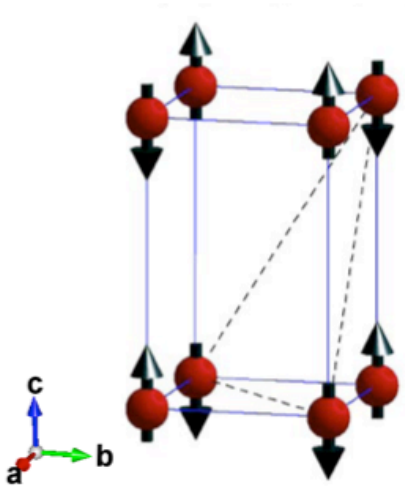
Preparing a magCIF file of a magnetic Structure for MAGNDATA. Example 1: $UNiGa_5$

Reference:
Kaneko et al., PHYSICAL REVIEW B **68**, 214419 (2003)
DOI: 10.1103/PhysRevB.68.214419

Parent P4/mmm structure at 9K in file: UNiGa5_9K_PRB68-214419.cif
The article reports the positional structure at several temperatures, but forgetting to state the underlying space group (!). However, other structural models for this compound can be found in the ICSD database, and the relevant space group can therefore be identified there as P4/mmm. We will then use the positional structure at 9K, including cell parameters, as given in the paper, under this space group. It is provided in the attached cif file indicated above.

The magnetic structures at 3.2K as reported in the reference:

The propagation vector is identified as **k**=(1/2,1/2,1/2) and as there is only a single U atom in the primitive unit cell, this example is extremely simple, as shown in Figure 1 of the paper, where only the spins in the parent unit cell are shown:



The structure and its MSG only depends on the orientation of the moment of the U atom at the origin, and this is along **c**. The relative orientation of the moments in all the other U atoms at the lattice vectors **T** is equal or opposite, being fully determined by the value of the propagation vector **k**. It depends on the value of $\exp(i2\pi\mathbf{k}.\mathbf{T})$ being +1 or -1.

Moment modulus: 0.75(5) μB at 3.2K (Table II of the reference) and T_N= 86K
The information above taken from the mentioned article, together with the provided CIF file is sufficient to produce a magCIF file that can be uploaded in MAGNDATA.

First of all, if you do not have them, download the instructions for uploading a magCIF file available in the webpage of MAGNDATA. There you will obtain a zip file that includes the pdf file: "instructions_to_prepare_mcif_file_v6.5.pdf". According to these instructions this example corresponds to "Case 3", as we do not have yet any magCIF file.

For the simple magnetic structure of this example the most rapid approach is to follow the 1st Procedure, which is recommended in the instructions for case "Case 3". That means: use the program MAXMAGN. This will be sufficient to produce an initial magCIF file and then follow the steps explained in the instructions for "Case 1", i.e. when one has already a magCIF file consistent with the MSG of the structure:

1) Open MAXMAGN, introduce the k-vector and tick the option "Structure data of the paramagnetic phase will be included". In the next step upload the cif file with the reported position structure at 9K. The program will show that three maximal symmetries are compatible with the observed propagation vector, described by three different magnetic space groups (MSGs). By clicking on the last column "Magnetic Structure" identify the MSG, which corresponds to the reported structure. Fill manually a value to the U moment (it can be arbitrary for the moment). Produce the corresponding .mcif file and visualize with the available option of the program, in order to check that the structure is the correct one. Save the corresponding mcif file, for further processing.

2) You have saved in the previous step a magCIF file of the model corresponding to the magnetic structure that is proposed in the paper. You have therefore the necessary file to go now to the process that is explained in the instructions as "Case 1", and obtain following the indications there the desired complete magCIF file ready for uploading in MAGNDATA.

3) The magCIF to be introduced in MAGNDATA has a small part about information on the irreps that are active. It is can be left untouched, without information, but it is recommended that you fill it using Get_mirreps. You should obtain with this program that only one 1-dim irrep is compatible with the magnetic arrangement of the structure.