ZTF-FCT
Zientzia eta Teknologia Fakultatea
Facultad de Ciencia y Tecnología

eman ta zabal zazu
Universidad del País Vasco
Euskal Herriko Unibertsitatea

How to properly report a magnetic structure in publications and prepare a magCIF file for MAGNDATA

J. Manuel Perez-Mato
Facultad de Ciencia y Tecnología
Universidad del País Vasco, UPV-EHU
BILBAO, SPAIN

Acta Cryst B
STRUCTURAL SCIENCE
CRYSTAL ENGINEERING
MATERIALS

ISSN 2052-5206

Guidelines for communicating commensurate magnetic structures. A report of the International Union of Crystallography Commission on Magnetic Structures

Acta Cryst. (2024). B80, 219–234

J. M. Perez-Mato,[a]* B. J. Campbell,[b] V. O. Garlea,[c] F. Damay,[d] G. Aurelio,[e] M. Avdeev,[f,g] M. T. Fernández-Díaz,[h] M. S. Henriques,[i] D. Khalyavin,[j] S. Lee,[k] V. Pomjakushin,[l] N. Terada,[m] O. Zaharko,[l] J. Campo,[n] O. Fabelo,[h] D. B. Litvin,[o] V. Petricek,[i] S. Rayaprol,[p] J. Rodriguez-Carvajal[h] and R. Von Dreele[q]

[a]Facultad de Ciencia y Tecnología, Universidad del País Vasco, UPV/EHU, Apartado 644, Bilbao, E-48080, Spain, [b]Department of Physics and Astronomy, Brigham Young University, Provo, Utah 84602, USA, [c]Neutron Scattering Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA, [d]Université Paris-Saclay, CEA-CNRS UMR12, Laboratoire Léon Brillouin, 91191 Gif-sur-Yvette Cedex, France, [e]Comisión Nacional de Energia Atómica and CONICET, Laboratorio Argentino de Haces de Neutrones, Centro Atómico Bariloche, Av. Bustillo 9500 R8402AGP, S. C. de Bariloche, Argentina, [f]Australian Nuclear Science and Technology Organisation, New Illawarra Rd, Lucas Heights, New South Wales 2234, Australia, [g]School of Chemistry, University of Sydney, Sydney, New South Wales 2006, Australia, [h]Institut Laue-Langevin (ILL), 71 avenue des Martyrs, F-38042 Grenoble Cedex 9, France, [i]FZU - Institute of Physics of the Czech Academy of Sciences, Na Slovance 2, 182 21 Prague, Czechia, [j]ISIS Pulsed Neutron and Muon Source, STFC Rutherford Appleton Laboratory, Harwell Campus, Didcot, Oxon OX11 0QX, United Kingdom, [k]Advanced Quantum Materials Research Center, Korea Atomic Energy Research Institute, 111, Daedeok-daero 989 beon-gil, Yuseong-gu, Daejeon, 34057, Republic of Korea, [l]Laboratory for Neutron Scattering and Imaging, Paul Scherrer Institut PSI, CH-5232 Villigen, Switzerland, [m]National Institute for Materials Science, Sengen 1-2-1, Tsukuba, Ibaraki 305-0047, Japan, [n]Aragón Nanoscience and Materials Institute (CSIC – University of Zaragoza) and Condensed Matter Physics Department, C/Pedro Cerbuna 12, 50009 Zaragoza, Spain, [o]Department of Physics, Eberly College, Penn State University, Penn State Berks, Reading, Pennsylvania 19610, USA, [p]UGC-DAE Consortium for Scientific Research, Mumbai Centre, BARC Campus, Trombay, Mumbai, 400085, India, and [q]Advanced Photon Source, Argonne National Laboratory, Lemont, IL 60439, USA. *Correspondence e-mail: jm.perezmato@gmail.com

This article is part of a collection of articles in a focused issue on Magnetic Structures.[wording ok?]

Keywords: IUCr Commission on Magnetic Structures; magnetic structures; magnetic space groups; representation analysis; magnetic CIF; guidelines.

A report from the International Union of Crystallography Commission on Magnetic Structures outlining the recommendations for communicating commensurate magnetic structures.

Summary: ***Independently of how a commensurate magnetic structure has been determined the final model should reported making full use of the MSG of the structure***

- **The description of a magnetic structure using its MSG of the structure is a direct simple extension of ordinary crystallography and therefore:**

simple, compact, standardized and robust…

This is the description used in the **CIF file format**, extended to magnetic structures (**magCIF**), which is now supported by many programs.

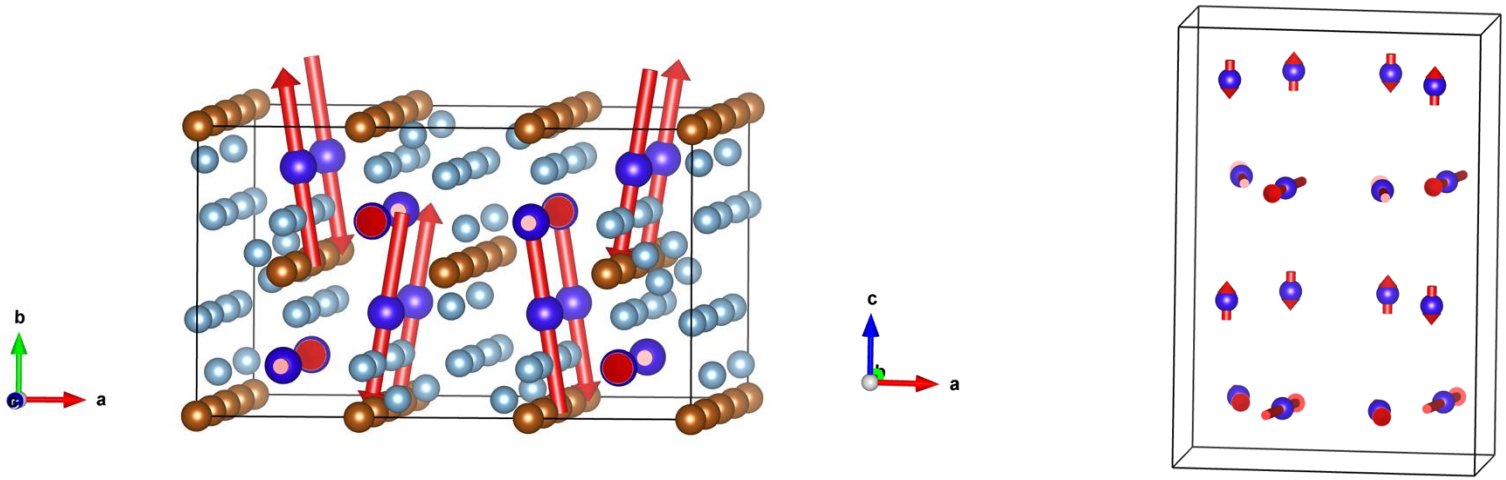
It has allowed the development of **MAGNDATA**

Example 1 (Commensurate):

$Dy_2Co_3Al_9$ Gorbunov et al. , 2018 (magndata #1.267)

(Single crystal neutron diffraction)

$Cmcm.1'$ —k=(0,0,1/2)→ A_amm2 (2c, a, b; 0,0,-1/4)



The MSG of this magnetic structure is only compatible with one irrep, namely the 2-dim irrep mZ1.

(only spin arrangements according to this irrep are allowed by the MSG, but restricted to a special combinations of the irrep basis vectors. No degrees of freedom corresponding to other irreps are permitted)

How to report… when only one irrep is compatible with the MSG

fundamental information:

Compound	$Dy_2Co_3Al_9$
Parent space group	*Cmcm* (N. 63)
Propagation vector(s)	(0, 0, ½)
Transformation from parent basis to the one used	(**a**,**b**,2**c**;0,0,0)
MSG symbol	A_amm2 (UNI: $Amm2.1'_a$)
MSG number	38.192
Transformation from basis used to standard setting of MSG	(**c**,**a**,**b**;0,0,-1/8)
Magnetic point group	*mm2.1'* (**c**,**a**,**b**) *or m2m.1'*
Unit cell parameters (Å)	a=12.72390 α=90º b=7.45860 β =90º c=18.59880 γ =90º
MSG symmetry operations	x,y,z,+1 -x,y,-z+3/4,+1 -x,y,z,+1 x,y,-z+3/4,+1
MSG symmetry centering operations	x,y,z,+1 x+1/2,y+1/2,z,+1 x,y,z+1/2,-1 x+1/2,y+1/2,z+1/2,-1
Positions of magnetic atoms	Dy1_1 Dy 0.33940 0.33290 0.12500 Dy1_2 Dy 0.66060 0.66710 0.37500
Positions of non-magnetic atoms	Co1 Co 0.32880 0.00000 0.00000 Co2 Co 0.00000 0.00000 0.00000 Al1_1 Al 0.00000 0.1249 0.125 Al1_2 Al 0.00000 0.8751 0.375 Al2_1 Al 0.1079 0.4459 0.125 Al2_2 Al 0.8921 0.5541 0.375 Al3_1 Al 0.0000 0.3322 0.2714 Al3_2 Al 0.00000 0.6678 0.5214 Al4_1 Al 0.1686 0.3330 0.03585 Al4_2 Al 0.8314 0.6670 0.28585
Magnetic moments components (μ_B) of magnetic atoms, symmetry constraints and moment magnitudes	Dy1_1 1.34(2) 8.35(2) 0.0 (mx,my,0) 8.46(2) Dy1_2 0.0 0.0 1.38(1) (0,0,mz) 1.38(1)

How to report… when only one irrep is compatible with the MSG

fundamental information:

Compound	$Dy_6Co_3Al_9$
Parent space group	*Cmcm* (N. 63)
Propagation vector(s)	(0, 0, ½)
Transformation from parent basis to the one used	(**a**,**b**,2**c**;0,0,0)
MSG symbol	*Amm2* (UNI: *Amm2.1'$_a$*)
MSG number	38.192
Transformation from basis used to standard setting of MSG	(**c**,**a**,**b**;0,0,-1/8)
Magnetic point group	*mm2 1'* (**c a b**) *or m2m 1'*
Unit cell parameters (Å)	a=12.72390 α=90º b=7.45860 β =90º c=18.59880 γ =90º
MSG symmetry operations	x,y,z,+1 -x,y,-z+3/4,+1 -x,y,z,+1 x,y,-z+3/4,+1
MSG symmetry centering operations	x,y,z,+1 x+1/2,y+1/2,z,+1 x,y,z+1/2,-1 x+1/2,y+1/2,z+1/2,-1

Basic relation with the parent paramagnetic structure

unit cell

How to report… when only one irrep is compatible with the MSG

fundamental necessary information:

Compound	$Dy_2Co_3Al_9$
Parent space group	*Cmcm* (N. 63)
Propagation vector(s)	(0, 0, ½)
Transformation from parent basis to the one used	(**a**,**b**,2**c**;0,0,0)
MSG symbol	*$A_a$mm2* (UNI: *Amm2.1'*)
MSG number	38.192
Transformation from basis used to standard setting of MSG	(**c**,**a**,**b**;0,0,-1/8)
Magnetic point group	*mm2.1'* (**c**,**a**,**b**) *or m2m.1'*
Unit cell parameters (Å)	a=12.72390 α=90º b=7.45860 β =90º c=18.59880 γ =90º
MSG symmetry operations	x,y,z,+1 -x,y,-z+3/4,+1 -x,y,z,+1 x,y,-z+3/4,+1
MSG symmetry centering operations	x,y,z,+1 x+1/2,y+1/2,z,+1 x,y,z+1/2,-1 x+1/2,y+1/2,z+1/2,-1

MSG identification

equivalent information

How to report… when only one irrep is compatible with the MSG

fundamental necessary information:

Compound	$Dy_2Co_3Al_9$	
Parent space group	*Cmcm* (N. 63)	
Propagation vector(s)	(0, 0, ½)	
Transformation from parent basis to the one used	(**a**,**b**,2**c**;0,0,0)	
MSG symbol	$A_a mm2$ (UNI: $Amm2.1'_a$)	
MSG number	38.192	
Transformation from basis used to standard setting of MSG	(**c**,**a**,**b**;0,0,-1/8)	
Magnetic point		
Unit cell parameters (Å)	a=12.72390 α=90º b=7.45860 β =90º c=18.59880 γ =90º	
MSG symmetry operations	x,y,z,+1 -x,y,-z+3/4,+1 -x,y,z,+1 x,y,-z+3/4,+1	{1|0,0,0} {2_{010}|0,0,¾} {m_{100}|0,0,0} {m_{001}|0,0,¾}
MSG symmetry centering operations	x,y,z,+1 x+1/2,y+1/2,z,+1 x,y,z+1/2,-1 x+1/2,y+1/2,z+1/2,-1	{1|0,0,0} {1|½,½,0} {1'|0,0,½} {1'|½,½,½ }

MSG identification

For Tables and text, the Seitz notation is highly recommended **as ALTERNATIVE !!!**

- **The identification and assignment the magnetic space group (MSG) is a "must"**

- Whatever the method employed to determine a commensurate magnetic structure, its MSG must be identified and reported.

- Representation analysis can be an efficient method for the determination of a commensurate magnetic structure but it is NOT an "alternative" to the identification of its MSG.

- **For a full identification of the MSG the transformation from the unit cell used to one where the MSG has its standard form must also be reported.**

- The magnetic point group (MPG) can be derived from the MSG, but it is so important that it is recommendable to report it explictly.

- **If you fear that the referees will think your paper is not enough "cutting hedge" research, because it includes too much detail and Tables, you can always submit the information as supplemental material, and your magnetic structure will be fully unambiguous, and easily portable for other studies (include a magCIF file as supplemental material !!!).**

How to report when only one irrep is compatible with the MSG ….

fundamental **NECESSARY** information

Positions of magnetic atoms	Dy1_1 Dy 0.33940 0.33290 0.12500 Dy1_2 Dy 0.66060 0.66710 0.37500
Positions of non-magnetic atoms	Co1 Co 0.32880 0.00000 0.00000 Co2 Co 0.00000 0.00000 0.00000 Al1_1 Al 0.00000 0.1249 0.125 Al1_2 Al 0.00000 Al2_1 Al 0.1079 0 Al2_2 Al 0.8921 0 Al3_1 Al 0.0000 0 Al3_2 Al 0.00000 0.6678 0.5214 Al4_1 Al 0.1686 0.3330 0.03585 Al4_2 Al 0.8314 0.6670 0.28585
Magnetic moments components (μ_B) of magnetic atoms, symmetry constraints and moment magnitudes	Dy1_1 1.34(2) 8.35(2) 0.0 (mx,my,0) 8.46(2) Dy1_2 0.0 0.0 1.38(1) (0,0,mz) 1.38(1)

Positions and moments of the magnetic atoms in the asymmetric unit referred to the MSG unit cell

MSG constraints on the magnetic moments

moment moduli

How to report when only one irrep is compatible with the MSG ….

fundamental necessary i

Positions of the set of of non-magnetic atoms of the asymmetric unit in the MSG unit cell

Positions of magnetic atoms	Dy1_1 Dy 0.339 Dy1_2 Dy 0.66(
Positions of non-magnetic atoms	Co1 Co 0.32880 0.00000 0.00000 Co2 Co 0.00000 0.00000 0.00000 Al1_1 Al 0.00000 0.1249 0.125 Al1_2 Al 0.00000 0.8751 0.375 Al2_1 Al 0.1078 0.4459 0.125 Al2_2 Al 0.8921 0.5541 0.375 Al3_1 Al 0.0000 0.3322 0.2714 Al3_2 Al 0.00000 0.6678 0.5214 Al4_1 Al 0.1686 0.3330 0.03585 Al4_2 Al 0.8314 0.6670 0.28585
Magnetic moments components (μ_B) of magnetic atoms, symmetry constraints and moment magnitudes	Dy1_1 1.34(2) 8.35(2) 0.0 (mx,my,0) 8.46(2) Dy1_2 0.0 0.0 1.38(1) (0,0,mz) 1.38(1)

- **Information on the positions of the NON-magnetic atoms is also necessary for a full knowledge of the magnetic structure**

- Even if the positions of the non-magnetic atoms were not needed for the determination of the spin arrangement, their knowledge is necessary for a full description of the structure.

- The MSG depends on the positions of the non-magnetic atoms.

- Enough information should be given from which to get a description (at least approximate) of the positional structure of all atoms; either appealing to some reference or including a full listing .

- Positional structure of all atoms, described using the MSG make explicit all magneto structural effects that may happen: split sites, atomic positions components that become free in the magnetic phase. **If you want to detect structural effects induced by the magnetic ordering this is the first step!**

How to report when only one irrep is compatible with the MSG ….

complementary information on representation analysis

	$Dy_2Co_3Al_9$
Primary irrep(s) label(s) with dimension	mZ1 (2-dim) (special direction)
Description of the primary irrep	mZ1: $\{2_{001}\|0, 0, ½\}$: (0 ,-1 ; 1 , 0) $\{2_{010}\|0 , 0 , ½\}$: (1, 0 ; 0,- 1) {-1|0,0,0}: (0, -1 ; -1, 0) {1|0,0,1}: (-1, 0 ; 0,- 1) {1|0,1,0}: (1, 0 ; 0,1) {1|1,0,0}: (1, 0 ; 0, 1) {1| ½ , ½ ,0}: (1, 0 ; 0, 1)
Secondary irrep(s) label(s)	Not allowed

NOT NECESSARY if the irrep labels used are those of standard listings (CDML or Kovalev)

How do we know the structure does not allow secondary magnetic irreps? for example, using Get_mirreps:

Input data

Group→subgroup	Transformation matrix
*Cmcm*1' (N. 63.458)→$A_a mm2$ (N. 38.192)	$\begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 2 & 0 & 0 & -1/4 \end{pmatrix}$

Representations and order parameters

Show the graph of isotropy subgroups

k-vectors	irreps and order parameters	isotropy subgroup transformation matrix	link to the irreps
GM: **(0,0,0)**	GM_1^+: (a)	*Cmcm*1' (No. 63.458) a,b,c;0,0,0	matrices of the irreps
	GM_4^-: (a)	*Amm*21' (No. 38.188) c,-a,-b;0,0,1/4	
Z: **(0,0,1/2)**	mZ_1: (0,a)	$A_a mm2$ (No. 38.192) 2c,-a,-b;0,0,-1/4	matrices of the irreps

ABOUT LABELS OF IRREDUCIBLE REPRESENTATIONS (IRREPS)

- **The irrep notation lacks a standard, but there is a couple of alternative unambiguous irrep labeling systems, supported with computer listings, that can be recommended:**

  - CDML notation (A. P. Cracknell, B. L. Davies, S. C. Miller and W. F. Love (1979)):

  software: ISOTROPY, Bilbao Crystallographic Server, JANA, FullProf (Basirreps)

  - **Kovalev notation** (O.V. Kovalev 1965-1993)**:**

  software: SARAh

- **It is strongly advised against using arbitrary irrep labels (like those of traditional software), but if done, then full unambiguous listings of the irrep characters must be necessarily included. Otherwise the irrep labels mean NOTHING!**

The irreps are mathematical constructs. They are tabulated or calculated by programs. They do not depend on you specific system. **You do not need to know how to calculate them but you need to know how to use them.**

On the use of irreps as an “alternative” description to the use of the MSG

- **if the MSG of the structure is only compatible with a single irrep (the majority of cases): A description using irrep spin basis vectors does NOT bring any advantage:**

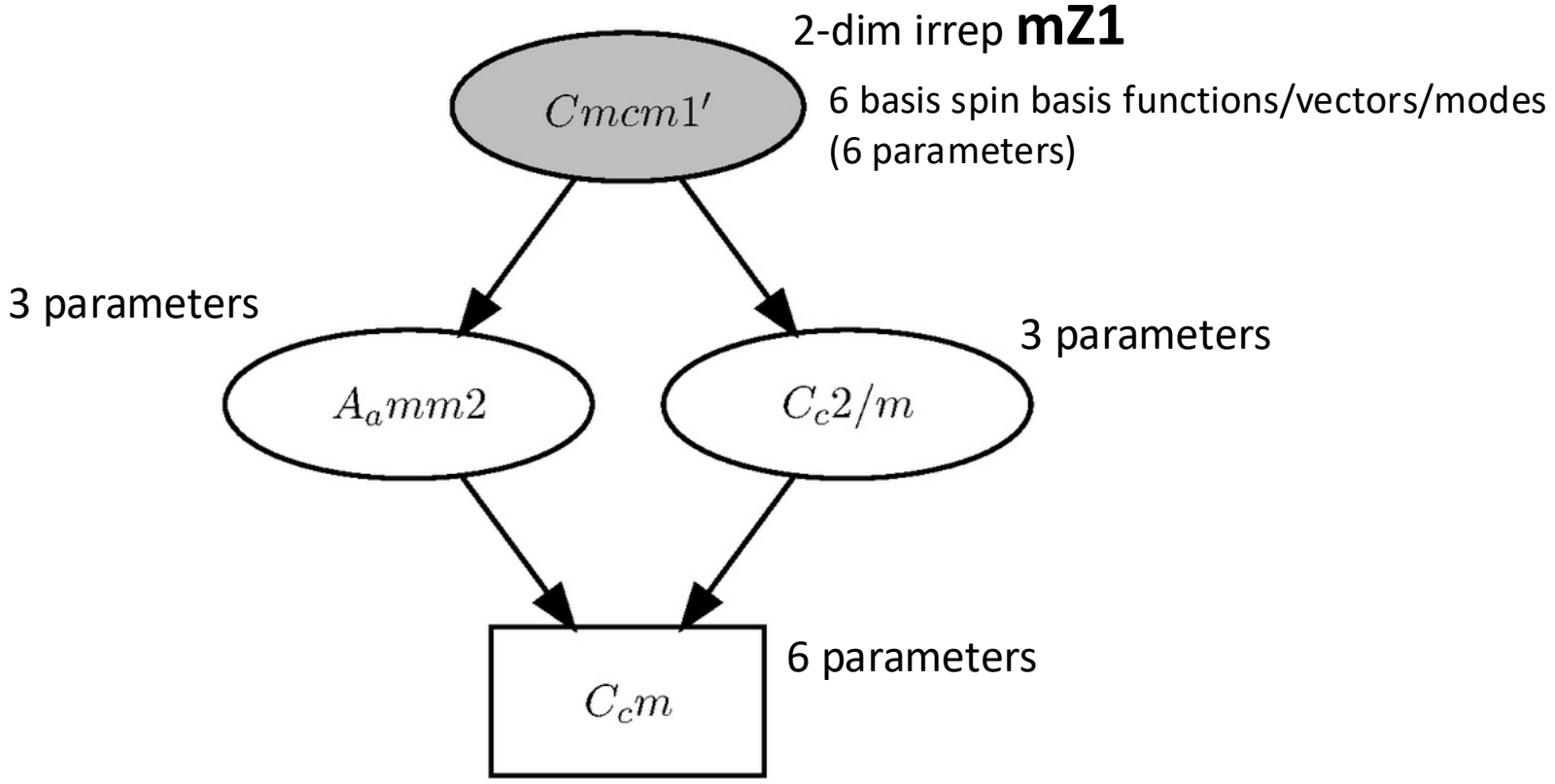
  - If the irrep is 1-dim, the two descriptions will be fully equivalent: the irrep basis functions will reproduce the same moment relationships among the magnetic atoms as the MSG.

  - If the irrep is multidimensional, in most cases several alternative MSGs can realized for the same irrep and the description using the actual MSG automatically introduces additional constraints that are not included when only restricting to the basis vectors of the irrep.

Our example 1:

$Dy_2Co_3Al_9$

Cmcm1' —k=(0,0,1/2)→ $A_a mm2$ (2c, a, b; 0,0,-1/8)



On the use of irreps as an "alternative" description to the use of the MSG

- **Only in the less frequent case that the MSG of the structure is compatible WITH MORE THAN ONE IRREP, the crystallographic description under the MSG can be further restricted by the particular irrep(s) being involved, since in many cases not all are present.**

How to report then when more than one irrep is compatible with the MSG?:

No standard exists yet for the inclusion of additional irrep restrictions…

(the magCIF standard does not support it yet….)

The guidelines paper just show with one example how it could be done….

Example 2 (Commensurate):

Mn_3Sn P.J. Brown et al. , 1990 (magndata #0.199)

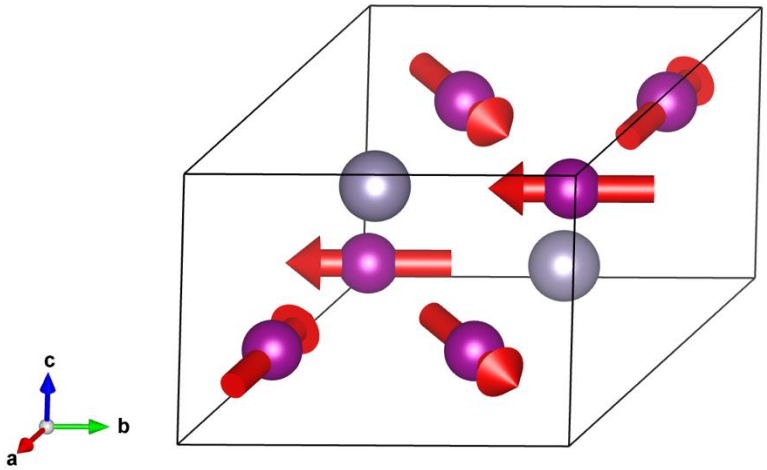
(Single crystal neutron diffraction)

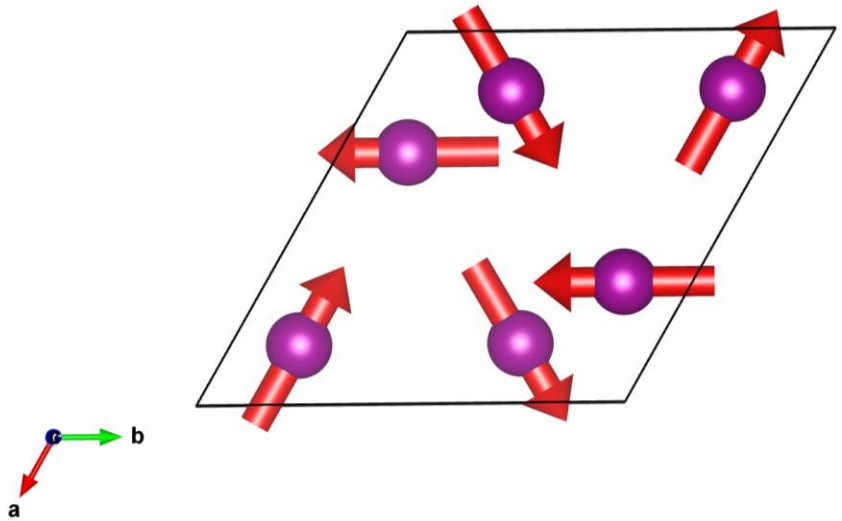
Mn at 6h Wyckoff position

k=(0,0,0)
2-dim irrep mGM6+

$P6_3/mmc.1'$ → *Cmc'm'* (-b, 2a+b, c; 0,0,0)

(N. 194) (N. 63.463)





The MSG of this magnetic structure is compatible with TWO irreps
(spin arrangements according to any of the two irreps are allowed by the MSG, no degrees of freedom corresponding to other irreps than these two are permitted)

k=(0,0,0)

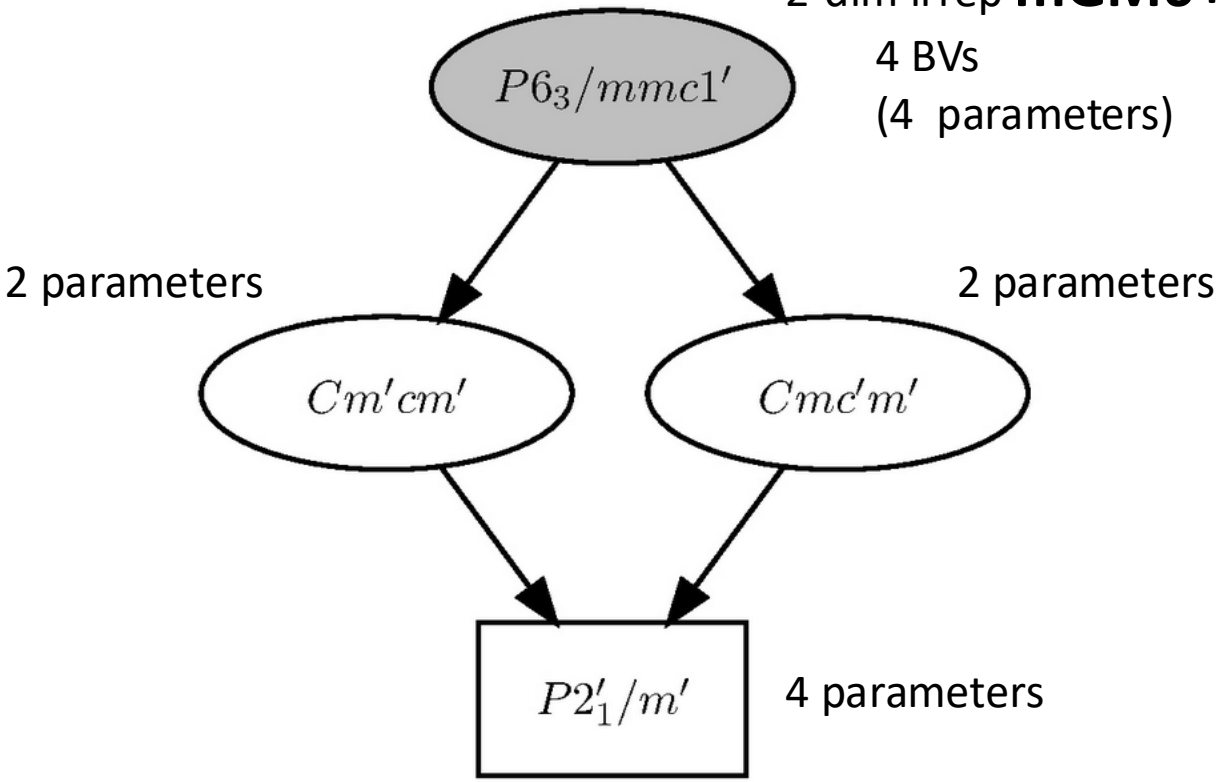
2-dim irrep mGM6+

$P6_3/mmc1'$ → $Cmc'm'$ (-b, 2a+b, c; 0,0,0)

2-dim irrep **mGM6+**

4 BVs

(4 parameters)



2 parameters

2 parameters

4 parameters

How to report when more than one irrep is compatible with the MSG ….

fundamental information **(the same as in the previous case)**

	Mn_3Sn
Parent space group	*P6₃/mmc* (N. 194)
Propagation vector(s)	(0, 0, 0)
Transformation from parent basis to the one used	(**a**, **b**, **c**;0,0,0)
MSG symbol	*Cmc'm'*
MSG number	63.463
Transformation from basis used to standard setting of MSG	(**-b**,2**a+b**,**c**;0,0,0)
Magnetic point group	*m'm'm* (2**a+b**,**c**,**-b**)
Unit cell parameters (Å)	a=5.665 α=90º b=5.665 β =90º c=4.531 γ =120º
MSG symmetry operations	x,y,z,+1 -x,-x+y,-z,+1 -x,-y,-z,+1 x,x-y,z,+1 x,x-y,-z+1/2,-1 -x,-y,z+1/2,-1 -x,-x+y,z+1/2,-1 x,y,-z+1/2,-1
Positions of magnetic atoms	Mn1_1 Mn 0.8388 0.6776 0.25 Mn1_2 Mn 0.3224 0.1612 0.25
Positions of non-magnetic atoms	Sn1 Sn 0.33333 0.66667 0.25
Magnetic moment components (μ_B) of magnetic atoms, symmetry constraints and moment magnitudes	Mn1_1 3.00(1) 3.00 0.0 (mx,my,0) 3.00(1) Mn1_2 0.0 -3.00 0.0 (0,my,0) 3.00(1)

Mn_3Sn

non-standard setting for the description

How to report when more than one irrep is compatible with the MSG ….

fundamental necessary information **(the same as in the previous case)**

	Mn_3Sn
Parent space group	*P6₃/mmc* (N. 194)
Propagation vector(s)	(0, 0, 0)
Transformation from parent basis to the one used	(**a**, **b**, **c**;0,0,0)
MSG symbol	*Cmc'm'*
MSG number	63.463
Transformation from basis used to standard setting of MSG	(**-b**,2**a+b**,**c**;0,0,0)
Magnetic point group	*m'm'm* (2**a+b**,**c**,**-b**)
Unit cell parameters (Å)	a=5.665 α=90º b=5.665 β =90º c=4.531 γ =120º
MSG symmetry operations	x,y,z,+1 {1|0,0,0} -x,-x+y,-z,+1 {2_{010}|0,0,0} -x,-y,-z,+1 {-1|0,0,0} x,x-y,z,+1 {m_{010}|0,0,0} x,x-y,-z+1/2,-1 {$2'_{210}$|0,0,½} -x,-y,z+1/2,-1 {$2'_{001}$|0,0,½} -x,-x+y,z+1/2,-1 {m'_{210}|0,0,½} x,y,-z+1/2,-1 {m'_{001}|0,0,½}
Positions of magnetic atoms	Mn1_1 Mn 0.8388 0.6776 0.25 Mn1_2 Mn 0.3224 0.1612 0.25
Positions of non-magnetic atoms	Sn1 Sn 0.33333 0.66667 0.25
Magnetic moment components (μ_B) of magnetic atoms, symmetry constraints and moment magnitudes	Mn1_1 3.00(1) 3.00 0.0 (mx,my,0) 3.00(1) Mn1_2 0.0 -3.00 0.0 (0,my,0) 3.00(1)

3 free parameters

How to report when more than one irrep is compatible with the MSG ….

complementary information on representation analysis

	Mn_3Sn
Primary *irrep*(*s*) label(s) with dimension	mGM6+ (2-dim) special direction
Description of primary *irrep*(*s*)	mGM6+: $\{6_{001}\|0,0,1/2\}$: (½ ,-√3/2 ; √3/2 , ½) {-1|0,0,0}: (1, 0 ; 0, 1) $\{m_{010}\|0,0,0\}$: (½ ,√3/2 ; √3/2 , -½)
Secondary *irrep*(*s*) label(s) with dimension	mGM3+ (1-dim)
Description of secondary *irrep*(*s*)	mGM3+: $\{6_{001}\|0,0,1/2\}$: -1 {-1|0,0,0}: 1 $\{m_{010}\|0,0,0\}$: 1
Primary basis mode(s) and amplitude(s) C_i (in μ_B)	mGM6+, mode 1: Mn1_1 (1, 1 , 0) C_1= 3.00(1) Mn1_2 (0, -1, 0) mGM6+, mode 2: C_2=0.0 Mn1_1 (0, 1, 0) Mn1_2 (0, 1, 0)
Secondary basis mode(s) and amplitude(s) C_i (in μ_B)	mGM3+, mode 3: Mn1_1 (1, 0, 0) C_3=0.0 Mn1_2 (0, 1, 0)

Second(ary) irrep allowed by the MSG

How to report when more than one irrep is compatible with the MSG ….

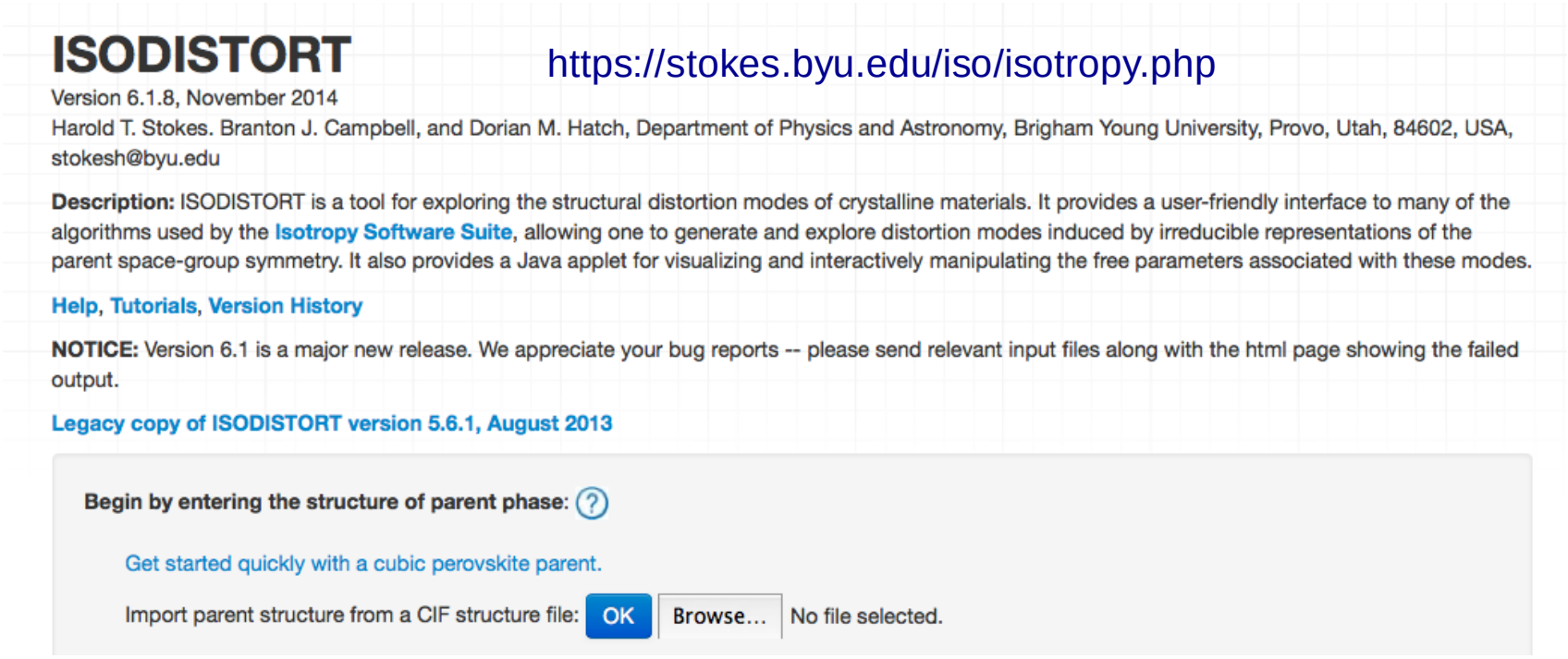
complementary information on representation analysis

	Mn_3Sn
Primary *irrep*(*s*) label(s) with dimension	mGM6+ (2-dim) special direction
Description of primary *irrep*(*s*)	mGM6+: $\{6_{001}\|0,0,1/2\}$: (½ ,-√3/2 ; √3/2 , ½) {-1|0,0,0}: (1, 0 ; 0, 1) $\{m_{010}\|0,0,0\}$: (½ ,√3/2 ; √3/2 , -½)
Secondary *irrep*(*s*) label(s) with dimension	mGM3+ (1-dim)
Description of secondary *irrep*(*s*)	mGM3+: $\{6_{001}\|0,0,1/2\}$: -1 {-1|0,0,0}: 1 $\{m_{010}\|0,0,0\}$: 1
Primary basis mode(s) and amplitude(s) C_i (in μ_B)	mGM6+, mode 1: Mn1_1 (1, 1 , 0) C_1= 3.00(1) Mn1_2 (0, -1, 0) mGM6+, mode 2: C_2=0.0 Mn1_1 (0, 1, 0) Mn1_2 (0, 1, 0)
Secondary basis mode(s) and amplitude(s) C_i (in μ_B)	mGM3+, mode 3: Mn1_1 (1, 0, 0) C_3=0.0 Mn1_2 (0, 1, 0)

Descomposition in amplitudes of irrep spin basis modes/

(as far as I know…)

The only program for mode analysis: (with irrep mode decomposition!)



Stokes & Campbell, Provo

FullProf can refine under a MSG the amplitudes of the irrep modes compatible with the MSG using output of ISODISTORT

Part of the pcr file created by ISODISTORT:

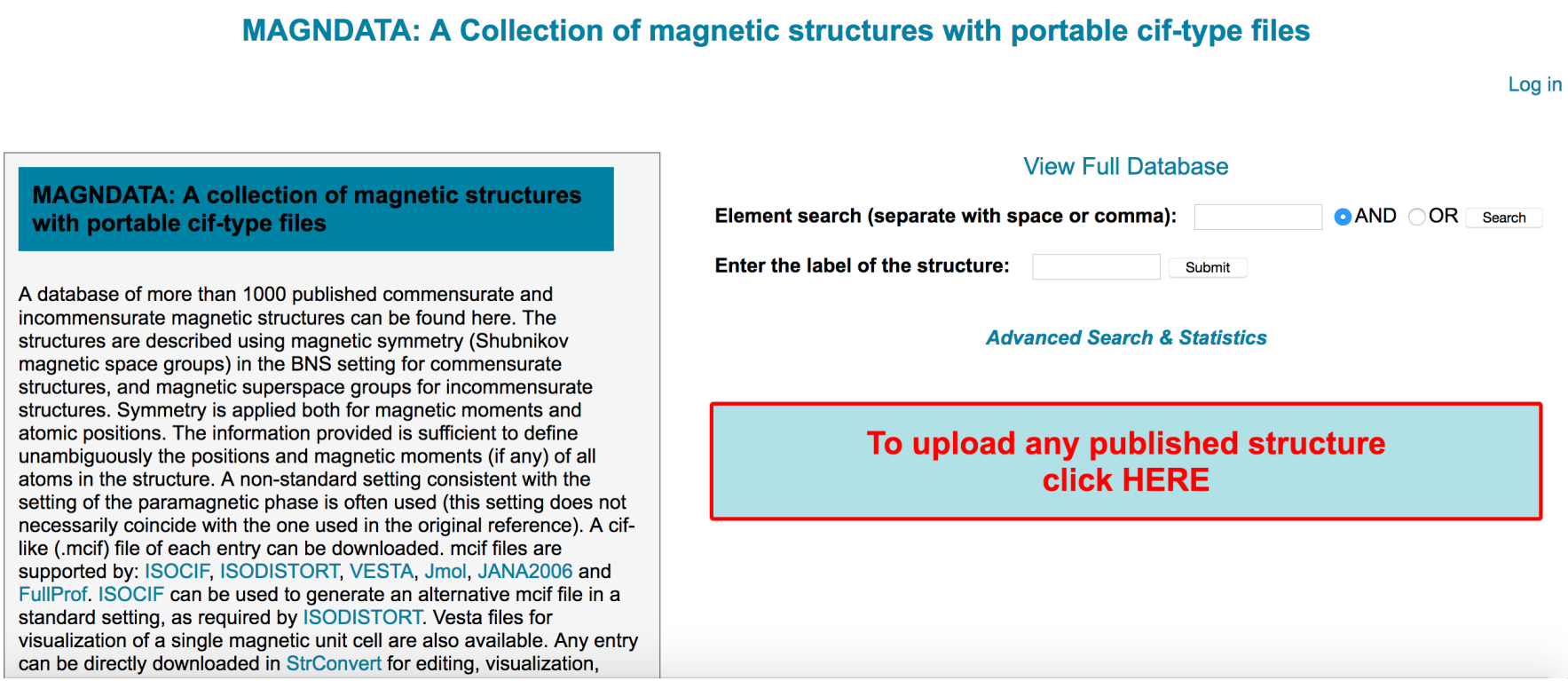
This is the future and is already available!

```
!-------------------------------------------------------------------------------
AMPLIMODES for FullProf          FIX xyz
!
!Nat Dis Ang Pr1 Pr2 Pr3 Jbt Irf Isy Str Furth       ATZ    Nvk Npr More
  3   0   0   0.0 0.0 1.0  -6   0   2   0    3       1000.0  0   7   0
Cmc'm'  number:  63.463   <--Magnetic Space Group Symbol (UNI symbol and BNS number)
Transform to standard:  b,-2a-b,c;0,0,0  <--Basis transformation from alt setting to standard BNS
Parent space group:  P6_3/mmc  IT_number:  194  <--Nonmagnetic Parent Group
Transform from Parent:  a,b,c;0,0,0  <--Basis transformation from parent to current setting
!
! Atom Typ    Mag Vec      X         Y         Z        Biso      Occ  N_type  Spc/Fftype
!       Rx        Ry        Rz        Ix        Iy        Iz     MagPh
Mn1_1  MMN2     1    0  -0.16120  0.67760   0.25000   0.50000  0.50000      1    1
                           0.00      0.00      0.00      0.00     0.00
     0.00000   0.00000   0.00000   0.00000   0.00000   0.00000  0.00000
                           0.00      0.00      0.00      0.00     0.00
Mn1_2  MMN2     1    0  -1.67760 -0.83880   0.25000   0.50000  0.25000      1    1
                           0.00      0.00      0.00      0.00     0.00
     0.00000   0.00000   0.00000   0.00000   0.00000   0.00000  0.00000
                           0.00      0.00      0.00      0.00     0.00
Sn1    SN       0    0  -0.66667 -0.33333   0.25000   0.50000  0.25000      0    2
                           0.00      0.00      0.00      0.00     0.00
! Basis vectors of magnetic symmetry modes for each atom
M_MODES    6
! Nm Atom   Irrep      Mx       My       Mz       Coeff
   1 Mn1_1   mGM3+      0.0721   0.0000   0.0000   1.00     } mode 1 mGM3+
   1 Mn1_2   mGM3+      0.0000   0.0721   0.0000   1.00
   2 Mn1_1   mGM6+      0.0510   0.1019   0.0000   1.00     } mode 2 mGM6+
   2 Mn1_2   mGM6+      0.0000   0.0000   0.0000   1.00
   3 Mn1_1   mGM6+      0.0510   0.0000   0.0000   1.00     } mode 3 mGM6+
   3 Mn1_2   mGM6+      0.0000  -0.1019   0.0000   1.00
! Amplitudes of Magnetic Symmetry Modes
MA_MODES    3    2
     A1_mGM3+          0.00000    1.00   }
     A2_mGM6+          0.00000    1.00   } mode amplitudes to refine
     A3_mGM6+          0.00000    1.00   }
!
```

In this form, one uses the representation method under a fixed MSG.

Things become much simpler!!!

How to prepare a magCIF file suitable for MAGNDATA



MAGNDATA File Upload Page

Welcome to MAGNDATA File Upload Section. Any published commensurate magnetic structure that is not already present in MAGNDATA can be uploaded here.

- The upload can be performed not only by the authors of the publication reporting the structure, but also by anybody, thinking that this structure should be in this database.
- The uploaded files, if consistent, will be processed and transformed by the Bilbao Crystallographic Server team into a more complete form to be included in the database.
- Once the structure has been finally included in MAGNDATA, the uploader will be informed by e-mail. Also, in case we encounter any problems / have some questions & comments about the data, it is essential that we have your e-mail information.
- The necessary upload process is limited to a zip file containing two files, that are:
  1. A PDF file of the publication, where the magnetic structure was reported.
  2. A CIF file of the magnetic structure using the magCIF format and having ".mcif" as its extension. This .mcif file must have certain features and information to be appropriate for MAGNDATA.

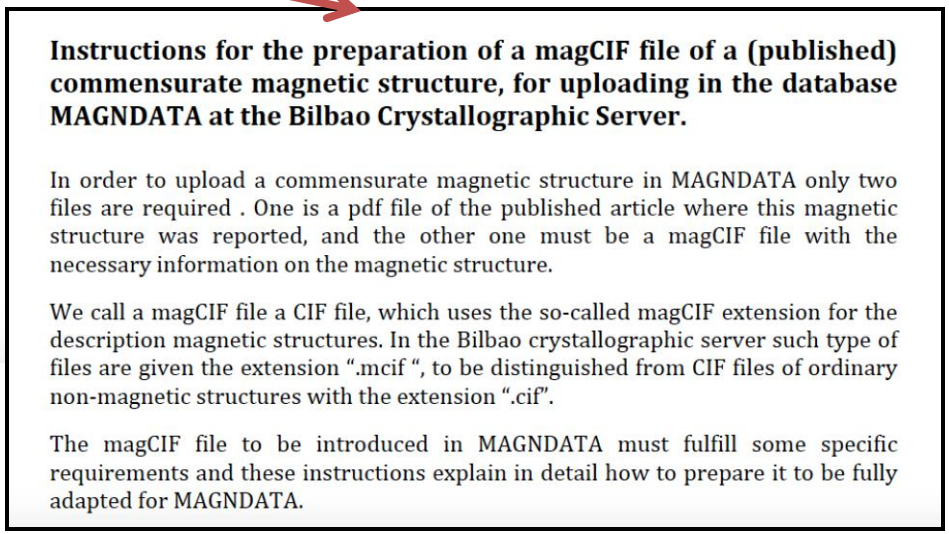
To download the instructions on how to prepare a .mcif file of the magnetic structure that can be uploaded in MAGNDATA click here.

Before proceeding to the file uploads, please provide your name, email and brief info *(info being optional)*. Once you have submitted these information, you'll be taken to the file submission page.

Your Name:
Your e-mail:

Brief info about the structure you are about to submit:

Proceed to File Uploads



Instructions for the preparation of a magCIF file of a (published) commensurate magnetic structure, for uploading in the database MAGNDATA at the Bilbao Crystallographic Server.

In order to upload a commensurate magnetic structure in MAGNDATA only two files are required . One is a pdf file of the published article where this magnetic structure was reported, and the other one must be a magCIF file with the necessary information on the magnetic structure.

We call a magCIF file a CIF file, which uses the so-called magCIF extension for the description magnetic structures. In the Bilbao crystallographic server such type of files are given the extension ".mcif ", to be distinguished from CIF files of ordinary non-magnetic structures with the extension ".cif".

The magCIF file to be introduced in MAGNDATA must fulfill some specific requirements and these instructions explain in detail how to prepare it to be fully adapted for MAGNDATA.

Instructions for the preparation of a magCIF file of a (published) commensurate magnetic structure, for uploading in the database MAGNDATA at the Bilbao Crystallographic Server.

In order to upload a commensurate magnetic structure in MAGNDATA only two files are required . One is a pdf file of the published article where this magnetic structure was reported, and the other one must be a magCIF file with the necessary information on the magnetic structure.

We call a magCIF file a CIF file, which uses the so-called magCIF extension for the description magnetic structures. In the Bilbao crystallographic server such type of files are given the extension ".mcif ", to be distinguished from CIF files of ordinary non-magnetic structures with the extension ".cif".

The magCIF file to be introduced in MAGNDATA must fulfill some specific requirements and these instructions explain in detail how to prepare it to be fully adapted for MAGNDATA.

How to prepare a magCIF file of your magnetic structure adequate for MAGNDATA

The best way:.

- ***Case 1***: **Use refinement software that supports .mcif files both for input and output: FullProf, GSAS-II, JANA, ….. (listed in alphabetical order!) to obtain a .mcif file of your structure fully consistent with its MSG.**

If you have solved however your structure with these programs or any other, but using a method that has not identified the MSG of the model, then there are two possible situations:

Case 2*: The refinement program can provide you a magCIF file of your final structure but "without symmetry", i.e. using the MSG P1, and listing all atoms and moments in the unit cell.*

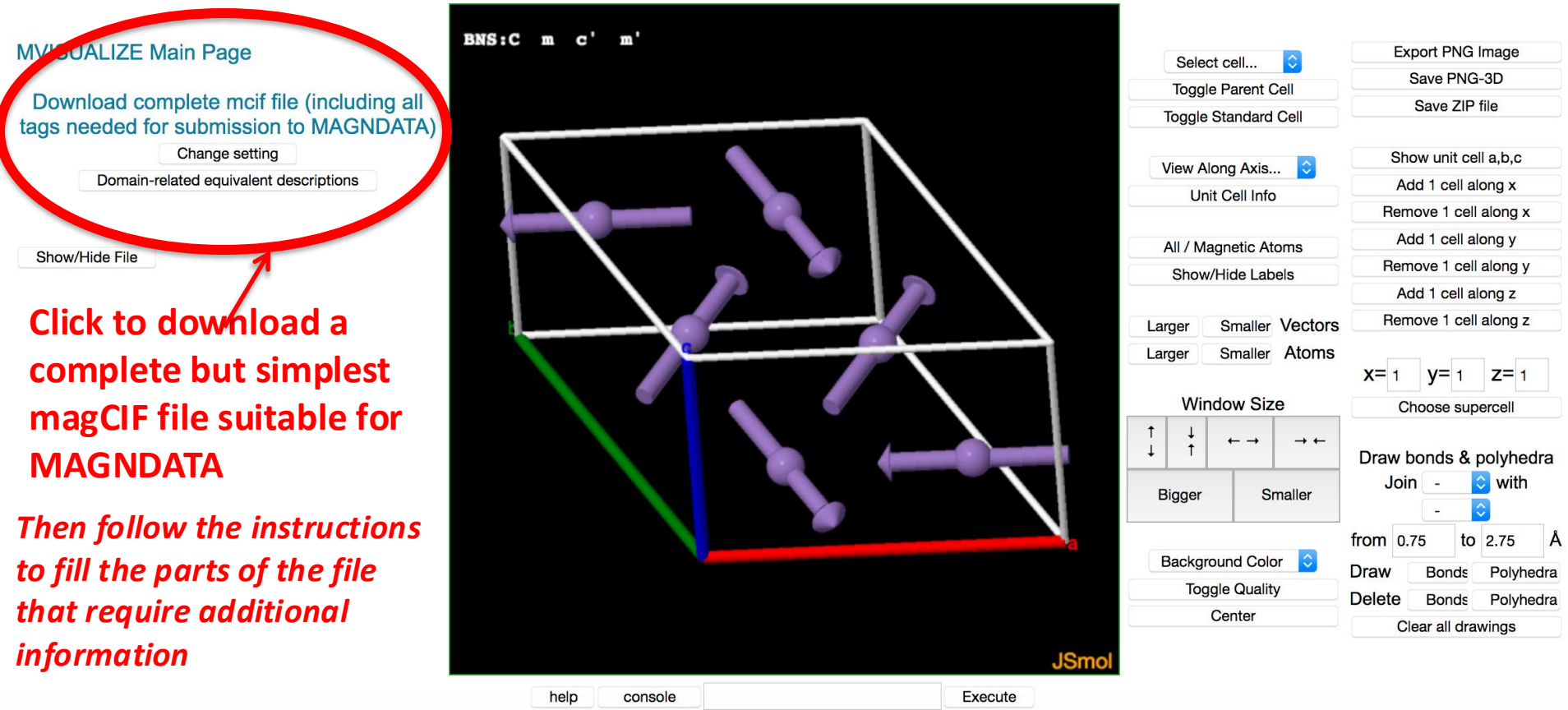
Case 3*: You know your magnetic structure so that you can calculate and list all atomic positions and magnetic moments in the unit cell, but you do not know its MSG.*

How to prepare a magCIF file suitable for MAGNDATA

Case 1: Your refinement program has generated a magCIF file of your structure consistent with its MSG

- Upload de .mcif file in **MVISUALIZE** to simplify the file and add items necessary for the database

Main Page of MVISUALIZE after uploading the mCIF file:



Click to download a complete but simplest magCIF file suitable for MAGNDATA

Then follow the instructions to fill the parts of the file that require additional information

How to prepare a magCIF file of your magnetic structure…

Case 2:You have a magCIF file of your structure but under MSG P1

Get from your refinement program a simple mCIF file in the lowest MSG P1, which only includes the lattice periodicity as symmetry and lists all atoms and moments within the unit cell.

If the program does not have this option, but you know your structure you should be able to prepare this file also either manually or with some computer script

A template file is included with the instructions that can be downloaded from MAGNDATA

All atoms in unit cell and their magnetic moments

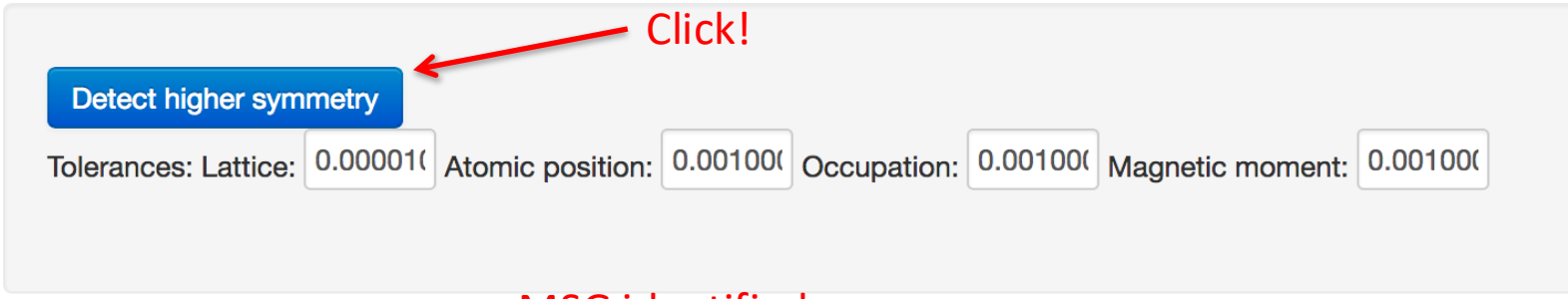
```
data_1
_cell_length_a                         5.66500
_cell_length_b                         5.66500
_cell_length_c                         4.53100
_cell_angle_alpha                      90.00000
_cell_angle_beta                       90.00000
_cell_angle_gamma                      120.00000

loop_
_space_group_symop_magn_operation.id
_space_group_symop_magn_operation.xyz
1    x,y,z,+1

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Mn1_1 Mn 0.83880 0.67760 0.25000 1.0000
Mn1_2 Mn 0.16120 0.83880 0.75000 1.0000
Mn1_3 Mn 0.16120 0.32240 0.75000 1.0000
Mn1_4 Mn 0.83880 0.16120 0.25000 1.0000
Mn1_5 Mn 0.32240 0.16120 0.25000 1.0000
Mn1_6 Mn 0.67760 0.83880 0.75000 1.0000
Sn1_1 Sn 0.33333 0.66667 0.25000 1.0000
Sn1_2 Sn 0.66667 0.33334 0.75000 1.0000

loop_
_atom_site_moment.label
_atom_site_moment.crystalaxis_x
_atom_site_moment.crystalaxis_y
_atom_site_moment.crystalaxis_z
Mn1_1 3.000 3.000 0.000
Mn1_2 -3.000 0.000 0.000
Mn1_3 3.000 3.000 0.000
Mn1_4 -3.000 0.000 0.000
Mn1_5 0.000 -3.000 0.000
Mn1_6 0.000 -3.000 0.000
```

No symmetry. Only the identity

How to prepare an magCIF file of your magnetic structure…

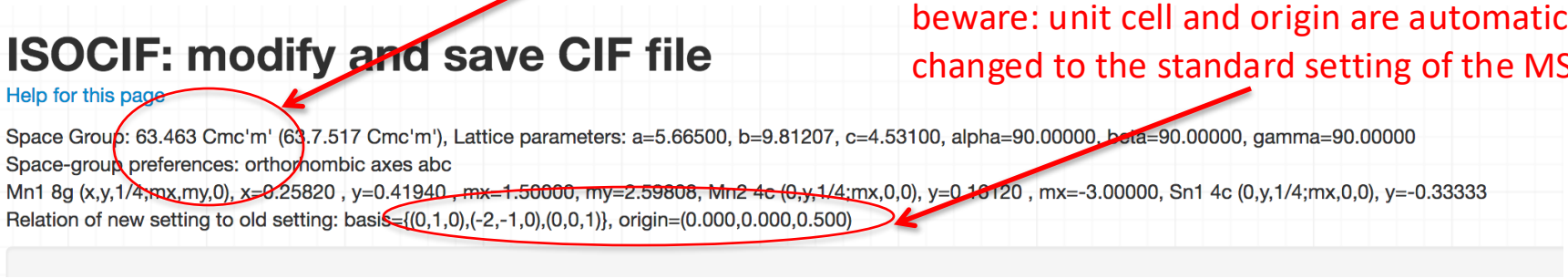
Case 2: You know your structure but you do not know (YET) its MSG…

Upload the P1 mCIF file of your structure in **ISOCIF**
from the ISOTROPY Software Suite.



MSG identified

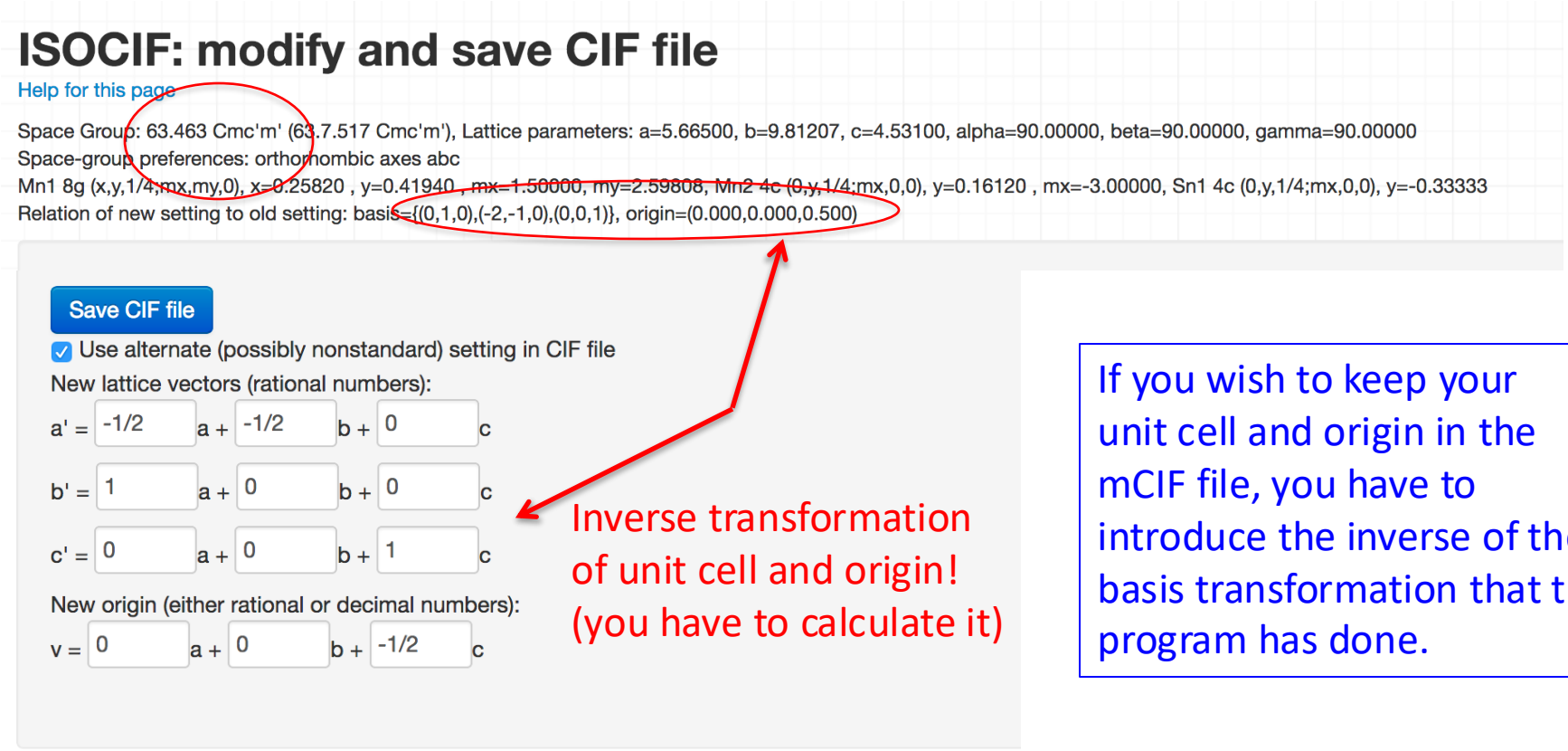
beware: unit cell and origin are automatically changed to the standard setting of the MSG!



How to prepare an magCIF file of your magnetic structure…

You know your structure but you do not know (YET) its MSG…

Save the new mCIF file with the correct MSG detected by ISOCIF. To keep the origin and unit cell of the input P1 file, care must be taken indicating the correct transformation from the standard basis chosen by the program.



If you wish to keep your unit cell and origin in the mCIF file, you have to introduce the inverse of the basis transformation that the program has done.

How to prepare a magCIF file of your magnetic structure…

Case 3:You know your structure but you do not know its MSG, and you do not have a magCIF file in P1

If you do not have a simple magCIF file in P1, provided by the refinement program, rather than preparing manually such type of file, it is more handy and much quicker in most cases, to use the tools in the Bilbao server (**MAXMAGN** or in more complex cases **k-SUBGROUPSMAG**) to enumerate probable spin arrangements for the known propagation vectors(s), identify the one that coincides with your structure, and produce the corresponding magCIF file with a fully consistent MSG.

In most cases a grahical comparison is sufficient for identifying the spin arrangement that corresponds to your structure. One can then download the corresponding mCIF file, and go then to the instructions of "Case 1", i.e. when one has a mCIF file consistent with the MSG of the structure.

Care must be taken of the fact however that these programs only list by default one of the possible equivalent domain-related MSGs and this may be not the one that corresponds to your model! One has then to use the option in both programs of enumerating all possible domain-related descriptions (conjugate MSGs) to be able to identify the one that describes your structure.

How to prepare a magCIF file of your magnetic structure…

You know your structure but you do not know its MSG…

Alternatively to **MAXMAGN** or **k-SUBGROUPSMAG,** you can use **ISODISTORT (Method 2)** to enumerate probable spin arrangements for the known propagation vectors(s), identify the one that coincides with your structure and produce the corresponding magCIF file with a fully consistent MSG.

ISODISTORT is in many aspects more powerful and certainly faster. But this program only provides the magCIF file for one of the domain-equivalent MSGs, and therefore in complex cases a direct comparison with your structure may fail.

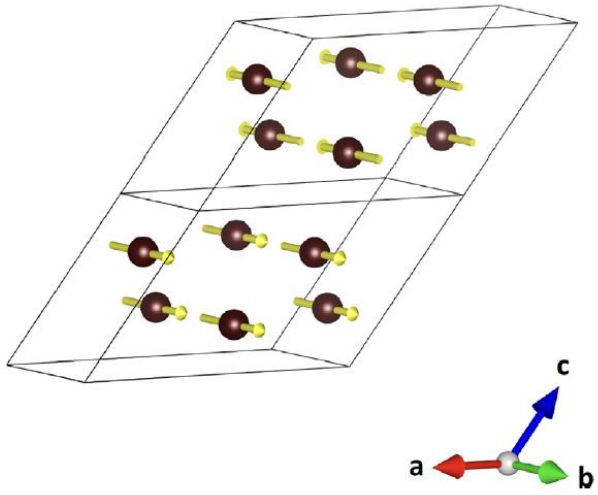


Fig. 6. The magnetic structure of $(Ho_{1-x}Lu_x)_2Fe_2Si_2C$ (x = 0.32 and 0.46). The Fe, Si and C atoms have been excluded for clarity.

Table 3
Crystallographic and magnetic parameters of $(Ho_{1-x}Lu_x)_2Fe_2Si_2C$ (x = 0.32 and 0.46) derived from refinements of the neutron diffraction patterns.

Parameters	$x = 0.32$		$x = 0.46$	
	30 K	3.5 K	30 K	3 K
$x_{Ho/Lu}$	0.5598(14)	0.5615(12)	0.5615(14)	0.5616(15)
$z_{Ho/Lu}$	0.293(2)	0.294(2)	0.298(3)	0.295(2)
x_{Fe}	0.204(1)	0.204(1)	0.204(1)	0.204(2)
z_{Fe}	0.098(2)	0.100(2)	0.097(2)	0.098(3)
x_{Si}	0.153(3)	0.155(3)	0.155(2)	0.158(3)
z_{Si}	0.705(4)	0.700(4)	0.701(4)	0.702(4)
a (Å)	10.4883(8)	10.4961(7)	10.4923(8)	10.4707(8)
b (Å)	3.8801(3)	3.8837(2)	3.8822(2)	3.8737(2)
c (Å)	6.6464(5)	6.6517(5)	6.6452(5)	6.6319(6)
β (°)	129.122(7)	129.101(5)	129.072(6)	129.076(6)
μ_{Ho} (μ_B)	–	8.8(2)	–	9.1(2)
R_p (%); R_{wp} (%)	15.5; 14.9	10.0; 10.9	13.3; 13.5	13.8; 14.8
R_{Bragg} (%); R_F (%)	8.1; 6.9	5.1; 3.5	4.7; 4.2	5.2; 3.5
R_{mag} (%)	–	5.1	–	7.1

Parent space group:

C2/m (N. 12)

8.8(2) μB

How to prepare a magCIF file of your INCOMMENSURATE magnetic structure…

And in the case of an incommensurate structure????

Well,…. it is not so easy as in the commensurate case

1. You'd better repeat the refinement using one of the programs that supports superspace symmetry groups for magnetic structures and produces the magCIF file of the refined model (JANA, FullProf, …)

or 2. As in the commensurate case, you can prepare a simple magCIF file without any symmetry except the identity, including ALL atoms in the unit cell, and all the determined modulations using cosine and sine functions, as defined in the superspace formalism.
Then upload in ISOCIF….then the program should be able to identify the actual symmetry as a magnetic superspace group (MSSG) and provide the corresponding mCIF file.

CONCLUSION

• There can be many different methods to determine magnetic structures (including just trial and error!), but we should have a UNIQUE STANDARD way for reporting them. This standard has been reached by means of extending the CIF format, a format promoted by the IUCr.

It only needs now some further extension for the inclusion of irrep modes information, to achieve its full completion!

FINALLY:
Please, when you publish a magnetic structure include a magCIF file as Suplemental Material of the publication (BUT FULLY CONSISTENT WITH WHAT IS IN THE PAPER!).

And….

When the article is published submit a magCIF file to MAGNDATA following the instructions in the database.