **The input files required for this tutorial are available in the Code files link**
- ▶ **Please download and extract the files**
- ▶ **Make a copy of all the files and then use them for practising**



About JSmol I

- ▶ **JSmol** is an open-source **HTML5** viewer for 3D chemical structures
- ▶ It is a JavaScript framework that allows web developers to create pages
- ▶ It runs in any web browser that supports **HTML5**



About JSmol II

- ▶ **JSmol** integrated web pages are interactive and excellent learning resources

- ▶ For more information, please refer to the link given below
<https://wiki.jmol.org/index.php/JSmol>



Steps to Create a Web Page I

1. Download the Jmol package and extract the contents
2. Extract **Jsmol.zip** file which is present inside the extracted Jmol package
3. Move the extracted **Jsmol** file to the **jspage** folder



Steps to Create a Web Page II

4. Open **nbutane.html** file in a text editor

5. Edit the path of **JSmol** file in **nbutane.html** document

This step will integrate the **JSmol** program with the web page



Steps to Create a Web Page III

6. Edit the **nbutane.html** text document to include 3D model files and text description
7. Run the completed **HTML** page locally using **HTTP** server, localhost 80



Installation of Apache Software

- ▶ We need to install **Apache** software in order to run the Jmol web pages locally on our computers
- ▶ **Apache** is an open source software
- ▶ It is used as a **http** web server to run the **HTML** web pages



Summary

We have,

- ▶ Created a **JSmol** integrated **HTML** text document
- ▶ Downloaded **Jmol** binary zip file
- ▶ Installed **Apache** software
- ▶ Ran the **HTML** page locally using **HTTP** server, localhost 80



Assignment

- ▶ Add a few more lines of text in the description for the conformers of **n-butane** in the **HTML** page
- ▶ Save the **HTML** page
- ▶ Run the **HTML** page as localhost and view the changes



Assignment

- ▶ Create models of conformations of **n-butane** using Jmol
- ▶ Save the 3D models as .mol files



About the Spoken Tutorial Project

- ▶ Watch the video available at https://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



Answers for THIS Spoken Tutorial

- ▶ **Questions in THIS Spoken Tutorial?**
- ▶ **Visit**
<https://forums.spoken-tutorial.org>
- ▶ **Choose the minute and second where you have the question**
- ▶ **Explain your question briefly**
- ▶ **The Spoken Tutorial project will ensure an answer**

You will have to register to ask questions



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 instructional material**



Acknowledgements

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