



Teaching molecular structure using Jmol

Robert M. Hanson
Department of Chemistry, St. Olaf College
Northfield, MN 55057

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238th ACS National Meeting
Washington, DC

The Jmol Project

- Jmol molecular visualization project
- Open-source
- Jmol.sourceforge.net
- Active user/developer community
 - about 400 “users”
 - about 150 “developers”
 - collectively 23,000 list messages

The Jmol Community

- Professional graphics designers
- Professional developers
- Professors, graduate students, undergraduates

The Jmol Community

- Generally one of three focal points:
 - Research
 - Publishing
 - Education

The Jmol Community

- Generally one of three focal points:
 - **Research**
 - Computational chemistry visualization
 - Structural biology
 - Electron microscopy/X-ray crystallography
 - Publishing
 - Education

47162: Cyclohexatriene, Molecular Orbitals - Gaussian

Status <<

guest
webmo
1:00
unlimited
0 jobs

Summary

- Cyclohexatriene
- Job # 47162
- 8/13/2009
- 3.3 sec

Actions

- Job Manager
- Raw output
- All files
- Print
- Help

Applet size

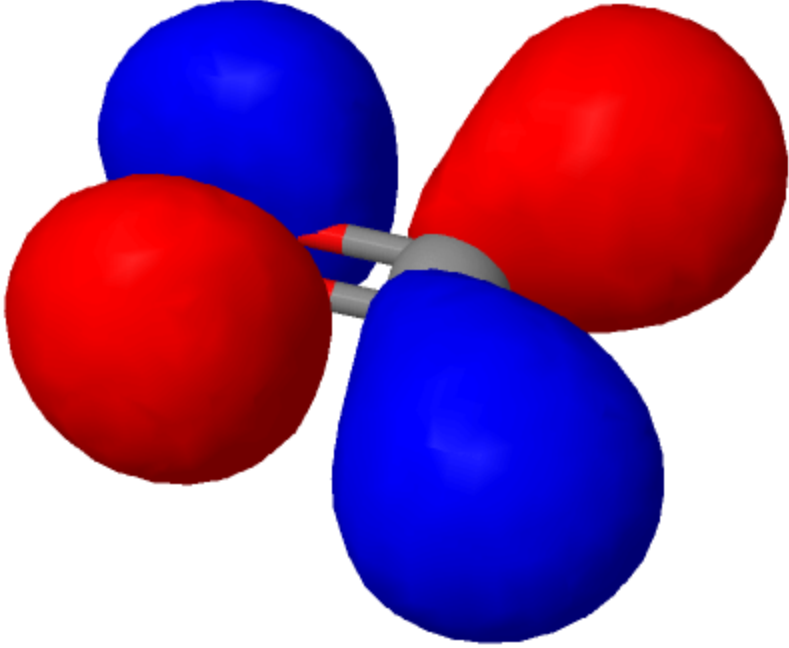
600 x 600
Resize

Notes >>

Molecule Viewer Data Viewer **MO Viewer**

File Edit View Help

ch2o_homo



- 1LDN
 - Download Files
 - FASTA Sequence
 - Display Files
 - Display Molecule
 - Image Gallery
 - Jmol Viewer
 - WebMol Viewer
 - Protein Workshop
 - FirstGlance
 - Asymmetric Unit
 - Assumed Biological Molecule 1
 - Assumed Biological Molecule 2
- Structural Reports
- External Links
- Structure Analysis
- Help
- Queries

STRUCTURE OF A TERNARY COMPLEX OF AN ALLOSTERIC LACTATE DEHYDROGENASE FROM BACILLUS STEAROTHERMOPHILUS AT 2.5 ANGSTROMS RESOLUTION

DOI:10.2210/pdb1ldn/pdb

Primary Citation

Structure of a ternary complex of an allosteric lactate dehydrogenase from *Bacillus stearothermophilus* at 2.5 Å resolution.
Wigley, D.B., Gamblin, S.J., Turkenburg, J.P., Dodson, E.J., Piontek, K., Muirhead, H., Holbrook, J.J.
(1992) J.Mol.Biol. 223: 317-335

PubMed: 1731077

Search Related Articles in PubMed

PubMed Abstract:

We report the refined structure of a ternary complex of an allosterically activated lactate dehydrogenase, including the important active site loop. Eightfold non-crystallographic symmetry averaging was utilized to improve the density maps. Interactions between the protein and bound coenzyme and ... [Read More & Search PubMed Abstracts]

Molecular Description

Hide

Classification: Oxidoreductase(choh(d) Nad(a))
Structure Weight: 285346.72
Molecule: L-LACTATE DEHYDROGENASE
Polymer: 1 Type: polypeptide(L) Length: 316
Chains: A, B, C, D, E, F, G, H
EC#: 1.1.1.27

1ldn

- Display Files
- Download Files
- Print this Page

Biological Molecule 1



More Images...

3-D Viewers:

- Jmol SimpleViewer
- Protein Workshop Other Viewers

STRUCTURE OF A TERNARY COMPLEX OF AN ALLOSTERIC LACTATE DEHYDROGENASE FROM BACILLUS STEAROTHERMOPHILUS AT 2.5 ANGSTROMS RESOLUTION

1ldn

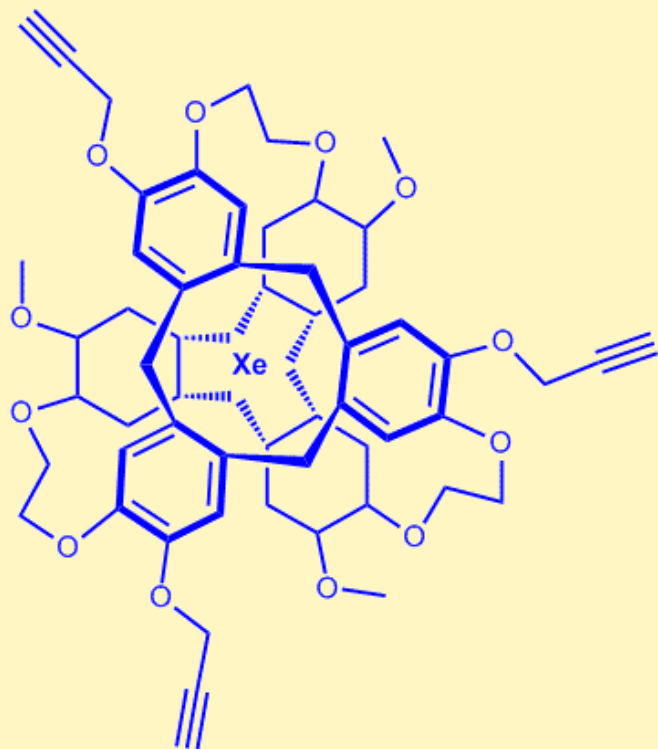
Display Files ▾
Download Files ▾



Jmol Version 11.6



The cryptophane cage:




has trapped a Xenon atom inside its interior cavity.

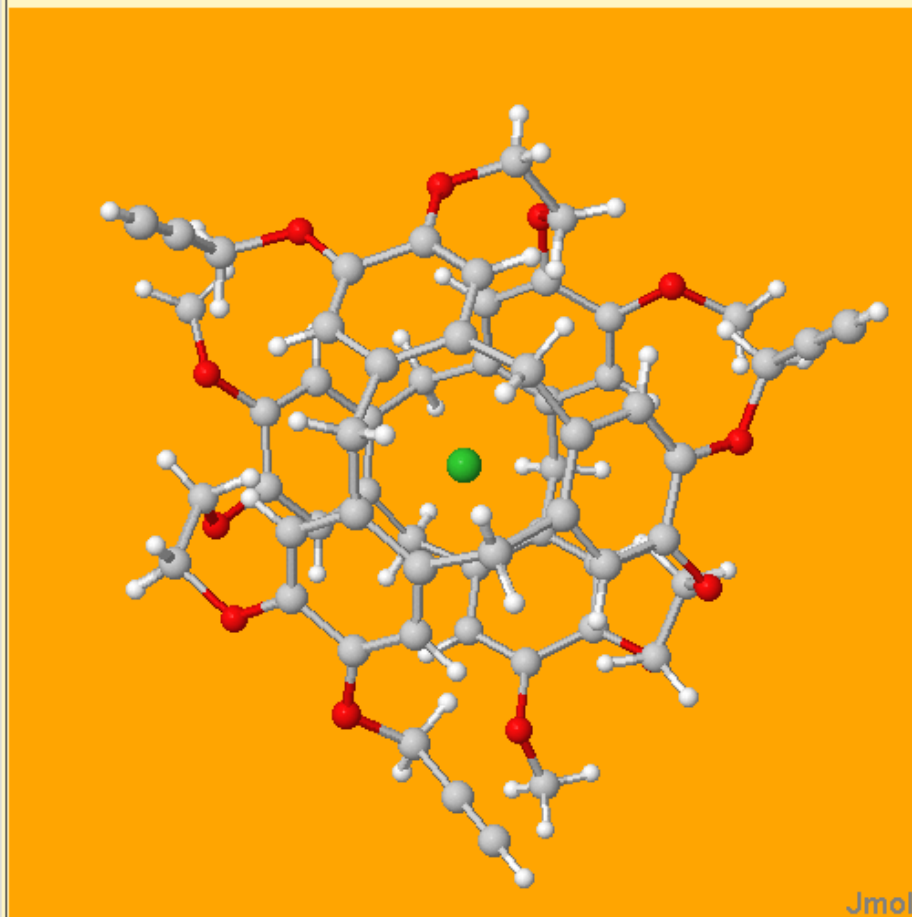
Hide Hydrogens Show Hydrogens VDW on Transparent VDW off

distance 1 distance 2 distance 3 Delete Measurements

plane 1 plane 2



Compound 9717



$C_{60}H_{54}O_{12}Xe$

The Jmol Community

- Generally one of three focal points:
 - Research
 - **Publishing**
 - Interactive website content
 - Professional graphics design
 - Database front ends
 - Education



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Articles

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HIV-1 Reverse Transcriptase Structure with RNase H Inhibitor Dihydroxy Benzoyl Naphthyl Hydrazone Bound at a Novel Site

Tools

★ Add to Favorites

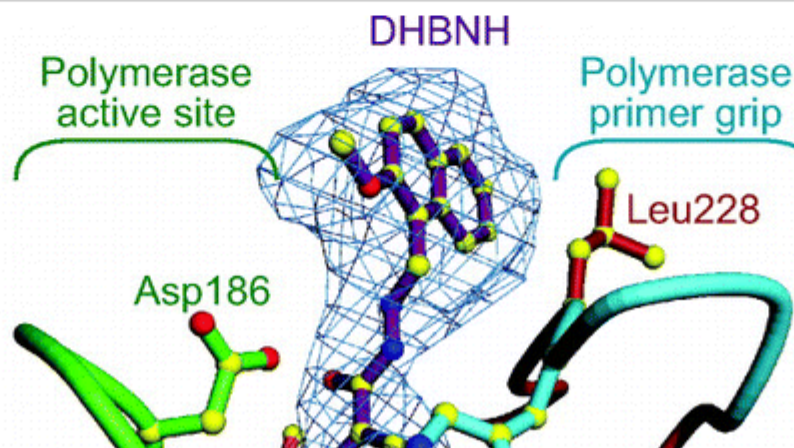
Related

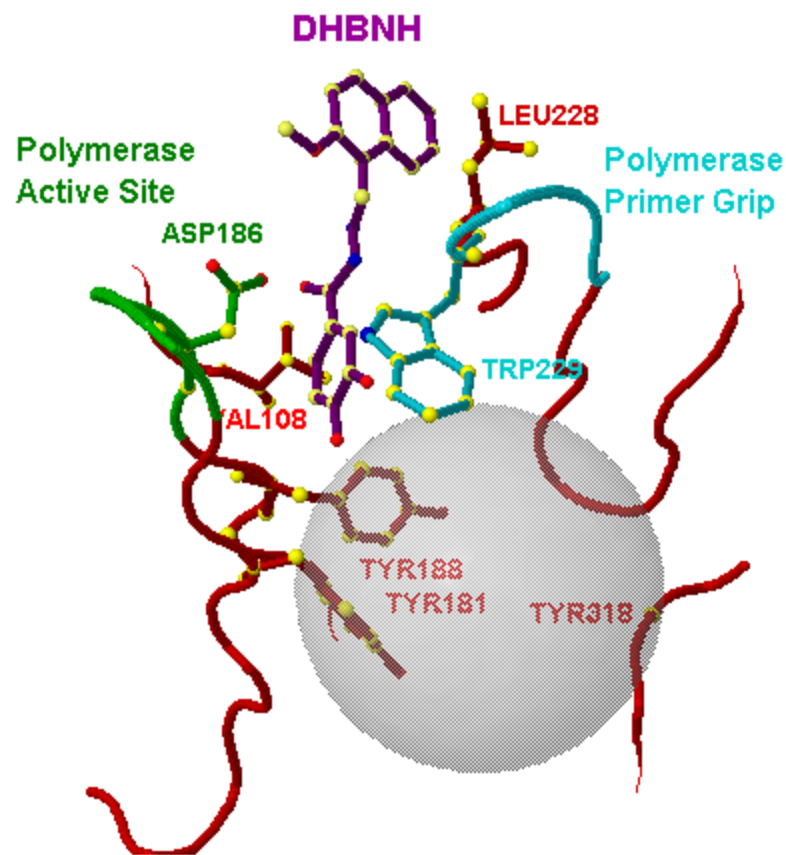
Illuminat
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Applicati
Related

« Previous Figure 3 of 8 Next »

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- download to MS PowerPoint





HIV-1 Reverse Transcriptase Structure with RNase H Inhibitor DHBNH Bound at a Novel Site

Figure 2 Options

Spacefill overlay:

- DHBNH
- Sidechains

Protein backbone:

- smoothed trace
- NNRTI binding site (gray)

Reset View

Explore this structure (215j) in [FirstGlance in Jmol](#)

Figure 2: The bound DHBNH inhibitor. The binding site of DHBNH is adjacent to the polymerase active site (green), the polymerase primer grip (cyan), and the NNRTI-binding pocket (translucent gray sphere). The

Jmol

spin 360° Y

spin 360° X

rock on

rock off

[Secondary Structure](#) [Cartoon](#) [N→C Rainbow](#)
[Composition](#) [Hydrophobic/Polar](#) [Charge](#)
[Contacts..](#) [Vines..](#) [All Models](#) [Hide..](#) [Find..](#)

Ligands+.. Background
 Water.. Spin
 Slab.. Zoom

[More Views..](#) 1LDN:
[Center Atom..](#) [Troubleshooting](#) [Reset](#) [Close](#)

Please click the button above to go to the *Introduction*.

NEW Share custom molecular views linked to explanations -- with ease -- at Proteopedia.Org!



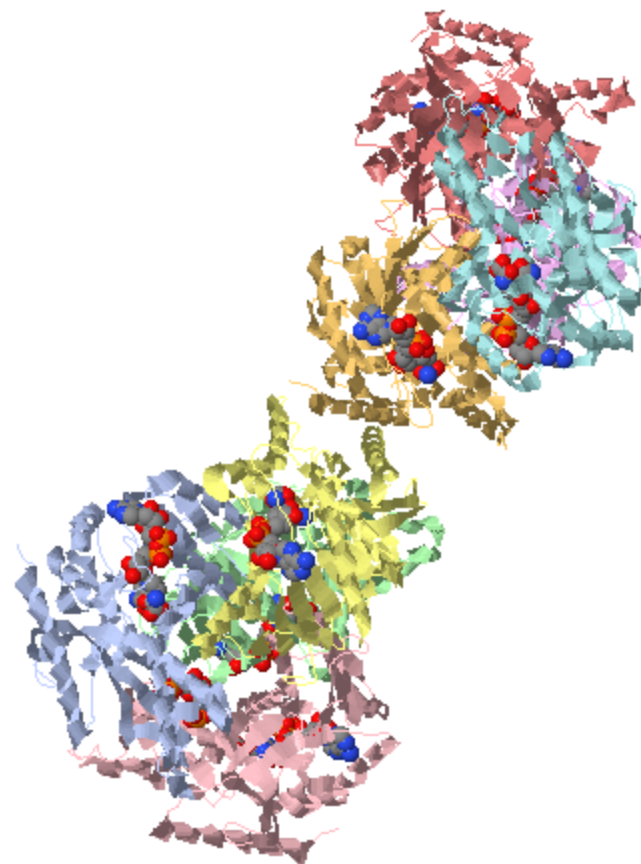
(Large molecules or multiple-model NMR data may need extra time to arrive.)

*Reloading/refreshing before you see the molecule sometimes prevents the molecule from ever appearing. To fix this, just close/quit your browser, and restart it.

196,491 Visitors

Since February 8, 2006

1LDN



Jmol

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[Query Management](#)
Introduction to ICSD Web

FIZ Karlsruhe provides the scientific and the industrial community with the world's largest database for inorganic crystal structures, ICSD, containing about 120,000 peer-reviewed data entries including their atomic coordinates dating back to 1913.

As the world's leading provider of scientific information on inorganic crystal structures, we take full responsibility for database production, maintenance and quality control, and we ensure that the ICSD database and our software solutions meet the highest possible quality standards.

At present, the ICSD contains:

- 1,400 crystal structures of the elements
- 23,000 records for binary compounds
- 42,500 records for ternary compounds
- 45,000 records for quarternary and quinquenary compounds
- About 90,000 entries (70,3%) have been assigned a structure type.

There are currently 4,860 structure prototypes. Detailed information on the ICSD may be found in the [scientific manual](#).

 ← [Select All](#) / [None](#) 2 Results

	Year ▲	Authors	Title	Struct. Formula	sgr	Mineral
<input checked="" type="checkbox"/>	2002	Post, J.E.; Heaney, P.J.; Hanson, J.;	Rietveld refinement of a triclinic structure for synthetic Na-birnessite using synchrotron powder diffraction data	Na _{0.58} Mn ₂ O ₄ (H ₂ O) _{1.5}	C1-	Birnessite
<input type="checkbox"/>	1994	Christensen, A.N.; Norby, P.; Hanson, J.C.;	A crystal structure determination fo Hg C ₂ O ₄ fom synchrotron, X-ray and neutron powder diffraction data	Hg C ₂ O ₄	P1211	

 Page : [1](2 results) results per page.

Na_{0.58}Mn₂O₄(H₂O)_{1.5}--Post, J.E. (2002)

C -1

a=5.175Å

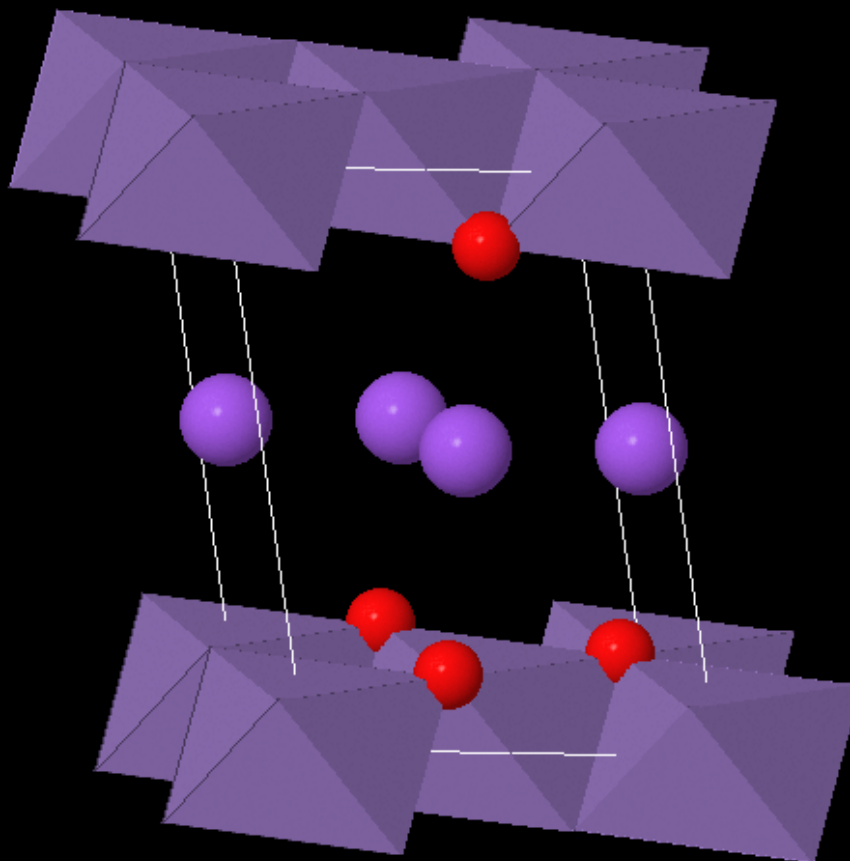
b=2.847Å

c=7.332Å

α=89.4°

β=103.2°

γ=89.9°



ICSD

Jmol

atoms 25% bond poly label persp stereo B/G Hbonds anim

cavities

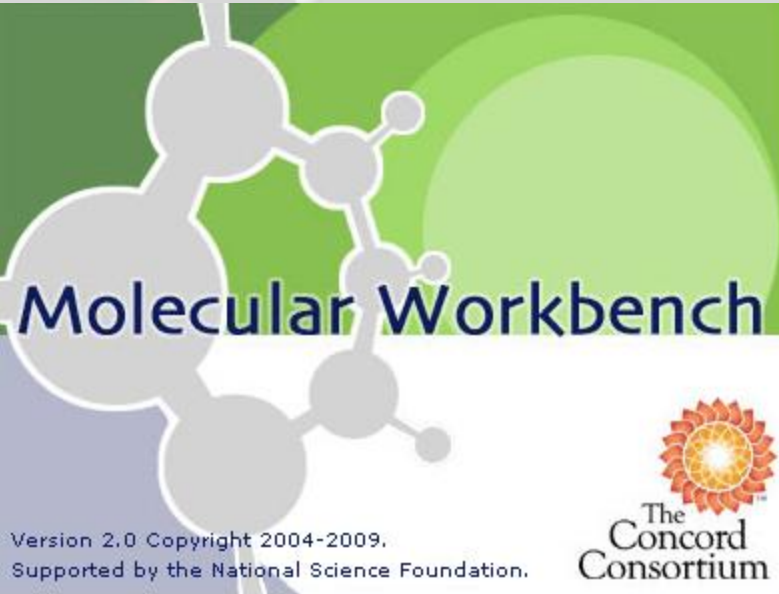
Select Create colour to a= b= c=

Local structure file: [HELP](#)

The Jmol Community


- Generally one of three focal points:
 - Research
 - Publishing
 - **Education**
 - High School
 - General chemistry
 - Organic chemistry
 - Biochemistry
 - Inorganic chemistry
 - Computational chemistry

The Molecular Workbench



Molecular Workbench

Version 2.0 Copyright 2004-2009.
Supported by the National Science Foundation.



The
Concord
Consortium

Testing connection to the main MW server...

The Molecular Workbench

Phase Change: Summary Questions

< PREV

PAGE

index

1

2

3

4

5

6

7

8

9



In this activity you have learned about the arrangement and movement of atoms and molecules in each state of matter, the role of the intermolecular attractions in phase change, and about how energy relates to changing phases of matter. Please answer the questions below to summarize what you have learned.

What to do?

- (1) Press the "Run" button.
- (2) Press the "Heat" or "Cool" button below to add energy.
- (3) Take snapshots that represent solid, gas, and liquid states.
- (4) Fill in snapshot images at the three questions below.

0 ps

Run Stop Reset

Heat Cool Take a snapshot

Symmetry Resources

- [Symmetry Tutorial](#)
- [Symmetry Gallery](#)
- [Symmetry Challenge](#)

Information

- [User's Guide](#)
- [Teaching Ideas](#)
- [References and Links](#)
- [Technical Details](#)

Feedback

- [Feature Request](#)
- [Molecule Request](#)

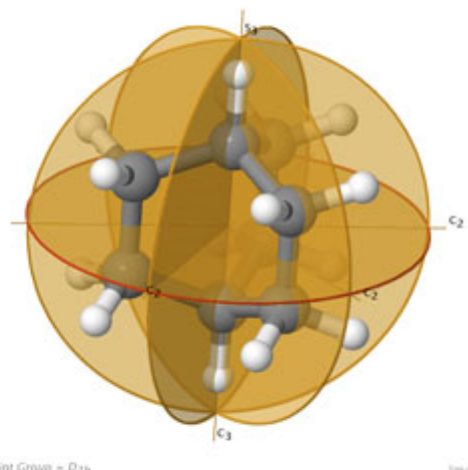


This project supported by
NSF-DUE #0536710

Symmetry Resources at Otterbein College

Welcome to the world of symmetry! The resources contained within this web site are designed to help students *learn* concepts of molecular symmetry and to help faculty *teach* concepts of molecular symmetry. The materials are designed for a variety of levels, so look around and see what we have to offer. Choose from the following pages:

- [Symmetry Tutorial](#) - An interactive point group symmetry tutorial. Guides students through all of the symmetry elements and operations, with interactive displays and animations.
- [The Symmetry Gallery](#) - A collection of nearly 70 unique molecules with interactive display of all symmetry elements and animation of all operations. The molecules are organized by point group, so you can select examples to demonstrate particular symmetry elements. Includes links to the chemical literature when available.
- [The Symmetry Challenge](#) - Using the same set of molecules from the Gallery, the Challenge includes a flow chart that details the process of determining the point group of each molecule. A great way to practice the point group determination process.



System Requirements: All pages require a modern browser with both Java and Javascript enabled. These pages have been extensively tested with Internet Explorer 6, 7 and 8 (PC), Safari 3 and 4 (Mac & Windows), and Firefox 1.x - 3.x (PC, Mac, Linux).

Updates: Some errors in various structures have been corrected (thanks Andy!). The "flickering" during animations in Safari has been fixed. Everything appears to now be working in IE8.

entry level ?

expanded valence ?

include metals ?

pi complexes ?

cool shapes ?

full database ?

CoolMolecules: A Molecular Structure Explorer

Search by...

atoms ?

bonds ?

shape ?

method ?

text ?

source ?

All of the 962 structures in **the full database** are actual, experimentally-determined structures. They are displayed TO SCALE (100 pm = 1 cm on my screen). You can rotate them around to see them from different angles, and you can double click on them to check bond lengths and angles right on the model itself. If the model doesn't display, you may

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	H																	He
2	Li	Be											B	C	N	O	F	Ne
3	Na	Mg	transition metals										Al	Si	P	S	Cl	Ar
4	K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
5	Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
6	Cs	Ba	Lu	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
7	Fr	Ra	Lr	Rf	Db	Sg	Bh	Hs	Mt									
lanthanides			La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb		
actinides			Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No		

PICK ALL

CLEAR

To begin, select one or more elements, rows, columns, or blocks of the periodic table.
Or you can choose to search by bonds, shape, experimental method, or text.

See <http://www.stolaf.edu/depts/chemistry/mo/struc> for more information about this database.

Teachers: See [the topics page](#) to get ideas for how to use this in class.

page last updated: 4/28/2006

Please report all problems to [Bob](#).

Thanks.

entry level ?

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cool shapes ?

full database ?

CoolMolecules: A Molecular Structure Explorer

Search by...

atoms ?

bonds ?

shape ?

method ?

text ?

source ?

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	H																	He
2	Li	Be											B	C	N	O	F	Ne
3	Na	Mg	transition metals										Al	Si	P	S	Cl	Ar
4	K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
5	Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
6	Cs	Ba	Lu	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
7	Fr	Ra	Lr	Rf	Db	Sg	Bh	Hs	Mt									
			lanthanides	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	
			actinides	Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	

PICK ALL

CLEAR

4 structures have nickel either in a central location or connected to it.
Of these, all have nickel in a central location.

sort by: center atom shape[View All](#) details

Ni <i>tetrahedral</i>	(CO) ₄ Ni	tetracarbonylnickel(0) (nickel carbonyl)	info view CCDC pdf
Ni <i>octahedral</i>	(C ₂ H ₈ N ₂) ₂ NiBr ₂	trans- dibromo- bis(ethylenediamine)nickel(II)	info view CCDC pdf
Ni <i>octahedral</i>	Ni(C ₁₂ H ₈ N ₂) ₃ ²⁺	tris(1,10- phenanthroline)nickel(II) cation	info view CCDC pdf
Ni <i>A(X-ar)2</i>	Ni(C ₅ H ₅) ₂	bis(<i>η</i> ⁵ - cyclopentadienyl)nickel(II) (nickelocene)	info view CCDC

All of the 962 structures in **the full database** are actual, experimentally-determined structures. They are displayed TO SCALE (100 pm = 1 cm on my screen). You can rotate them around to see them from different angles, and you can double click on them to check bond lengths and angles right on the model itself. If the model doesn't display, you may

$(C_2H_8N_2)_2NiBr_2$

name trans- dibromo- bis(ethylene diamine)nickel(II)
shape octahedral
method x-ray diffraction
reference M. Yamashita, E. Tsuruta, K. Inoue, M. Oyama,
K. Toriumi, Inorganic Chemistry, 32, 363, 1993

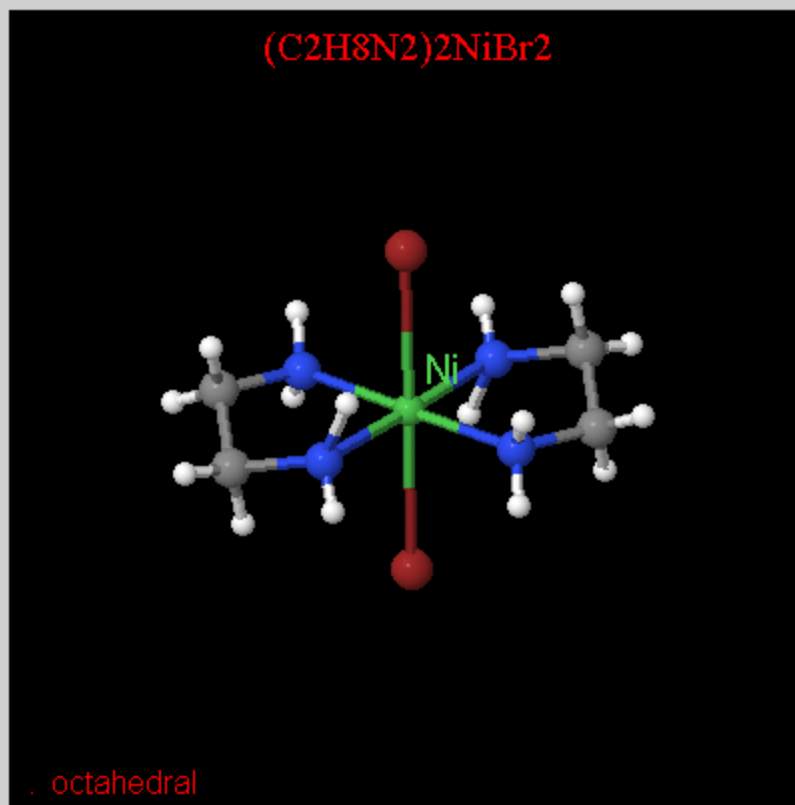
CCDC entry SUGSUI

filename [tNien2Br2.mol](#)

direct link [tNien2Br2&view=1](#)

distance Br-Ni = 263.5 pm
distance N-Ni = 193.6 pm
distance N-Ni = 195.2 pm

angle Br-Ni-Br = 180
angle Br-Ni-N = 89.1
angle Br-Ni-N = 89.8
angle Br-Ni-N = 90.2
angle Br-Ni-N = 90.9
angle N-Ni-N = 180
angle N-Ni-N = 86.5
angle N-Ni-N = 93.5



100 pm (1.00 Angstroms)

[\[clear labels\]](#) [\[zoom in\]](#) [\[zoom out\]](#)

[\[send script\]](#) [\[big model\]](#)

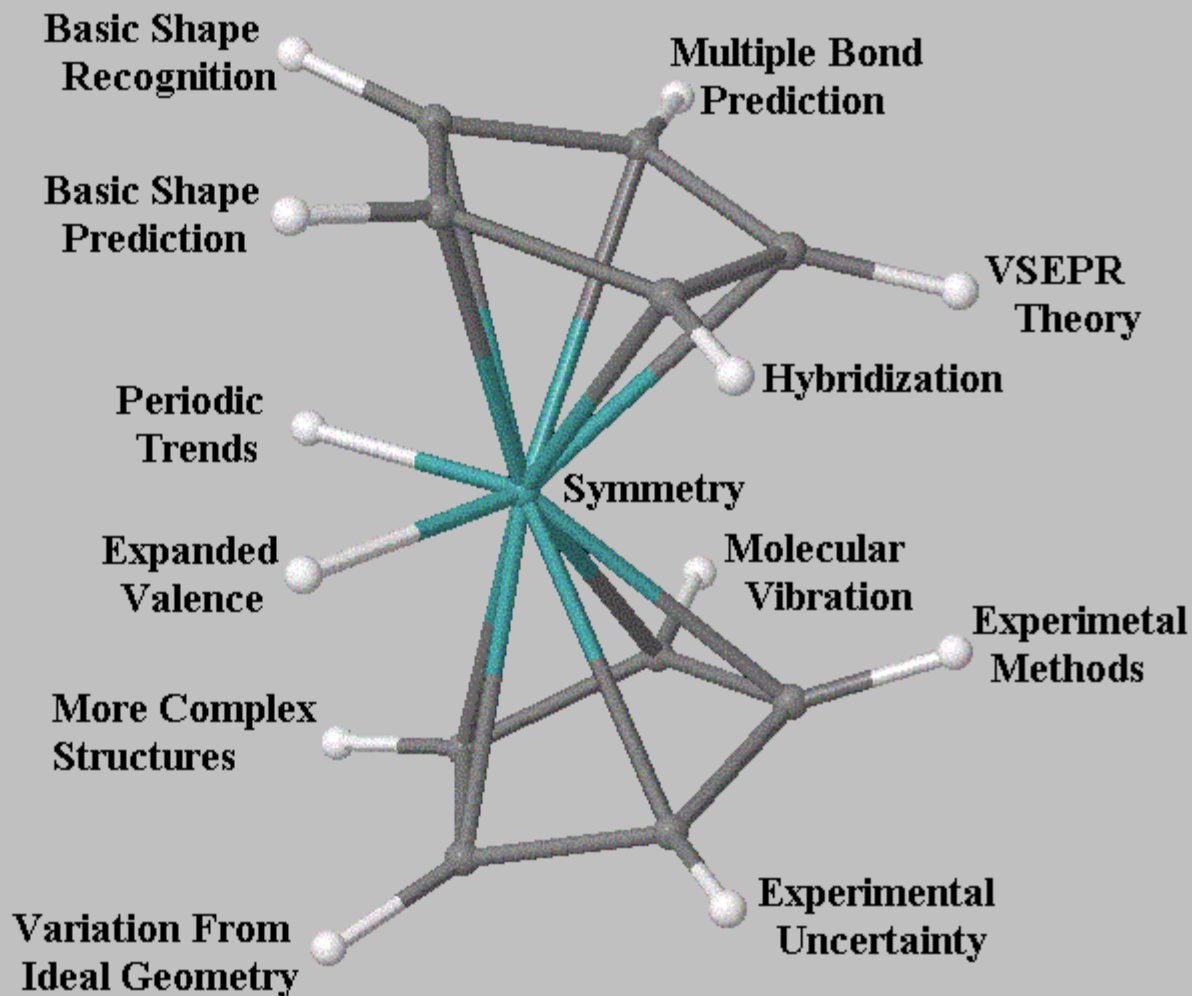
[\[previous\]](#)

2/4

[\[next\]](#)

CoolMolecules

Select a Topic to View
Suggested Class Activities



CoolMolecules



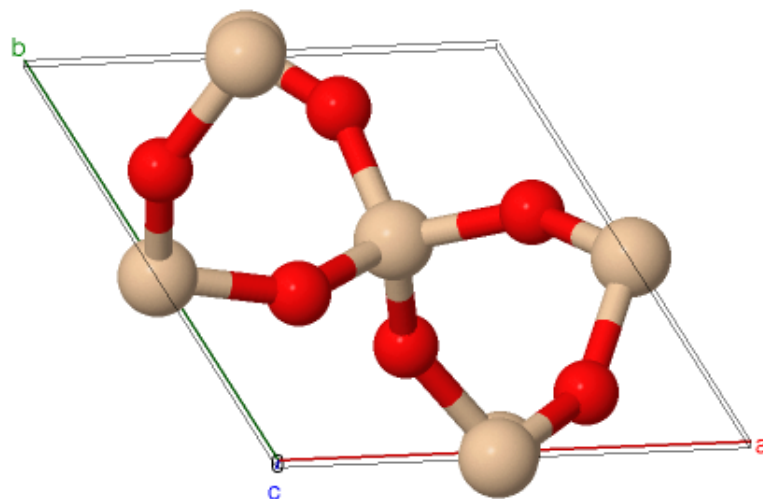
Mike McGuan

Melanie Casavant

P 32 2 1
 a=4.916Å
 b=4.916Å
 c=5.405Å
 $\alpha=90.0^\circ$
 $\beta=90.0^\circ$
 $\gamma=120.0^\circ$

Jmol Crystal Symmetry Explorer

load "" 1 packed
 load "" 1 {555 555 1
 load "" 1 {444 666 1
 load "" 1 {455 655 1
 load "" 1 {545 565 1
 load "" 1 {554 556 1
 load "" 1 {445 665 1
 load "" 1 {454 666 1
 load "" 1 {544 566 1
 background



quartz.cif

Hermann-Mauguin symbol: P 32
 2 1

international table number: 154

Hall symbol: P 32 2"

lattice type: P: primitive

6 operators

select a symmetry operation

show atoms

select an atom or position

Load URL or FILE

Load SCRIPT

Save FILE

Save STATE

Save JPG

Save PNG

console

Execute

Jmol

mol script terminated