

J-ICE : Mulliken Charges - 1

1. Load the desired output

The screenshot displays the J-ICE web interface. At the top, a navigation menu includes 'FILE', 'APP.', 'EDIT', 'BUILD', 'MEAS.', 'ORIENT.', 'CELL', 'POLY.', 'ISOSUR.', 'GEOM.', 'FREQ.', 'E&M', and 'MAIN'. The 'FILE' menu is highlighted with a yellow circle. On the left, crystallographic data is shown: 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 model shows Hematite (α-Fe₂O₃) with iron (Fe) atoms in orange and oxygen (O) atoms in red. A yellow banner at the bottom of the model reads 'Hematite or α-Fe₂O₃'. The energy is listed as -5499.5076871799 Hartree. The 'Jmol_S' logo is visible. On the right, a 'FILE MANAGER' panel is highlighted with a yellow circle, containing 'Load File' and 'Export File' dropdown menus. The JICE logo is also present. At the bottom right, a citation is provided: '*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] *'. A footer bar at the bottom contains buttons for 'Reload', 'Reset', 'Console', 'New window', 'File content', 'Save state', 'Restore state', and 'Feedback'.

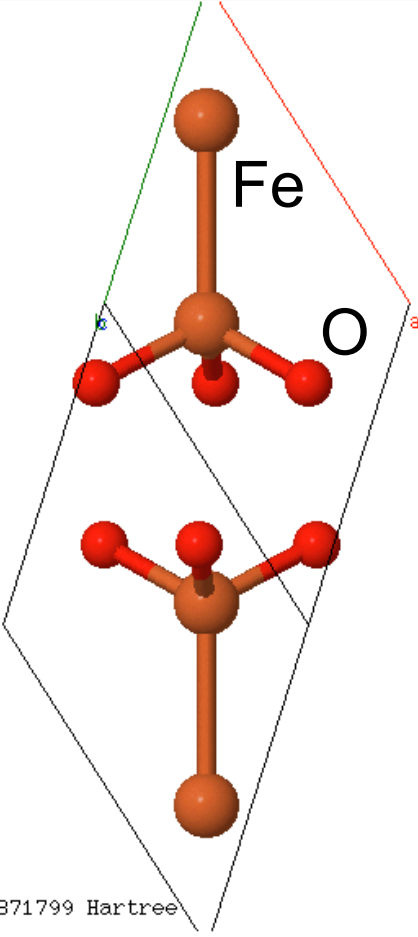
J-ICE : Mulliken Charges - 2

2. Move to E&M

Release 2.0 by Pieremanuele Canepa - powered by Jmol

FILE APP. EDIT BUILD MEAS. ORIENT. CELL POLY. ISOSUR. GEOM. FREQ. **Superimpose Mulliken Charges, Spin, Magnetic Moment Onto Your Structure.** Acknowledgments

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



Fe O

Energy = -5499.5076871799 Hartree

Jmol_S

Filename: [Reload](#) [Reset](#) [Console](#) [New window](#) [File content](#) [Save state](#) [Restore state](#) [Feedback](#)

ELECTRONIC - MAGNETIC PROPERTIES

Mulliken population analysis
[view Mulliken](#)

Colour-scheme

Spin arrangement
[view Spin](#) [view Magnetic Moment](#)

View only atoms with spin

[Remove](#)

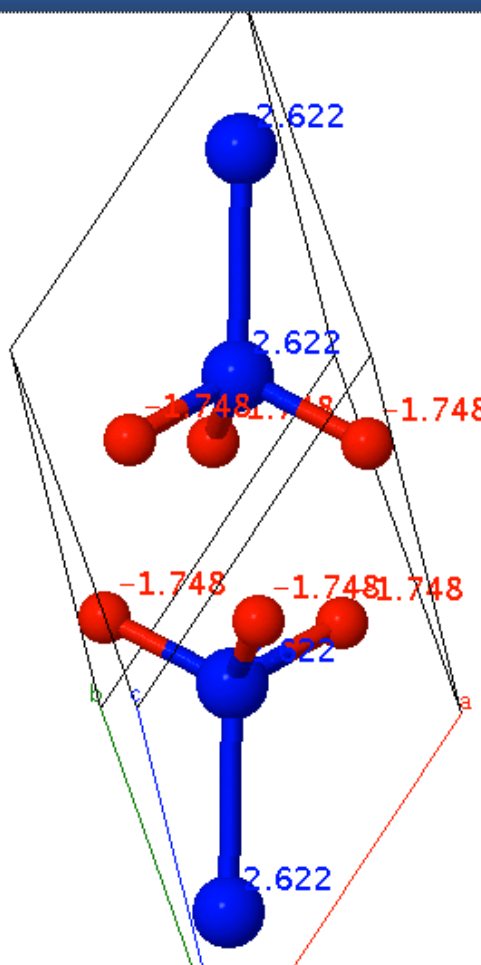
J-ICE : Mulliken Charges - 3

3. Superimpose Mulliken charges

Superimpose Mulliken Charges, Spin, Magnetic Moment Onto Your Structure. Acknowledgments

FILE APP. EDIT BUILD MEAS. ORIENT. CELL POLY. ISOSUR. GEOM. FREQ.

P 1 [P 1]
a=5.461Å
b=5.461Å
c=5.461Å
α=55.8°
β=55.8°
γ=55.8°



2.622
-1.748
-1.748
-1.748
-1.748
-1.748
2.622
2.622
2.622

ELECTRONIC - MAGNETIC PROPERTIES

Mulliken population analysis
view Mulliken

Colour-scheme Rainbow (default)

Spin arrangement
view Spin view Magnetic Moment

View only atoms with spin ↓ ↑

Remove

Mulliken Charges

Jmol_S

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

19th Jan 11 3