

Overview of Avogadro

Spoken Tutorial Project

<http://spoken-tutorial.org>

National Mission on Education through ICT

<http://sakshat.ac.in>

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Learning Objectives



Learning Objectives

- ▶ **About Avogadro software**



Learning Objectives

- ▶ **About Avogadro software**
- ▶ **Download and installation of Avogadro**



Learning Objectives

- ▶ **About Avogadro software**
- ▶ **Download and installation of Avogadro**
- ▶ **To open the documentation page**



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- ▶ **About Avogadro interface**



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- ▶ **Benefits of Avogadro**



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- ▶ **Download and installation of Avogadro**
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- ▶ **About Avogadro interface**
- ▶ **Benefits of Avogadro**
- ▶ **Play video clippings of Avogadro tutorials available on our website**



System Requirement



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- ▶ **Ubuntu Linux OS v 14.04**



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- ▶ **Avogadro v 1.1.1**



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- ▶ **Avogadro v 1.1.1**
- ▶ **Mozilla Firefox Browser 58.0.2**



System Requirement

- ▶ **Ubuntu Linux OS v 14.04**
- ▶ **Avogadro v 1.1.1**
- ▶ **Mozilla Firefox Browser 58.0.2**
- ▶ **A working internet connection**



Pre-requisites



Pre-requisites

- ▶ **High School Chemistry**



About Avogadro



About Avogadro

- ▶ **3D Molecular builder, editor and visualization tool**



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- ▶ **Free and Open Source software**



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- ▶ **Build, load and edit 3D structures of various molecules**



About Avogadro

- ▶ **3D Molecular builder, editor and visualization tool**
- ▶ **Free and Open Source software**
- ▶ **Build, load and edit 3D structures of various molecules**
- ▶ **Runs on Windows, Mac OSX and Linux OS**



Download Avogadro on Windows OS



Download Avogadro on Windows OS

- ▶ **We will download Avogadro on Windows operating system**



Install Avogadro on Mac OSX



Install Avogadro on Mac OSX

- ▶ Learn to install Avogadro on Mac OSX



Install Avogadro on Ubuntu Linux



Install Avogadro on Ubuntu Linux

- ▶ We will learn to install Avogadro on Ubuntu Linux machine



Installation of Java Virtual Machine



Installation of Java Virtual Machine

- ▶ **Install Java Virtual Machine for smooth working of Avogadro software**



Installation of Java Virtual Machine

- ▶ **Install Java Virtual Machine** for smooth working of Avogadro software
- ▶ **Here is the link to install Java**
<https://java.com/download>



Benefits of Avogadro



Benefits of Avogadro

- ▶ Offers flexible high quality rendering



Benefits of Avogadro

- ▶ **Offers flexible high quality rendering**
- ▶ **Energy minimisation can be done for the molecules to obtain stable conformations**



Benefits of Avogadro

- ▶ Offers flexible high quality rendering
- ▶ Energy minimisation can be done for the molecules to obtain stable conformations
- ▶ Huge fragment library to load inbuilt structures



Benefits of Avogadro



Benefits of Avogadro

- ▶ Files can be exported to png, jpg, bmp file formats



Benefits of Avogadro

- ▶ **Files can be exported to png, jpg, bmp file formats**
- ▶ **Two or more structures can be built or loaded on the panel**



Video Clippings



Video Clippings

- ▶ We will briefly go through the individual tutorials created in this series



Spoken Tutorial: Build Molecules



Spoken Tutorial: Build Molecules

Explains how to,

- ▶ **Import molecules from database**
- ▶ **Rotate, zoom in and zoom out**
- ▶ **Build molecules, show fragment library**
- ▶ **Set up force field & optimize geometry**
- ▶ **Measure bond lengths, bond angles and dihedral angles**



Spoken Tutorial: Edit Molecules



Spoken Tutorial: Edit Molecules

Explain about,

- ▶ **Add and delete atoms and bonds, rotate bonds**
- ▶ **Change length of the bond**
- ▶ **Change hydrogen to methyl group**
- ▶ **Copy, paste and join structures**



Spoken Tutorial: Create Surfaces



Spoken Tutorial: Create Surfaces

Explain about,

- ▶ **Properties of molecules, label the atoms with partial charge**
- ▶ **Create Van der waals surfaces**



SpokenTutorial: Hydrogen Bonding



SpokenTutorial: Hydrogen Bonding

Explain about,

- ▶ **How to configure Avogadro**
- ▶ **Show Hydrogen bonding in molecules**
- ▶ **Measure length of hydrogen bonds**
- ▶ **Show force display type and dipole moments in molecules**



Spoken Tutorial: General Features in Avogadro



Spoken Tutorial: General Features in Avogadro

- ▶ **Proton transfer in molecules by changing pH values**
- ▶ **Load crystal structures and show Miller planes**
- ▶ **Build super cells and nanotubes**
- ▶ **Show geometries in coordination compounds**



Spoken Tutorial: Stereoisomerism



Spoken Tutorial: Stereoisomerism

Explain about,

- ▶ **Conformational isomerism**
- ▶ **Geometrical isomerism**
- ▶ **R-S configuration with examples**



Spoken Tutorial: File Extensions



Spoken Tutorial: File Extensions

Explain about,

- ▶ **Prepare input files for computational chemistry programmes such as:**
GAMESS, Gaussian, MOPAC, NWChem
- ▶ **View molecular orbitals and calculate IR spectrum using output files generated from-** *GAMESS, Gaussian*



Summary

- ▶ **About Avogadro software**
- ▶ **Download and installation of Avogadro**
- ▶ **To open the documentation page**
- ▶ **About Avogadro interface**
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Assignment



Assignment

1. Install Avogadro on your machine



Assignment

1. **Install Avogadro on your machine**
2. **Open Avogadro interface and explore**



Assignment



Assignment

1. Go through the menus and tool bars



Assignment

1. **Go through the menus and tool bars**
2. **Change the background colour of the Panel**



About the Spoken Tutorial Project

- ▶ Watch the video available at http://spoken-tutorial.org/What_is_a_Spoken_Tutorial
- ▶ It summarises the Spoken Tutorial project



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- ▶ 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



Forum for specific questions

- ▶ **Do you have questions in THIS Spoken Tutorial?**
- ▶ **Please visit**
<http://forums.spoken-tutorial.org>
- ▶ **Choose the minute and second where you have the question**
- ▶ **Explain your question briefly**
- ▶ **Someone from our team will answer them**



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

- ▶ Spoken Tutorial Project is a part of the Talk to a Teacher project
- ▶ It is supported by the National Mission on Education through ICT, MHRD, Government of India
- ▶ More information on this Mission is available at <http://spoken-tutorial.org/NMEICT-Intro>

