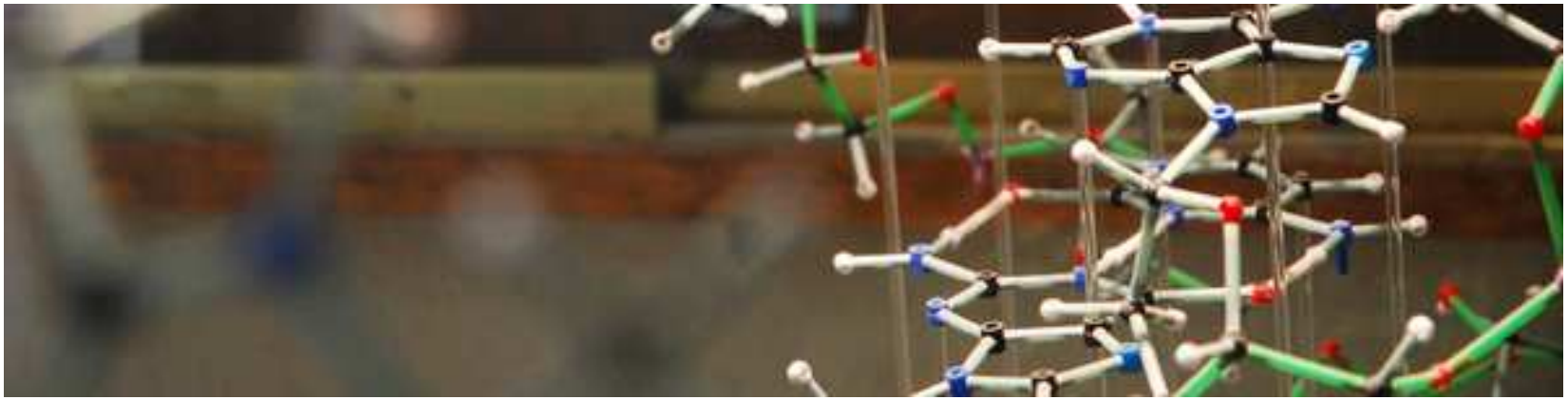

JMol tutorial

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General information on JMol

Operating System Support

A free and Open Source Molecular viewer for: Linux, Windows, Mac

Oriented to:

Creation and visualization of 3-dimensional models of Chemical Structures

...and also for:

Visualization of secondary structures of Proteins and Macromolecules

General information on JMol

Framework

Java (JRE) (Sun Microsystem)

Available for download

Most popular package manager for Linux
http://jmol.sourceforge.net

This tutorial has been tested on

Window 10, JMol 14.6.2, Java(JRE) 7
Linux Mint 17, Jmol 14.1, Java(JRE) 7

Molecular Structure

Learning Objectives 1

Jmol Application window and some basic operations

- Menu bar, Tool bar and Jmol panel
- Modify the size of the Jmol panel
- Create models of simple organic molecules
- Build molecules by substituting hydrogen with Methyl group
- Energy minimization to get a stable conformation
- Save the image as .mol file

Molecular Structure
Learning Objectives 2

- Substitute the hydrogen atom in a molecular model with a functional group
- Add and delete bonds
- Add and delete atoms
- Pop-up menu (Contextual menu)

Molecular Structure
Laboratory 1

- Create models of 2,4-dimethylpentane
- Create models of 3-ethyl-5-methylheptane
- Minimize energy to get the most stable conformation
- Save the image as .mol file
- Rotate the model using the “rotate molecule” in tool bar

Molecular Structure

Laboratory 2

- Create models of the following molecules:
  3-bromo-1-butanol and 2-amino-4-chloro-pentane
- Do energy minimization and Save the image in JPEG format

Molecular Structure

Summary 1

- About Jmol Appliction Window
- Resize the Jmol Panel
- Use the "Modelkit" function in the tool bar to create 3D models of simple organic moecules like Methane, Ethane and Propane
- Build molecules by substitution of hydrogen with Methyl group
- Energy minimization to get a stable conformation
- Save the image as .mol file

Molecular Structure
Summary 2

- Substitute the hydrogen atom in alkanes with a functional group
- Add bonds to convert alkanes to alkenes and alkynes
- Add and delete atoms
- Pop-up menu (Contextual menu)

Molecular Structure
Assignment

- Create models of 2-fluoro-1,3-butadiene and 2-pentyne
- Use the Pop-up menu to change the display of the model to wireframe
- Do energy minimization and Save the image in PDF format

Display and view
Learning Objective

- Rotate, zoom, move and spin the model
- Modify the view
- Change the style of display
- Change the color of atoms and bonds
- Display the model with 'Axes' and 'Boundbox'
- Save the image in various file formats

Display and view
Laboratory

- Create a model of 2-chloro-3-iodo-pentane
- Explore the 'Spin' option in the Pop-up menu
- Change the direction of spin to 'Z' axis and rate of spin to '40'

Display and view
Summary

- Rotate, zoom, move and spin the model
- View the model from various angles
- Change the style of display
- Change the color of atoms and bonds
- Display the model with ‘Axes’ and ‘Boundbox’
- Save the image in various file formats

Display and view
Assignment

- Create a model of 3-amino-1-propanol
- Change the display style to ‘Sticks’
- Change the color of hydrogens in the model to ‘Green’
- Change the color of all the bonds to ‘Yellow’

Mesurament and labelling

Learning Objectives

- Create models of `carboxylic acid` and `nitroalkane`
- Label atoms in a model with symbol and number
- Measure bond lengths, bond angles and dihedral angles (torsion angles)

Mesurament and labelling

Laboratory

- Create models of `1-butanoic acid` and `ethylacetate`
- Optimize the structure by doing energy minimization
- Save the image

Mesurament and labelling

Summary

- Create models of `carboxylic acid` and `nitroalkane`
- Label atoms in a model with symbol and number
- Measure bond lengths, bond angles and dihedral angles (Torsion angles)

Mesurament and labelling

Assignment

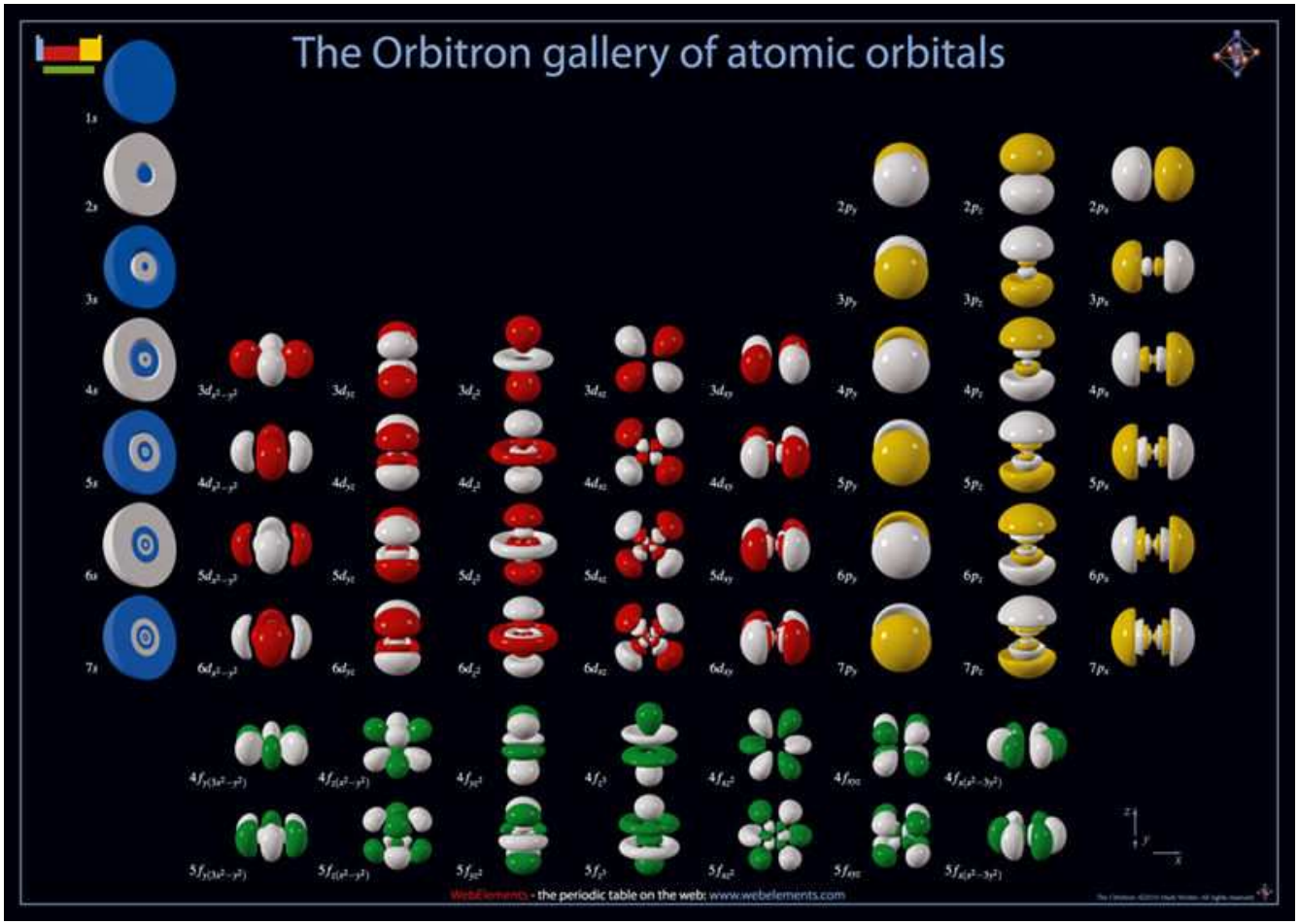
- Create models of molecules with single, double and triple bonds
- Measure bond lengths between the carbon atoms and compare them

Surface and Orbitals
Learning Objectives

- Create models of alicyclic and aromatic molecules
- Display different surfaces of molecules
- Display atomic and molecular orbitals

Surface and Orbitals

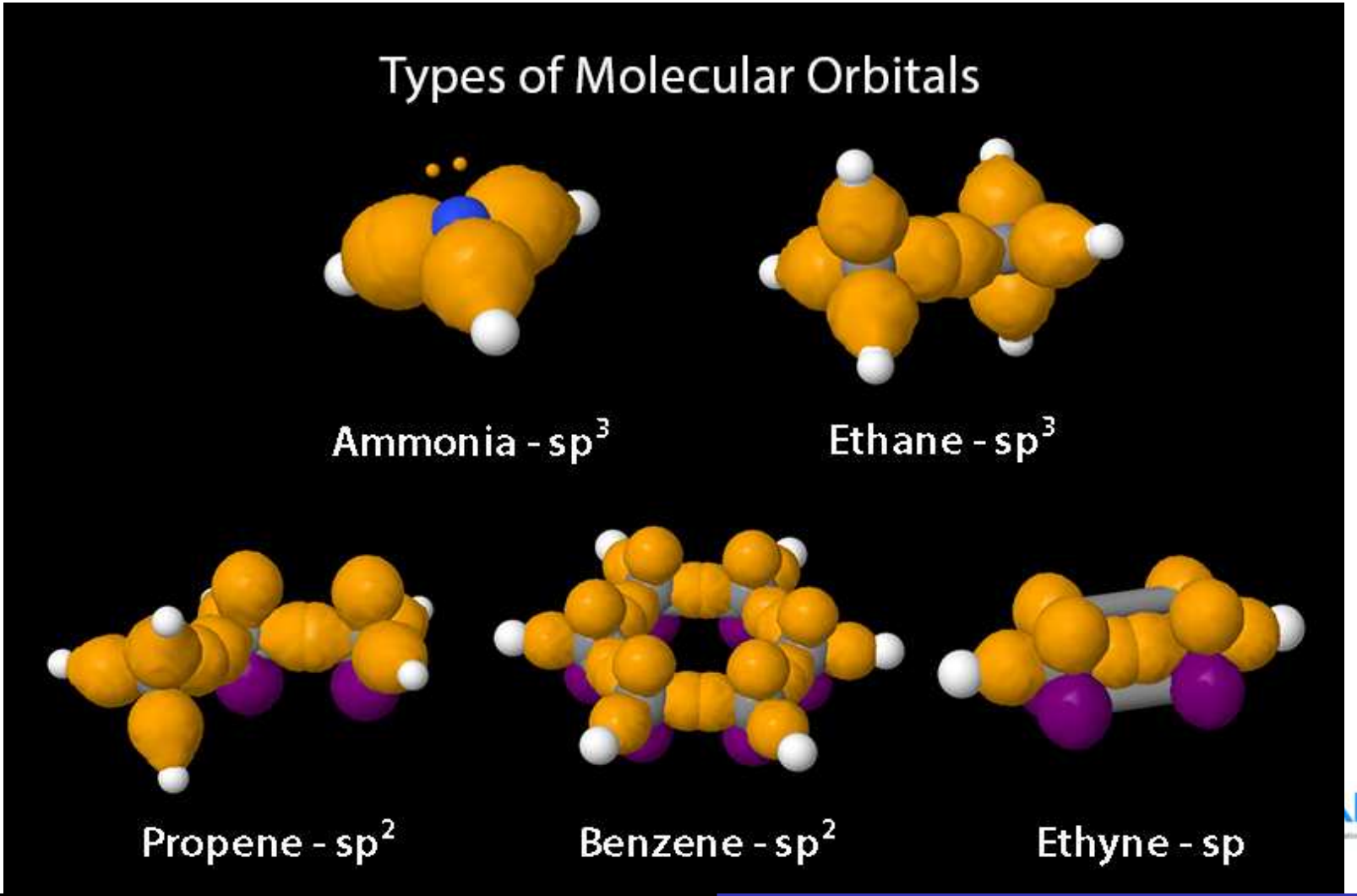
Types of Atomic Orbitals



Surface and Orbitals
Laboratory

- Linear Combination of Atomic Orbitals (LCAO) method is used to create Molecular Orbitals
- The Command line to create Molecular Orbitals: *lcaocartoon create*

Surface and Orbitals
Type of Molecular Orbitals



Surface and Orbitals
Summary

- Create a model of cyclohexane and cyclopentane
- Create a model of benzene
- Display surface topology of molecules
- Display atomic orbitals
  s, p, d and f
- Display molecular orbitals (LCAO)
  sp^3, sp^2 and sp

Surface and Orbitals
Assignment

- Create a model of 2-butene and display molecular orbitals (LCAO)
- Explore `lcaocartoon` command to change the color and size of molecular orbitals
- http://chemapps.stolaf.edu/jmol/docs/

Script Console
Learning Objectives

- About script commands
- `Script console` window
- Change display of the model by using script commands
- Display lines of text on the panel

Script Console

Modify Display in Jmol Application

Display on Jmol panel can be modified using

- Options in menu bar
- Options in the Pop-up menu
- Scripting commands on the `script console`

Script Console
Script Commands

- A set of commands is called a `script command`
- Script commands control the display of the model on screen
- Jmol uses a command language based on `Rasmol program`

Script Console
Script Commands

- Writing such commands is called `scripting`
- Documentation of Jmol's scripting language and list of `script commands` is available at this link

http://chemapps.stolaf.edu/jmol/docs/

Script Console
Using Commands

- Script commands are typed on `script console` window
- `Script console` is Jmol's command line interface
- It is available in the menu bar, under `File` and `Console` option

Script Console

How to write Commands

- Type the command at the `$` prompt on the `script console` window
- Script command starts with a `command word`
- Continues with a set of parameters, separated by `spaces`
- Is terminated by the `end of line character` or `semicolon (;)`
- The command will appear red, until you have completed typing the command
- Press `Enter` key on the keyboard, to activate the command

Script Console
Summary

- Script commands
- `Script console` window
- Change the display of the model using script commands
- Display lines of text on the panel

Script Console
Assignment

1. Create a model of `3-methyl pentane`
2. Use script commands to do the following
   - Change the color of all hydrogens to blue
   - Change the color of all the bonds to red
   - Set the molecule to spin

Molecular Structure from Database

Learning Objectives

- Load chemical structures from *Pubchem* database

Molecular Structure from Database

Identification of the Molecule

- Common name or IUPAC name
- CAS number (Chemical Abstracts Service registry number)
- CID number (Compound Identification Number)
- InChi identifier (IUPAC International Chemical Identifier)
- SMILES identifier (Simplified Molecular Input Line Entry System)

Molecular Structure from Database

Laboratory

- Load structure of *caffeine* from Pubchem database https://pubchem.ncbi.nlm.nih.gov
- Highlight the important features in the molecule
- Modify the display to *wireframe*
- Load and Modify the display of Phenol and Cholesterol

Molecular Structure from Database

Summary

- Load chemical structures from *Pubchem* database
- Modify the display of Caffeine, Phenol and Cholesterol

Protein
Learning Objectives

- Load structures of proteins from *Protein Data Bank (PDB)*
- Download .pdb files from PDB database
- Display secondary structure in various formats
- Highlight hydrogen bonds and disulfide bonds

Protein

Molecular Structure analysis of large biomolecules

JMol offer the possibility to explore:

- *Proteins and Macromolecules*
- *Nucleic acids (DNA and RNA)*
- *Crystal structures and Polymers*

Protein
Laboratory

- Load structures of protein from *Protein Data Bank (PDB)*
- Download .pdb files from the database
- View 3D structure of insulin using *PDB code (4EX1)*

Protein
Summary

- View protein structure without water molecules
- Display secondary structure in various formats
- Highlight hydrogen bonds and disulfide bonds

Protein
Assignment

- Download the .pdb file of human Hemoglobin from *PDB* database
- Show secondary structure in cartoon display
- Highlight the *Porphyrin* units of the protein
  http://www.rcsb.org/pdb/home/home.do

Enzyme
Learning Objectives

- Load structure of *Human Pancreatic Hexokinase* on Jmol panel
- Modify the display of *secondary structure*
- Highlight amino acid residues at the active site

Crystal Structure and Unit Cell

Learning Objectives

- Download CIF (Crystallographic Information File) from Crystallography Open Database (COD)
- Open CIF in Jmol
- Display unit cell and unit cell parameters on Jmol panel
- Display crystal structures of different crystal systems Example Cubic, Hexagonal and Rhombohedral

Crystal Systems

Table: The seven crystal systems[After Whittaker, 1981pp. 24]

Crystal system	Cell Shape	Cell axes	Characteristic Symmetry[1]	# classes
Triclinic	General parallelepiped	$a \neq b \neq c$ $\alpha \neq \beta \neq \gamma \neq 90°$	Monad	2
Monoclinic	Right prism with parallelogram as base	$a \neq b \neq c$ $\alpha = \gamma = 90° \neq \beta$	1 diad	3
Orthorhombic	Rectangular parallelepiped	$a \neq b \neq c$ $\alpha = \beta = \gamma = 90°$	3 diads	3
Tetragonal	Square prism	$a = b \neq c$ $\alpha = \beta = \gamma = 90°$	1 tetrad	7
Trigonal (Rhomohedral)	Cube deformed along one diagonal	$a = b = c$ $\alpha = \beta = \gamma \neq 90°$	1 triad	5
Hexagonal	Prism on a 60° paralleogram	$a = b \neq c$ $\alpha = \beta = 90°; \gamma = 120°$	1 hexad	5
Cubic	Cube	$a = b = c$ $\alpha = \beta = \gamma = 90°$	4 triads	7

Crystal Structure and Unit Cell

Crystallographic Information File (CIF)

- Crystallographic Information File (CIF) is a standard text file format for representing crystallographic information
- CIF format has the file extension .cif

Crystal Structure and Unit Cell

Crystallography Open Database (COD)

- Crystallography Open Database (COD) is an open-access database
- The downloadable CIF are available at COD website
- www.crystallography.net

Crystal Structure and Unit Cell
Unit Cell

- Unit cell is the smallest repeating unit in a crystal
- Stacking of these unit cells in 3 dimensions will form the basis of the crystal structure

Crystal Structure and Unit Cell

Laboratory

- Download CIF from Crystallography Open Database (COD)
- Open CIF in Jmol
- Display unit cell and unit cell parameters

Crystal Structure and Unit Cell
Summary

- Display crystal structures of sodium chloride, graphite and calcite

Crystal Structure and Unit Cell

Assignment

- Download CIF for quartz crystal from COD database
- Display unitcell on Jmol panel and explore the symmetry options

Symmetry
Learning Objectives

- Draw line (axis) through atoms in a molecule
- Spin and rotate the molecule along the axis
- Draw plane through atoms in a molecule
- Demonstrate point group classification

Symmetry
Symmetry Elements

- Axis of Symmetry
- Plane of Symmetry
- Center of Symmetry

Symmetry
Laboratory

- Draw line representing C_3 axis of symmetry in a model of ethane
- Spin the model along C_3 axis
- Draw lines (C_2 and C_3 rotational axes) through atoms in methane molecule
- Spin and rotate the molecule along the axis
- Draw reflection plane through atoms in methane molecule
- Jmol Script Commands at: www.chemapps.stolaf.edu/jmol/docs/

Symmetry
Summary

- Draw lines (C_2 and C_3 rotational axes) through atoms in methane molecule
- Spin and rotate the molecule along the axis
- Draw reflection plane through atoms in methane molecule
- Demonstrate point group classification using examples of methane

Symmetry
Assignment

- Draw reflection plane in a model of dichloromethane
- Find out the point group classification for ammonia and benzene

Animation
Learning Objectives

- Animations using Jmol script commands
- For demonstration: Ethane and Hemoglobin
- Keywords used for animations
  move, delay, slab, loop and capture

Animation
Commands

- move: Rotate, Zoom and Translate
- delay: Pause a script
- slab: Percentage of the molecule to be displayed on panel

Animation
Commands

- loop: Causes the script to restart at the beginning, with an optional time delay
- capture: Captures animations as animated GIF files
- http://chemapps.stolaf.edu/jmol/docs/

Animation
Move commands

move [x-rotation] [y-rotation] [z-rotation] [zoom-factor] [x-translation] [y-translation] [z-translation] [slab-cutoff] [seconds-total]

Animation
Summary

- Create animation of ethane and hemoglobin using script commands with key words move, delay, loop and slab
- Save the animation as GIF file using capture command