

# 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](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](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](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](mailto: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**

