

Bond Rotation in Jmol

Spoken Tutorial Project

<https://spoken-tutorial.org>

National Mission on Education through ICT

Script: Snehalatha Kaliappan

Video: Madhuri Ganapathi

IIT Bombay

21 November 2022



Learning Objectives



Learning Objectives

- ▶ Use tools in the modelkit menu to rotate bonds



Learning Objectives

- ▶ Use tools in the modelkit menu to rotate bonds
- ▶ Use script commands to rotate specific bonds in a model



Learning Objectives

- ▶ Use tools in the modelkit menu to rotate bonds
- ▶ Use script commands to rotate specific bonds in a model
- ▶ Create models of **anti**, **gauche** and **eclipsed** conformers of **1,2-dichloroethane**



System Requirements



System Requirements

- ▶ **Ubuntu Linux OS version 20.04**



System Requirements

- ▶ **Ubuntu Linux OS version 20.04**
- ▶ **Jmol version 14.32.80**



System Requirements

- ▶ **Ubuntu Linux OS version 20.04**
- ▶ **Jmol version 14.32.80**
- ▶ **Java version 11.0.16**



Pre-requisites



Pre-requisites

To follow this tutorial the learner,



Pre-requisites

- To follow this tutorial the learner,**
- ▶ **must have knowledge of high school chemistry**



Pre-requisites

To follow this tutorial the learner,

- ▶ must have knowledge of high school chemistry
- ▶ must be familiar with the basic operations of Jmol



Pre-requisites

To follow this tutorial the learner,

- ▶ must have knowledge of high school chemistry
- ▶ must be familiar with the basic operations of Jmol
- ▶ **Jmol Spoken Tutorials link:**
<https://spoken-tutorial.org>



Conformations of 1,2-dichloroethane

Conformations of **1,2 dichloroethane**:



Conformations of 1,2-dichloroethane

Conformations of 1,2 dichloroethane:

- ▶ anti and gauche



Conformations of 1,2-dichloroethane

Conformations of 1,2 dichloroethane:

- ▶ **anti** and **gauche**
- ▶ **Anti conformer is more stable when compared to gauche**



Conformations of 1,2-dichloroethane

Conformations of 1,2 dichloroethane:

- ▶ **anti** and **gauche**
- ▶ **Anti** conformer is more stable when compared to **gauche**
- ▶ **Eclipsed** conformer is unstable



Conformations of 1,2-dichloroethane

Conformations of 1,2 dichloroethane:

- ▶ **anti** and **gauche**
- ▶ **Anti** conformer is more stable when compared to **gauche**
- ▶ **Eclipsed** conformer is unstable
- ▶ **Conformers are interconvertible by C-C bond rotation**



Bond Rotation Tools

Bond rotation in Jmol:



Bond Rotation Tools

Bond rotation in Jmol:

- ▶ Using the bond rotating tool from the modelkit menu



Bond Rotation Tools

Bond rotation in Jmol:

- ▶ Using the bond rotating tool from the modelkit menu
- ▶ Typing Jmol script commands on the Console



Links to Jmol Script Commands

- ▶ **Jmol Script Commands**

<https://chemapps.stolaf.edu/jmol/docs>

- ▶ **Rotate Command**

<https://chemapps.stolaf.edu/jmol/docs/#rotate>



Link to Jmol Script Commands ST Video

Please watch the video on script commands

It is available on the Spoken Tutorial website in the Jmol Application series

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



Summary

- ▶ Used tools in the modelkit menu to rotate bonds
- ▶ Used script commands to rotate specific bonds in a model
- ▶ Created models of **anti**, **gauche** and **eclipsed** conformers of **1,2-dichloroethane**



Assignment

- ▶ Explore the **rotate** command to create the models of conformations of **n-butane**



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



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
- ▶ If you do not have good bandwidth, you can download and watch it



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



Acknowledgements

**Spoken Tutorial project is funded by
Ministry of Education (MoE), Govt. of
India**

