

# Creating an Input File

**Spoken Tutorial Project**

**<http://spoken-tutorial.org>**

**National Mission on Education through ICT**

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# Learning Objectives



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**We will learn to,**



# Learning Objectives

**We will learn to,**

- **Create a 3D model of a molecule in Avogadro**



# Learning Objectives

We will learn to,

- Create a 3D model of a molecule in Avogadro
- Optimize its geometry in Avogadro



# Learning Objectives

**We will learn to,**

- **Create a 3D model of a molecule in Avogadro**
- **Optimize its geometry in Avogadro**
- **Measure the bond length and bond angle of the optimized molecule**



# Learning Objectives



# Learning Objectives

- **Save the structure in XYZ file format in a folder**



# Learning Objectives

- **Save the structure in XYZ file format in a folder**
- **Generate Orca input file using Extensions menu**



# System Requirement



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- **Ubuntu Linux OS v20.04**



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- **Avogadro v1.2.0**



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- **Ubuntu Linux OS v20.04**
- **Avogadro v1.2.0**
- **Gedit Text Editor v3.36.2**



# Pre-requisites



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- To follow this tutorial, learners should be familiar with Avogadro software



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- To follow this tutorial, learners should be familiar with Avogadro software
- Please use the link below to access the tutorials on Avogadro

[https://spoken-tutorial.org/tutorial-search/?search\\_foss=Avogadro&search\\_language=English](https://spoken-tutorial.org/tutorial-search/?search_foss=Avogadro&search_language=English)



# ORCA Input File



# ORCA Input File

- **ORCA accepts the input in the form of coordinates in xyz format**



# ORCA Input File

- ORCA accepts the input in the form of coordinates in xyz format
- The input file in xyz format can be created using Avogadro or online servers



# ORCA Input File

- ORCA accepts the input in the form of coordinates in xyz format
- The input file in xyz format can be created using Avogadro or online servers
- You can use any other software such as Jmol to create the input file



# ORCA Input File



# ORCA Input File

- Information on how to create an xyz file using online servers is provided in the Additional reading material



# Summary

**We have,**

- **Created a 3D model of a molecule in Avogadro**
- **Optimized its geometry in Avogadro**
- **Measured the bond length and bond angle of the optimized molecule**



# Summary

- **Saved the structure in XYZ file format in a folder**
- **Generated Orca input file for geometry optimization using Extensions menu**



# Assignment

- 1 Practise drawing the structures of benzene and cyclohexane in Avogadro
- 2 Optimize the geometry of the molecules in Avogadro
- 3 Save the structures in XYZ file format
- 4 Generate Orca input files for geometry optimization of the molecules



# 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



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- 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



# Acknowledgements

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