

Tutorial: DyFeO₃

Nuclear and Magnetic Structures refinement of DyFeO₃.

DyFeO₃

Summary of the provided data

Powder data collected at ILL on high-flux diffractometer D20 with $\lambda = 2.41123 \text{ \AA}$, at 1.6K and 5K.

Powder data collected at ILL on high-resolution diffractometer D2B with $\lambda = 1.594636 \text{ \AA}$, at 78K and 5K.

All the data are in the format Ins=10 for FullProf and are within the subdirectory **Data-files**

All the data contain a second phase, which is Aluminium powder that has been mixed with the DyFeO₃ sample in order to minimize the global absorption of the sample

Crystal structure of DyFeO₃ is summarized in the file DyFeO₃.cif. This file can be used to start sessions in the Bilbao Crystallographic Serve or in ISODISTORT.

The PCR files are in the **PCR-files** subdirectory. They are ready for making refinements with the appropriate data file.

Moreover, the article in which the magnetic and crystal structures are described is provided in the root directory of the tutorial, the name of the file being:

616_Ritter_DyFeO₃_2022_J._Phys._Condens._Matter_34_265801.pdf.

In order to tackle the tasks involved in the exercises described below, the user of this tutorial is encouraged to read this paper in detail to know about the physics of the problem.

In summary, DyFeO₃ at 78K is already magnetically ordered but at 5K, the magnetic structure is

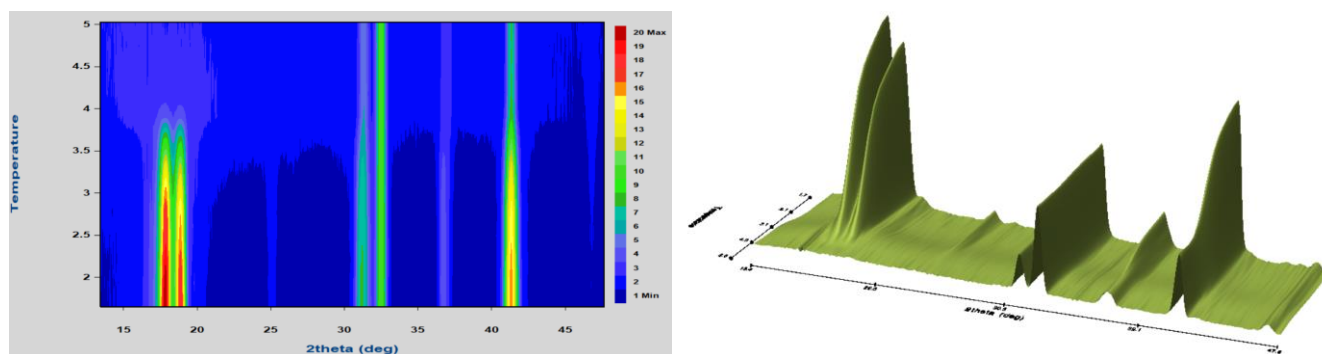


Figure 1: Evolution of the low-angle part of powder diffraction patterns of DyFeO₃ at low temperature

not the same as that at 78K. In both cases (commensurate structures), only the Fe atoms are

magnetically ordered. Below 5K, the Dy ions get ordered with an incommensurate structure. See the figure 1.

Values of U, V, W for D2B:

U	V	W	X	Y
0.053590	-0.161820	0.159698	0.000000	0.042017

Values of U, V, W for D20:

U	V	W	X	Y
3.031798	-1.827277	0.518409	0.000000	0.000000

The unit cell parameters of DyFeO₃ described in the *Pbnm* space group at 78K are:

a	b	c	alpha	beta	gamma
5.297677	5.590787	7.606675	90.0000	90.0000	90.0000

The crystal structure of DyFeO₃ described in the *Pbnm* space group at 78K is:

Atom	Formf	x	y	z	Biso	Occ.
Dy	Dy	0.98156	0.06782	0.25000	0.09882	0.50000
Fe	Fe	0.50000	0.00000	0.00000	0.36447	0.50000
O1	O	0.10684	0.45926	0.25000	0.56716	0.50000
O2	O	0.69282	0.30383	0.05455	0.41702	1.00000

With this information, the user of the tutorial may start from the scratch to construct PCR files to solve the magnetic structures.

Exercises

In this tutorial, the user is not guided systematically for doing the work. Essentially the way of working is the same as in the other tutorials, so the methods and actions are similar to those already known by the user. In the **PCR-files** subdirectory, the user have the final solutions for the refinements. If the user prefer to start with the already known PCR it is better to make a copy.

1: With the above information, make a refinement of the structure of the D2B data at 78K without putting any magnetic contribution. A completely new PCR file can be prepared using **CIFs_to_PCR** program by providing an IRF file for D2B from the distribution of the FullProf Suite.

2: Verify that the propagation vector of the magnetic structure is $\mathbf{k}=(0, 0, 0)$. Try to solve the magnetic structure using symmetry analysis with the help of the **BCS** program **k-SUBGROUPSMAG**, MAXMAGN or with the program **Baslreps**. What is the magnetic space group of the 78K magnetic structure of DyFeO₃?

- 3:** Repeat the exercises 1 and 2 for the data of D2B at 5K. Determine the magnetic space group of the magnetic structure at 5K.
- 4:** Do a refinement of the data from D20 using the magnetic structure already determined at 5K with the data of D2B. You can fix the crystal and magnetic structures and refine only the scale factor, the background and the profile parameters.
- 5:** Treat the data of D20 at 1.6K. Notice that new peaks appear that are originated by the long range ordering of Dy ions. Determine the propagation vector using **k-Search**. For that do a refinement using the same model as in 5K fixing all structural and magnetic parameters. Use the generated PRF file to get the peak positions for determining the propagation vector of the Dy ordering. Notice that there are some small peaks corresponding to the third harmonic of the primary propagation vector.
- 6:** Use Baslreps to obtain the basis vectors for the determined propagation vector for Dy ions. You may prepare a PCR file using these basis vectors, by copying the adequate parts of the *.fp file generated by Baslreps.
- 7:** Use **ISODISTORT** to explore the possible magnetic superspace groups. Export CIF files to be converted into PCR files using **mCIF_to_PCR** program.