CICLO DE TALLERES

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

(II) Quimica ogánica

Bob Hanson
St. Olaf College, Northfield, MN
hansonr@stolaf.edu
http://www.stolaf.edu/people/hansonr

Universidad Mayor de San Simón
Cochabamba, Bolivia

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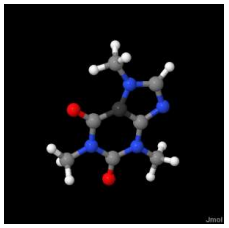
Temas para el Debate

- una breva 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

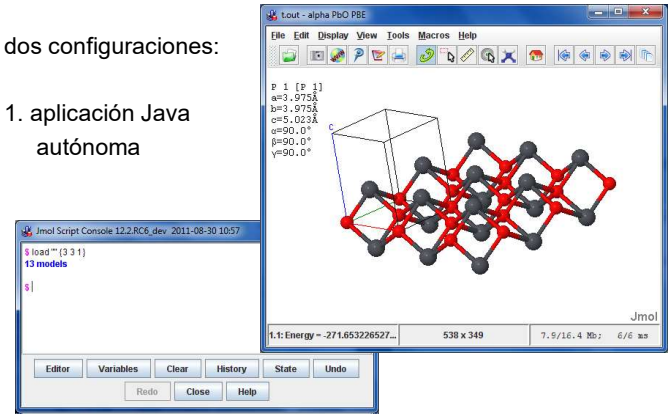
interdisciplinario

principalmente desarrollado con la entrada de los usuarios

introducción general a Jmol

dos configuraciones:

1. aplicación Java autónoma



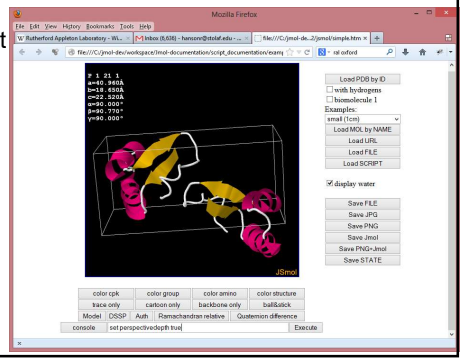
introducción general a Jmol

dos configuraciones:

2. “JSmol” JavaScript aplicación

tiene fácil acceso a cualquier navegador web

fácilmente adaptable a cualquier interés particular



capacidades generales

varios archivos con milliones de estructuras

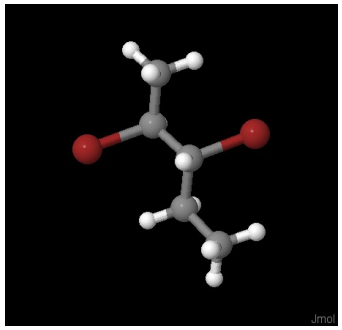
en particular, para las moléculas pequeñas:

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

Especialmente importante para la química orgánica

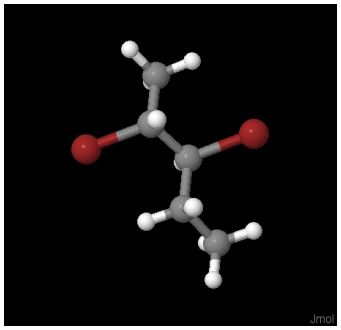
Capacidades generales - estereoquímica

load $2,3-dibromopentane



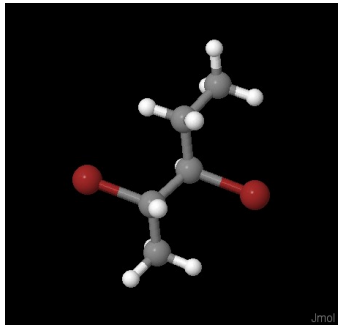
capacidades generales - estereoquímica

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



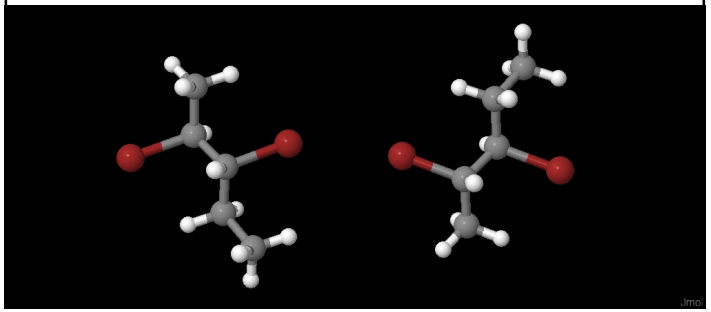
capacidades generales - estereoquímica

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



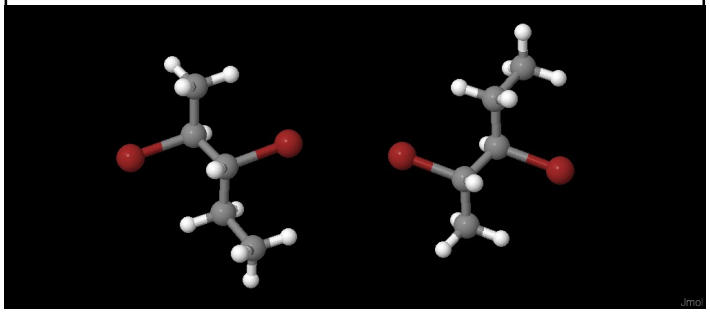
capacidades generales - estereoquímica

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



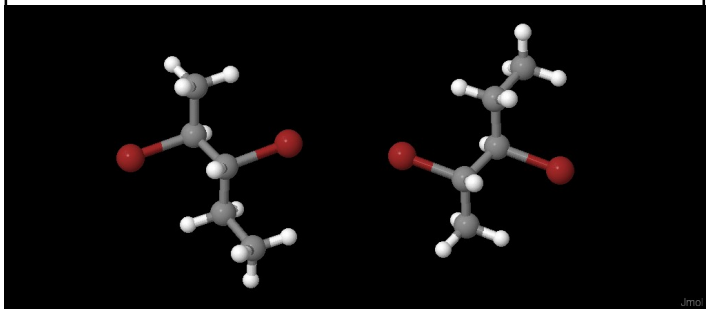
capacidades generales - estereoquímica

compare {1.1} {2.1} rotate translate



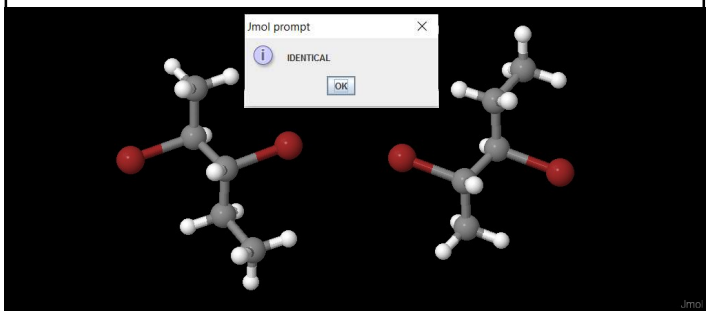
capacidades generales - estereoquímica

compare {1.1} {2.1} ***atoms { !_H}*** *rotate translate*

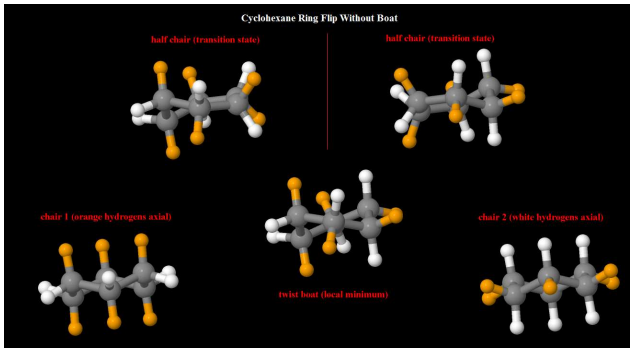


capacidades generales - estereoquímica

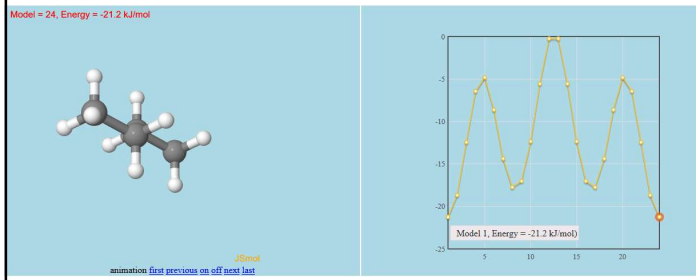
load files "$2,3-dibromopentane" "$(2S,3R)-2,3-dibromopentane"
prompt compare({1.1}, {2.1}, "isomer")



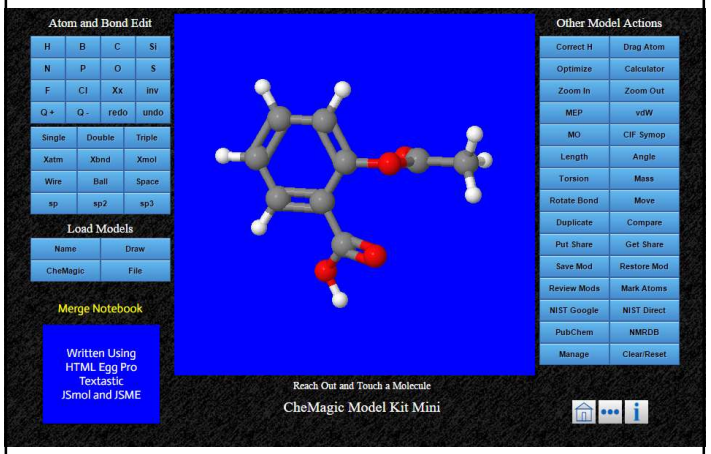
capacidades generales - conformaciónes



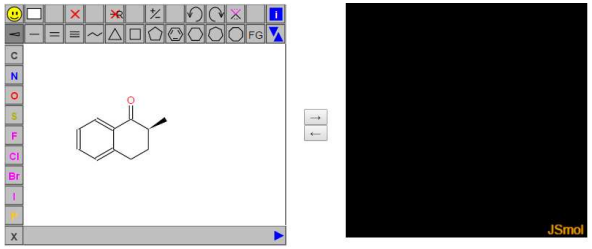
capacidades generales - conformaciónes



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



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



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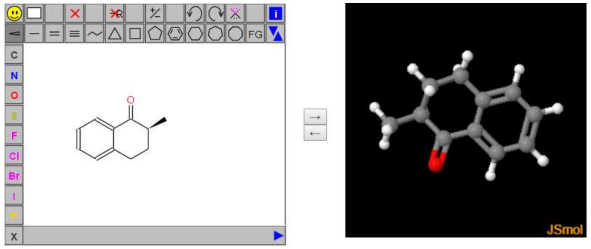

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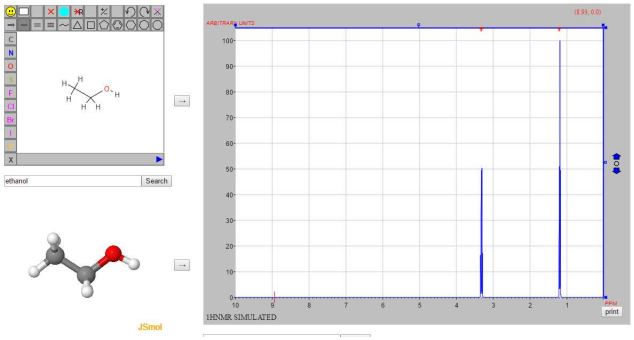

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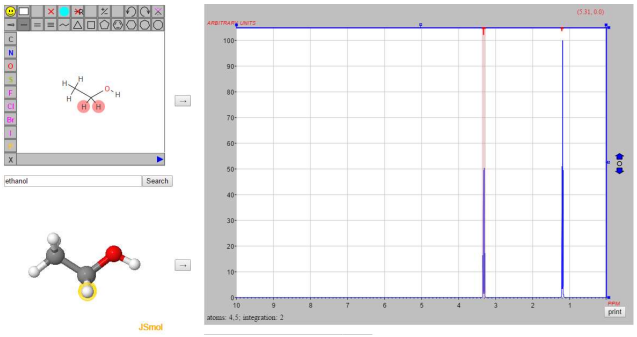

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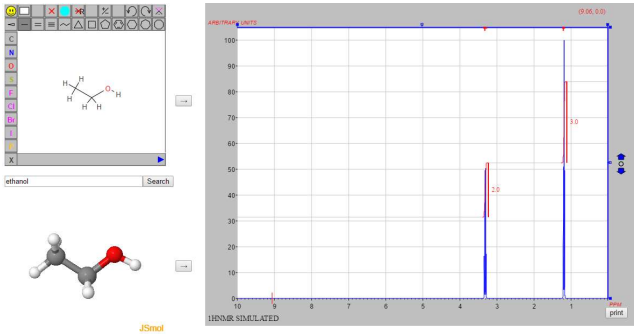

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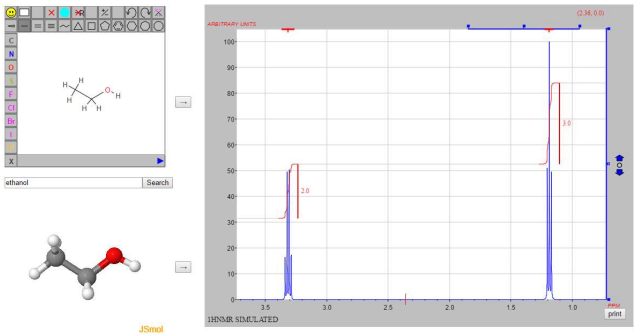

http://chemapps.stolaf.edu/jmol/jsmol/jsv_predict2.htm

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