

J-ICE : Follow Geometry OPT. - 1

1. Load the desired output

Release 2.0 by P. Canepa - powered by **Jmol** Help | Acknowledgments

FILE APP. EDIT BUILD MEAS. ORIENT. CELL POLY. ISOSUR. GEOM. FREQ. E&M MAIN

P 1 [P 1]
a=5.435Å
b=5.435Å
c=5.435Å
α=55.2°
β=55.2°
γ=55.2°

Energy = -5499.5076871799 Hartree

Filename:
Reload **Reset** **Console** **New window** **File content** **Save state** **Restore state** **Feedback**

Jmol_S

FILE MANAGER

Load File
Load New FILE

Upload/Save File
Export File

JICE

Please DO CITE:

*J-ICE: a new Jmol interface for handling and visualizing Crystallographic and Electronics properties.
P. Canepa, R.M. Hanson, P. Ugliengo, M. Alfredsson, J. Appl. Cryst., (2011), 44 [doi] *

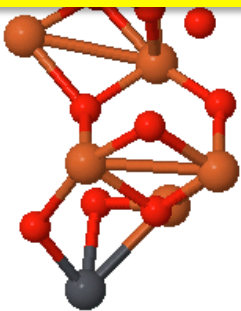
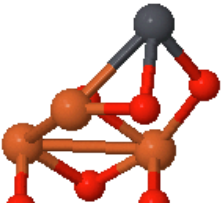
J-ICE : Follow Geometry OPT. - 2

2. Move to GEOM.

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FILE APP. EDIT BUILD MEAS. ORIENT. CELL POLY. ISOSURF **GEOM.** FREQ. E&M MAIN

slab
a=5.084Å
b=5.083Å
γ=120.0°



Energy = -16522.799492072 Hartree

Filename: file:/Users/pieremanuelecanepa/PhD-Kent/J-ICE/Sample-files/CRYSTAL/GEOM/Pb_top_triangle_rex

Reload Reset Console New window File content Save state Restore state Feedback

show Geometry Optimizations. Help Acknowledgments

GEOMETRY OPTIMIZATION

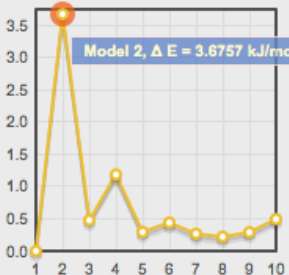
<< > || >> loop palindrome

select motion speed | save video frames

Energy unit measure: Hartree

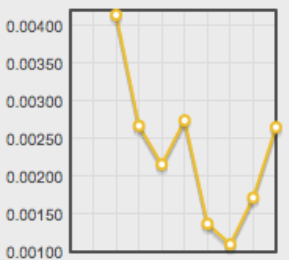
1	Energy = -16522.799310171 Hartree
2	Energy = -16522.799492072 Hartree
3	Energy = -16522.79994405 Hartree
4	Energy = -16522.800056578 Hartree
5	Energy = -16522.800224483 Hartree
6	Energy = -16522.800326359 Hartree
7	Energy = -16522.800410605 Hartree
8	Energy = -16522.800521357 Hartree
9	Energy = -16522.800710205 Hartree
10	Energy = -16522.800710205 Hartree

ΔE (kJ/mol)



Model 2, ΔE = 3.6757 kJ/mol

ForceMax



Jmol_S

J-ICE : Follow Geometry OPT. - 3

3. Select specific geom. point, watch geom. opt., etc.

The screenshot shows the Jmol web interface for following geometry optimizations. The interface includes a menu bar (FILE, APP, EDIT, BUILD, MEAS., ORIENT., CELL, POLY, ISOSUR., GEOM., FREQ., E&M, MAIN) and a title bar (Release 2.0 by Pieremanuele Canepa - powered by Jmol, Follow Geometry Optimizations., Help | Acknowledgments). The main content area is titled 'GEOMETRY OPTIMIZATION' and features several controls and data displays:

- Geometry controls:** A set of navigation buttons (back, forward, play, stop) and options for 'loop' and 'palindrome' are circled in yellow.
- Selectable models list:** A list of optimization steps with their corresponding energy values in Hartrees. The second step is highlighted in orange. This list is also circled in yellow.
- Selectable ΔE chart:** A line graph showing the energy difference (ΔE) in kJ/mol over 10 optimization steps. A blue box highlights the second step with a value of $\Delta E = 3.6757$ kJ/mol. This chart is circled in yellow.
- Selectable Force dumping chart:** A line graph showing the maximum force (ForceMax) over 10 optimization steps. This chart is also circled in yellow.

Annotations on the left side of the interface include:

- A blue box labeled 'Geometry controls' with an arrow pointing to the navigation buttons.
- A blue box labeled 'Selectable models list' with an arrow pointing to the optimization steps list.
- A blue box labeled 'Selectable ΔE chart' with an arrow pointing to the energy difference graph.
- A blue box labeled 'Selectable Force dumping chart' with an arrow pointing to the force graph.

A yellow box on the right side contains the text: 'Forces dumping is only available for CRYSTAL geometry optimizations'. A red arrow points from this box towards the force dumping chart.

At the bottom of the interface, there is a status bar with buttons for 'Reload', 'Reset', 'Console', 'New window', 'File content', 'Save state', 'Restore state', and 'Feedback'. The text 'CRYSTAL/GEOM/Pb_top_triangle_re' is visible in the status bar.