

CICLO DE TALLERES

VISUALIZACION INTERACTIVA DE MOLECULAS EN 3D Y USO DE LOS RECURSOS Jmol

(II) Quimica orgánica

Bob Hanson
St. Olaf College, Northfield, MN

hansonr@stolaf.edu

<http://www.stolaf.edu/people/hansonr>

Universidad Mayor de San Simón
Cochabamba, Bolivia

29 Jun 2016

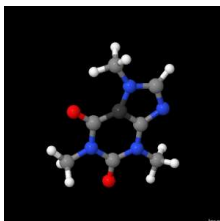
Temas para el Debate

- una breve introducción a Jmol
- discusión de los grupos
- capacidades generales de Jmol
- algunos ejemplos de la web
- discusión de los grupos
- tiempo para experimentar
- discusión

introducción general a Jmol

Misión : visualización en tiempo real de la estructura molecular, la dinámica y la energía.

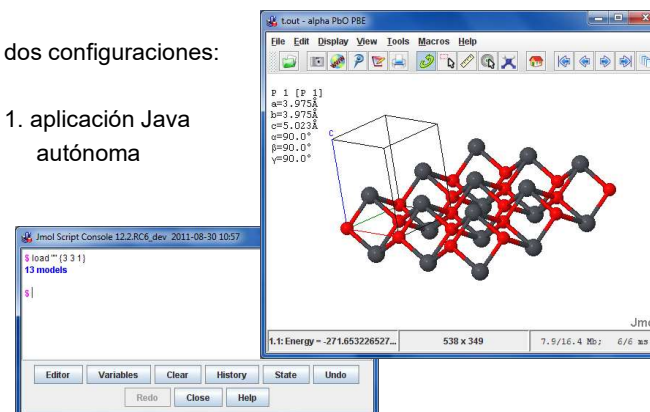
Jmol es :
código abierto
interdisciplinario
principalmente desarrollado
con la entrada de los usuarios



introducción general a Jmol

dos configuraciones:

1. aplicación Java autónoma



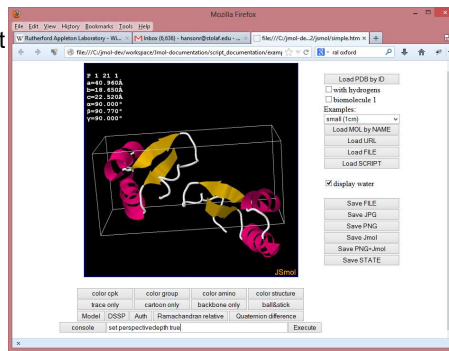
introducción general a Jmol

dos configuraciones:

2. "JSmol" JavaScript aplicación

tiene fácil acceso a cualquier navegador web

fácilmente adaptable a cualquier interés particular



capacidades generales

varios archivos con millones de estructuras

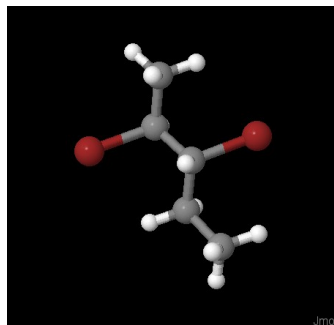
en particular, para las moléculas pequeñas:

NCI Resolver *load \$3-bromotoluene*
 PubChem *load :Tylenol*

Especialmente importante para la química orgánica

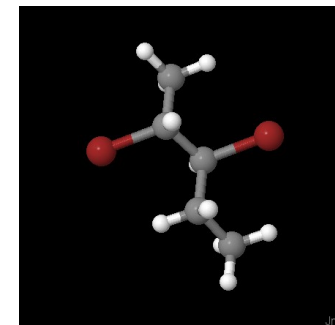
Capacidades generales - estereoquímica

load \$2,3-dibromopentane



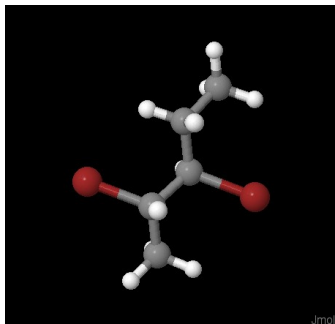
capacidades generales - estereoquímica

load \$(2R,3S)-2,3-dibromopentane



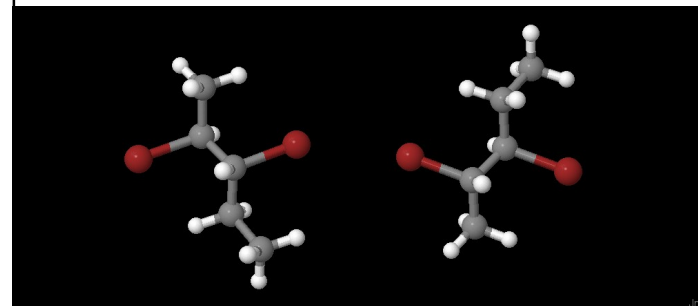
capacidades generales - estereoquímica

load \$(2S,3R)-2,3-dibromopentane



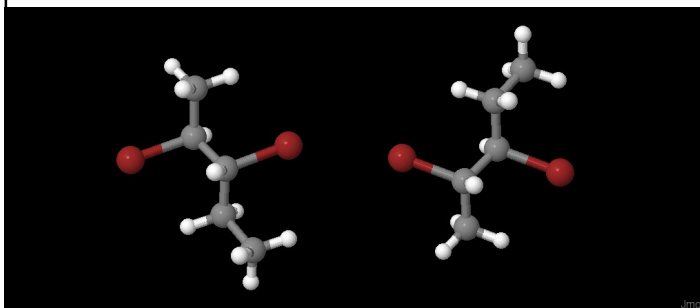
capacidades generales - estereoquímica

load files "\$2,3-dibromopentane" "\$(2S,3R)-2,3-dibromopentane"



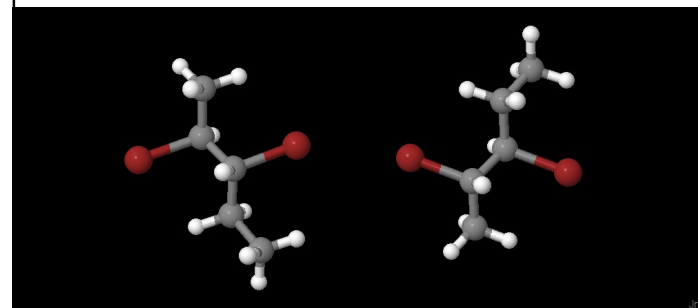
capacidades generales - estereoquímica

compare {1.1} {2.1} rotate translate



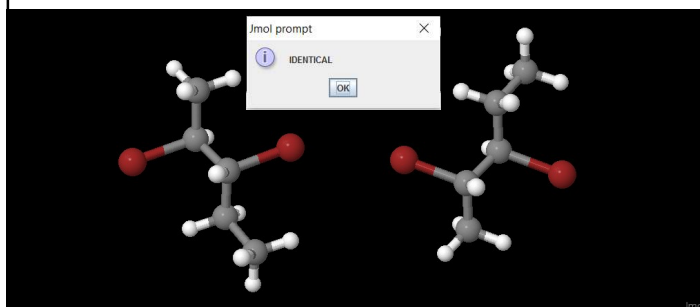
capacidades generales - estereoquímica

compare {1.1} {2.1} atoms {1_H} rotate translate

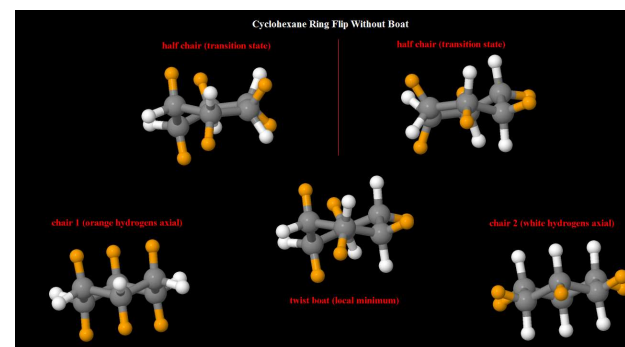


capacidades generales - estereoquímica

load files "\$2,3-dibromopentane" "\$2S,3R)-2,3-dibromopentane"
prompt compare({1.1}, {2.1}, "isomer")



capacidades generales - conformaciones



capacidades generales - conformaciones



<http://chemapps.stolaf.edu/jmol/jsmol/jmol-flot-energy.htm>

Atom and Bond Edit

H	B	C	Si
N	P	O	S
F	Cl	Xx	inv
Q+	Q-	redo	undo
Single	Double	Triple	
Xatm	Xbond	Xmol	
Wire	Ball	Space	
sp	sp2	sp3	

Load Models

Name	Draw
CheMagic	File

Merge Notebook

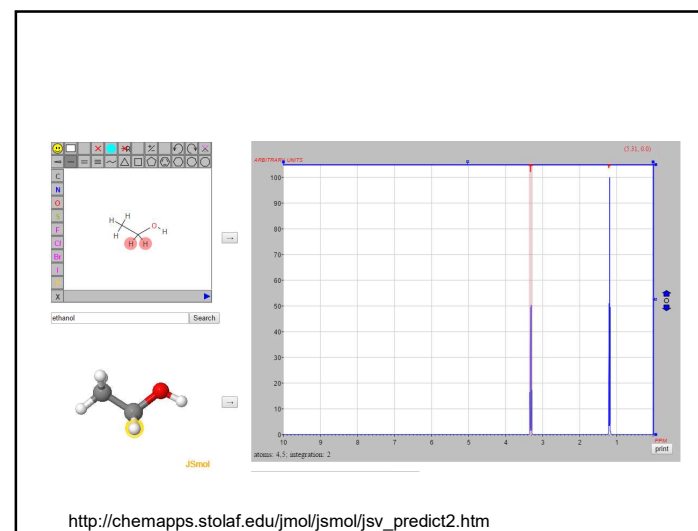
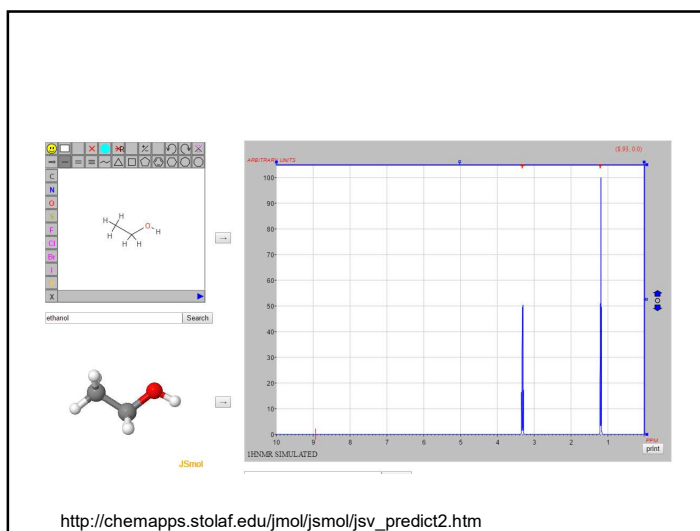
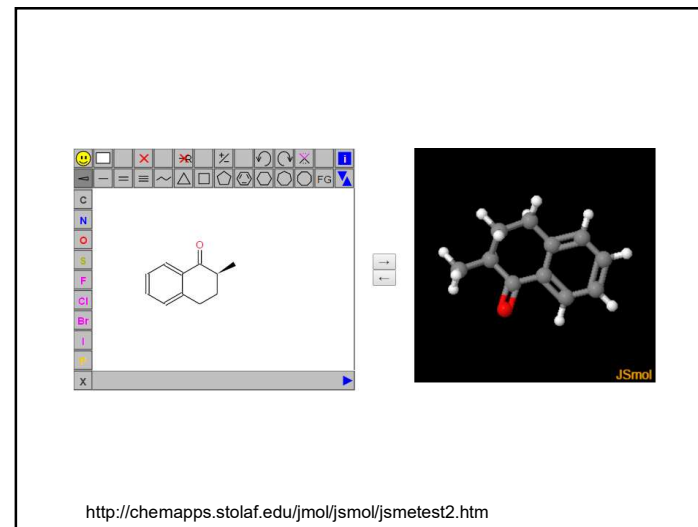
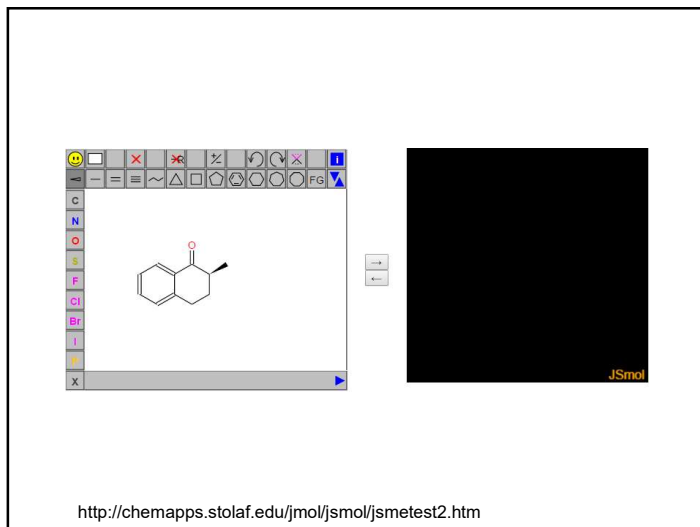
Written Using
HTML Egg Pro
Textastic
JSmol and JSME

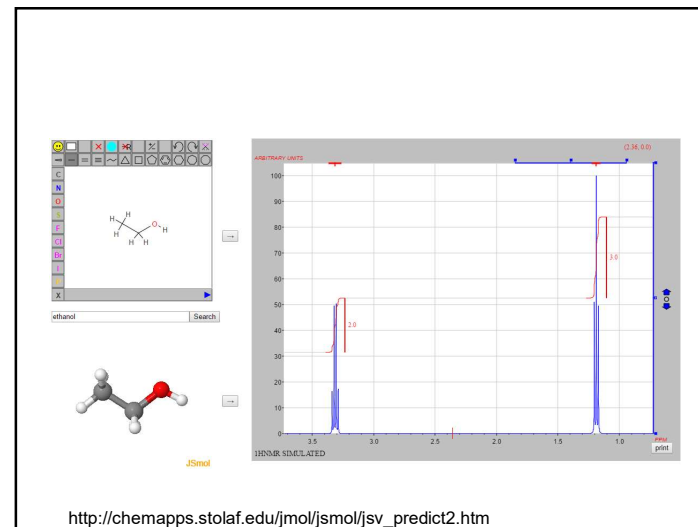
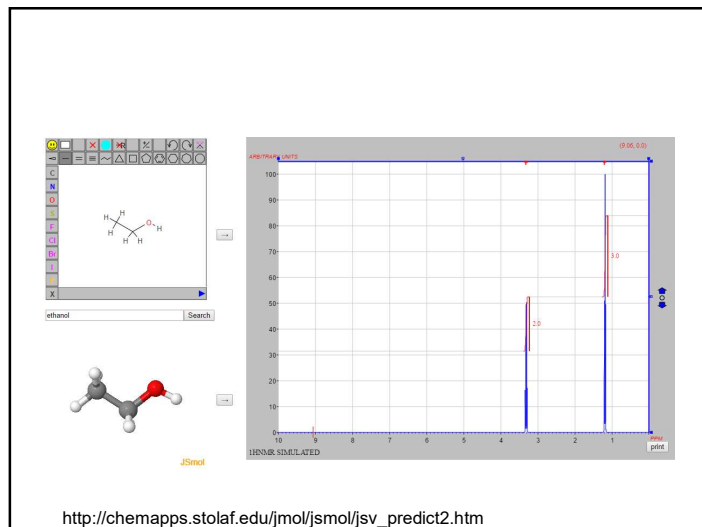
Other Model Actions

Correct H	Drag Atom
Optimize	Calculator
Zoom In	Zoom Out
MEP	vdW
MO	CIF Symop
Length	Angle
Torsion	Mass
Rotate Bond	Move
Duplicate	Compare
Put Share	Get Share
Save Mod	Restore Mod
Review Mods	Mark Atoms
NIST Google	NIST Direct
PubChem	NMRDB
Manage	Clear/Reset

Reach Out and Touch a Molecule
CheMagic Model Kit Mini

<http://chemagic.org/molecules/mini.html>





ChemTube3D

www.chemtube3d.com/ Traducir esta página

ChemTube3D contains interactive 3D animations and structures, with supporting information for some of the most important topics covered during an ...

Organic Chemistry Animations

Organic Chemistry Animations.
Welcome to the Introductory ...

ChemTube3D: Solid State

Basic Solid State Structures. Cubic
close packed / Face-centred ...

Organic Structure and Bonding

Organic Structure and Bonding.
Welcome to the Introductory ...

A Level Organic Chemistry ...

Organic reaction mechanisms
relevant to UK ... A Level ...

Polymers

Polymers are formed by joining large
numbers of small ...

Stereochemistry Home Page

Stereochemistry Home Page ... The
Stereochemistry section ...

Organic Reactions

C=O nucleophilic addition
C=O nucleophilic substitution
C=O addition - loss of carbonyl
oxygen
Stereochemistry
Nucleophilic substitution
Elimination
**Electrophilic addition to
alkenes**
• Ethylene and Bromine
• Stereospecific addition
• Epoxidation peracid
• Epoxidation of E-Allyl silane
• Unsymmetrical alkenes HBr
• Regioselective addition
• Diene bromination
• Stereoisomers
Electrophilic aromatic substitution
Electrophilic alkenes
Oxidation
Enols and Enolates as
nucleophiles
Conjugate addition
Aromatic heterocycles
Diels-Alder reactions
Pericyclic reactions
Rearrangements
Radical reactions
Fragmentations
Carbene chemistry
Stereochemistry

Electrophilic addition to alkenes

Ethylene and Bromine

Background Colour:



Small (300 px) Larger View

Click the structures and reaction arrows in sequence to view the 3D models and animations respectively.

