

Crystal Structure:

Dy (Hexagonal Closed Pack)

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CIF Source:

Spedding F H, Daane A H, Herrmann K W

Acta Crystallographica 9 (1956) 559-563

The crystal structures and lattice parameters of high-purity scandium, yttrium and the rare earth metals

Locality: synthetic

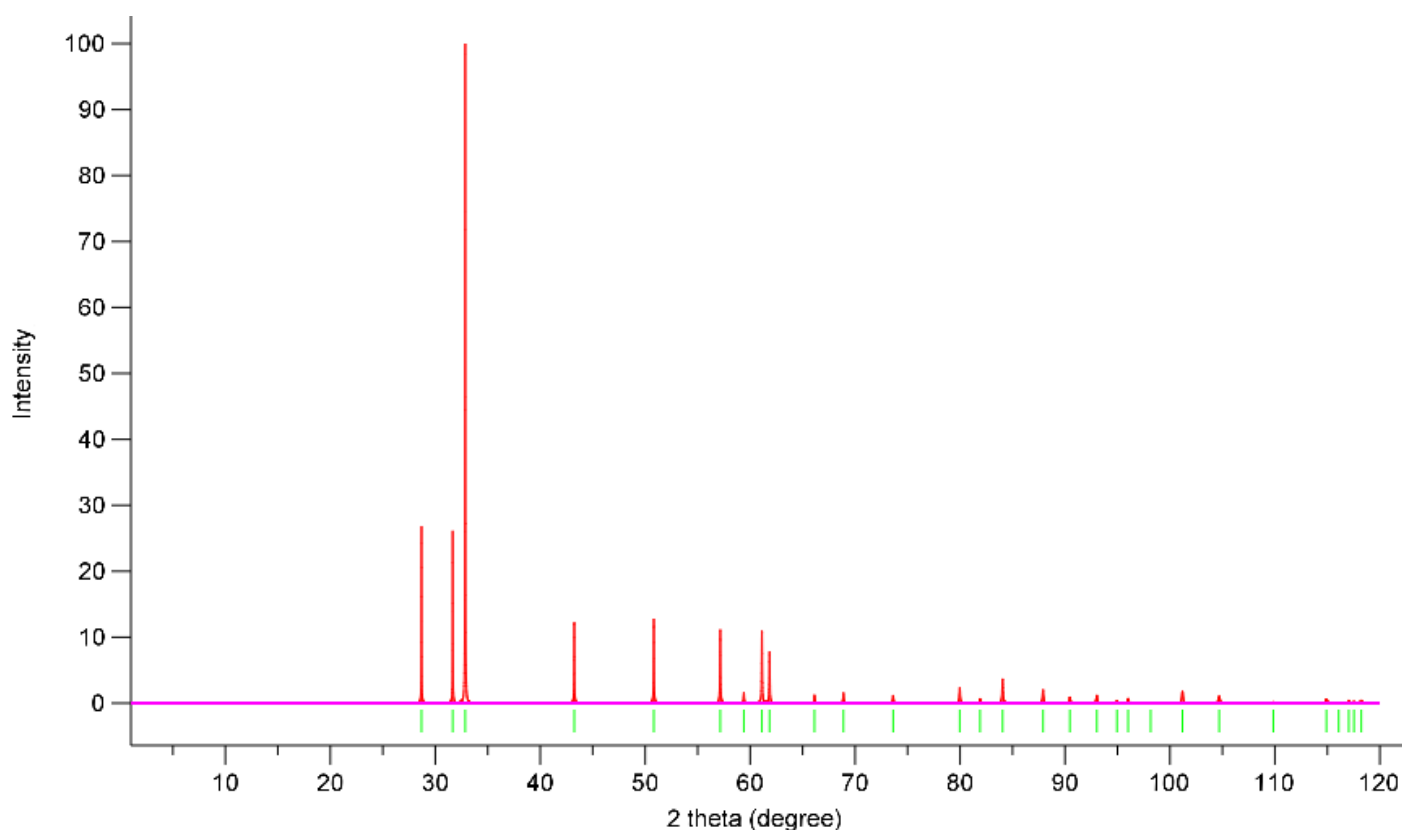
Note: sample 99.8% pure

_database_code_amcsd 0009175

<http://rruff.geo.arizona.edu/AMS/download.php?id=10420.cif&down=cif>

Simulated Powder XRD using VESTA:

X-Ray Wavelength: 1.54059 Angstrom



Powder XRD pattern simulation of Dysprosium (Hexagonal)

Simulation 1: GGA-Spin Polarized

Pseudopotential Used:

Dy.pbe-spdn-rrkjus_psl.1.0.0.UPF

PP Type: Ultrasoft

Exchange Correlation Functional: PBE-GGA Spin Polarized
Non-linear core corrections are used.

Wavefunction Energy Cutoff: 35 Ry
Charge Density Energy Cutoff: 385 Ry
k - mesh: 8x8x8
Run Type: GGA-PBE
Starting Magnetization: 0.4

Total Energy vs Cutoff:

Cutoff(Ry)	Total Energy(Ry)
10	-247.31269578
15	-249.39216615
20	-249.80984740
25	-249.88662023
30	-249.89774501
35	-249.89854612
37	-249.89874195

In order to perform spin polarized calculations set the `nspin` parameter to 2.

Then as explained [here](#), set a starting magnetization to break the symmetry. The calculation should find the lowest-energy spin state compatible with the given crystal structure and not orthogonal to initial conditions (e.g.: if you start with a FM alignment, you will hardly find an AFM final state even if it exists). Perform several calculations at different starting magnetizations, choose the one with smaller energy as ground state. The system must be in all cases treated as a metal, whether it is or not. In principle, you should use pseudopotentials with the nonlinear core correction.

The following shows the total energy for different values of starting magnetization. NOTE: Starting magnetization is given in fractions, ranging between -1 (all spins down for the valence electrons of atom type 'i') to 1 (all spins up).

Total Energy vs Starting Magnetization:

SM	Total Energy (Ry)	Tot. Magnetic Mom/Abs. Mg. Mom. (Bohr Magneton)
0.1	-249.89851578	0.16/0.16
0.2	-249.89854612	0.10/0.10
0.3	-249.89856050	0.01/0.01
0.4	-249.89856057	0.01/0.01
0.5	-249.89855980	0.01/0.01
0.6	-249.89855985	0.01/0.01
0.7	-249.89855995	0.02/0.02
0.8	-249.89855872	0.03/0.03
0.9	-249.89856010	0.01/0.01
1.0	-249.89853780	0.12/0.12

Here we can see that the magnetic moments are pretty small, and therefore, a spin polarized calculation may or may not be necessary.

Clearly, a starting magnetization value of 0.4 gives the lowest energy.

Now, we perform optimization of geometry.

Optimized Coordinates and Lattice Parameters:

CELL_PARAMETERS {angstrom}

3.614257	0.000003	0.000000
-1.807126	3.130034	0.000000
0.000000	0.000000	5.618172

ATOMIC_POSITIONS {angstrom}

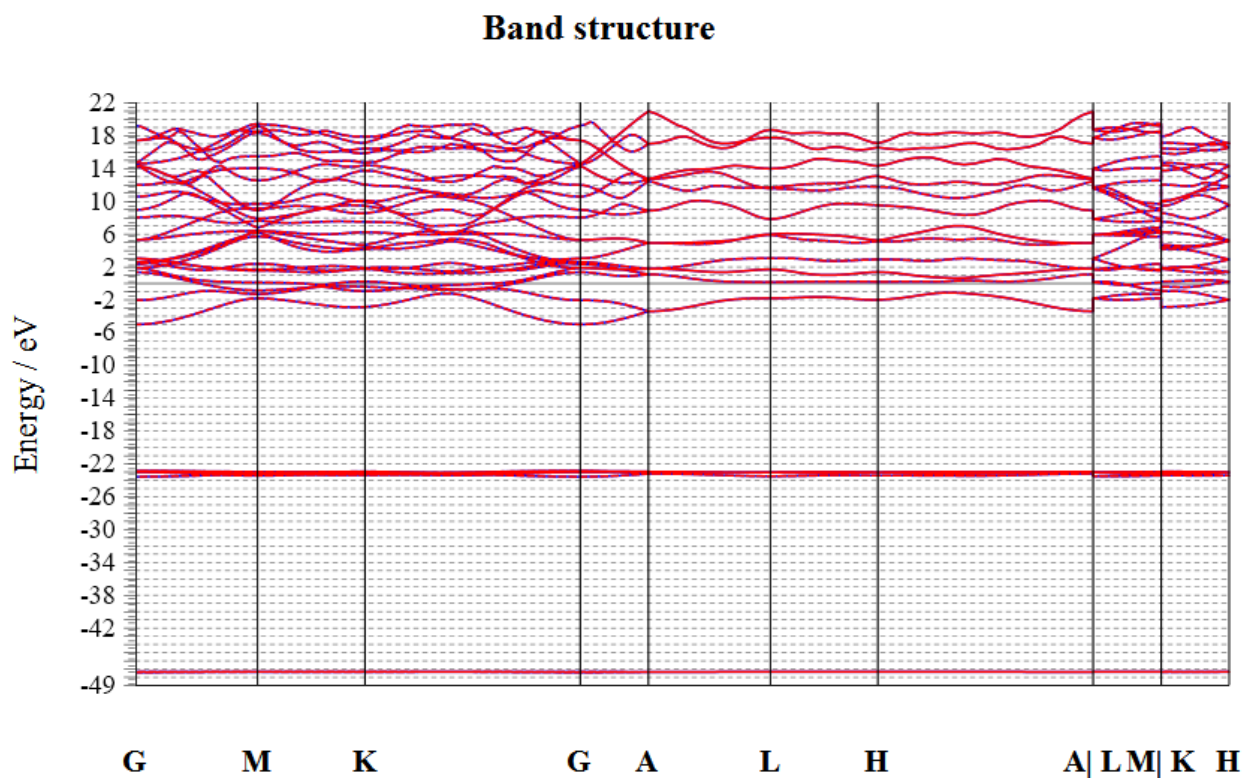
Dy	-0.000010	2.086705	1.404543
Dy	1.807122	1.043363	4.213629

Total magnetic moment for optimized system: 0.00 Bohr Magneton.

This shows the that GGA-DFT is insufficient to predict the correct experimental magnetic moment value of 7-10 B.M.

Magnetic moment per atom= 0.00 B.M.

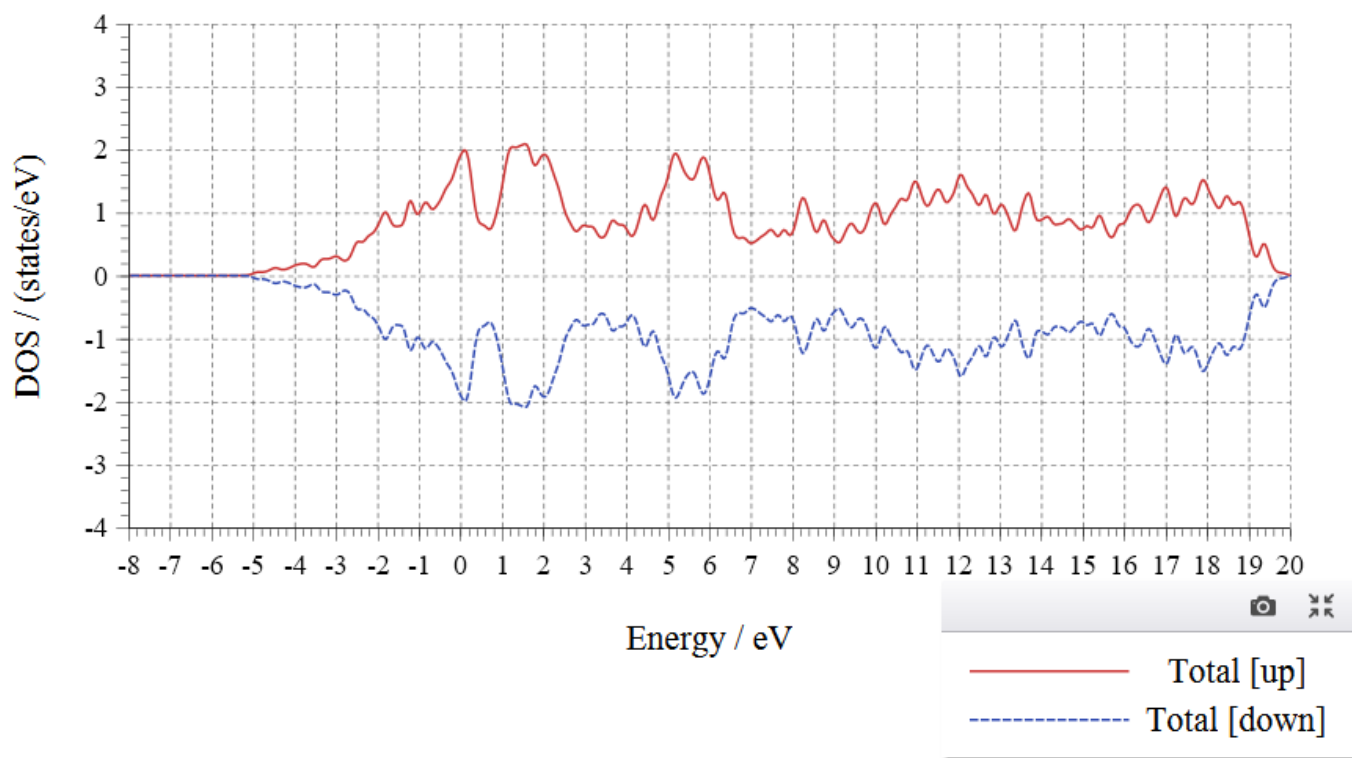
Bandstructure:



Bandstrucutre of Dysprosium (HCP) along high symmetry points

Density of States(DOS):

Density of states



Total Density of Stated (DOS) of Dysprosium (HCP)

Input Files:

Acknowledgements:

I acknowledge the use of the following tools and packages in order to produce the above simulations.

Quantum Espresso(for DFT based simulations): <http://www.quantum-espresso.org/>

BURAI(for visualization and as a GUI for QE): <http://nisihara.wixsite.com/burai>

VESTA(for visualization and XRD simulations): <http://jp-minerals.org/vesta/en/>

References and Resources

<https://en.wikipedia.org/wiki/Dysprosium>

<http://www-rjn.physics.ox.ac.uk/lectures/magnetismnotes10.pdf>

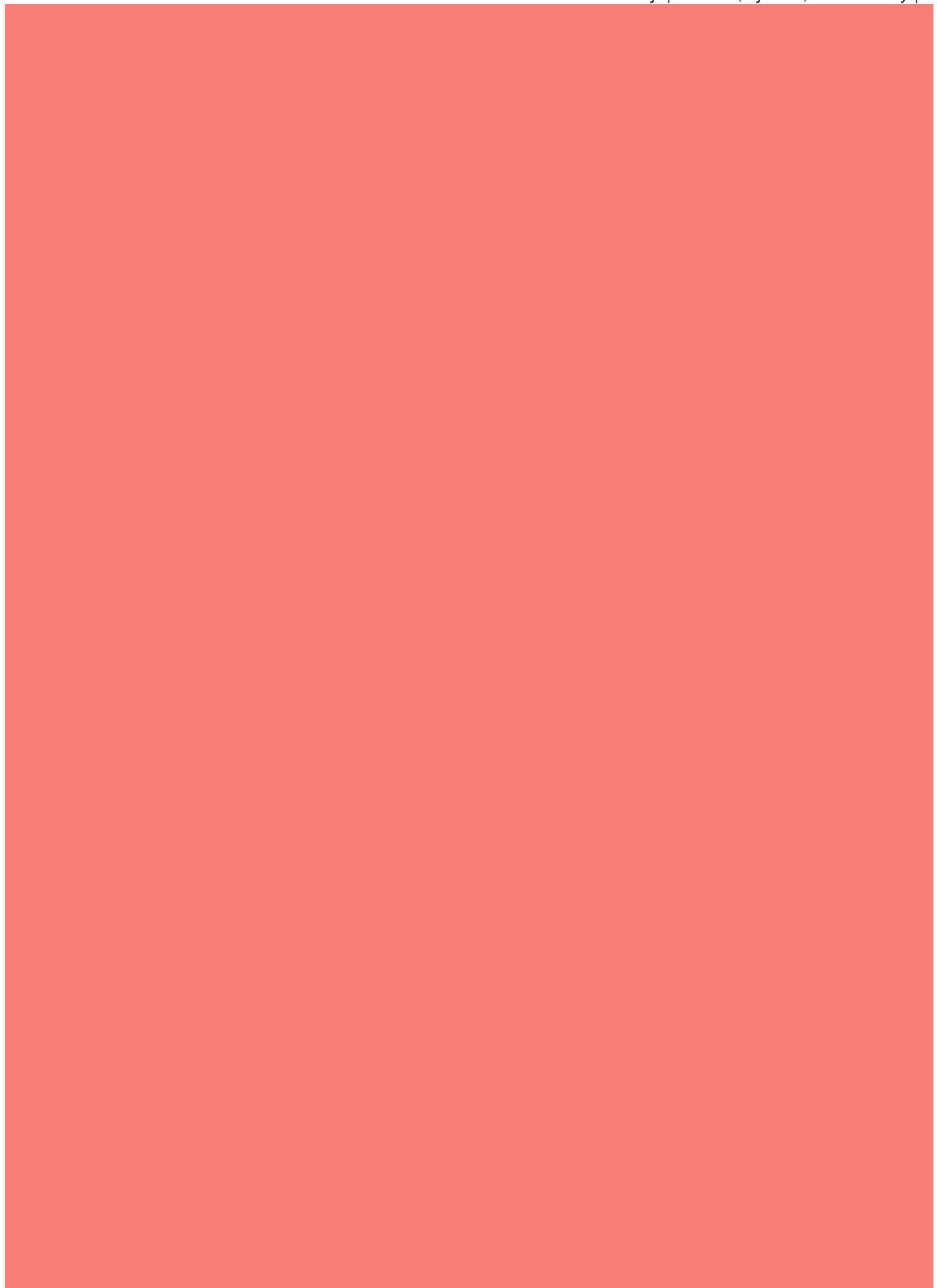
<http://146.141.41.27/Lectures/Omololu-Wednesday-21-MetalsMagnetism2.pdf>



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I'm a physicist specializing in computational material science with a PhD in Physics from Friedrich-Schiller University Jena, Germany. I write efficient codes for simulating light-matter interactions at atomic scales. I like to develop Physics, DFT, and Machine Learning related apps and software from time to time. Can code in most of the popular languages. I like to share my knowledge in Physics and applications using this Blog and a YouTube channel.

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