

Run an Input File

Spoken Tutorial Project

<https://spoken-tutorial.org>

National Mission on Education through ICT

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Learning Objectives



Learning Objectives

- **Run an input file in the ORCA environment**



Learning Objectives

- Run an input file in the ORCA environment
- Generate an output file



Learning Objectives

- Run an input file in the ORCA environment
- Generate an output file
- Compare the bond length and bond angle before and after optimization in ORCA



Learning Objectives

- Run an input file in the ORCA environment
- Generate an output file
- Compare the bond length and bond angle before and after optimization in ORCA
- Analyse the generated output



System Requirement



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- **Ubuntu Linux OS v20.04**



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- **ORCA v5.0.4**



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- **Gedit text editor v3.36.2**



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- **Ubuntu Linux OS v20.04**
- **ORCA v5.0.4**
- **Gedit text editor v3.36.2**
- **Avogadro v1.2.0**



Pre-requisites



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To follow this tutorial,



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To follow this tutorial,

- **Learner should be familiar with Avogadro software**



Pre-requisites

To follow this tutorial,

- Learner should be familiar with Avogadro software
- Learner should have installed ORCA version 5.0.4



Pre-requisites

To follow this tutorial,

- Learner should be familiar with Avogadro software
- Learner should have installed ORCA version 5.0.4
- If not please access the relevant tutorials <https://spoken-tutorial.org>



Code Files



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- The files used in this tutorial are provided in the Code files link



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- Please download and extract the files



Code Files

- The files used in this tutorial are provided in the Code files link
- Please download and extract the files
- Make a copy and then use them while practising



Summary

- Ran an input file in the ORCA environment using the terminal
- Generated an output file
- Compared the bond length and bond angle before and after optimization in ORCA
- Analysed the generated output



Assignment I

- 1 Open the input files of cyclohexane and benzene generated in the previous assignment
- 2 Run the input files in the ORCA environment using the terminal



Assignment II

- 3 **Generate the output files**
- 4 **Compare the bond lengths and bond angles before and after optimization in ORCA**



About 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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