

Molecular Sophie Computer Simulation Software Suite Version 2.0.96-0.1 Build Date : 23-Oct-2007 09:51: [Simulation]

File Edit Project Simulation Molecule Atom Bond Experiment Log Help

Project Explorer Tree:

- Simulation 1
 - Mo Enzyme
 - Cytochrome C
 - N1
 - N2
 - N3
 - N4
 - N5
 - N6
 - N7
 - N8
 - Fe1
 - Fe2
 - Fe1-N1
 - Fe1-N2
 - Fe1-N3
 - Fe1-N4
 - Fe2-N5
 - MoCo
 - H1
 - O1
 - O2
 - S1
 - S2
 - Mo1
 - Mo1-O1
 - Mo1-S1
 - Mo1-S2
 - Mo1-O2
 - Mo1-H1
 - Iron Sulfur Cluster
 - S1

Atom Properties (Mo1):

Atomic Number: 42
Atomic Mass: 95.94
Isotopes: 24

Description: []

Electron Spin: 1/2

Spin Hamiltonian View Matrix

Linewidth Isotopes Position

Electron Zeeman Fine Structure Hyperfine Quadrupole

Hyperfine Name: []

Representation: Axial

Units: MHz

Axial

Parameter	Value	Vary	Minimum	Maximum
A_{\perp}	0.00800	<input type="checkbox"/>	0.00000	0.00610
A_{\parallel}	0.00800	<input type="checkbox"/>	0.00000	0.00610
α	0.00000	<input type="checkbox"/>	-0.0001	0.00010
β	0.00000	<input type="checkbox"/>	-0.0001	0.00010

Simulation % Completion / Isotope Combination

Atom Node: Use MB3 to Delete|Cut|Copy the Atom from the Molecule.

Figure 15. Molecular Sophie Graphical User Interface showing the Explorer Tree and the Axial Hyperfine Interaction Form.