

Surfaces and Orbitals

Talk to a Teacher

<http://spoken-tutorial.org>

National Mission on Education through ICT

<http://sakshat.ac.in>

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Learning Objectives



Learning Objectives

- ▶ **Create models of alicyclic and aromatic molecules**



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- ▶ Create models of alicyclic and aromatic molecules
- ▶ Display different surfaces of molecules



Learning Objectives

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



Pre-requisites

You should know how to



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- ▶ **Create and edit molecular models in Jmol Application**



Pre-requisites

You should know how to

- ▶ Create and edit molecular models in Jmol Application
- ▶ If not, watch the relevant tutorials available at <http://spoken-tutorial.org>



System Requirements



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- ▶ Ubuntu OS version 12.04



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- ▶ **Jmol version 12.2.2**



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- ▶ **Jmol version 12.2.2**
- ▶ **Java (JRE) version 7
(Sun Microsystems)**



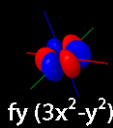
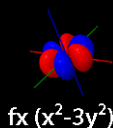
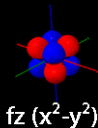
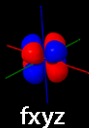
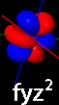
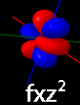
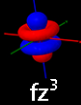
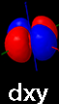
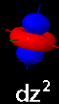
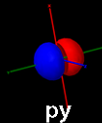
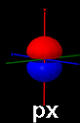
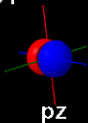
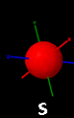
Script Commands

Type of orbital	Script command
	\$ command line n l m
s	\$ isosurface phase atomicorbital 2 0 0
px	\$ isosurface phase atomicorbital 2 1 0
py	\$ isosurface phase atomicorbital 2 1 1
pz	\$ isosurface phase atomicorbital 2 1 -1
dz2	\$ isosurface phase atomicorbital 3 2 0
dxz	\$ isosurface phase atomicorbital 3 2 1
dyz	\$ isosurface phase atomicorbital 3 2 -1
dxy	\$ isosurface phase atomicorbital 3 2 2
$d(x^2-y^2)$	\$ isosurface phase atomicorbital 3 2 -2
fx^3	\$ isosurface phase atomicorbital 4 3 0
fxz^2	\$ isosurface phase atomicorbital 4 3 1
fyz^2	\$ isosurface phase atomicorbital 4 3 -1
$fxyz$	\$ isosurface phase atomicorbital 4 3 2
$fz(x^2-y^2)$	\$ isosurface phase atomicorbital 4 3 -2
$fx(x^2-y^2)$	\$ isosurface phase atomicorbital 4 3 3
$fy(x^2-y^2)$	\$ isosurface phase atomicorbital 4 3 -3



Types of Atomic Orbitals

Types of Atomic Orbitals



Molecular Orbitals



Molecular Orbitals

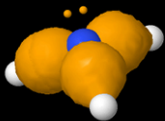
- ▶ **Linear Combination of Atomic Orbitals (LCAO) method is used to create Molecular Orbitals**
- ▶ **The Command line to create Molecular Orbitals:**

lcaocartoon create



Types of Molecular Orbitals

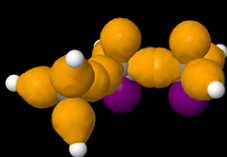
Types of Molecular Orbitals



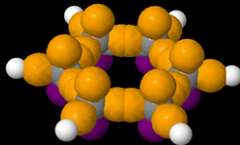
Ammonia - sp^3



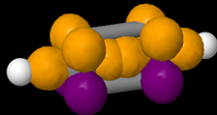
Ethane - sp^3



Propene - sp^2



Benzene - sp^2



Ethyne - sp



Talk to a Teacher



Summary

- ▶ Create a model of cyclohexane and cyclopentane
- ▶ Create a model of benzene
- ▶ Display surface topology of molecules



Summary

- ▶ **Display atomic orbitals**
 s , p , d and f
- ▶ **Display molecular orbitals**
 sp^3 , sp^2 and sp



Assignment

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



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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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



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>

