

# J-ICE - Tutorial: Look and feeling

File

App.

Edit

Build

Meas.

Orient.

Cell

Poly.

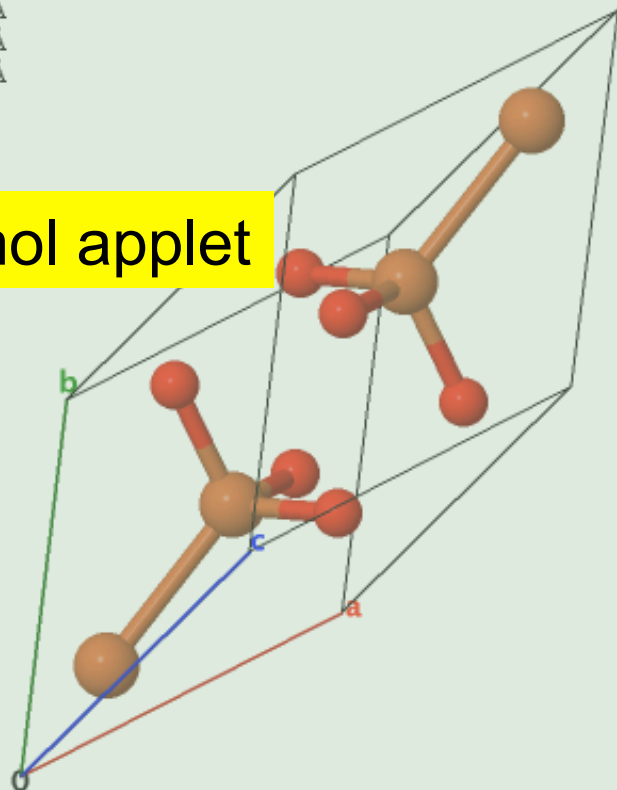
IsoSur.

2

Widget Menu

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

Jmol applet



1

File manager

Load File

Load New FILE

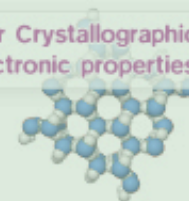
3

Export/Save File

Export File



Jmol Interface for Crystallographic and Electronic properties



release 1.0.5  
by Pieremanuele Canepa

powered by Jmol

Interactive Palette

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, submitted to J. Appl. Cryst., (2011), 44 [doi] "

Jmol\_S

Control Bar

Filename: <http://j-ice.sourceforge.net/ondemand/output/hematite.out>

Reload

Reset

Console

New window

File content

Save state

Restore state

Feedback

Acknowledgement

4

# J-ICE - Tutorial: Import & Export

**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  
 $\alpha=55.2^\circ$   
 $\beta=55.2^\circ$   
 $\gamma=55.2^\circ$

**Import Export**

**File manager**

Load File  
Load New FILE

Export/Save File  
Export File

Jmol Interface for Crystallographic and Electronic properties

**J-ICE**

release 1.0.5  
by Pieremanuele Canepa

powered by Jmol

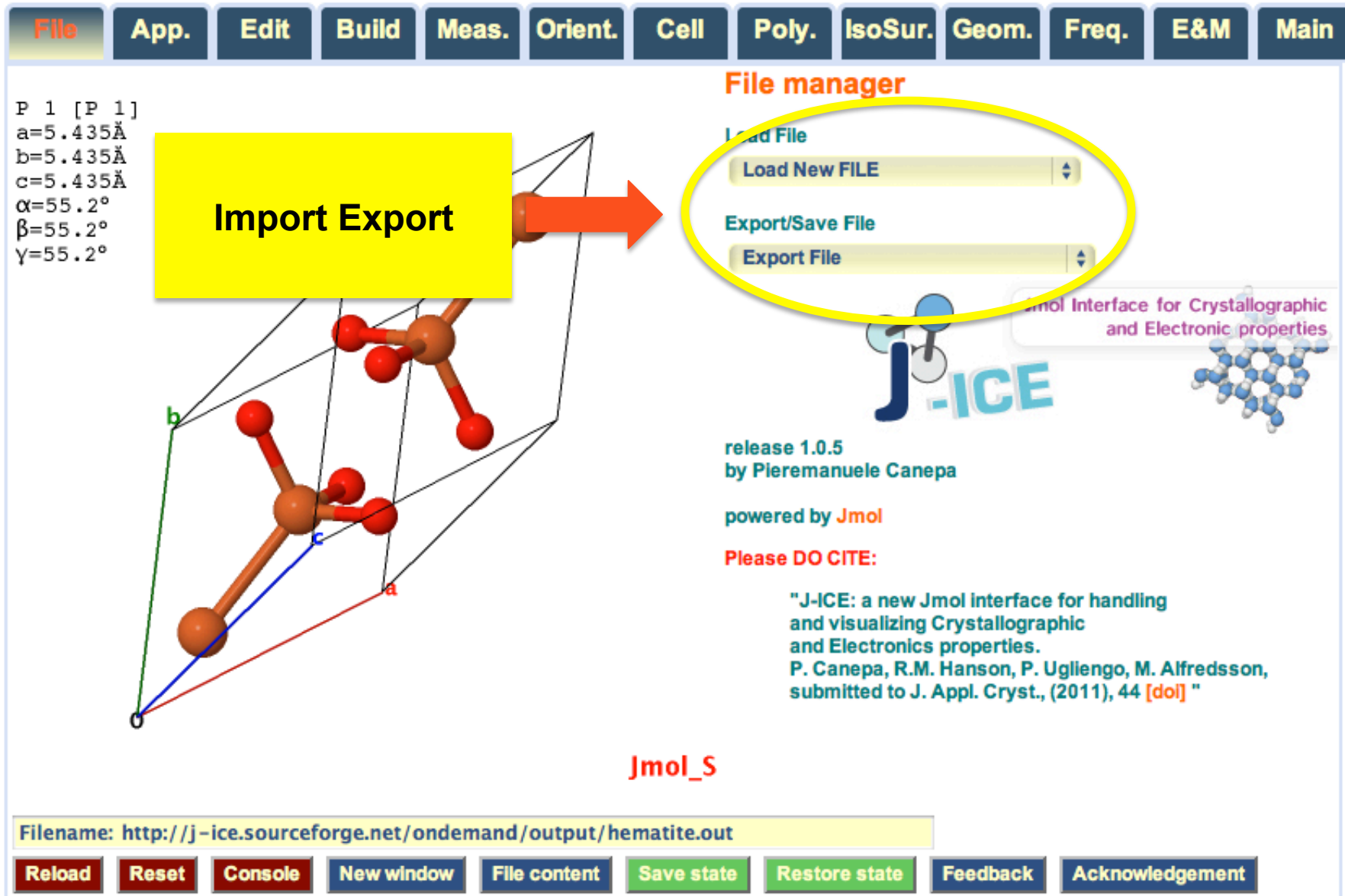
Please DO CITE:

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

**Jmol\_S**

Filename: <http://j-ice.sourceforge.net/ondemand/output/hematite.out>

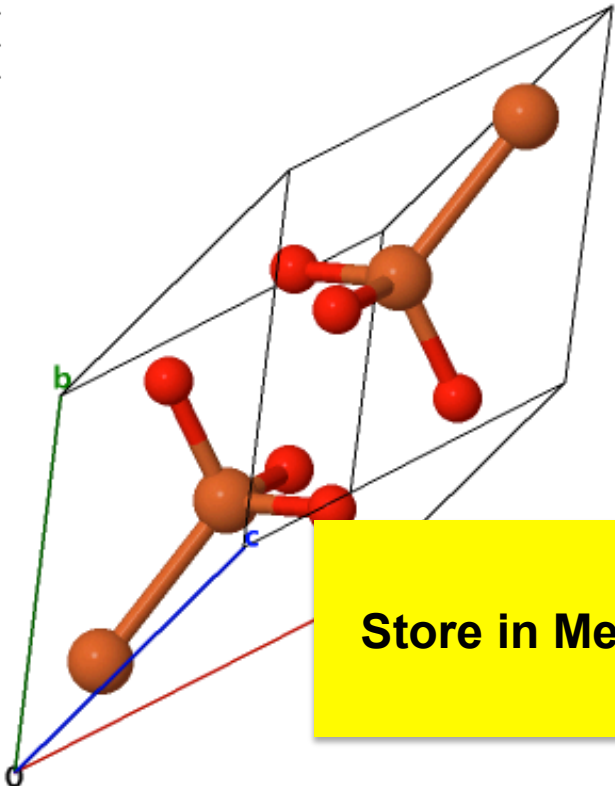
**Reload** **Reset** **Console** **New window** **File content** **Save state** **Restore state** **Feedback** **Acknowledgement**



# J-ICE - Tutorial: Save temporary

**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  
 $\alpha=55.2^\circ$   
 $\beta=55.2^\circ$   
 $\gamma=55.2^\circ$



**File manager**

Load File  
Load New FILE

Export/Save File  
Export File

Jmol Interface for Crystallographic and Electronic properties

release 1.0.5  
by Pieremanuele Canepa

powered by Jmol

Please D

Alfredsson,  
Submitted to: Appl. Cryst., (2011), 44 [doi]

**Store in Memory**

**Re-store**

1

2

Filename: <http://j-ice.sourceforge.net/ondemand/output/hemite1000>

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

# J-ICE - Tutorial: Save permanently - 1

**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°
```

**1**

Carry out changes to your structures, maps or whatsoever

Save current state

**2**

**File manager**

Load File

Load New FILE

Export/Save File

Export File

- Export File
- CASTEP (\*.cell)
- CRYSTAL (\*.d12)
- GULP (\*.gln)
- GROMACS (\*.gro)
- PWscf QUANTUM espresso (\*.inp)
- VASP (POSCAR)
- coordinates XYZ (\*.XYZ)
- frac. coordinates (\*.XYZfrac)
- image PNG (\*.png)
- coordinates PDB (\*.PDB)
- image POV-ray (\*.pov)
- current state (\*.spt)**

Interface for Crystallographic and Electronic properties

Jmol\_S

Filename: <http://j-ice.sourceforge.net/ondemand/output/hematite.out>

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

# J-ICE - Tutorial: Reload - 2

**File** **App.** **Edit** **Build** **Meas.** **Orient.** **Cell** **Poly.** **IsoSur.** **Geom.** **Freq.** **E&M** **Main**

```
P 1
a=5
b=5
c=5
α=5
β=5
γ=55.2°
set pdbSequential false;
set percentVdwAtom 23;
set smallMoleculeMolMass 10000;
set smartAromatic true;
load /*file*/"file:/Users/pieremanuelecane/HAP_fullopt_40_r1.fullopt.out" /*options*/ {555 555 -1} PACKED;
}

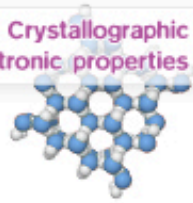
function _setVariableState() {
set defaultanglelabel "%VALUE %UNITS";
set defaultcolorscheme "jmol";
}
```

**File manager**


Load File

- Load New FILE
- Load New FILE
- Load generic (\*.\*)
- Load CIF (\*.cif)

Interface for Crystallographic and Electronic properties



Reload prev. state



- Load VASP (OUTCAR)
- Load VASP (\*.xml)
- Load WIEN2k (\*.struct)
- Load map (\*.cube)
- Load map (\*.jvxl)
- Load state (\*.spt)

P. Canepa, R.M. Hanson, P. Ugliengo, M. Alfredsson, Submitted to Appl. Cryst., (2011), 44 [doi]

**Jmol\_S**

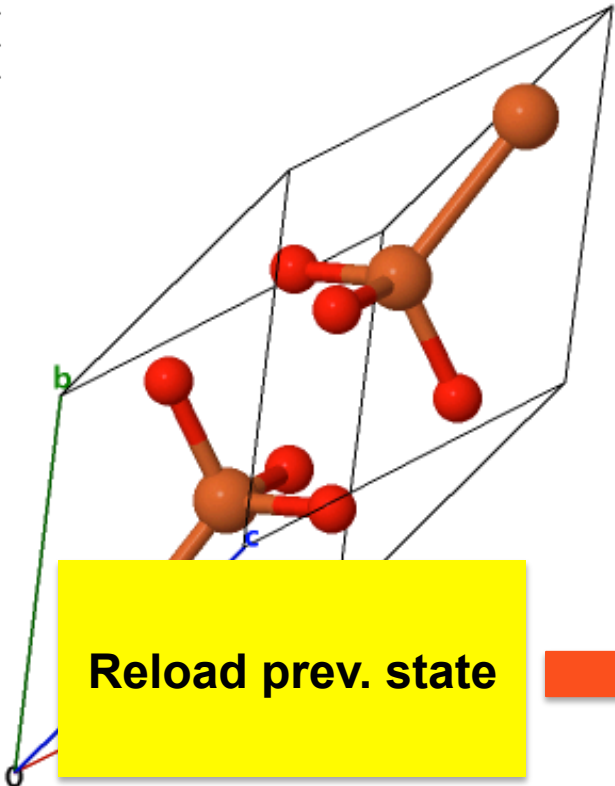
Filename: <http://j-ice.sourceforge.net/ondemand/output/hematite.out>

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

# J-ICE - Tutorial: Reload - 3

**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  
 $\alpha=55.2^\circ$   
 $\beta=55.2^\circ$   
 $\gamma=55.2^\circ$

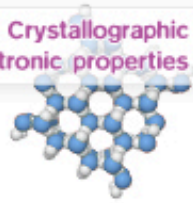


**File manager**

Load File

- Load New FILE
- Load New FILE
- Load generic (\*.\*)
- Load CIF (\*.cif)
- Load XYZ (\*.XYZ)
- Load CASTEP (\*.cell)
- Load CRYSTAL (\*.out)
- Load FHI-aims (\*.in)
- Load GAUSSIAN0X (\*.\*)
- Load GROMACS (\*.gro)
- Load GULP (\*.gout)
- Load Material Studio (\*.\*)
- Load PDB (\*.pdb)
- Load QuantumESPRESSO (\*.out)
- Load ShelX (\*.\*)
- Load VASP (OUTCAR)
- Load VASP (\*.xml)
- Load WIEN2k (\*.struct)
- Load map (\*.cube)
- Load map (\*.jvxl)
- Load state (\*.spt)**

Interface for Crystallographic and Electronic properties



P. Canepa, R.M. Hanson, P. Ungaro, M. Alfredsson, Submitted to Appl. Cryst., (2011), 44 [doi]

**Jmol\_S**

Filename: <http://j-ice.sourceforge.net/ondemand/output/hematite.out>

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