

FullProf exercises on magnetic structure of $\text{KTb}_3\text{F}_{12}$

The proposed exercises below may serve as a tutorial for learning the use of FullProf as a tool for investigating magnetic structures. This is a very simple case but it is a good example for beginners.

To know about the physics of this compound see the article:

Magnetic properties of a mixed-valence (III/IV) terbium fluoride $\text{KTb}_3\text{F}_{12}$, by M. Gillot, M. El-Ghozzi, D. Avignan, G. Andre, F. Bouree and A. Cousson
Journal of Applied Physics **91**(10), 8519 (2002)

Exercises:

Given the information below, do the exercises 1-9. The PCR files that are distributed with this tutorial are ready for working. The best, for a beginner, is to save the PCR files in another directory and try to construct the PCR files from the scratch using the method proposed in the manual of FullProf.

Crystallographic structure:

SPGR	I 4/m						
CELL	a=7.721339	c=7.535282					
			x	y	z	Biso	Wyckoff
ATOM	K	K	0.00000	0.00000	0.00000	1.40185	2a
ATOM	Tba	TB	0.00000	0.00000	0.50000	0.31639	2b
ATOM	Tbb	TB	0.00000	0.50000	0.25000	0.31254	4d
ATOM	F1	F	0.34598	0.02055	0.00000	0.94306	8h
ATOM	F2	F	0.23804	0.03291	0.68006	1.26930	16i

Approx. U,V,W parameters of 3T2: 0.3287 -0.4975 0.2475
" " " of G41: 0.7920 -0.2800 0.0800

1) Refine the crystal structure of $\text{KTb}_3\text{F}_{12}$ using the data from 3T2 at 5K in order to get the proper structural parameters in the paramagnetic state near the Néel temperature ($T_N=3.65\text{K}$)

PCR file: ktbk5.pcr

DAT file: ktbk5.dat

From Bond-Valence calculations verify that the Tba corresponds to Tb^{3+} and Tbb to Tb^{4+}

2) Refine the scale factor and profile parameters using the data from G41 at 4.94K.

PCR file: 4p94.pcr

DAT file: 4p94.dat

The peak shape of Bragg reflections in G41 is quite complex for angles higher than $2\theta=70$ degrees. The model used in the PCR file is not totally adequate but it is enough for getting a proper value of the scale factor.

3) Determine the propagation vector of the magnetic structure using the low temperature data from G4.1. This can be done easily, in this case, just testing simple cases using an additional phase (fixing completely the nuclear phase) in profile matching (Le Bail fit) mode.

PCR file: **1p4-pm.pcr**

DAT file: **1p4.dat**

In the above PCR file we have put More=1 and Jvi=11 so that an integrated magnetic reflections file suitable for simulated annealing is generated.

4) Prepare a simulated annealing PCR file and run the program without taking into account the possible symmetries. In this case, the magnetic structure is easily obtained from the scratch by just using a trial and error method; however, it is instructive to prepare a SAnn. run for learning purposes.

PCR file: **simann.pcr**

INT file: **1p4-pm2.int** (coming from the run in step 3)

We can use Fp-Studio for monitoring the behaviour of the simulated annealing run putting **Ls2=5** and **Jview=3**. Run FullProf in console mode invoking the program as:

```
My_directory> fp2k simann 1p4-pm2
```

Open Fp-Studio and read the file "simann.fst". Click on the red arrow button to follow the evolution of the magnetic structure solution.

5) Make a symmetry analysis of G_k , determine the IRreps of G_k and classify the possible magnetic structures. Use BasIreps to do the work. Determine the possible magnetic space groups.

Already prepared *.smb files: **Ktb.smb** and **Ktb-sub.smb**

Verify that the Irrep corresponding to the ordering of Tb^{4+} site corresponds to Irep(3) that is not allowed for the site of Tb^{3+}

Verify that the magnetic space group of the solution found by simulated annealing corresponds to I_{P4}/m .

7) Refine the magnetic structure.

8) Use ISODISTORT to obtain a PCR file with symmetry modes and do the refinement of amplitudes. Start by loading the CIF file KTb3F12.cif into the ISODISTORT web page.

9) Give a qualitative physical explanation of the observed facts