

J-ICE : Cell properties - 1

1. Load the desired output

Import, Export Files.
Release 2.0.0 by Pieremanuele Canepa - powered by Jmol [Help](#) | [Acknowledgments](#)

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

Load File
Load New FILE

Export/Save File
Export File

JICE

Hematite or $\alpha\text{-Fe}_2\text{O}_3$

Energy = -5499.5076871799 Hartree

Jmol_S

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] *

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

J-ICE : Cell properties - 2

2. Move to Cell

Release 2.0 by Pieremanuele Canepa - powered by Jmol

Modify Cell Features And Symmetry. Help | Acknowledgments

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

CELL PROPERTIES

P 1 [P 1]
a=5.4
b=5.4
c=5.4
α=55.
β=55.
γ=55.

CRYSTAL CALCULATION
(INPUT ACCORDING TO THE INTERNATIONAL TABLES FOR X-RAY CRYSTALLOGRAPHY)

CRYSTAL FAMILY : HEXAGONAL

CRYSTAL CLASS (GROTH - 1921) : DITRIGONAL SCALENOHEDRAL

SPACE GROUP (CENTROSYMMETRIC) : R -3 C

Common sets 0 0 0
+ Advanced cell-offset options

Cell parameters (selected model)
Unit: Å Bohr
a 5.4345846 b 5.4345846 c 5.4345846
α 55.22805 β 55.22805 γ 55.22805 degrees

Volume cell 100.90737 Å³

+ Advanced options

Symmetry operators

Hermann-Mauguin symbol: P 1
International number: 1
lattice type: Primitive
Symmetry operators: 1

The screenshot shows the Jmol software interface. The 'CELL' menu item is highlighted with a yellow circle. A yellow box highlights the crystallographic data: 'CRYSTAL FAMILY : HEXAGONAL', 'CRYSTAL CLASS (GROTH - 1921) : DITRIGONAL SCALENOHEDRAL', and 'SPACE GROUP (CENTROSYMMETRIC) : R -3 C'. A 3D ball-and-stick model of a Hematite molecule is shown with a red arrow pointing upwards. A yellow box highlights the 'Cell parameters (selected model)' section, which includes unit, a, b, c, α, β, γ values. A red arrow points to the 'Advanced options' section.

Hematite or $\alpha\text{-Fe}_2\text{O}_3$ has a rhombohedral primitive cell

J-ICE : Cell properties - 3

3. Conventional and primitive cell

The screenshot displays the Jmol software interface. At the top, the title bar reads "Release 2.0 by Pieremanuele Canepa - powered by Jmol" and "Modify Cell Features And Symmetry." The menu bar includes FILE, APP., EDIT, BUILD, MEAS., ORIENT., CELL, POLY., ISOSUR., GEOM., FREQ., E&M, and MAIN. The main window shows a 3D ball-and-stick model of a crystal structure with axes labeled a, b, and c. A yellow box highlights the cell parameters in the top-left corner:

```
-R 3 2" c [R -3 c:h]
a=5.038Å
b=5.038Å
c=13.772Å
α=90.0°
β=90.0°
γ=120.0°
```

On the right, the "CELL PROPERTIES" panel is visible. A yellow box highlights the "Set cell:" section, which includes radio buttons for "primitive" and "conventional" (selected), and checkboxes for "Auto Pack" and "Choose Pack Range". A red arrow points from this section to the 3D model. Below the model, a yellow box contains the text: "Hexagonal primitive cell: useful for representations". Another red arrow points from the "Set cell:" section to the "Supercell:" section, which has a yellow box around it. Below the supercell section, another yellow box contains the text: "Swap between primitive and convectional cell". The bottom of the interface shows a "Filename:" field and buttons for "Reload", "Reset", "Console", "New window", "File content", "Save state", "Restore state", and "Feedback".

J-ICE : Cell properties - 4

4. Represent operators which allow to build the entire lattice

Release 2.0 by Pieremanuele Canepa - powered by **Jmol**

Modify Cell Features And Symmetry

Help | Acknowledgments

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

`-R 3 2" c [R -3 c:h]`
a=5.038Å
b=5.038Å
c=13.772Å
α=90.0°
β=90.0°
γ=120.0°

24: x,x-y,z+1/2
c-glide plane
translation: 0 0 1/2

View Cell View axes
Cell style: size 1 dotted dotted, color
Set cell: primitive conventional
 Auto Pack Choose Pack Range

Supercell:
a: b: c: A force supercell (P1)
pack

Offset unitcell
Common sets 0 0 0
+ Advanced cell-offset options

Cell parameters (selected model)
Unit: Å Bohr
a 5.038 b 5.038 c 13.771999
α 90 β 90 γ 120 degrees
Volume cell 302.722 Å³
+ Advanced cell options

Symmetry operators
Hermann-Mauguin symbol: R -3 c:h
International table number: 167:h
lattice type: -R: centrosymmetric rhombohedral
Symmetry operators: 36
24: c-glide plane (x,x-y,z+1/2)
#3 Fe3 { 0.67 0.33 0.98/1 }
 superimpose atoms opacity: 20%

Overlay operators representations on the current structure

Jmol's

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

J-ICE : Cell properties - 5

5. Many other options

The screenshot displays the Jmol software interface. At the top, a menu bar includes FILE, APP, EDIT, BUILD, MEAS., ORIENT., CELL, POLY., ISOSUR., GEOM., FREQ., E&M, and MAIN. A sub-menu 'Modify Cell Features And Symmetry.' is open. The left panel shows crystallographic data: P 1 [P 1], a=5.435Å, b=5.435Å, c=5.435Å, α=55.2°, β=55.2°, γ=55.2°. The central 3D view shows a unit cell with axes a, b, and c, and a central iron atom (Fe) with its neighbors. The energy is -5499.5076871799 Hartree. The bottom bar contains buttons: Reload, Reset, Console, New window, File content, Save state, Restore state, and Feedback.

CELL PROPERTIES

- View Cell View axes
- Cell style: size 1 dotted dotted, color
- Set cell: primitive conventional
- Auto Pack Choose Pack Range
- Supercell:
a: b: c: Å force supercell (P1)
- Offset unitcell
Common sets 0 0 0
 Advanced cell-offset options
- Cell parameters (selected model)
Unit: Å Bohr
a 5.4345846 b 5.4345846 c 5.4345846
α 55.22805 β 55.22805 γ 55.22805 degrees
Volume cell 100.90737 Å³
 Advanced cell options
- Symmetry operators
Hermann-Mauguin symbol: P 1
International table number: 1
lattice type: P: primitive
Symmetry operators: 1
select a symmetry operation
#1 Fe { 0.36 0.36 0.36/1 }
 superimpose atoms opacity: 20%