File Extensions

Spoken Tutorial Project
http://spoken-tutorial.org
National Mission on Education through ICT
http://sakshat.ac.in

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Learning Objectives

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We will learn to:

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- **Prepare input files for computational chemistry programmes such as: GAMESS, Gaussian, MOPAC, NWChem etc**

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- View **molecular orbitals** and **calculated IR spectrum** using output files generated from **GAMESS** and **Gaussian** software

System Requirement

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- **Ubuntu Linux OS v 14.04**

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- **Avogadro version 1.1.1**

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- **The example files required for this tutorial are provided as code files**

About Gaussian

- **Gaussian is a computer programme for computational chemistry**
- **It is a commercial software, developed and licensed by Gaussian Inc.**
- **http://www.gaussian.com/**

About GAMESS

- The General Atomic and Molecular Electronic Structure System (GAMESS)
- It is a general ab initio quantum chemistry package

About GAMESS

- **It is available at no cost to both academic and industrial users**
- **http://www.msg.ameslab.gov/gamess/download.html**

Note to viewers

Viewers please note;

- **Gaussian is a commercial software**
- **Hence I will not be able to show the interface to load the input file**

Note to viewers

- **Those interested can download GAMESS software from the given link**
- **Load the input file to generate the output file**
- **http://www.msg.ameslab.gov/gamess/download.html**

Summary

- Prepare input files for computational chemistry programmes such as: GAMESS and Gaussian
- View molecular orbitals for benzene and water molecules

Summary

- View calculated IR spectrum for molecules using log files generated from Gaussian

Assignment

1. **Open the log file for benzene molecule (Benzene.log) from the code files provided**
2. **Display any Molecular Orbital(HOMO/LUMO) from the list**
3. **Change the display and color of the lobes**
4. **Save the image in JPEG format**

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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- More information on this Mission is available at http://spoken-tutorial.org/NMEICT-Intro