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How to report magnetic structures & prepare magCIF files

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Example (Commensurate):

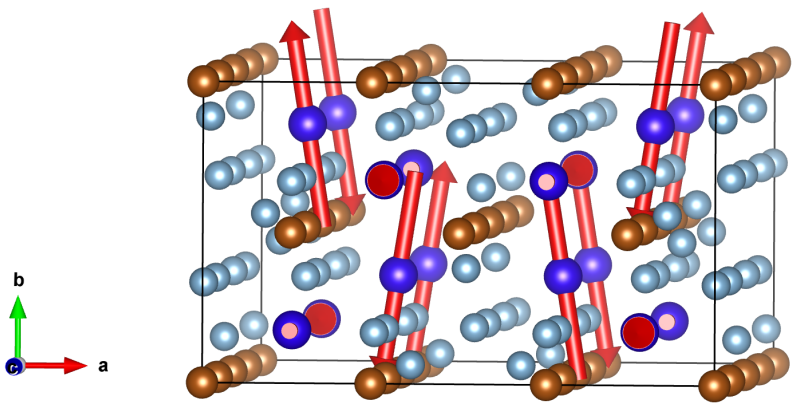
$Dy_2Co_3Al_9$ Gorbunov et al. , 2018 (magndata #1.267)

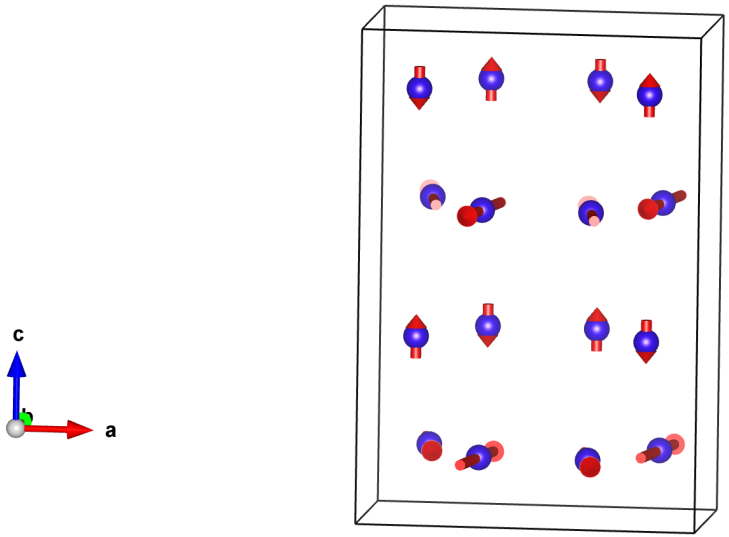
(Single crystal neutron diffraction)

k=(0,0,1/2)

2-dim irrep mZ1

Cmcm1' → *$A_a$mm2* (c, a, b; 0,0,7/8)





The MSG of this magnetic structure is only compatible with one irrep (only spin arrangements according to this irrep are allowed by the MSG, no degrees of freedom corresponding to other irreps are permitted)

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

(A kind of standard based on the magCIF extension of the CIF format)

fundamental necessary information

BNS OG

		$Dy_2Co_3Al_9$ (#1.267) (BNS setting)		$Dy_2Co_3Al_9$ (OG setting)	
1.1	MSG symbol	*A_amm2*		*$A_{2a}mm2$*	
1.2	MSG number	38.192		38.6.270	
1.3	Transformation to standard setting of MSG	(**c**,**a**,**b**;0,0,7/8)		(**c**,**a**,**b**;0,0,-1/4)	
1.4	Magnetic point group	*mm21'* (**c**,**a**,**b**) *or m2m1'*		*mm21'* (**c**,**a**,**b**) *or m2m1'*	
1.5	Unit cell parameters (Å)	a=12.72390 α=90º b=7.45860 β =90º c=18.59880 γ =90º		a=12.72390 α=90º b=7.45860 β =90º c=9.2994 γ =90º	
1.6	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}	x,y,z,+1 -x,y,-z+1/2,-1 -x,y,z,+1 x,y,-z+1/2,-1	{1|0,0,0} {$2'_{010}$|0,0,½} {m_{100}|0,0,0} {m'_{001}|0,0,½}
1.7	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}	x,y,z x+1/2,y+1/2,z	{1|0,0,0} {1|½,½,0}
1.8	OG wavevector k OG	------		(0,0,1/2)	
1.9	Positions of magnetic atoms	Dy1_1 Dy 0.33940 0.33290 0.12500 Dy1_2 Dy 0.66060 0.66710 0.87500		Dy1_1 Dy 0.33940 0.33290 0.250 Dy1_2 Dy 0.66060 0.66710 0.750	

- **Two alternative settings and notations of the MSGs can be considered standard : the Belov-Neronova-Smirnova (BNS) and the Opechowschi-Guccione (OG), but at present only software for the BNS setting is available.**

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

fundamental necessary information

		$Dy_2Co_3Al_9$ (#1.267) (BNS setting)		$Dy_2Co_3Al_9$ (OG setting)	
1.1	MSG symbol	*A_amm2*		*$A_{2a}mm2$*	
1.2	MSG number	38.192		38.6.270	
1.3	Transformation to standard setting of MSG	(**c**,**a**,**b**;0,0,7/8)		(**c**,**a**,**b**;0,0,1/4)	
1.4	Magnetic point group	*mm21'* (**c**,**a**,**b**) *or m2m1'*		*mm21'* (**c**,**a**,**b**) *or m2m1'*	
1.5	Unit cell parameters (Å)	a=12.72390 α=90º b=7.45860 β =90º c=18.59880 γ =90º		a=12.72390 α=90º b=7.45860 β =90º c=9.2994 γ =90º	
1.6	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}	x,y,z,+1 -x,y,-z+1/2,-1 -x,y,z,+1 x,y,-z+1/2,-1	{1|0,0,0} {$2'_{010}$|0,0,½} {m_{100}|0,0,0} {m'_{001}|0,0,½}
1.7	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}	x,y,z x+1/2,y+1/2,z	{1|0,0,0} {1|½,½,0}
1.8	OG wavevector k OG	------		(0,0,1/2)	
1.9	Positions of magnetic atoms	Dy1_1 Dy 0.33940 0.33290 0.12500 Dy1_2 Dy 0.66060 0.66710 0.87500		Dy1_1 Dy 0.33940 0.33290 0.250 Dy1_2 Dy 0.66060 0.66710 0.750	

- **The identification and the report of 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.

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

.... fundamental necessary information

		$Dy_2Co_3Al_9$ (#1.267) (BNS setting)		$Dy_2Co_3Al_9$ (OG setting)	
1.1	MSG symbol	*$A_a mm2$*		*$A_{2a} mm2$*	
1.2	MSG number	38.192		38.6.270	
1.3	Transformation to standard setting of MSG	(**c**,**a**,**b**;0,0,7/8)		(**c**,**a**,**b**;0,0,1/4)	
1.4	Magnetic point group	*mm21'* (**c**,**a**,**b**) *or m2m1'*		*mm21'* (**c**,**a**,**b**) *or m2m1'*	
1.5	Unit cell parameters (Å)	a=12.72390 α=90º b=7.45860 β =90º c=18.59880 γ =90º		a=12.72390 α=90º b=7.45860 β =90º c=9.2994 γ =90º	
1.6	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}	x,y,z,+1 -x,y,-z+1/2,-1 -x,y,z,+1 x,y,-z+1/2,-1	{1|0,0,0} {$2'_{010}$|0,0,½} {m_{100}|0,0,0} {m'_{001}|0,0,½}
1.7	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}	x,y,z x+1/2,y+1/2,z	{1|0,0,0} {1|½,½,0}
1.8	OG wavevector k OG	------		(0,0,1/2)	
1.9	Positions of magnetic atoms	Dy1_1 Dy 0.33940 0.33290 0.12500 Dy1_2 Dy 0.66060 0.66710 0.87500		Dy1_1 Dy 0.33940 0.33290 0.250 Dy1_2 Dy 0.66060 0.66710 0.750	

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

fundamental necessary information

		$Dy_2Co_3Al_9$ (#1.267) (BNS setting)		$Dy_2Co_3Al_9$ (OG setting)	
1.1	MSG symbol	*A_amm2*		*$A_{2a}mm2$*	
1.2	MSG number	38.192		38.6.270	
1.3	Transformation to standard setting of MSG	(**c**,**a**,**b**;0,0,7/8)		(**c**,**a**,**b**;0,0,1/4)	
1.4	Magnetic point group	*mm21'* (**c**,**a**,**b**) *or m2m1'*		*mm21'* (**c**,**a**,**b**) *or m2m1'*	
1.5	Unit cell parameters (Å)	a=12.72390 α=90º b=7.45860 β =90º c=18.59880 γ =90º		a=12.72390 α=90º b=7.45860 β =90º c=9.2994 γ =90º	
1.6	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}	x,y,z,+1 -x,y,-z+1/2,-1 -x,y,z,+1 x,y,-z+1/2,-1	{1|0,0,0} {$2'_{010}$|0,0,½} {m_{100}|0,0,0} {m'_{001}|0,0,½}
1.7	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}	x,y,z x+1/2,y+1/2,z	{1|0,0,0} {1|½,½,0}
1.8	OG transformation k OG			(0,0,1/2)	
1.9	Positions of magnetic atoms	Dy1_1 Dy 0.33940 0.33290 0.12500 Dy1_2 Dy 0.66060 0.66710 0.87500		Dy1_1 Dy 0.33940 0.33290 0.250 Dy1_2 Dy 0.66060 0.66710 0.750	

equivalent information

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

fundamental necessary information

		$Dy_2Co_3Al_9$ (#1.267) (BNS setting)		$Dy_2Co_3Al_9$ (OG setting)	
1.1	MSG symbol	*$A_a$mm2*		*A_{2a}mm2*	
1.2	MSG number	38.192		38.6.270	
1.3	Transformation to standard setting of MSG	(**c**,**a**,**b**;0,0,7/8)		(**c**,**a**,**b**;0,0,1/4)	
1.4	Magnetic point group	*mm21'* (**c**,**a**,**b**) *or m2m1'*		*mm21'* (**c**,**a**,**b**) *or m2m1'*	
1.5	Unit cell parameters (Å)	a=12.72390 α=90º b=7.45860 β =90º c=18.59880 γ =90º			
1.6	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}	x,y,z,+1 -x,y,-z+1/2,-1 -x,y,z,+1 x,y,-z+1/2,-1	{1|0,0,0} {$2'_{010}$|0,0,½} {m_{100}|0,0,0} {m'_{001}|0,0,½}
1.7	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}	x,y,z x+1/2,y+1/2,z	{1|0,0,0} {1|½,½,0}
1.8	OG transformation k OG			(0,0,1/2)	
1.9	Positions of magnetic atoms	Dy1_1 Dy 0.33940 0.33290 0.12500 Dy1_2 Dy 0.66060 0.66710 0.87500		Dy1_1 Dy 0.33940 0.33290 0.250 Dy1_2 Dy 0.66060 0.66710 0.750	

MSG as set of symmetry operations compulsory in the magCIF file

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

fundamental necessary information

		$Dy_2Co_3Al_9$ (#1.267) (BNS setting)		$Dy_2Co_3Al_9$ (OG setting)	
1.1	MSG symbol	*A_amm2*		*$A_{2a}mm2$*	
1.2	MSG number	38.192		38.6.270	
1.3	Transformation to standard setting of MSG	(**c**,**a**,**b**;0,0,7/8)		(**c**,**a**,**b**;0,0,1/4)	
1.4	Magnetic point group	*mm21'* (**c**,**a**,**b**) *or m2m1'*			
1.5	Unit cell parameters (Å)	a=12.72390 α=90º b=7.45860 β =90º c=18.59880 γ =90º		a=12.72390 α=90º b=7.45860 β =90º c=4.2994 γ =90º	
1.6	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}	x,y,z,+1 -x,y,-z+1/2,-1 -x,y,z,+1 x,y,-z+1/2,-1	{1|0,0,0} {$2'_{010}$|0,0,½} {m_{100}|0,0,0} {m'_{001}|0,0,½}
1.7	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}	x,y,z x+1/2,y+1/2,z	{1|0,0,0} {1|½,½,0}
1.8	OG propagation k OG			(0,0,1/2)	
1.9	Positions of magnetic atoms	Dy1_1 Dy 0.33940 0.33290 0.12500 Dy1_2 Dy 0.66060 0.66710 0.87500		Dy1_1 Dy 0.33940 0.33290 0.250 Dy1_2 Dy 0.66060 0.66710 0.750	

For Tables and text, the Seitz notation to be highly recommended

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

fundamental necessary information

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

1.9	Positions of magnetic atoms	Dy1_1 Dy 0.33940 0.33290 0.12500 Dy1_2 Dy 0.66060 0.66710 0.87500	Dy1_1 Dy 0.33940 0.33290 0.250 Dy1_2 Dy 0.66060 0.66710 0.750
1.10	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	Co1 Co 0.32880 0.00000 0.00000 Co2 Co 0.00000 0.00000 0.00000 Al1_1 Al 0.00000 0.12490 0.250 Al1_2 Al 0.00000 0.87510 0.750 Al2_1 Al 0.10790 0.44590 0.250 Al2_2 Al 0.89210 0.55410 0.750 Al3_1 Al 0.00000 0.33220 0.5428 Al3_2 Al 0.00000 0.66780 0.0428 Al4_1 Al 0.16860 0.33300 0.0717 Al4_2 Al 0.83140 0.66700 0.5717
1.11	Magnetic moments (μ_B) of magnetic atoms and their symmetry constraints	Dy1_1 1.34(2) 8.35(2) 0.00000 (mx,my,0) 8.46 Dy1_2 0.0 0.0 -1.38(1) (0,0,mz) 1.38	Dy1_1 1.34(2) 8.35(2) 0.0 (mx,my,0) 8.46 Dy1_2 0.0 0.0 1.38(1) (0,0,mz) 1.38

moment moduli

MSG constraints on the magnetic moments

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

Simple, Compact and Robust…

It is the description used in the CIF file format, extended to magnetic structures, which is supported now by many programs.

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

fundamental necessary information

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

1.9	Positions of magnetic atoms	Dy1_1 Dy 0.33940 0.33290 0.12500 Dy1_2 Dy 0.66060 0.66710 0.87500	Dy1_1 Dy 0.33940 0.33290 0.250 Dy1_2 Dy 0.66060 0.66710 0.750
1.10	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	Co1 Co 0.32880 0.00000 0.00000 Co2 Co 0.00000 0.00000 0.00000 Al1_1 Al 0.00000 0.12490 0.250 Al1_2 Al 0.00000 0.87510 0.750 Al2_1 Al 0.10790 0.44590 0.250 Al2_2 Al 0.89210 0.55410 0.750 Al3_1 Al 0.00000 0.33220 0.5428 Al3_2 Al 0.00000 0.66780 0.0428 Al4_1 Al 0.16860 0.33300 0.0717 Al4_2 Al 0.83140 0.66700 0.5717
1.11	Magnetic moments (μ_B) of magnetic atoms and their symmetry constraints	Dy1_1 1.34(2) 8.35(2) 0.00000 (mx,my,0) Dy1_2 0.0 0.0 -1.38(1) (0,0,mz)	Dy1_1 1.34(2) 8.35(2) 0.0 (mx,my,0) Dy1_2 0.0 0.0 1.38(1) (0,0,mz)

- **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 effects induced by the magnetic ordering this the first step!

- In many cases, even if the MSG implies a decrease of symmetry of the positional structure, magneto-structural effects are very weak and within experimental resolution the positional structure keeps the constraints of the space group of the paramagnetic phase. Then the positional structure of the non-magnetic atoms can be reported using this space group instead of the MSG (in the CIF file as a second phase).

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

complementary information

		$Dy_2Co_3Al_9$ (#1.267) (BNS or OG setting)
2.1	Parent space group	*Cmcm* (N. 63)
2.2	Propagation vector(s)	k1=(0,0,1/2)
2.3	Transformation from parent setting to the one used	(**a**,**b**,2**c**;0,0,0)
2.4	Primary irrep(s) labels with dimension	mZ1(2)
2.5	Secondary irrep(s) labels if allowed	-------
2.6	Description of the primary irrep(s)	mZ1: $\{2_{001}\|0,0,1/2\}$: (0 ,-1 ; 1 , 0) $\{2_{010}\|0,0,1/2\}$: (1, 0 ; 0,- 1) {-1|0,0,0}: (0, -1 ; -1, 0)
2.7	Description of the secondary irrep(s) if allowed	---------

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

complementary information

Relation with the paramagnetic structure

		$Dy_2Co_3Al_9$ (#1.267) (BNS or OG setting)
2.1	Parent space group	*Cmcm* (N. 63)
2.2	Propagation vector(s)	k1=(0,0,1/2)
2.3	Transformation from parent setting to the one used	(**a**,**b**,2**c**;0,0,0)
2.4	Primary irrep(s) labels with dimension	mZ1(2)
2.5	Secondary irrep(s) labels if allowed	-------
2.6	Description of the primary irrep(s)	mZ1: $\{2_{001}\|0,0,1/2\}$: (0 ,-1 ; 1 , 0) $\{2_{010}\|0,0,1/2\}$: (1, 0 ; 0,- 1) {-1|0,0,0}: (0, -1 ; -1, 0)
2.7	Description of the secondary irrep(s) if allowed	---------

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

complementary information

Information on the irreducible representations (irreps) involved

		$Dy_2Co_3Al_9$ (#1.267) (BNS or OG setting)
2.1	Parent space group	*Cmcm* (N. 63)
2.2	Propagation vector(s)	k1=(0,0,1/2)
2.3	Transformation from parent setting to the one used	(**a**,**b**,2**c**;0,0,0)
2.4	Primary irrep(s) labels with dimension	mZ1(2)
2.5	Secondary irrep(s) labels if allowed	-------
2.6	Description of the primary irrep(s)	mZ1: $\{2_{001}\|0,0,1/2\}$: (0 ,-1 ; 1 , 0) $\{2_{010}\|0,0,1/2\}$: (1, 0 ; 0,- 1) {-1|0,0,0}: (0, -1 ; -1, 0)
2.7	Description of the secondary irrep(s) if allowed	---------

Only supplemental information!

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, ….
  - **Kovalev notation** (O.V. Kovalev 1965-1993)**:**
    software: SARAh

- **It is strongly advised against using arbitrary irrep labels, but if done, then full unambiguous listings of the irrep characters must be necessarily included.**

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:**

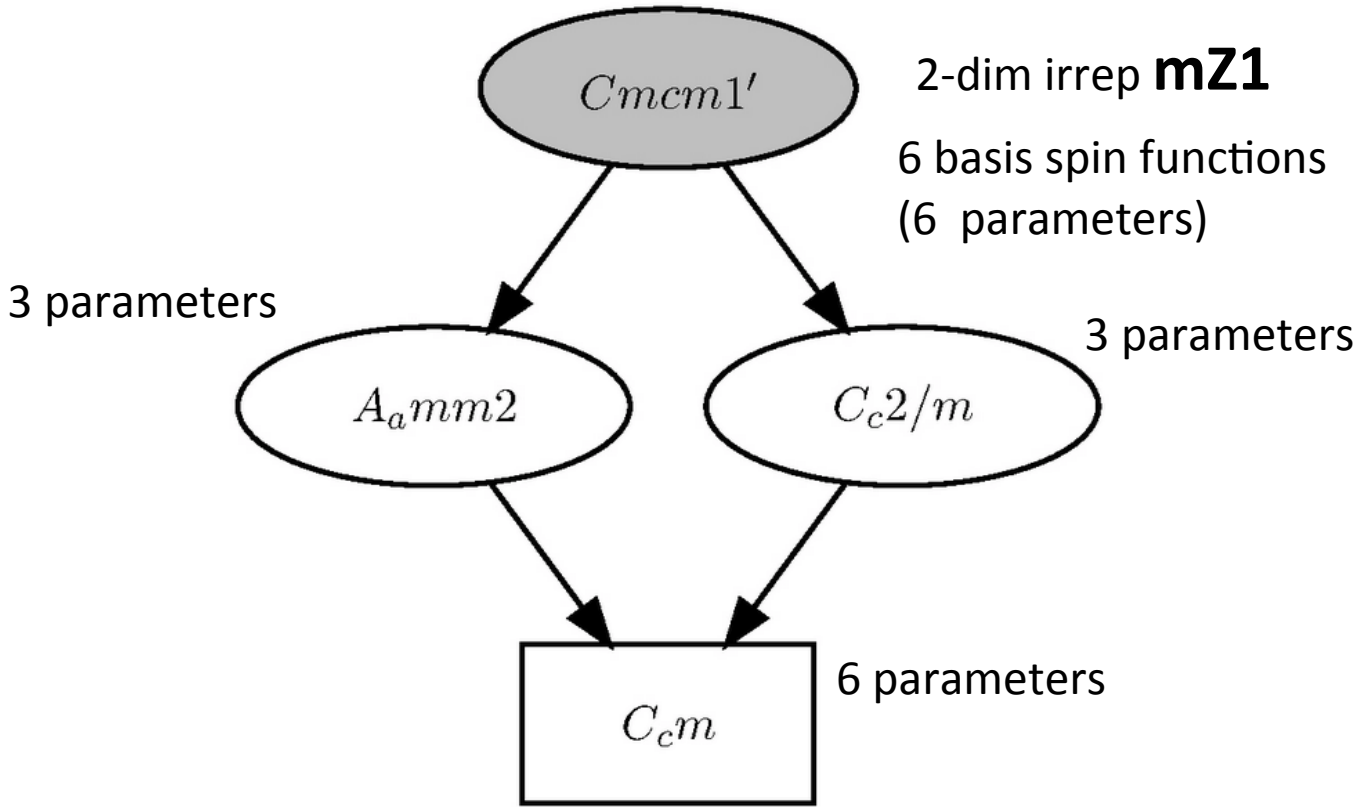
  - If the irrep is 1-dim, the two descriptions will be fully equivalent: the irrep basis functions will reproduce the same moment relationships among the magnetic atoms as the MSG.

  - If the irrep is multidimensional, several alternative MSGs can realized for the same irrep and the description using the actual MSG automaticaly introduces additional constraints that must be taken into account.

Our example:

k=(0,0,1/2)

Cmcm1' → $A_a mm2$ (c, a, b; 0,0,7/8)



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 in the spin arrangement.**

How to report then when <u>more than one</u> irrep is compatible with the MSG ?

Unfortunately, no standard yet for the inclusion of additional irrep restrictions…

What follows is just a proposal

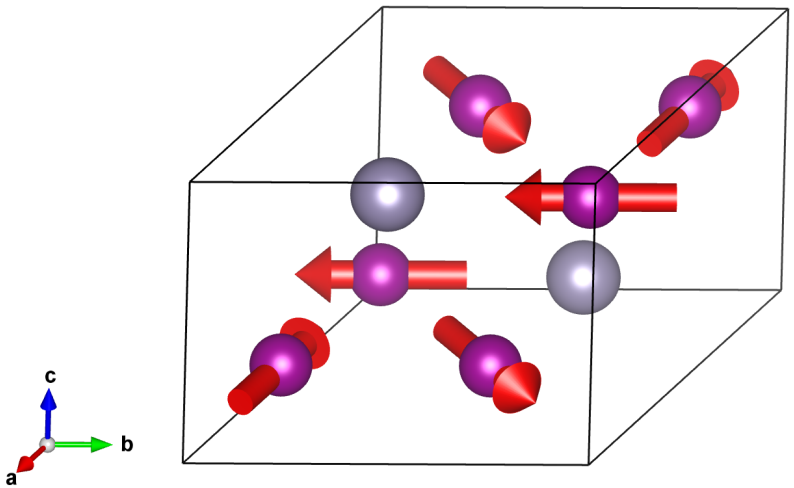
Example (Commensurate):

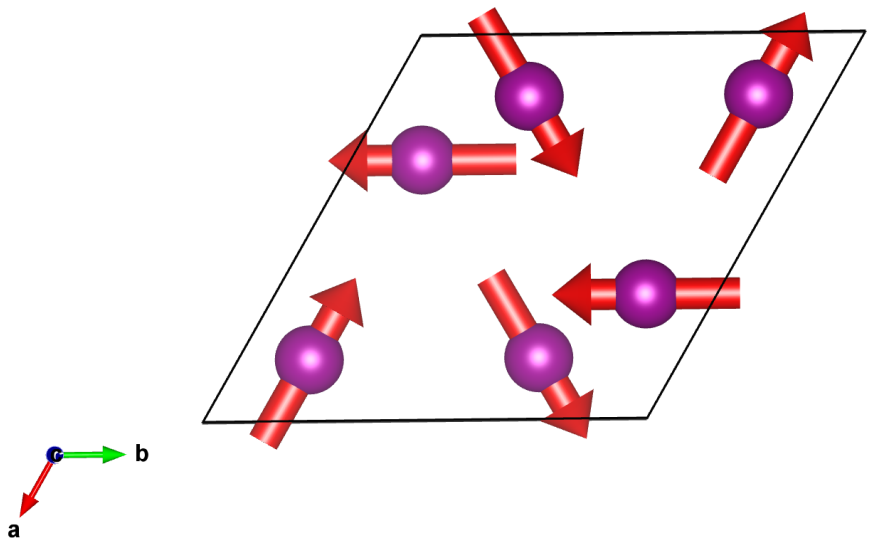
Mn_3Sn P.J. Brown et al. , 1990 (magndata #0.199)

(Single crystal neutron diffraction)

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

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





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)

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

fundamental necessary information (the same as before)

		Mn_3Sn (#0.199) (BNS setting)	
1.1	MSG symbol	*Cmc'm'*	
1.2	MSG number	63.463	
1.3	Transformation to standard setting of MSG	(**-b**,2**a+b**,**c**;0,0,0)	
1.4	Magnetic point group	*mm21'* (**c**,**a**,**b**) *or m2m1'*	
1.5	Unit cell parameters (Å)	a=5.665 α=90º b=5.665 β =90º c=4.531 γ=120º	
1.6	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	{1|0,0,0} {2_{010}|0,0,0} {-1|0,0,0} {m_{010}|0,0,0} {$2'_{210}$|0,0,½} {$2'_{001}$|0,0,½} {m'_{210}|0,0,½} {m'_{001}|0,0,½}
1.7	MSG symmetry centering operations	x,y,z,+1	{1|0,0,0}
1.9	Positions of magnetic atoms	Mn1_1 Mn 0.8388 0.6776 0.25 Mn1_2 Mn 0.3224 0.1612 0.25	
1.10	Positions of non-magnetic atoms	Sn1 Sn 0.333333 0.666667 0.25	
1.11	Magnetic moments (μ_B) of magnetic atoms and their symmetry constraints	Mn1_1 3.00(1) 3.0 0.0 (mx,my,0) Mn1_2 0.0 -3.0 0.0 (0,my,0)	

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

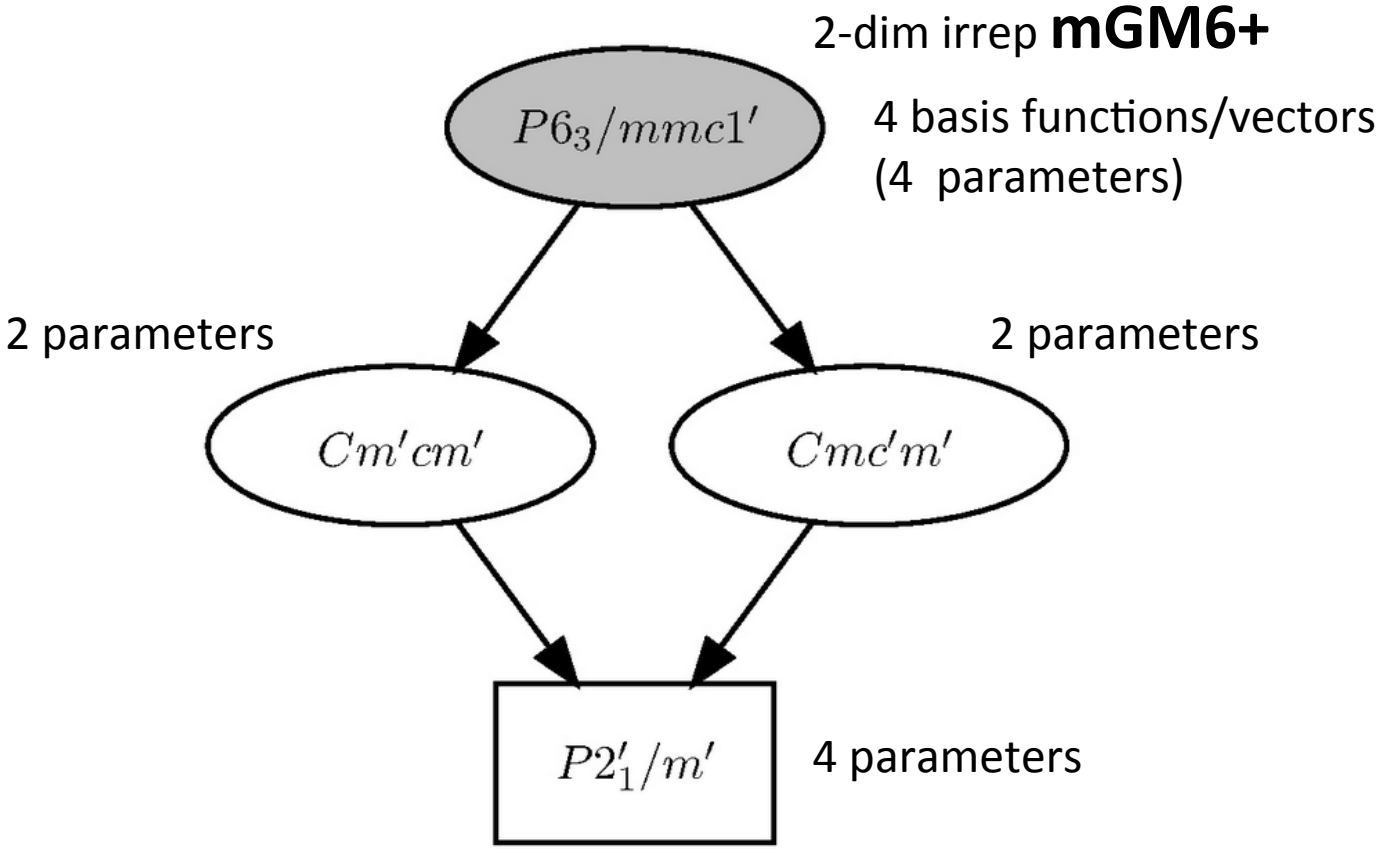
fundamental necessary information (the same as before)

		Mn_3Sn (#0.199) (BNS setting)	
1.1	MSG symbol	*Cmc'm'*	
1.2	MSG number	63.463	
1.3	Transformation to standard setting of MSG	(**-b**,2**a+b**,**c**;0,0,0)	
1.4	Magnetic point group	*mm21'* (**c**,**a**,**b**) *or m2m1'*	
1.5	Unit cell parameters (Å)	a=5.665 α=90º b=5.665 β =90º c=4.531 γ=120º	
1.6	MSG symmetry operations	x,y,z,+1 -x,-x -x,-y 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	{1|0,0,0} {m_{010}|0,0,0} {$2'_{210}$|0,0,½} {$2'_{001}$|0,0,½} {m'_{210}|0,0,½} {m'_{001}|0,0,½}
1.7	MSG symmetry centering operations	x,y,z,+1	{1|0,0,0}
1.9	Positions of magnetic atoms	Mn1_1 Mn 0.8388 0.6776 0.25 Mn1_2 Mn 0.3224 0.1612 0.25	
1.10	Positions of non-magnetic atoms	Sn1 Sn 0.333333 0.666667 0.25	
1.11	Magnetic moments (μ_B) of magnetic atoms and their symmetry constraints	Mn1_1 3.00(1) 3.0 0.0 (mx,my,0) Mn1_2 0.0 -3.0 0.0 (0,my,0)	

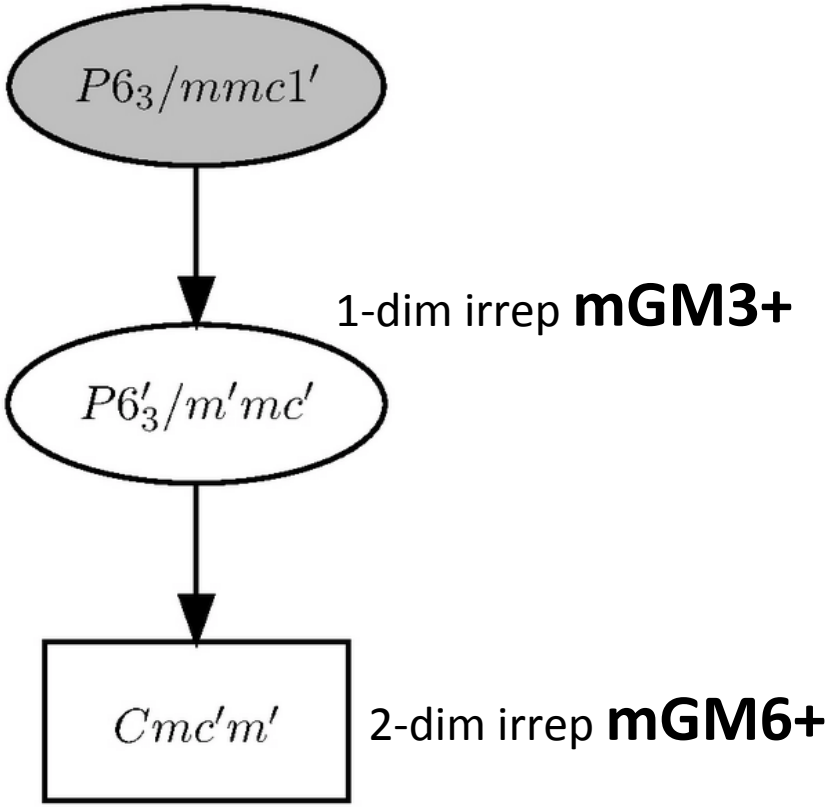
3 free parameters

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

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



Why 3 freee parameters when described using the MSG Cm'cm' instead of 2 parameters?



Von Neumann principle:
Everything that keeps the symmetry Cmc'm' is allowed and can happen…
Anything that keeps the symmetry P6'$_3$/m'mc' keeps the symmetry of its subgroup Cmc'm'
Therefore…. a spin arrangement according to the irrep mGM3+ is also allowed in the structure with MSG Cmc'm'

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

fundamental information (different than in previous case!)

2.1	Parent space group	*P63/mmc* (N. 194)
2.2	Propagation vector(s)	k1=(0,0,0)
2.3	Transformation from parent setting to the one being used	(**a**,**b**,**c**;0,0,0)
2.4	Primary irrep(s) labels with dimension	mGM6+(2)
2.5	Secondary irrep(s) labels with dimension (if symmetry allowed)	mGM3+(1)
2.6	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)
2.7	Description of secondary irrep(s) if allowed	mGM3+: $\{6_{001}\|0,0,1/2\}$: -1 {-1|0,0,0}: 1 $\{m_{010}\|0,0,0\}$: 1
3.1	Description of primary mode(s)	mGM6+: Mn1_1 (a+b,2b,0) Mn1_2 (0,-2a,0)
3.2	Description of secondary mode(s)	mGM3+: Mn1_1 (c,0,0) Mn1_2 (0,c,0)

Second(ary) irrep allowed by the MSG

1.9	Positions of magnetic atoms	Mn1_1 Mn 0.8388 0.6776 0.25 Mn1_2 Mn 0.3224 0.1612 0.25
1.11	Magnetic moments (μ_B) of magnetic atoms and their symmetry constraints	Mn1_1 3.00(1) 3.0 0.0 (mx,my,0) Mn1_2 0.0 -3.0 0.0 (0,my,0)

2.1	Parent space group	*P63/mmc* (N. 194)
2.2	Propagation vector(s)	k1=(0,0,0)
2.3	Transformation from parent setting to the one being used	[illegible]
2.4	Primary irrep(s) labels with dimension	[illegible]
2.5	Secondary irrep(s) labels with dimension (if symmetry allowed)	[illegible]
2.6	Description of primary irrep(s)	[illegible] $\{m_{010}\|0,0,0\}$: (½ ,√3/2 ; √3/2 , -½)
2.7	Description of secondary irrep(s) if allowed	mGM3+: $\{6_{001}\|0,0,1/2\}$: -1 {-1|0,0,0}: 1 $\{m_{100}\|0,0,0\}$: 1
3.1	Description of primary mode(s)	mGM6+: Mn1_1 (a+b,2b,0) Mn1_2 (0,-2a,0) 2 parameters
3.2	Description of secondary mode(s)	mGM3+: Mn1_1 (c,0,0) Mn1_2 (0,c,0) 1 parameter

Separation of the 3 magnetic degrees of freedom within the MSG into the two allowed irreps.

Only the constraints for the atoms in the aymmetric unit are needed !!! (the rest is generated by the MSG).

Description of the irrep basis vectors involved

1 basis vector for **mGM3+**:

Mn1_1 c (1,0,0) c=0
Mn1_2 (0,1,0)

The form of the moments of all atoms in the unit cell is NOT needed! The MSG operations takes care of that

2 basis vectors for **mGM6+**:

	basis vector 1:		basis vector 2:
Mn1_1	a (1,0,0)	+	b (1,2,0)
Mn1_2	(0,2,0)		(0,0,0)

The form of the moments of all atoms in the unit is NOT needed! The MSG operations takes care of that

3.1	Description of primary mode(s)	mGM6+: Mn1_1 (a+b,2b,0) Mn1_2 (0,-2a,0)	2 parameters
3.2	Description of secondary mode(s)	mGM3+: Mn1_1 (c,0,0) Mn1_2 (0,c,0)	1 parameter

When defined under the MSG symmetry of the structure, the description of the basis vectors does not require complex functions…

- The secondary irrep mGM3+ spin mode is absent.
- Only the irrep mGM6+ mode is present, but the model includes an additional constraint (a=b), which is not forced by the restriction to this single irrep. (additional ad-hoc restriction of equal modulus for the two split sites).

a=b → equal moment modulus
not forced by symmetry
but assumed

1.9	Positions of magnetic atoms	Mn1_1 Mn 0.8388 0.6776 0.25 Mn1_2 Mn 0.3224 0.1612 0.25
1.11	Magnetic moments (μ_B) of magnetic atoms and their symmetry constraints	Mn1_1 3.00(1) 3.0 0.0 (mx,my,0) Mn1_2 0.0 -3.0 0.0 (0,my,0)

3.1	Description of primary mode(s)	mGM6+: Mn1_1 (a+b,2b,0) Mn1_2 (0,-2a,0)
3.2	Description of secondary mode(s)	mGM3+: Mn1_1 (c,0,0) Mn1_2 (0,c,0)

a = b ; a=1.5

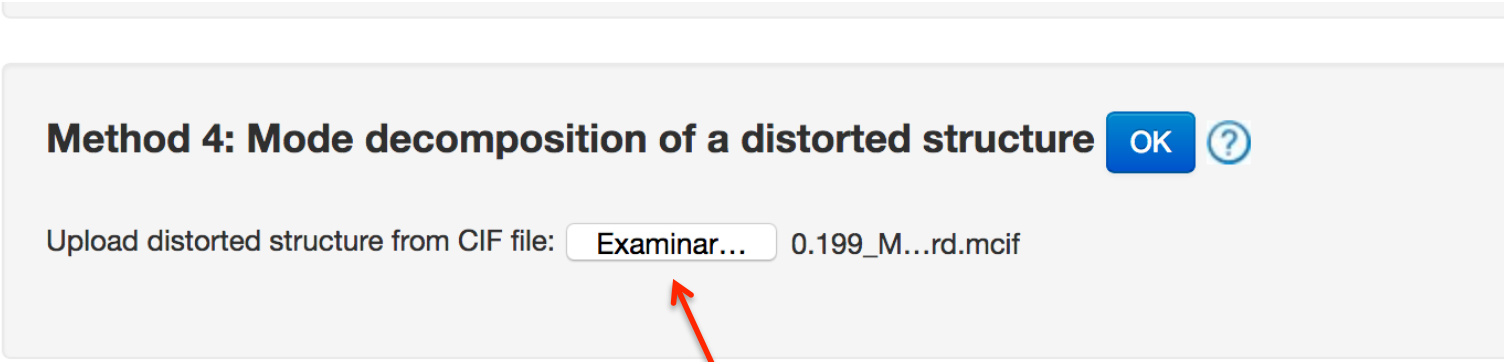
c = 0

How do I know that more than one irrep is compatible with the symmetry of my structure and therefore allowed within the phase?

Method 1: Use ISODISTORT (Method 4) to decompose your structure in irrep modes

Input: CIF and mCIF files of parent and magnetic structure

standard setting ! (use ISOCIF to transform to a standard setting if needed)



mCIF file of your structure in standard setting

How do I know that more than one irrep is compatible with the symmetry of my structure and therefore allowed within the phase?

Method 1: Use ISODISTORT (Method 4) to decompose your structure in irrep modes

Input: CIF and mCIF files of parent and magnetic structure

ISODISTORT: distortion

Space Group: 194 P6_3/mmc D6h-4, Lattice parameters: a=5.66500, b=5.66500, c=4.53100, alpha=90.00000, beta=90.00000, gamma=120.00000
Default space-group preferences: monoclinic axes a(b)c, monoclinic cell choice 1, orthorhombic axes abc, origin choice 2, hexagonal axes, SSG standard setting
Mn1 6h (x,2x,1/4), x=-0.16120, Sn1 2c (1/3,2/3,1/4)
Include magnetic Mn distortions
Reading CIF file...
Done.
Distorted structure: Magnetic Space group: 63.463 Cmc'm', Lattice parameters: a=5.66500, b=9.81207, c=4.53100, alpha=90.00000, beta=90.00000, gamma=90.00000 Atomic positions: Mn1_1 8g (x,y,1/4;mx,my,0), x=-0.24180, y=0.08060 , mx=1.50000, my=-2.59808, Mn1_2 4c (0,y,1/4;mx,0,0), y=-0.16120 , mx=-3.00000, Sn1 4c (0,y,1/4;mx,0,0), y=0.33333

Subgroup: 63.463 Cmc'm', basis={(1,0,0),(1,2,0),(0,0,1)}, origin=(0,0,0), s=1, i=6
Lattice parameters of undistorted supercell: a=5.66500, b=9.81207, c=4.53100, alpha=90.00000, beta=90.00000, gamma=90.00000

Save interactive distortion ? Save interactive diffraction ? CIF file ? Distortion file ? Domains ? Primary order parameters ? Modes details Complete modes details ?
TOPAS.STR ? FULLPROF.pcr ? IR matrices Subgroup tree OK

Enter mode and strain amplitudes: ?

P6_3/mmc[0,0,0]mGM3+ (a) 194.269 P6_3'/m'mc', basis={(0,-1,0),(1,1,0),(0,0,1)}, origin=(0,0,0), s=1 i=2, k-active= (0,0,0)
0.00000 [Mn1:h:mag]B1(a)

P6_3/mmc[0,0,0]mGM6+ (0,a) 63.463 Cmc'm', basis={(1,0,0),(1,2,0),(0,0,1)}, origin=(0,0,0), s=1 i=6, ferromagnetic, k-active= (0,0,0)
-5.19616 [Mn1:h:mag]A2(a)
-5.19616 [Mn1:h:mag]B1(a)

Decomposition into irrep components for mGM6+ and mGM3+ with zero amplitude for mGM3+

How do I know that more than one irrep is compatible with the symmetry of my structure and therefore allowed within the phase?

Method 2: Use Get_mirreps and MAGNETIC REP in the Bilbao Server

Input: Parent SG, Wyckoff position(s) of magnetic atom(s) and MSG

List of physically irreducible representations and order parameters between a parent group and a given subgroup.

Input data

Get_mirreps input

Group→subgroup	Transformation matrix
$P6_3/mmc1'$ (N. 194.264)→$Cmc'm'$ (N. 63.463)	$\begin{pmatrix} 0 & 2 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$

Representations and order parameters

Get_mirreps output

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)	$P6_3/mmc1'$ (No. 194.264) a,b,c;0,0,0	matrices of the irreps
	GM_3^+: (a,-(√3 a))	$Cmcm1'$ (No. 63.458) -b,2a+b,c;0,0,0	
	mGM_3^+: (a)	$P6_3'/m'mc'$ (No. 194.269) a,b,c;0,0,0	
	mGM_6^+: (a,a/√3)	$Cmc'm'$ (No. 63.463) -b,2a+b,c;0,0,0	

2 magn. irreps allowed

How do I know that more than one irrep is compatible with the symmetry of my structure and therefore allowed within the phase?

Method 2: Use Get_mirreps and MAGNETIC REP in the Bilbao Server

Input: Parent SG, Wyckoff position(s) of magnetic atom(s) and MSG

MAGNETIC REP output:

Decomposition of the magnetic representation of the magnetic space group $P6_3/mmc1'$ (No. 194.264)

(gray group of the paramagnetic phase)

Wave-vector: GM:(0,0,0)

Wave-vectors of the star (1 vector):

GM:(0,0,0)

Wyckoff position	Decomposition into irreps
6h:(x,2*x,1/4)	mGM1-(1) ⊕ mGM2+(1) ⊕ mGM2-(1) ⊕ mGM3+(1) ⊕ mGM3-(1) ⊕ mGM4+(1) ⊕ mGM5+(2) ⊕ 2 mGM5-(2) ⊕ 2 mGM6+(2) ⊕ mGM6-(2)

In parentheses the dimensions of the irreducible representations of the little group of k

The 2 irreps are possible for the WP 6h

How to prepare an (m)CIF file of your magnetic structure…

The best way:.

- **Use for your refinement software that supports mCIF files both for input and output: FullProf, GSAS-II, JANA, TOPAS (?) ….. (listed in alphabetical order!)**

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 two approaches are possible to obtain a correct mCIF of your structure…

How to prepare an (m)CIF file of your magnetic structure…

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

First Method: Use the tools in the Bilbao server (MAXMAGN or in more complex cases k-SUBGROUPSMAG restricted to one single irrep) to enumerate probable spin arrangements for the known propagation vectors(s) and compare with your structure. (If by refining you have used the representation method and you know the irrep(s) involved, restrict to this irrep or these irreps in the program).

In most cases a grahical comparison will be sufficient for identifying the spin arrangement that corresponds to your structure. Then, download the corresponding mCIF file and fill by hand the missing data that corresponds to your structure.

Take care of the fact however that these program 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 corresponds to your structure.

You can use alternatively ISODISTORT. But this program only provides the mCIF file for one of the domain-equivalent MSGs, and therefore in complex cases a direct comparison may fail.

How to prepare an (m)CIF file of your magnetic structure…

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

Second Method: Prepare a very 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 you know your structure you should be able to do that either by hand or with some computer tool !)

How to prepare an (m)CIF file of your magnetic structure…

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

Second Method: Prepare a very 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, and upload in **ISOCIF**

No symmetry. Only the identity

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
```

How to prepare an (m)CIF file of your magnetic structure…

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

Second Method: Prepare a very simple mCIF file in the lowest MSG P1, which only includes the lattice periodicity and lists all atoms and moments within the unit cell. Upload in **ISOCIF**

Click!

Detect higher symmetry

Tolerances: Lattice: 0.00001(Atomic position: 0.00100(Occupation: 0.00100(Magnetic moment: 0.00100(

MSG identified

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

ISOCIF: modify and save CIF file

Help for this page

Space Group: 63.463 Cmc'm' (63.7.517 Cmc'm'), Lattice parameters: a=5.66500, b=9.81207, c=4.53100, alpha=90.00000, beta=90.00000, gamma=90.00000
Space-group preferences: orthorhombic axes abc
Mn1 8g (x,y,1/4;mx,my,0), x=0.25820 , y=0.41940 , mx=1.50000, my=2.59808, Mn2 4c (0,y,1/4;mx,0,0), y=0.16120 , mx=-3.00000, Sn1 4c (0,y,1/4;mx,0,0), y=-0.33333
Relation of new setting to old setting: basis={(0,1,0),(-2,-1,0),(0,0,1)}, origin=(0.000,0.000,0.500)

How to prepare an (m)CIF file of your magnetic structure…

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

Second Method: Prepare a very simple mCIF file in the lowest MSG P1, which only includes the lattice periodicity and lists all atoms and moments within the unit cell. Upload in **ISOCIF**

ISOCIF: modify and save CIF file

Help for this page

Space Group: 63.463 Cmc'm' (63.7.517 Cmc'm'), Lattice parameters: a=5.66500, b=9.81207, c=4.53100, alpha=90.00000, beta=90.00000, gamma=90.00000
Space-group preferences: orthorhombic axes abc
Mn1 8g (x,y,1/4;mx,my,0), x=0.25820 , y=0.41940 , mx=-1.50000, my=2.59808, Mn2 4c (0,y,1/4;mx,0,0), y=0.16120 , mx=-3.00000, Sn1 4c (0,y,1/4;mx,0,0), y=-0.33333
Relation of new setting to old setting: basis={(0,1,0),(-2,-1,0),(0,0,1)}, origin=(0.000,0.000,0.500)

Save CIF file

☑ Use alternate (possibly nonstandard) setting in CIF file

New lattice vectors (rational numbers):

a' = -1/2 a + -1/2 b + 0 c

b' = 1 a + 0 b + 0 c

c' = 0 a + 0 b + 1 c

New origin (either rational or decimal numbers):

v = 0 a + 0 b + -1/2 c

Inverse transformation of unit cell and origin!

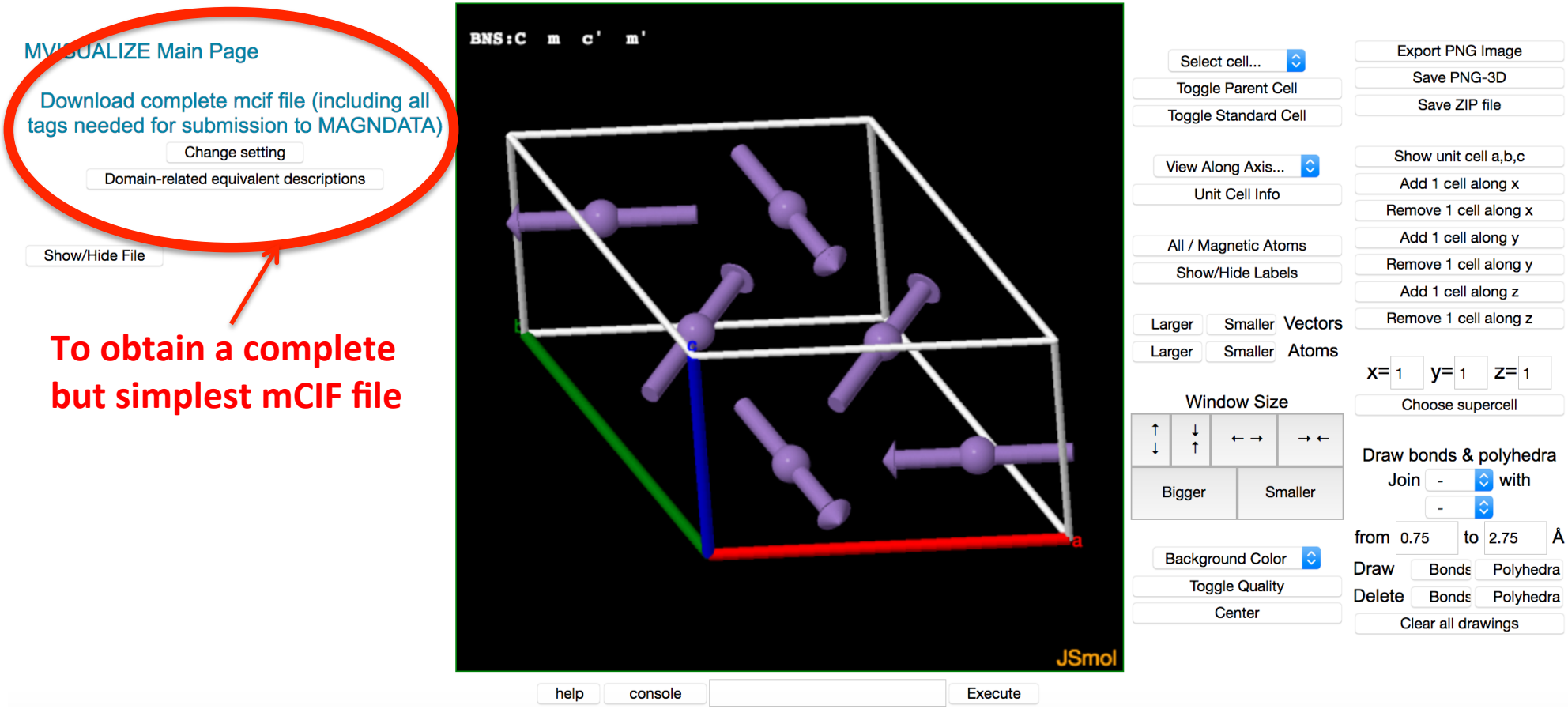
If you wish to keep your unit cell and origin in the (m)CIF file, you have to introduce the inverse of the basis transformation that the program has done.

How to prepare an (m)CIF file of your magnetic structure…

Finally, to simplify the obtained (m)CIF file and add items needed for submission to a database like MAGNDATA, you can use **MVISUALIZE**

MainPage of MVISUALIZE after the mCIF file:

MVISUALIZE: 3D Visualization of magnetic structures with Jmol



To obtain a complete but simplest mCIF file

How to prepare an (m)CIF file of your 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 mCIF file of the refined model (JANA, FullProf(?),…)

or 2. In the worst case, as in the commensurate case, you can prepare a simple mCIF 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.
(For INC structures is a recently added feature, I have not tried it yet myself!)

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, and we are close to reach this goal, by means of extending the CIF format (its extension to irrep modes information is the final step that is still missing).**