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Euskal Herriko Unibertsitatea

Symmetry of incommensurate magnetic structures
Magnetic superspace groups

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

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TOPICAL REVIEW

Magnetic superspace groups and symmetry constraints in incommensurate magnetic phases

J M Perez-Mato[1], J L Ribeiro[2], V Petricek[3] and M I Aroyo[1]

[1] Departamento de Física de la Materia Condensada, Facultad de Ciencia y Tecnología, Universidad del País Vasco, UPV/EHU, Apartado 644, E-48080 Bilbao, Spain
[2] Centro de Física da Universidade do Minho, P-4710-057 Braga, Portugal
[3] Institute of Physics, Academy of Sciences of the Czech Republic v.v.i., Na Slovance 2, CZ-18221 Praha 8, Czech Republic

E-mail: jm.perez-mato@ehu.es

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Abstract
Superspace symmetry has been for many years the standard approach for the analysis of non-magnetic modulated crystals because of its robust and efficient treatment of the structural constraints present in incommensurate phases. For incommensurate magnetic phases, this generalized symmetry formalism can play a similar role. In this context we review from a practical viewpoint the superspace formalism particularized to magnetic incommensurate phases.

SYMMETRY OF COMMENSURATE CRYSTALS

A symmetry operation fullfills two conditions:

- the operation keeps the **energy invariant**: **rotations**
  translations
  space inversion
  time reversal

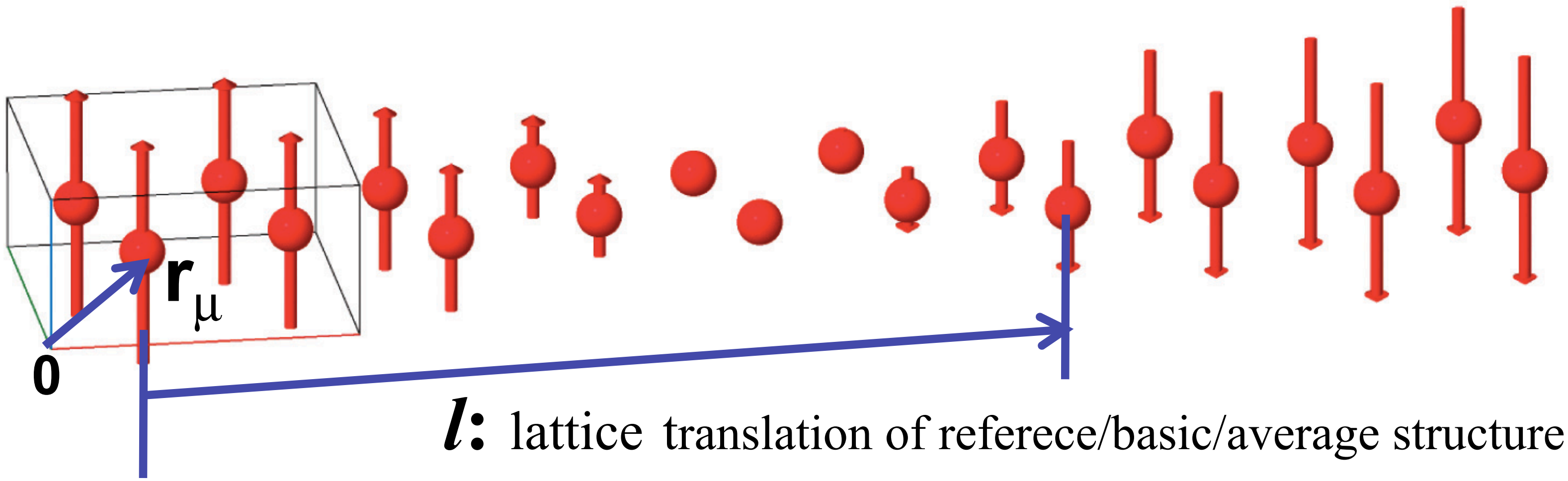
- the system is **undistinguishable** after the transformation

Symmetry operations in commensurate magnetic crystals:

magnetic space group: $\{ \{\mathbf{R}_i | \mathbf{t}_i\} , \{\mathbf{R'}_j | \mathbf{t}_j\} \}$

or $\{ \{\mathbf{R}_i , \theta | \mathbf{t}_i\}\}$ $\theta = +1$ without time reversal
$\theta = -1$ with time reversal

Incommensurate modulated structures



$\boldsymbol{l}$: lattice translation of referece/basic/average structure

Harmonic Modulation with propagation vector k of "quantity" A of atom μ:

$$A(\boldsymbol{l},\mu) = A_\mu\, e^{i2\pi \mathbf{k}.(\boldsymbol{l}+\mathbf{r}\mu)} + A^*_\mu\, e^{-i2\pi \mathbf{k}.(\boldsymbol{l}+\mathbf{r}\mu)}$$

How do we describe a modulated structure without periodicity?

Simplest case: single-k modulated structures

(One incommensurate propagation vector k (and its opposite **-k**!) **:**

general anharmonic case

μ= 1,…,n atoms in unit cell of basic structure

$$A(\boldsymbol{l},\mu) = \sum_n A_{\mu,n}\, e^{i2\pi n \mathbf{k}.(\boldsymbol{l}+\mathbf{r}\mu)} + A^*_{\mu,n} e^{-i2\pi n \mathbf{k}.(\boldsymbol{l}+\mathbf{r}\mu)}$$

$$\boxed{A_\mu(x4) = \sum_n A_{\mu,n}\, e^{i2\pi n x4} + A^*_{\mu,n} e^{-i2\pi n x4}}$$

$$A_\mu(x_4) = A_{\mu 0} + \sum_{n=1,\ldots} A_{\mu,ns} \sin(2\pi n x_4) + A_{\mu,nc} \cos(2\pi n x_4)$$

$$\boxed{A(\boldsymbol{l},\mu) = A_\mu(x4 = \mathbf{k}.(\boldsymbol{l}+\mathbf{r}\mu))}$$

How do we describe a modulated structure without periodicity?

Simplest case: single-k modulated structures

(One incommensurate propagation vector k (and its opposite **-k**!) **:**

Incommensurate Structure	**=**	**Basic (periodic) structure** **+** **set of atomic modulation functions** $A_\mu(x_4)$

μ= 1,…,n atoms in unit cell of basic structure

$$A_\mu(x_4) = A_{\mu 0} + \sum_{n=1,\ldots} A_{\mu,ns}\sin(2\pi n x_4) + A_{\mu,nc}\cos(2\pi n x_4)$$

$$\boxed{A(\boldsymbol{l},\mu) = A_\mu(x4 = \mathbf{k}.(\boldsymbol{l}+\mathbf{r}\mu))}$$

Description of an incommensurate modulated structure

1) Basic structure: $\mathbf{r}_{l\mu} = \boldsymbol{l} + \mathbf{r}_{\mu}$ $\boldsymbol{l}$: basic lattice/periodicity

μ= 1,…,n atoms in unit cell of basic structure

2) Modulations (magnetic moments, atomic displacements,..):

modulation functions: $\mathbf{A}_{\mu}(x_4)$ with period 1: $\mathbf{A}_{\mu}(x_4) = \mathbf{A}_{\mu}(x_4 + 1)$

$$A_{\mu}(x_4) = A_{\mu 0} + \sum_{n=1,\dots} A_{\mu,ns} \sin(2\pi n x_4) + A_{\mu,nc} \cos(2\pi n x_4)$$

$$\boxed{\textbf{Value of A for atom } (l,\mu)\textbf{:} \quad \mathbf{A}(\boldsymbol{l},\mu) = \mathbf{A}_{\mu}(x_4 = \mathbf{k}.\,\mathbf{r}_{l\mu})}$$

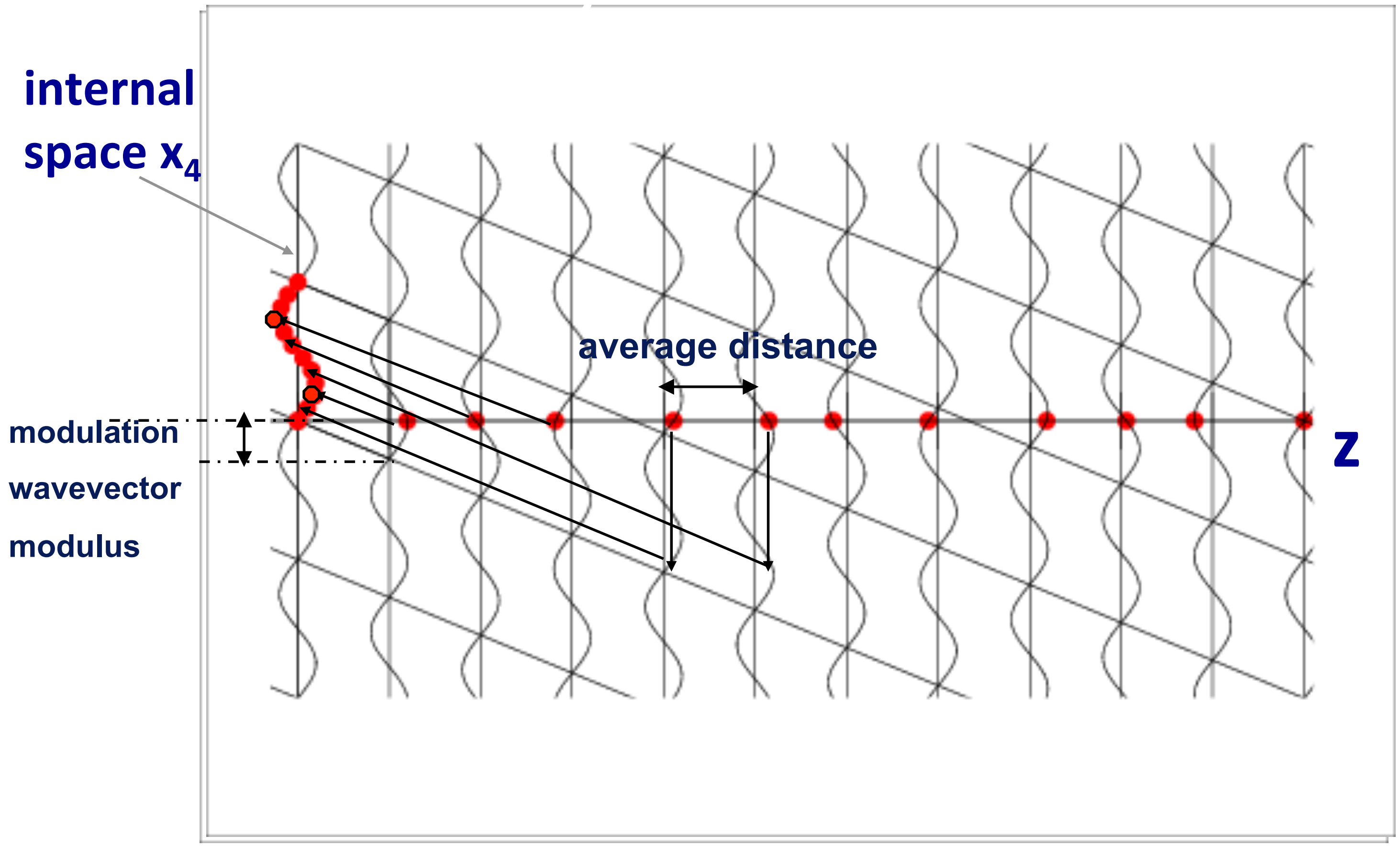
k = incommensurate propagation vector

fourth coordinate in superspace

example: 1.1.9

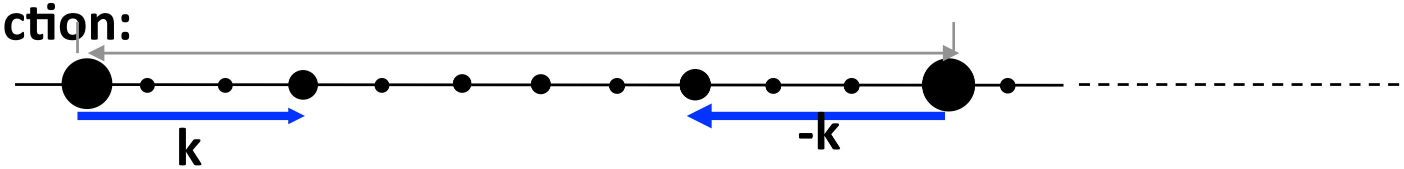
A global shift of the modulation functions along x_4 keeps the energy invariant

Superspace description of modulated structures (*displacive modulation*)



variable of modulation function: x_4=k.r

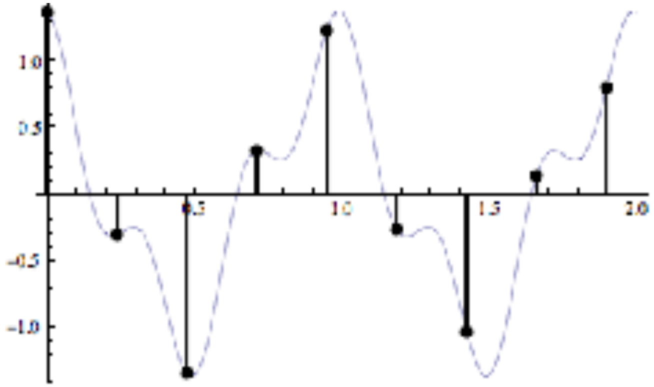
Diffraction:



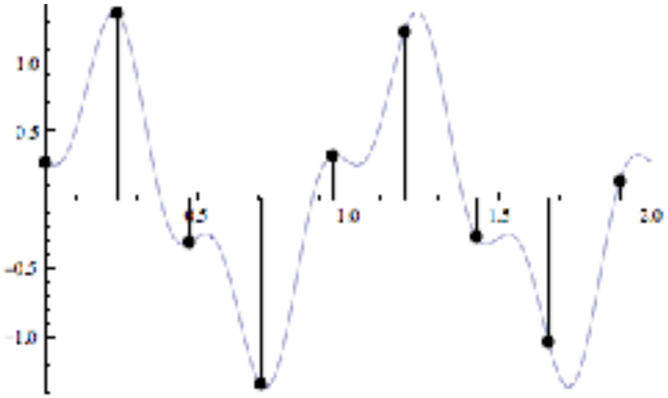
Superspace translational symmetry: **{E|T, -q.T}**
real spac. lat. translation + phase shift (internal space translation)

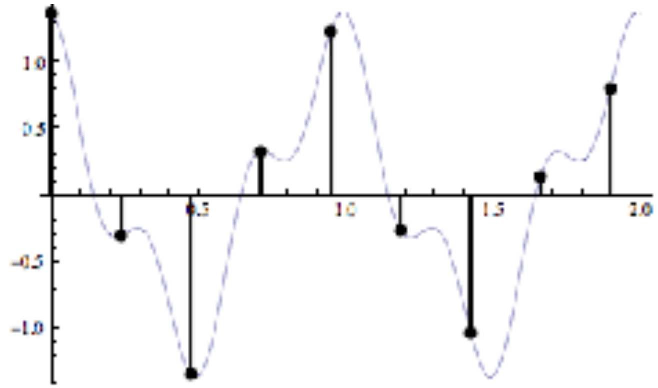
(combination of transformations that keep energy invariant)

"lost" real space translation translation:{E|T, 0}



phase shift translation:{E|0, -q.T}





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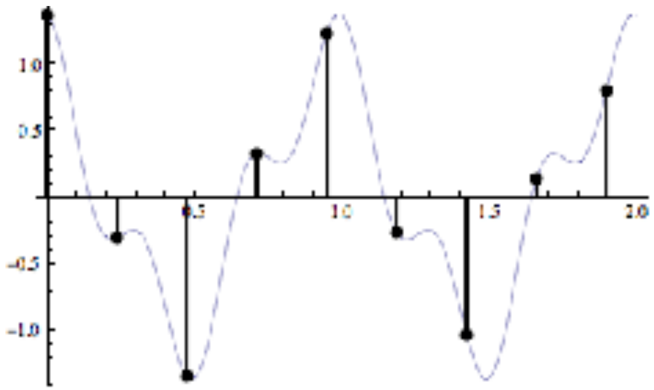
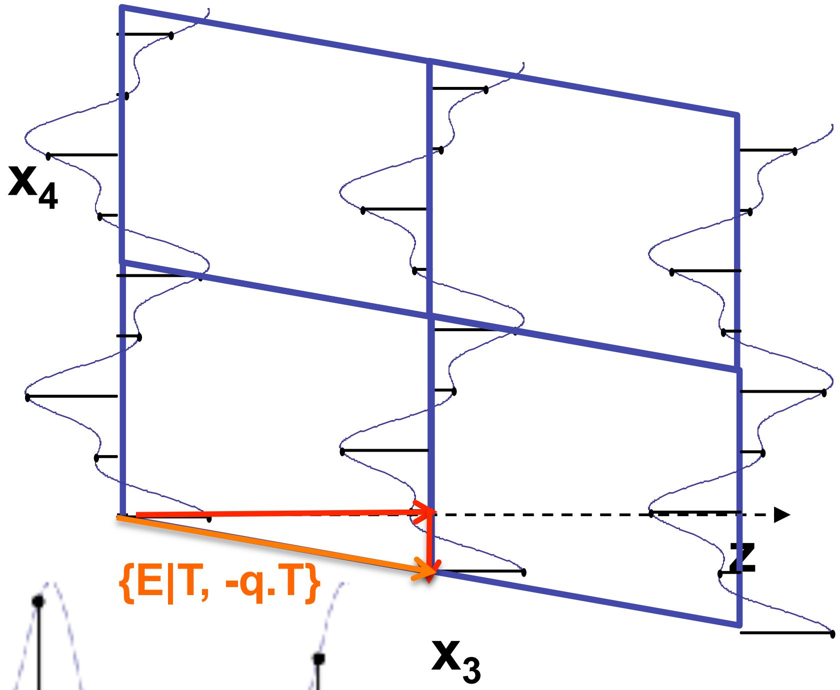
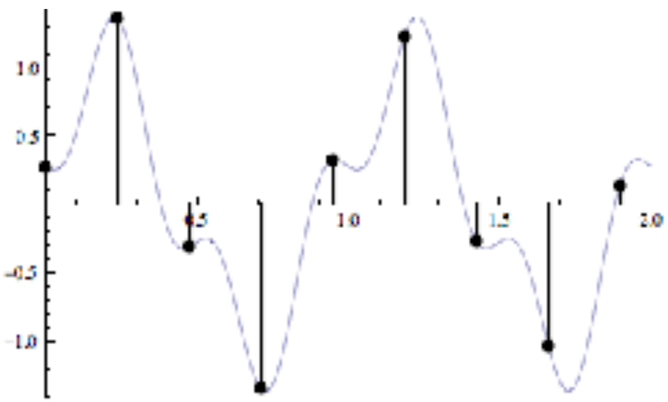
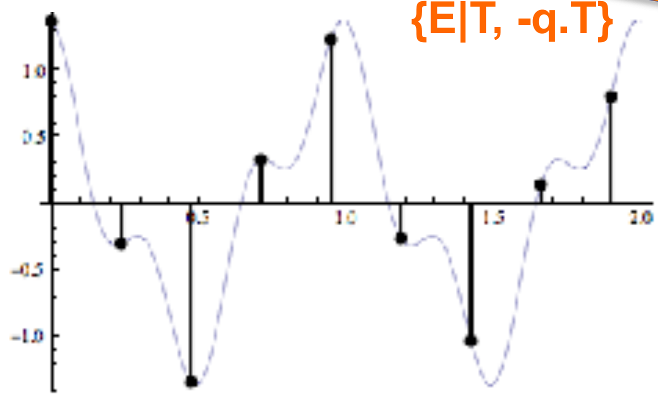




phase shift translation:{E|0, -q.T}





SYMMETRY OF INCOMMENSURATE PHASES

(Phase) global shift of all modulations along x_4 is energy invariant!

Symmetry operations in 1k incommensurate crystals:

sym. operations: space group operations

+ phase shifts of all modulations along x4

magnetic superspace group: $\{ \{\mathbf{R}_i |\ \mathbf{t}_i\ ,\ \tau_i\}\ ,\ \{\mathbf{R'}_j|\mathbf{t}_j\ ,\ \tau_j\}\ \}$

SYMMETRY OF INCOMMENSURATE PHASES

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magnetic superspace group: $\{ \{\mathbf{R}_i | \ \mathbf{t}_i \ , \ \tau_i\} \ , \{\mathbf{R'}_j | \mathbf{t}_j \ , \ \tau_j\} \ \}$

magnetic point group: set of all roto-inversion and roto-inversion+time inversion operations **{R, R'}** in its magnetic **superspace group!**

Incommensurate magnetic structures have an unambiguous magnetic point group symmetry

Symmetry relations between the modulation functions of different atoms in the basic unit cell due to a symmetry operation.

Superspace symmetry operation: $\{\mathbf{R},\theta|\mathbf{t},\tau\}$

$\{\mathbf{R}|\mathbf{t}\}$: is a space group operation of the basic (periodic) structure

$A_\nu(x_4)$ **atom** (l,ν) $\xrightarrow{\{R|t\}}$ **atom'** (l',μ) $A_\mu(x_4)$

Symmetry relations between the modulation functions of different atoms in the basic unit cell due to a symmetry operation.

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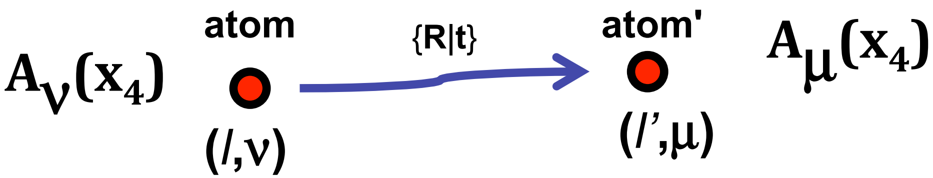
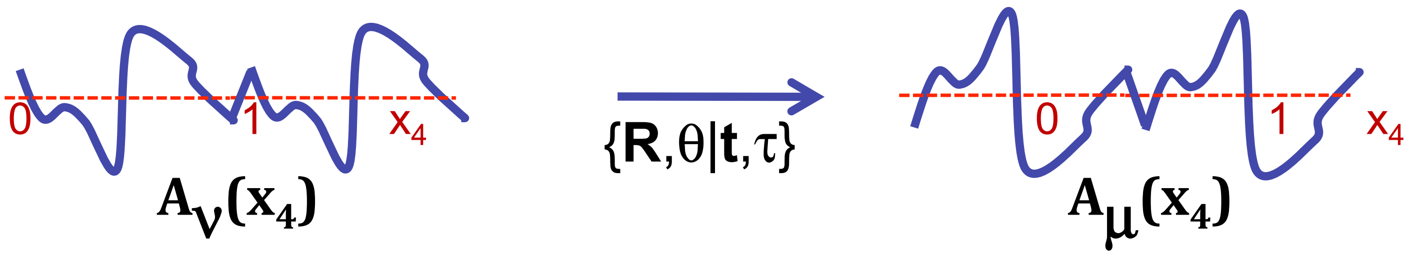


superspace symmetry operation $(\mathbf{R},\theta|\mathbf{t},\tau)$ implies a relation among the modulation functions of the atoms ν and μ of the basic structure:



Symmetry relations between the modulation functions of different atoms in the basic unit cell due to a symmetry operation.

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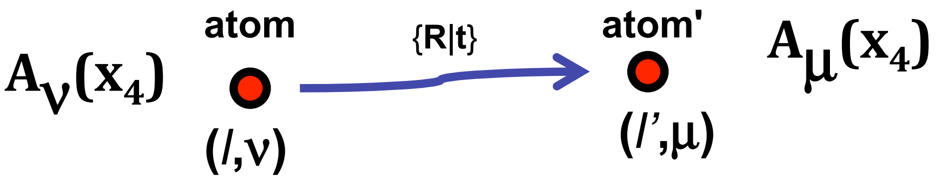

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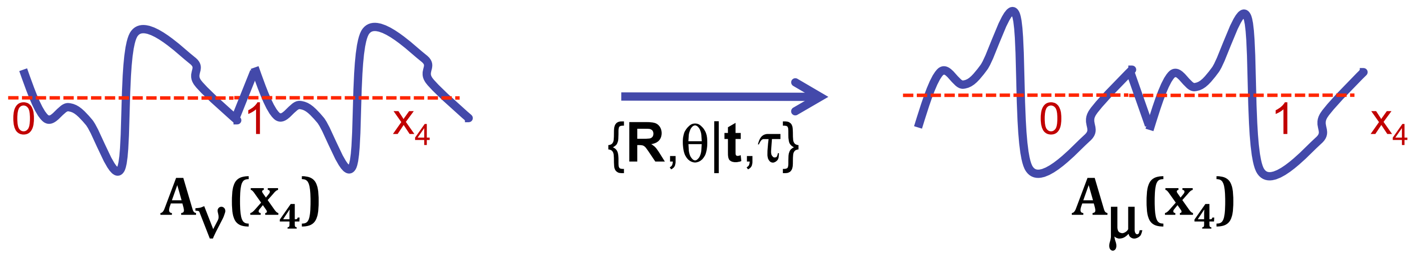

For the modulation of magnetic moments:

$$\boxed{\mathbf{M}_\mu(R_I x_4+\tau_o + \mathbf{H}_R.\mathbf{r}_\nu) = \theta\,\det(\mathbf{R})\mathbf{R}\,.\,\mathbf{M}_\nu(x_4)}$$

R_I, τ_o , $\mathbf{H}_R$ defined by $\{\mathbf{R},\theta|\mathbf{t},\tau\}$

If $\mu = \nu$ $\longrightarrow$ $\mathbf{M}_\nu(x_4)$ **symmetry restricted!**

Symmetry relations between the modulation functions of different atoms in the basic unit cell.

$$\boxed{\mathbf{M}_{\mu}(R_I x_4+\tau_o + \mathbf{H}_R.\mathbf{r}_{\nu}) = \theta \det(\mathbf{R})\mathbf{R} \,.\, \mathbf{M}_{\nu}(x_4)}$$

R_I, τ_o , $\mathbf{H}_R$ defined by $\{\mathbf{R},\theta|\mathbf{t},\tau\}$:

$$\boldsymbol{k}\cdot\boldsymbol{R} = R_I\boldsymbol{k} + \boldsymbol{H}_R \quad R_I = +1 \text{ or } -1$$

$$\tau_o = \tau + \boldsymbol{k}.\mathbf{t}$$

τ_o is independent of the translation **t** !
operations are then rather given and listed as $\{\mathbf{R},\theta|\mathbf{t},\tau_o\}$, the **t** implying a translation in superpace that includes the $-\mathbf{k}.\mathbf{t}$ along x_4

Symmetry relations between the modulation functions of different atoms in the basic unit cell.

$$\boxed{\mathbf{M}_{\mu}(R_I x_4+\tau_o + \mathbf{H}_R.\mathbf{r}_{\nu}) = \theta \det(\mathbf{R})\mathbf{R} \,.\, \mathbf{M}_{\nu}(x_4)}$$

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$$\tau_o = \tau + \boldsymbol{k}.\mathbf{t}$$

Example and notation of operation $\{\mathbf{R},\theta|\mathbf{t},\tau_o\}$ with $\mathbf{H}_R\neq 0$:

$$\boldsymbol{k} = (\alpha\ ,\ ½,\ 0) \xrightarrow{m_y} \boldsymbol{k}' = (\alpha\ ,\ -½,\ 0) = \boldsymbol{k} + (0,\ -1,\ 0)$$

$\{m'_y|1/2\ 1/2\ 0\ 1/2\ \}$

$R_I = +1 \quad \mathbf{H}_R = (0,\ -1,\ 0)$

$$\left[\begin{array}{ccc|c} & \mathbf{R}\ (3x3) & & \begin{matrix}0\\0\\0\end{matrix} \\ \hline H_{Rx} & H_{Ry} & H_{Rz} & R_i \end{array}\right] \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \hline x_4 \end{bmatrix} + \begin{bmatrix} t_1 \\ t_2 \\ t_3 \\ \hline \tau_o \end{bmatrix} = \left[\begin{array}{ccc|c} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ \hline 0 & -1 & 0 & 1 \end{array}\right] \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \hline x_4 \end{bmatrix} + \begin{bmatrix} 1/2 \\ 1/2 \\ 0 \\ \hline 1/2 \end{bmatrix} = \mathbf{x1+1/2,-x2+1/2,x3,-x2+x4+1/2,-1}$$

Symmetry relations between the atomic modulations

$M_i(x_4) = M_{i\,\sin 1}\sin(2\pi x_4) + M_{i\,\cos 1}\cos(2\pi x_4)$ $\quad i=x,y,z$

Example: inversion

$(x\ y\ z)$ atom 1 $\xrightarrow{\{\mathbf{-1}|000\}}$ $(-x\ -y\ -z)$ atom 2

superspace operation

$(\mathbf{-1}|000,0)$: **-x1 –x2 –x3 –x4 +1**

$\mathbf{k} \xrightarrow{\mathbf{-1}} \mathbf{-k}$

$R_I = -1 \quad \mathbf{H}_R = 0$

$\tau_o = 0 + \boldsymbol{k}.\mathbf{t} = 0$

$$\boxed{\mathbf{M}_\mu(R_I x_4 + \tau_o + \mathbf{H}_R.\mathbf{r}_\nu) = \theta\,\det(\mathbf{R})\mathbf{R}\,.\,\mathbf{M}_\nu(x_4)}$$

$$\boxed{\mathbf{M}_2(-x_4) = \mathbf{M}_1(x_4)}$$

Relation between the modulation of their magnetic moments

Symmetry relations between the atomic modulations

$M_i\,(x_4) = M_{i\,\sin 1}\,\sin(2\pi x_4) + M_{i\,\cos 1}\,\cos(2\pi x_4) \qquad i=x,y,z$

Example: inversion

$$\boxed{\text{atom 1}}\ (x\ y\ z) \xrightarrow{\{\mathbf{-1}|000\}} \boxed{\text{atom 2}}\ (-x\ -y\ -z)$$

superspace operation

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Relation between the modulation of their magnetic moments

$$\boldsymbol{M}^2_{\sin n} = -\boldsymbol{M}^1_{\sin n} \qquad \boldsymbol{M}^2_{\cos n} = \boldsymbol{M}^1_{\cos n}$$

Symmetry relations between the atomic modulations

$M_i(x_4) = M_{i\,\sin 1}\sin(2\pi x_4) + M_{i\,\cos 1}\cos(2\pi x_4) \qquad i=x,y,z$

Example: inversion

$$\underset{\text{atom 1}}{(x\ y\ z)} \xrightarrow{\{\mathbf{-1}|000\}} \underset{\text{atom 2}}{(-x\ -y\ -z)}$$

superspace operation

$(\mathbf{-1}|000{,}0)$: $\mathbf{-x1\ -x2\ -x3\ -x4\ +1}$

$$\mathbf{k} \xrightarrow{\mathbf{-1}} \mathbf{-k}$$

$R_I = -1 \qquad \mathbf{H}_R=0$

$\tau_o = 0 + \boldsymbol{k}.\mathbf{t}=0$

$$\boxed{\mathbf{M}_\mu(R_I x_4+\tau_o + \mathbf{H}_R.\mathbf{r}_\nu) = \theta \det(\mathbf{R})\mathbf{R} \,.\, \mathbf{M}_\nu(x_4)}$$

$$\boxed{\mathbf{M}_2(-x_4) = \mathbf{M}_1(x_4)}$$

Relation between the modulation of their magnetic moments

$$\boldsymbol{M}^2_{\sin n} = -\boldsymbol{M}^1_{\sin n} \qquad \boldsymbol{M}^2_{\cos n} = \boldsymbol{M}^1_{\cos n}$$

If atom 1= atom 2:

$$\boxed{\mathbf{M}^1_{\sin n} = 0}$$

only cosine terms

all modulations In phase

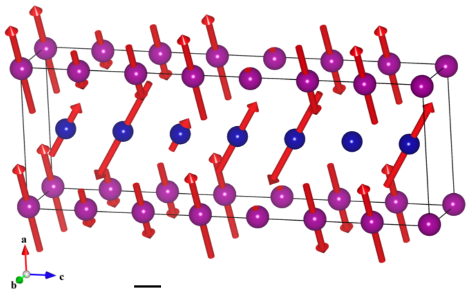
$$M_{1\alpha}(x_4) = M^1_{\alpha 0} + \sum_n M^1_{\alpha,\cos n}\cos(2\pi n x_4)$$

α= ***x, y, z***

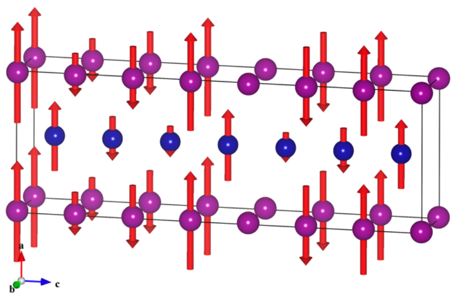
(collinear)

A centrosymmetric incommensurate modulation

A non-centrosymmetric incommensurate modulation



$P\bar{1}1'(\alpha\beta\gamma)0s$



$P11'(\alpha\beta\gamma)0s$

propagation vector:

***k*=(α,β,γ)**

$\{1|0000\}$ **: x1 x2 x3 x4 +1**

$\{\bar{1}|0000\}$ **: -x1 –x2 –x3 –x4 +1**

$\{1'|000\tfrac{1}{2}\}$ **: x1 x2 x3 x4+1/2 -1**

$\{\bar{1}'|000\tfrac{1}{2}\}$ **: -x1 -x2 -x3 -x4+1/2 -1**

$\{1|0000\}$ **: x1 x2 x3 x4 +1**

$\{1'|000\tfrac{1}{2}\}$ **: x1 x2 x3 x4+1/2 -1**

Translation into FullProf parameters:

$$\boldsymbol{M}^{\nu}(x_4) = M_o^{\nu} + \sum_{n=1,\dots} [\boldsymbol{M}_{\sin n}^{\nu} \sin(2\pi n x_4) + \boldsymbol{M}_{\cos n}^{\nu} \cos(2\pi n x_4)]$$

atom v at cell L:

$$M^{\nu}{}_{\boldsymbol{L}} = M^{\nu}\left(x_4 = \boldsymbol{q}\cdot(\boldsymbol{L}+\boldsymbol{r}_{\nu})\right)$$

Superspace (JANA2006)

$$\boldsymbol{M}^{\nu}{}_{L} = M_o^{\nu} + \sum_{\boldsymbol{k}} [\boldsymbol{S}_k^{\nu} \exp(-i2\pi\boldsymbol{k}\cdot\boldsymbol{L}) + \boldsymbol{S}_k^{\nu *} \exp(i2\pi\boldsymbol{k}\cdot\boldsymbol{L})]$$

FullProf

$$\boxed{\boldsymbol{S}_{\boldsymbol{k}}^{\nu}\, e^{i2\pi\boldsymbol{k}\cdot\boldsymbol{r}_{\nu}} = \boldsymbol{M}_{\cos 1}^{\nu} + i\,\boldsymbol{M}_{\sin 1}^{\nu}}$$

Translation into FullProf parameters:

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atom ν at cell L:

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$$\boldsymbol{M}^{\nu}{}_{L} = M_o^{\nu} + \sum_{\boldsymbol{k}} [\boldsymbol{S}_k^{\nu} \exp(-i2\pi\boldsymbol{k}\cdot \boldsymbol{L}) + \boldsymbol{S}_k^{\nu *} \exp(i2\pi\boldsymbol{k}\cdot \boldsymbol{L})]$$

FullProf

$$\boxed{\boldsymbol{S}_{\boldsymbol{k}}^{\nu}\, e^{i2\pi\boldsymbol{k}\cdot\boldsymbol{r}_{\nu}} = \boldsymbol{M}_{\cos 1}^{\nu} + i\, \boldsymbol{M}_{\sin 1}^{\nu}}$$

Symmetry relation for the FullProf parameters:

{**R**,θ|**t**,τ} : (*l*,ν) ⟶ (*l*,μ) **same cell: t must be a specific one**

$$\boldsymbol{S}_k^{\mu} = \theta\ det(\boldsymbol{R})\boldsymbol{R}\cdot\ \boldsymbol{S}_k^{\nu} \exp(-i2\pi\boldsymbol{k}\cdot\ \boldsymbol{t})\exp(i2\pi\tau_o) \qquad \textbf{if } R_I=+1$$

$$\boldsymbol{S}_k^{\mu} = \theta\ det(\boldsymbol{R})\boldsymbol{R}\cdot\ \boldsymbol{S}_k^{\nu *} \exp(-i2\pi\boldsymbol{k}\cdot\ \boldsymbol{t})\exp(i2\pi\tau_o) \qquad \textbf{if } R_I=-1$$

t must be such that μ atom is in zero cell !

Symmetry relations between the atomic modulations if described with FullProf parameterization

Example: inversion

superspace operation

$(\bar{\mathbf{1}}|000,0)$: **-x1 –x2 –x3 –x4 +1**

(x y z)		(-x -y -z)
atom 1	$\xrightarrow{(\bar{\mathbf{1}}\|000)}$	atom 2

$$\boxed{\boldsymbol{S}_{nk}^{2} = \boldsymbol{S}_{nk}^{1*}\exp(-i2\pi n\boldsymbol{k}\cdot\boldsymbol{l})}$$

The lattice translation ***l*** depends on which cell goes the atom 2, directly related with atom 1 by the inversion (-1|000)

Description of an incommensurate structure using superspace symmetry: $RbFe(MoO_4)_2$ magndata 1.1.2

Basic unitcell:
(not necessarily the paramgn one).

5.5955(6), 5.5955(6), 7.4377(7)
90, 90, 120

Propagation (wave) vector:

1 0.333333 0.333333 0.458

Superspace group: P31'(1/3,1/3,g)ts

x1,x2,x3,x4 ,+1
-x2,x1-x2,x3,-x2+x4+1/3,+1
-x1+x2,-x1,x3,-x1+x4+2/3, +1
x1,x2,x3,x4+1/2, -1
-x2,x1-x2,x3,-x2+x4+5/6,-1
-x1+x2,-x1,x3,-x1+x4+1/6,-1

Asymmetric unit (positions):

Rb1 Rb 0.00000 0.00000 0.50000
Fe1 Fe 0.00000 0.00000 0.50000
Mo1 Mo 0.333333 0.666667 0.234(3)
Mo2 Mo -0.333333 -0.666667 -0.234(3)
O1 O 0.333333 0.666667 0.463(6)
O2 O -0.333333 -0.666667 -0.463(6)
O3 O 0.103(4) -0.218(3) 0.158(4)
O4 O -0.103(4) 0.218(3) -0.158(4)

Asymmetric unit (moments):

Fe1 0 0 0

Asymmetric unit (moment modulations):

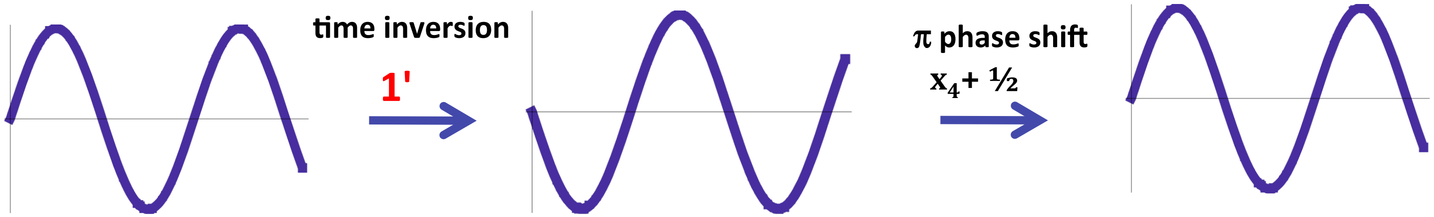
			cosine	sine
Fe1	x	1	-3.9/√3	3.9(5)
Fe1	y	1	-3.9*2/√3	0

Asymmetric unit (position modulations): ???
They may exist! (subject to the same superspace group)

A simple general "Theorem":

(1'| 0 0 0 ½) is a superspace symmetry operation of any single-k INC magnetic modulation.

Invariance of (sinusoidal) irrep magnetic modulations for (1'| 0 0 0 ½):

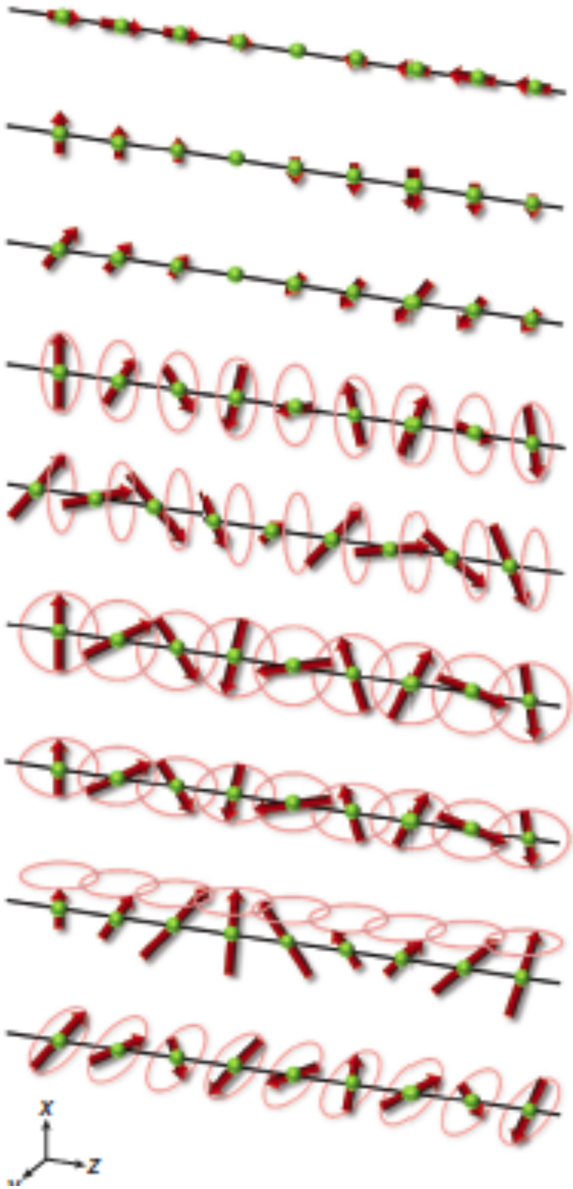


time inversion belongs to the symmetry point group of a single-k INC phase (grey point group)

Consequences of (1'| 0 0 0 ½) : $\boxed{A_\mu(x_4+\tfrac{1}{2}) = 1' A_\mu(x_4)}$

modulation of magnetic moments	$M_\mu(x_4+\tfrac{1}{2}) = -M_\mu(x_4)$	odd-harmonics : 1k, 3k ,5k ...
modulation of atomic displac.	$u_\mu(x_4+\tfrac{1}{2}) = u_\mu(x_4)$	even-harmonics : 2k, 4k ...

Point group symmetry of spin chains

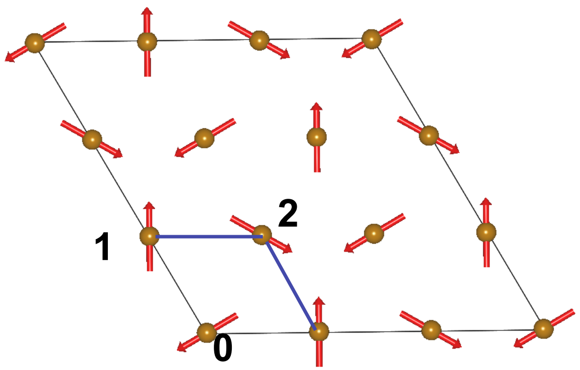


	Point group		
	No lattice	Cubic lattice	Hexagonal lattice
Collinear longitudinal	$\infty/mm1'$	$4/mmm1'$	$6/mmm1'$
Collinear transversal	$mmm1'$	$mmm1'$	$mmm1'$
Collinear transversal oblique	$12/m11'$	$12/m11'$	$12/m11'$
Proper screw	$\infty 21'$	$4221'$	$6221'$
Conical screw	$\infty 2'$	$42'2'$	$62'2'$
Cycloid	$2mm1'$	$2mm1'$	$2mm1'$
Elliptical cycloid	$2mm1'$	$2mm1'$	$2mm1'$
Transverse cone	$2'mm'$	$2'mm'$	$2'mm'$
Elliptical oblique cycloid	$1m11'$	$1m11'$	$1m11'$

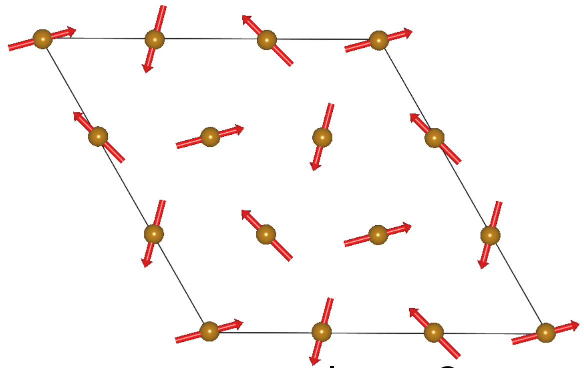
Mulferroic $RbFe(MoO_4)_2$: Superspace group: P31’(1/3 1/3 γ) ts

A “120º spin arrangement” forced by the superspace group:

example 1.1.2



layer 1



layer 2

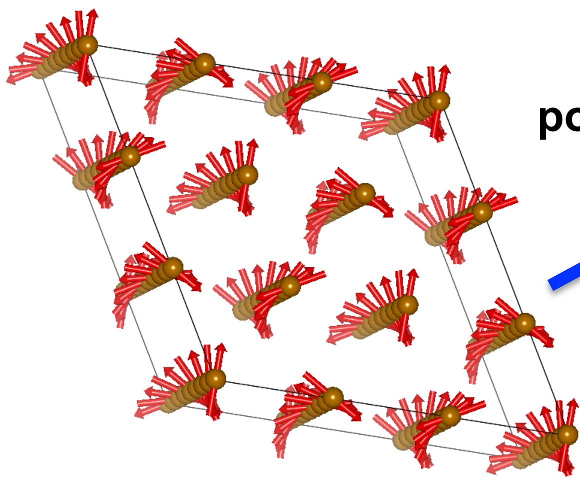
***k*=(1/3 1/3 γ)**

$$\{3_z^+ \mid 000\tfrac{1}{3}\} \rightarrow \boxed{\boldsymbol{M}\left(x_4+\tfrac{1}{3}\right)=3_z^- . \boldsymbol{M}(x_4)}$$

atom 0: $\boldsymbol{M}(x_4=0)$

atom 1: $\boldsymbol{M}\left(x_4=\boldsymbol{k}.\,\boldsymbol{r}_1=\tfrac{1}{3}\right)=3_z^- .\, \boldsymbol{M}(0)$

atom 2: $\boldsymbol{M}\left(x_4=\boldsymbol{k}.\,\boldsymbol{r}_2=\tfrac{2}{3}\right)=3_z^- .\, \boldsymbol{M}\left(\tfrac{1}{3}\right)$



perspective

point group: 31'

$\mathbf{P_z}$

$CeCuAl_3$: **Superspace group: I41'(0 0 γ) qs** **point group: 41'**

magndata 1.1.33

$\boldsymbol{k}$ =(0 0 0.52) Parent space group: I4mm

helical configuration is symmetry dictated (and protected!):

Ce site at (0,0,0) : invariant for { $\mathbf{4}^{+}_{001}$ | 0 0 0 1/4 }

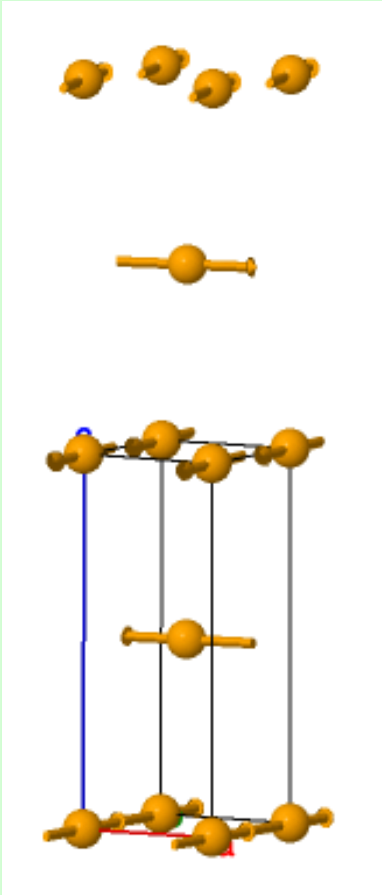
$$\boxed{\mathbf{M}_{\mu}(R_I x_4+\tau_o + \mathbf{H}_R.\mathbf{r}_{\nu}) = \theta\,\det(\mathbf{R})\mathbf{R}\,.\,\mathbf{M}_{\nu}(x_4)}$$

{ $\mathbf{4}^{+}_{001}$ | 0 0 0 1/4 } $\longrightarrow$ $\boxed{\mathbf{M}(x_4 + 1/4) = \mathbf{4}^{+}_{z}\,.\mathbf{M}(x_4)}$

$M_i(x_4) = M_{i\,sin1}\sin(2\pi x_4) + M_{i\,cos1}\cos(2\pi x_4)$ i=x,y,z

$M_i(x_4 + 1/4) = M_{i\,sin1}\cos(2\pi x_4) - M_{i\,cos1}\sin(2\pi x_4)$

$\mathbf{4}^{+}_{z}\,.(M_x(x_4), M_y(x_4), M_z(x_4)) = (-M_y(x_4), M_x(x_4), M_z(x_4))$



$CeCuAl_3$: **Superspace group: I41'(0 0 γ) qs** **point group: 41'**

magndata 1.1.33

$\boldsymbol{k}$ =(0 0 0.52) Parent space group: I4mm

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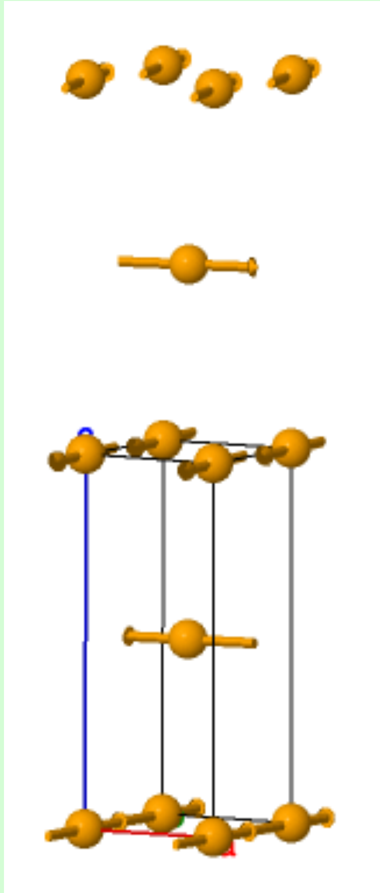
{ $\mathbf{4}^{+}_{001}$ | 0 0 0 1/4 } $\longrightarrow$ $\boxed{\mathbf{M}(x_4 + 1/4) = \mathbf{4}^{+}_{z}\,.\mathbf{M}(x_4)}$



$M_i(x_4) = M_{i\,\sin1}\sin(2\pi x_4) + M_{i\,\cos1}\cos(2\pi x_4)$ i=x,y,z

$M_i(x_4 + 1/4) = M_{i\,\sin1}\cos(2\pi x_4) - M_{i\,\cos1}\sin(2\pi x_4)$

$\mathbf{4}^{+}_{z}.(M_x(x_4), M_y(x_4), M_z(x_4)) = (-M_y(x_4), M_x(x_4), M_z(x_4))$

$M_{z\,\sin1}\sin(2\pi x_4) + M_{z\,\cos1}\cos(2\pi x_4) = M_{z\,\sin1}\cos(2\pi x_4) - M_{z\,\cos1}\sin(2\pi x_4)$

$$\boxed{M_{z\,\sin1} = M_{z\,\cos1} = 0}$$

$CeCuAl_3$: Superspace group: I41'(0 0 γ) qs point group: 41'

magndata 1.1.33

$\boldsymbol{k}$ =(0 0 0.52) Parent space group: I4mm

helical configuration is symmetry dictated (and protected!):

Ce site at (0,0,0) : invariant for { $\mathbf{4}^+_{001}$ | 0 0 0 1/4 }

$$\boxed{\mathbf{M}_{\mu}(R_I x_4+\tau_o + \mathbf{H}_R.\mathbf{r}_{\nu}) = \theta \det(\mathbf{R})\mathbf{R} \,.\, \mathbf{M}_{\nu}(x_4)}$$

{ $\mathbf{4}^+_{001}$ | 0 0 0 1/4 } $\longrightarrow$ $\boxed{\mathbf{M}(x_4 + ¼) = \mathbf{4}^+_z .\mathbf{M}(x_4)}$

$M_i (x_4) = M_{i\ sin1} \sin(2\pi x_4) + M_{i\ cos1} \cos(2\pi x_4)$ i=x,y,z

$M_i (x_4 + ¼) = M_{i\ sin1} \cos(2\pi x_4) - M_{i\ cos1} \sin(2\pi x_4)$

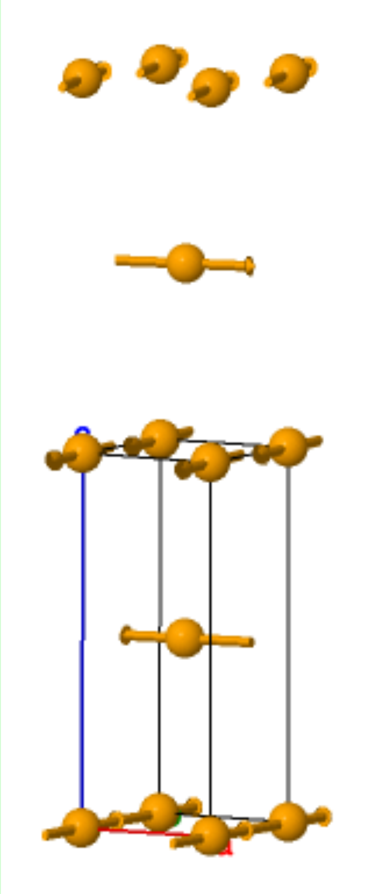
$\mathbf{4}^+_z .(M_x(x_4), M_y(x_4), M_z(x_4)) = (-M_y(x_4), M_x(x_4), M_z(x_4))$

$M_{z\ sin1} \sin(2\pi x_4) + M_{z\ cos1}\cos(2\pi x_4)=M_{z\ sin1} \cos(2\pi x_4) - M_{z\ cos1} \sin(2\pi x_4)$

$$\boxed{\mathbf{M_{z\ sin1} = M_{z\ cos1} = 0}}$$

$-M_{y\ sin1} \sin(2\pi x_4) - M_{y\ cos1}\cos(2\pi x_4)=M_{x\ sin1} \cos(2\pi x_4) - M_{x\ cos1} \sin(2\pi x_4)$

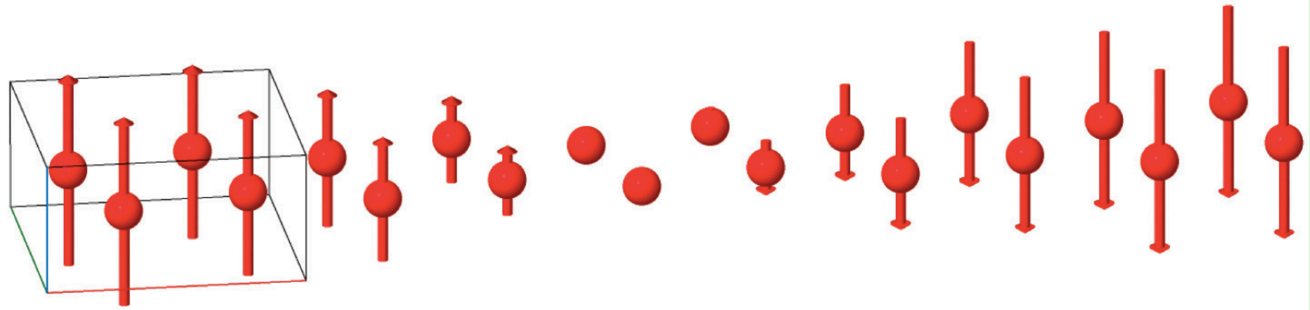
$$\boxed{\mathbf{M_{y\ cos1} = -M_{x\ sin1}\ ;\ M_{x\ cos1} = M_{ysin1}}}$$



Ce_2Pd_2Sn magndata 1.1.9 space inversion is maintained

superspace group: Pbam1'(a00)0s0s parent space group: P4/mbm

4 magnetic atoms per primitive unit cell



Average atomic positions

Atom	x	y	z
1	0.17810	0.67810	0.50000
2	0.82190	0.32190	0.50000
3	0.32190	0.17810	0.50000
4	0.67810	0.82190	0.50000

irrep basis modes: 3 parameters

refined model: all modulations in phase (1 parameter)

superspace symmetry constraint: 2 parameters
(same amplitude for the 4 atoms, but atoms related by inversion, not in phase but with opposite phases)

Atom	Magnetic moment Fourier Cos coeffs						Magnetic moment Fourier Sin coeffs					
	Symmetry constraints			Numerical values			Symmetry constraints			Numerical values		
	x	y	z	x	y	z	x	y	z	x	y	z
1	0	0	$M_z$cos1	0.0	0.0	1.70000	0	0	$M_z$sin1	0.0	0.0	0.0
2	0	0	$M_z$cos1	0.0	0.0	1.70000	0	0	-$M_z$sin1	0.0	0.0	0.0
3	0	0	$M_z$cos1	0.0	0.0	1.70000	0	0	-$M_z$sin1	0.0	0.0	0.0
4	0	0	$M_z$cos1	0.0	0.0	1.70000	0	0	$M_z$sin1	0.0	0.0	0.0

Representation analysis vs superspace magnetic symmetry

How to calculate the superspace group (single-***k*** structures) for an irrep magnetic mode:

(isotropy subgroups (*epikernels and kernel*) of an irrep)

Global (complex) amplitudes of a frozen sinusoidal spin wave with propagation vector **k:**

$$M(\mu,\boldsymbol{l}) = \sum_{i=1,\dots,N} S_i(\boldsymbol{k})\sigma_i(\mu)e^{-i2\pi\boldsymbol{k}.(\boldsymbol{l}+\boldsymbol{r}_\mu)} + S_i(-\boldsymbol{k})\sigma_i^*(\mu)e^{i2\pi\boldsymbol{k}.(\boldsymbol{l}+\boldsymbol{r}_\mu)}$$

Generalized invariance equation:

phase shift

N-dim

(R,θ|t,τ) belongs to superspace group if :

$$\begin{bmatrix} \mathbf{1}e^{i2\pi\tau} & 0 \\ 0 & \mathbf{1}\,e^{-i2\pi\tau} \end{bmatrix} T[(\mathbf{R},\theta|\mathbf{t})] \begin{bmatrix} \mathbf{S}(k) \\ \mathbf{S}(-k) \end{bmatrix} = \begin{bmatrix} \mathbf{S}(k) \\ \mathbf{S}(-k) \end{bmatrix}$$

(R|t) is an operation of the grey paramagnetic space group

Additional term in an incommensurate phase

magnetic space group operation with R**q** =±**q** (transformation represented by a a NxN matrix)

Possible subgroups (isotropy subgroups) for any irrep are derived both by ISODISTORT (stokes.byu.edu/isotropy.html) or by JANA2006

Superspace magnetic symmetry produced by an irrep magnetic mode:

Generalized invariance equation:

N-dim

$$\begin{bmatrix} \mathbf{1}e^{i2\pi\tau} & 0 \\ 0 & \mathbf{1}e^{-i2\pi\tau} \end{bmatrix} T[(\mathbf{R}|\mathbf{t})] \begin{bmatrix} \mathbf{S}(k) \\ \mathbf{S}(-k) \end{bmatrix} = \begin{bmatrix} \mathbf{S}(k) \\ \mathbf{S}(-k) \end{bmatrix}$$

N =1 **one to one correspondance irrep – superspace group**

But including constraints of operations changing *k* into –*k*

Example: paraelectric phase : Pbnm1'

Inc. propagation vector: (0,β,0)

irrep	1	m_x	2_y	m_z	$1'$	Superpace group	Generators **plus**
$m\Delta_1$	1	1	1	1	-1	$Pbnm1'(0\beta 0)000s$	$\{m_x \mid \frac{1}{2}0\frac{1}{2}0\}, \{m_z \mid 00\frac{1}{2}0\}$
$m\Delta_2$	1	-1	1	-1	-1	$Pbnm1'(0\beta 0)s0ss$	$\{m_x \mid \frac{1}{2}0\frac{1}{2}\frac{1}{2}\}, \{m_z \mid 00\frac{1}{2}\frac{1}{2}\}$
$m\Delta_3$	1	-1	-1	1	-1	$Pbnm1'(0\beta 0)s00s$	$\{m_x \mid \frac{1}{2}0\frac{1}{2}\frac{1}{2}\}, \{m_z \mid 00\frac{1}{2}0\}$
$m\Delta_4$	1	1	-1	-1	-1	$Pbnm1'(0\beta 0)00ss$	$\{m_x \mid \frac{1}{2}0\frac{1}{2}0\}, \{m_z \mid 00\frac{1}{2}\frac{1}{2}\}$

{1'|000½ }
and {-1|0000}

$TbMnO_3$ magndata 1.1.6

Superspace magnetic symmetry produced by an irrep magnetic mode:

Generalized invariance equation:

N-dim

$$\begin{bmatrix} \mathbf{1}e^{i2\pi\tau} & 0 \\ 0 & \mathbf{1}e^{-i2\pi\tau} \end{bmatrix} T[(\mathbf{R}|\mathbf{t})] \begin{bmatrix} \mathbf{S}(k) \\ \mathbf{S}(-k) \end{bmatrix} = \begin{bmatrix} \mathbf{S}(k) \\ \mathbf{S}(-k) \end{bmatrix}$$

N =1 **one to one correspondance irrep – superspace group**

But including constraints of operations changing *k* into –*k*

Example: paraelectric phase : Pbnm1'

Inc. propagation vector: (0,β,0)

space inversion conserved

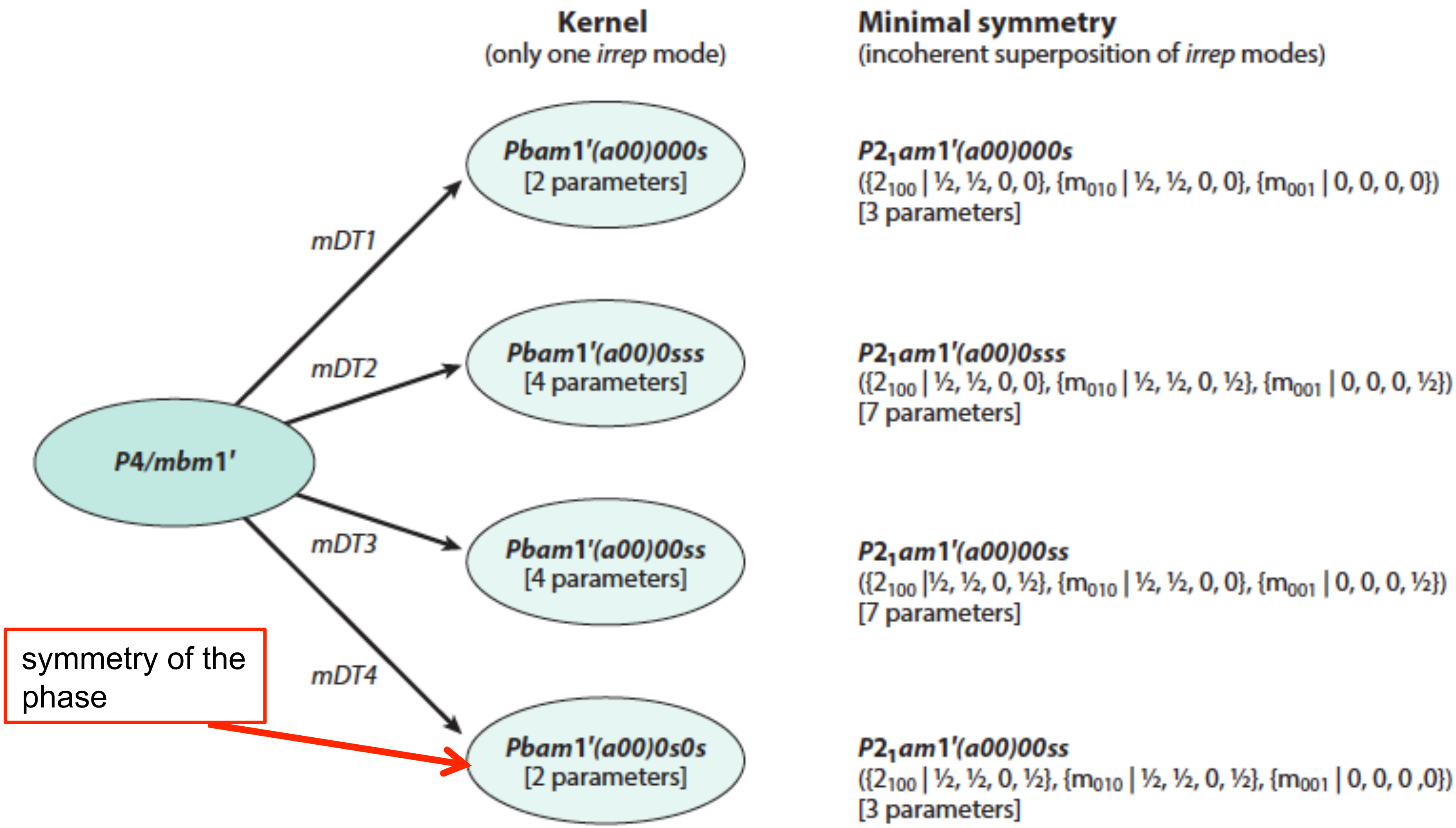
{1'|000½ } and {-1|0000}

irrep	1	m_x	2_y	m_z	$1'$	Superpace group	Generators **plus**
$m\Delta_1$	1	1	1	1	-1	$Pbnm1'(0\beta 0)000s$	$\{m_x \mid \frac{1}{2}0\frac{1}{2}0\}, \{m_z \mid 00\frac{1}{2}0\}$
$m\Delta_2$	1	-1	1	-1	-1	$Pbnm1'(0\beta 0)s0ss$	$\{m_x \mid \frac{1}{2}0\frac{1}{2}\frac{1}{2}\}, \{m_z \mid 00\frac{1}{2}\frac{1}{2}\}$
$m\Delta_3$	1	-1	-1	1	-1	$Pbnm1'(0\beta 0)s00s$	$\{m_x \mid \frac{1}{2}0\frac{1}{2}\frac{1}{2}\}, \{m_z \mid 00\frac{1}{2}0\}$
$m\Delta_4$	1	1	-1	-1	-1	$Pbnm1'(0\beta 0)00ss$	$\{m_x \mid \frac{1}{2}0\frac{1}{2}0\}, \{m_z \mid 00\frac{1}{2}\frac{1}{2}\}$

$TbMnO_3$ magndata 1.1.6

Ce_2Pd_2Sn magndata 1.1.9 space inversion is maintained

superspace group: Pbam1'(a00)0s0s parent space group: P4/mbm



Superspace magnetic symmetry produced by an irrep magnetic mode:

Generalized invariance equation:

N-dim

$\boxed{N > 1}$

$$\begin{bmatrix} \mathbf{1}e^{i2\pi\tau} & 0 \\ 0 & \mathbf{1}e^{-i2\pi\tau} \end{bmatrix} T[(\mathbf{R}|\mathbf{t})] \begin{bmatrix} \mathbf{S}(k) \\ \mathbf{S}(-k) \end{bmatrix} = \begin{bmatrix} \mathbf{S}(k) \\ \mathbf{S}(-k) \end{bmatrix}$$

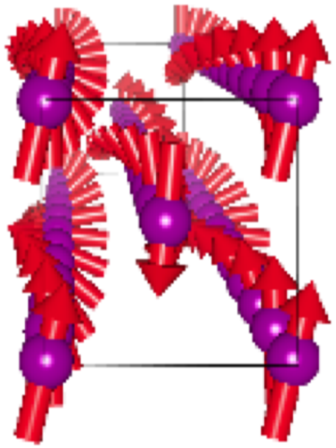
One irrep with N>1 ➔ several possible superspace groups

Example: paraelectric phase : Im-3m Inc. propagation vector: $(0,0,\gamma)$

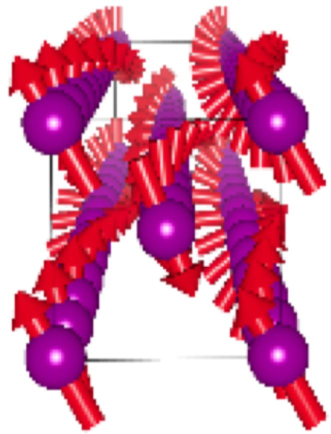
Irrep mDT5: Seven different possible magnetic symmetries for the same irrep

Possible transversal spin waves with different superspace symmetries on a bcc structure (Im-3m):

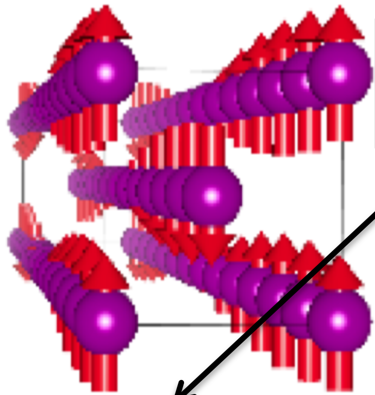
All correspond to a single 4dim irrep



$I4221'(00\gamma)q00s$

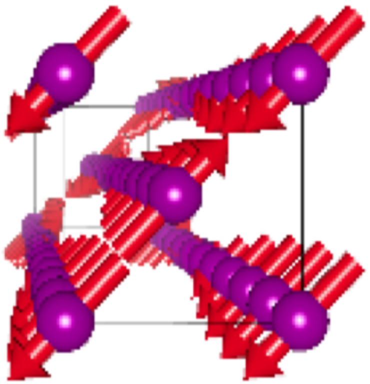


$I4221'(00\gamma)\bar{q}00s$

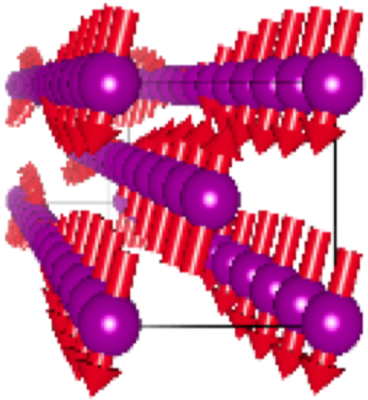


Phase I of Chromium

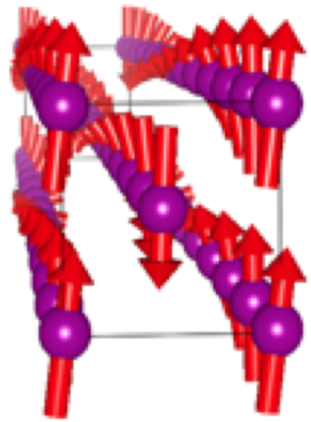
$Immm1'(00\gamma)s00s$



$Fmmm1'(00\gamma)s00s$



$I112/m1'(00\gamma)s0s$



$I2221'(00\gamma)00ss$

$CeCuAl_3$: **Superspace group:** I41'(0 0 γ) qs

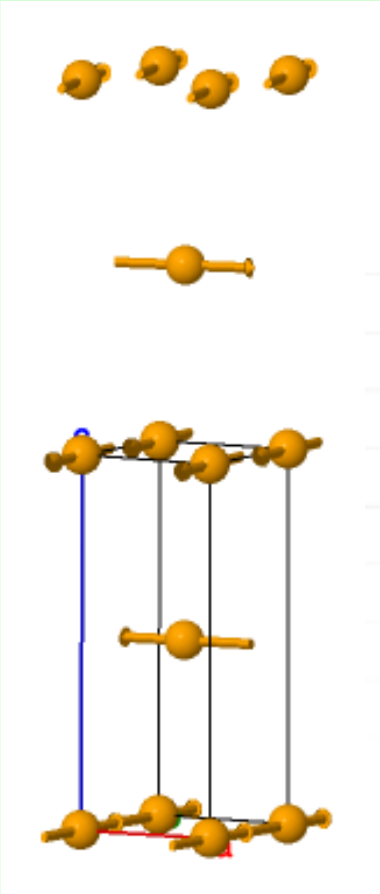
example 1.1.33

k =(0 0 0.52)

Parent space group: I4mm

What are the possible superspace groups that can result from spin ordering restricted to a **single irrep**?

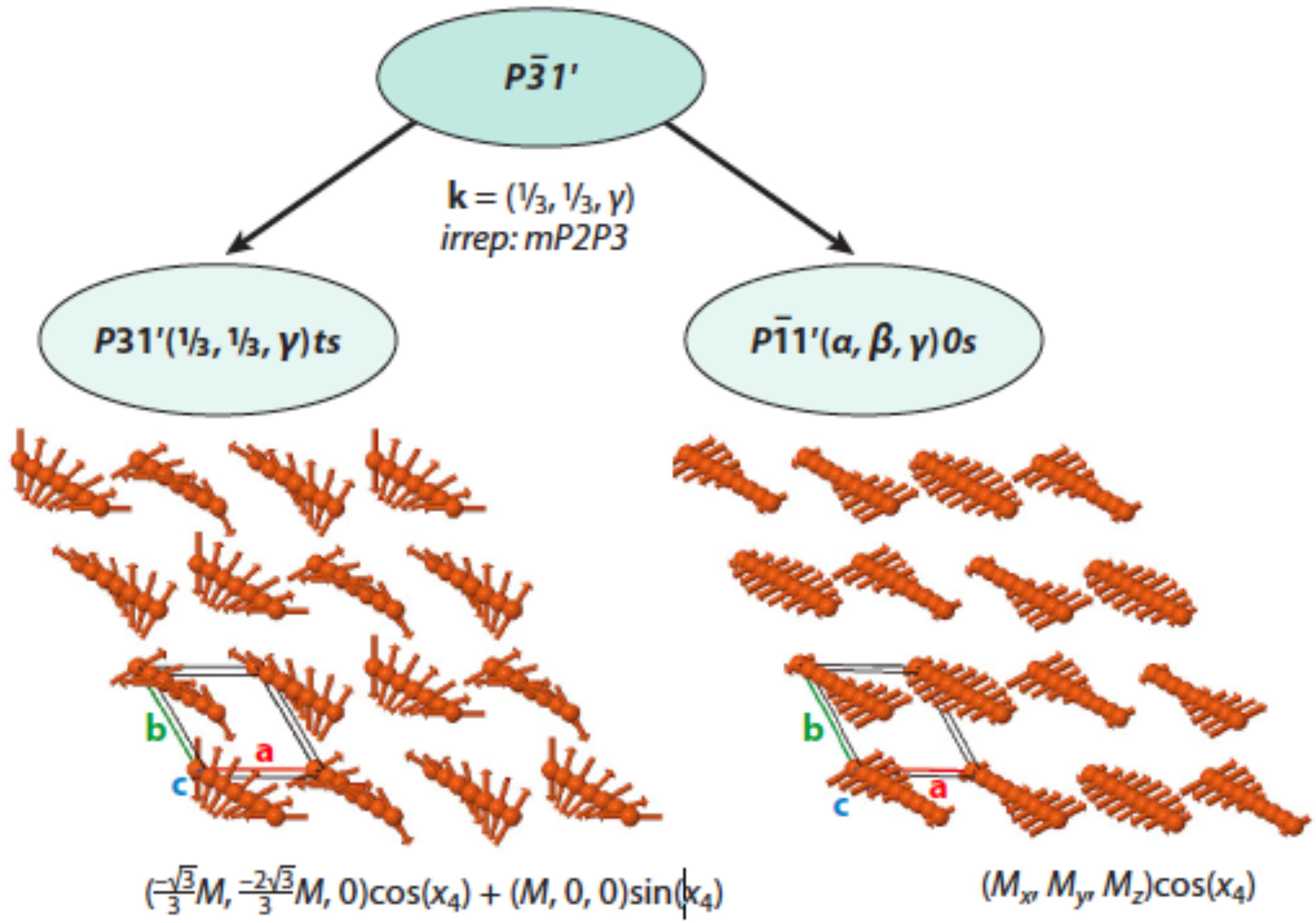
Use of ISODISTORT or JANA2006 to obtain possible superspace groups for a given irrep(s)



k point: LD (0,0,g), g=0.52000 (1 incommensurate modulation/1 arm)
IR: mLD5LE5

Finish selecting the distortion mode by choosing an order parameter direction ?

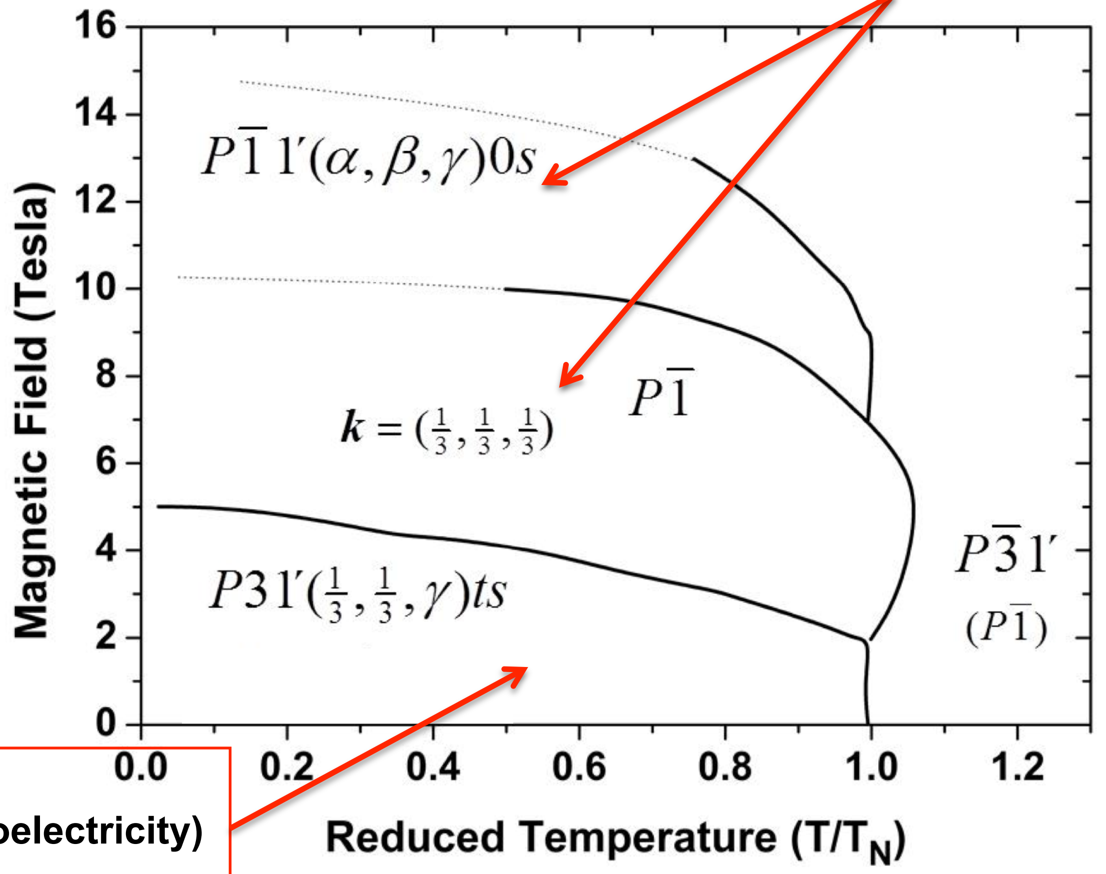
- ⦿C (a,0,b,0) 79.1.21.2.m26.? I41'(0,0,g)qs, basis={(0,1,0,0),(-1,0,0,0),(0,0,1,0),(0,0,0,1)}, ori
- ○C (a,a,b,b) 44.1.12.2.m230.? Imm21'(0,0,g)s0ss, basis={(0,1,0,0),(1,0,0,0),(0,0,-1,0),(0,0,0
- ○C (a,b,b,-a) 42.1.17.2.m220.? Fmm21'(0,0,g)s0ss, basis={(-1,1,0,0),(1,1,0,0),(0,0,-1,0),(0,
- ○4D (a,b,c,d) 5.1.7.3.m14.? B21'(0,0,g)ss, basis={(-1,1,0,0),(1,-2,0,0),(0,0,1,0),(0,0,0,1)}, or


$P\bar{3}1'$
$\mathbf{k} = (1/3, 1/3, \gamma)$
irrep: mP2P3
$P31'(1/3, 1/3, \gamma)ts$
$P\bar{1}1'(\alpha, \beta, \gamma)0s$
b
a
c
b
a
c
$(\frac{-\sqrt{3}}{3}M, \frac{-2\sqrt{3}}{3}M, 0)\cos(x_4) + (M, 0, 0)\sin(x_4)$
$(M_x, M_y, M_z)\cos(x_4)$

$RbFe(MoO_4)_2$: A phase diagram with phases and symmetries caused by a single active 4-dim magnetic irrep

Magnetic field along [1,-1,0]

Non-polar symmetry:
No polarization



Phase diagram after Kenzelmann et al.

PRL 2007

Polar symmetry:
induced (improper ferroelectricity)
Multiferroic phase

The case of $TbMnO_3$

Pbnm --- INC1 --- INC2 (P_z)

$\mathbf{k} = \beta\, \mathbf{b}^*$

spin modes (Kenzelmann et al. 2005):

$\mathbf{S}_3\mathbf{e_3}(j)\exp[i\mathbf{q.l}] + \mathbf{S}_3{}^*\mathbf{e_3}(j)\exp[-i\mathbf{q.l}]$ irrep $m\Delta_3$

$\mathbf{S}_2\mathbf{e_2}(j)\exp[i\mathbf{q.l}] + \mathbf{S}_2{}^*\ \mathbf{e_2}(j)\exp[-i\mathbf{q.l}]$ irrep $m\Delta_2$

Pbnm1'

$\xrightarrow{S_3}$ **Pbnm1'(0b0)s00s**

$\xrightarrow{S_2}$ **Pbnm1'(0b0)s0ss**

$\xrightarrow{P_z}$ **Pbn2$_1$1'**

→ **Pbn2$_1$1'(0b0)s00s** $\phi_3 - \phi_2 = \pm\, \pi/2$

$\mathbf{S}_3 = S_3\exp[i\phi_3]$
$\mathbf{S}_2 = S_2\exp[i\phi_2]$

Symmetry and magnetic structure depends on phase shift $\phi_3 - \phi_2$

Pbnm1' $\xrightarrow{S_3}$ **Pbnm1'(0b0)s00s** $\xrightarrow{S_2}$ **Pbn2$_1$1'(0b0)s00s** (induced P_z)

Trilinear coupling: $iP_z(S_3S_2{}^* - S_3{}^*S_2)$ ➔ $P_z \sim S_3S_2\ \mathrm{Sin}(\phi_3 - \phi_2)$ induced polarization

Pbnm1'(0b0)s00s + **Pbnm1'(0b0)s0ss** → **P2$_1$/b1'(0bg)0ss**

collinear spin wave

$\phi_3 - \phi_2 = 0$

Pbnm1'(0b0)s00s + **Pbnm1'(0b0)s0ss** → **Pbn2$_1$1'(0b0)s00s**

cycloidal spin wave

$\phi_3 - \phi_2 = \pm\, \pi/2$

The case of $TbMnO_3$

Pbnm --- INC1 --- INC2 (P_z)

k= β b*

spin modes (Kenzelmann et al. 2005):

$\mathbf{S}_3\mathbf{e_3}(j)\exp[i\mathbf{q.l}] + \mathbf{S}_3^*\mathbf{e_3}(j)\exp[-i\mathbf{q.l}]$ irrep $m\Delta_3$

$\mathbf{S}_2\mathbf{e_2}(j)\exp[i\mathbf{q.l}] + \mathbf{S}_2^* \mathbf{e_2}(j)\exp[-i\mathbf{q.l}]$ irrep $m\Delta_2$

$$\begin{array}{ccccc} & & \text{Pbnm1'} & & \\ & \swarrow^{S_3} & \downarrow^{S_2} & \searrow^{P_z} & \\ \text{Pbnm1'(0b0)s00s} & & \text{Pbnm1'(0b0)s0ss} & & \text{Pbn}2_1\text{1'} \\ & \searrow & \downarrow & \swarrow & \\ & & \text{Pbn}2_1\text{1'(0b0)s00s} & & \end{array}$$

$\phi_3 - \phi_2 = \pm \pi/2$

$\mathbf{S}_3 = S_3\exp[i\phi_3]$
$\mathbf{S}_2 = S_2\exp[i\phi_2]$

Symmetry and magnetic structure depends on phase shift $\phi_3 - \phi_2$

induced P_z

$$\text{Pbnm1'} \xrightarrow{\mathbf{S}_3} \text{Pbnm1'(0b0)s00s} \xrightarrow{\mathbf{S}_2} \text{Pbn}2_1\text{1'(0b0)s00s}$$

Trilinear coupling: $iP_z(S_3S_2^* - S_3^*S_2)$ $\rightarrow$ $P_z \sim S_3S_2 \sin(\phi_3 - \phi_2)$ induced polarization

$$\begin{array}{ccc} \text{Pbnm1'(0b0)s00s} & \searrow & \\ & & \text{P}2_1\text{/b1'(0bg)0ss} \\ \text{Pbnm1'(0b0)s0ss} & \nearrow & \end{array} \qquad \begin{array}{ccc} \text{Pbnm1'(0b0)s00s} & \searrow & \\ & & \text{Pbn}2_1\text{1'(0b0)s00s} \\ \text{Pbnm1'(0b0)s0ss} & \nearrow & \end{array}$$

collinear spin wave

$\phi_3 - \phi_2 = 0$

cycloidal spin wave

$\phi_3 - \phi_2 = \pm \pi/2$

Incommensurate phases of delafossites

Table 3. Possible superspace symmetries (magnetic superspace groups) of incommensurate phases resulting from the in-phase and in-quadrature superposition of two irreducible magnetic modulations with a single propagation vector $\vec{k}_i = (\alpha, \alpha, \frac{3}{2})$ in a $R\bar{3}m1'$ structure.

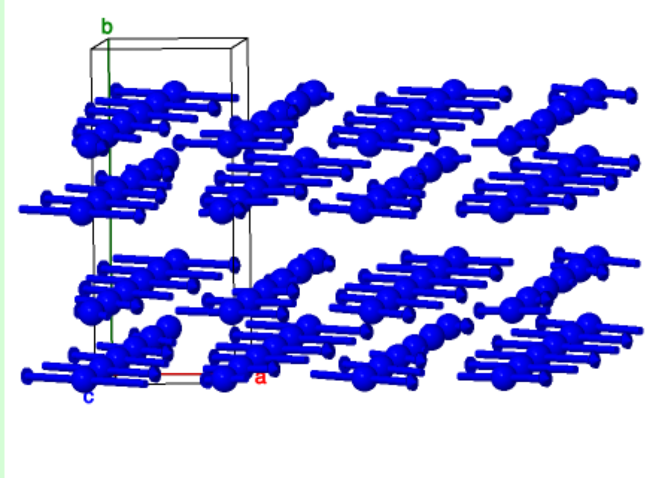
	$S_x(mY_1)$	$S_y(mY_2)$	$S_z(mY_1)$
$S_x(mY_1)$		$Cm1'(1\beta\frac{1}{2})0s$ ($\Delta\phi=\frac{\pi}{2}$)	$C21'(1\beta\frac{1}{2})0s$ ($\Delta\phi=\frac{\pi}{2}$)
$S_y(mY_2)$	$P\bar{1}1'(1\beta\frac{1}{2})0s$ ($\Delta\phi=0$)		$Cm1'(1\beta\frac{1}{2})0s$ ($\Delta\phi=\frac{\pi}{2}$)
$S_z(mY_1)$	$C\frac{2}{m}1'(1\beta\frac{1}{2})sss$ ($\Delta\phi=0$)	$P\bar{1}1'(1\beta\frac{1}{2})0s$ ($\Delta\phi=0$)	

$MnWO_4$ magndata 1.12

parent SG: P2/c **k** = (-0.214, ½ ,0.457)

MSSG: X2/c1'(α0γ)0ss

Transformation from parent structure: (**a**,2**b**,**c**;0,0,0)



X centering: {1|0 ½ 0, ½ }

elliptical cycloidal/helical arrangement
is symmetry allowed, but close to negligible

Atom	Magnetic moment Fourier Cos coeffs						Magnetic moment Fourier Sin coeffs					
	Symmetry constraints			Numerical values			Symmetry constraints			Numerical values		
	x	y	z	x	y	z	x	y	z	x	y	z
Mn1	$M_x$cos1	0	$M_z$cos1	1.46(3)	0.0	1.18(2)	0	$M_y$sin1	0	0.0	0.05(3)	0.0

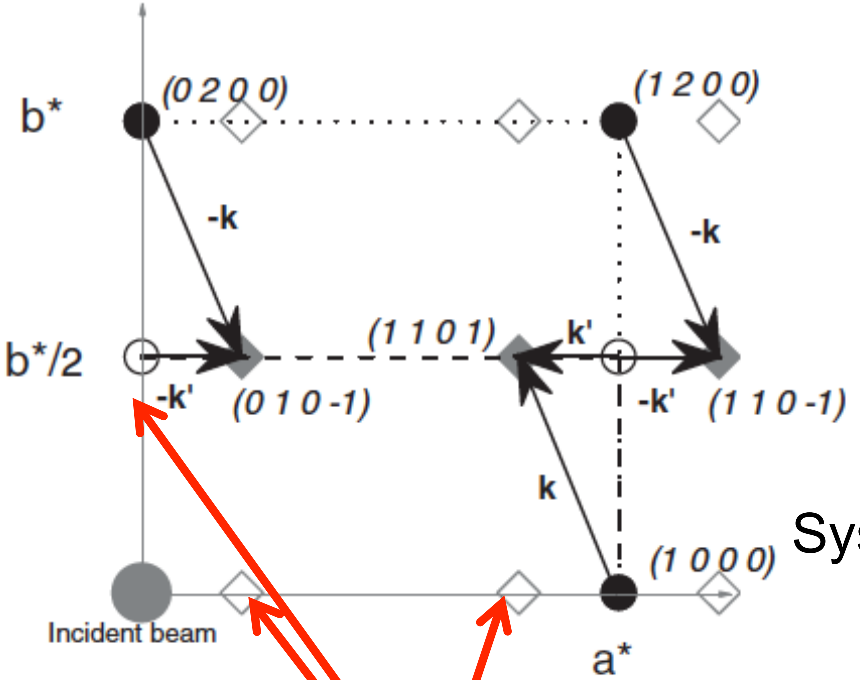
relation of the modulations of the two symmetry related Mn atoms:

opposite chirality

Atom	Magnetic moment Fourier Cos coeffs						Magnetic moment Fourier Sin coeffs					
	Symmetry constraints			Numerical values			Symmetry constraints			Numerical values		
	x	y	z	x	y	z	x	y	z	x	y	z
1	$M_x$cos1	0	$M_z$cos1	1.46000	0.0	1.18000	0	$M_y$sin1	0	0.0	0.05000	0.0
2	$M_x$cos1	0	$M_z$cos1	1.46000	0.0	1.18000	0	-$M_y$sin1	0	0.0	-0.05000	0.0

X-centerings: avoiding complex descriptions of the modulations

Example: **(a^*, b^*, c^*) k= (α, ½,0)**



systematic absences if indexed with **b***/2 and **k'**

Indexation Bragg peaks:

$(h,k,l,m) = (h,k,l) + m\,\mathbf{k}$

Alternative with X centering:

(a^*, $b^*/2$, c^*) k'= (α, 0,0)

$\mathbf{(h,k',l,m') = (h,k',l) + m'\,k'}$

$k'=2k \quad m'=m$

Systematic absence: (h,k',l,m'), $k'+m'$ = odd

working basic unit cell: (**a,2b,c**)

with centering operation: {1'| 0, ½, 0 ½ }

which only means modulations of atoms separated by **b** are in antiphase (as they should be):

$$\boxed{\mathbf{M}_{i+\mathbf{b}}(x_4 + ½) = \mathbf{M}_i(x_4)}$$

Diffraction symmetry (non-polarized)

$$\boldsymbol{H} = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^* + m\boldsymbol{k} \quad = \quad (h, k, l, m)$$

Consequences of a symmetry operation $\{\mathbf{R}, \theta | \mathbf{t}, \tau_o\}$:

non-magnetic: $F(\boldsymbol{H}) = e^{i2\pi \boldsymbol{H}.\boldsymbol{t}_s} F(\boldsymbol{H}.\boldsymbol{R}_S)$ Intensity($\boldsymbol{H}.\boldsymbol{R}_s$)=Intensity($\boldsymbol{H}$)

magnetic: $\boldsymbol{F}_M(\boldsymbol{H}) = e^{i2\pi \boldsymbol{H}.\boldsymbol{t}_s} \theta\, det(\boldsymbol{R}) \boldsymbol{R}.\boldsymbol{F}_M(\boldsymbol{H}.\boldsymbol{R}_S)$, Intensity($\boldsymbol{H}.\boldsymbol{R}_s$)=Intensity($\boldsymbol{H}$)

$\boldsymbol{H}.\boldsymbol{t}_s$ represents $ht_1 + kt_2 + lt_3 + m\tau_o$

$\boldsymbol{H}.\boldsymbol{R}_S$ stands for $(hklm).\boldsymbol{R}_S$

Systematic absences or extinction rules coming from superspace symmetry operations occur when *H* = *H.R*$_s$ …

Diffraction symmetry (non-polarized)

$$H = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^* + m\mathbf{k} \quad = \quad (h,k,l,m)$$

Extinction rules: ("trivial" cases)

{1'| 0 0 0 0 }

(non-magnetic structures)

$$F(H) = e^{i2\pi H.t_s} F(H.R_s) \rightarrow F(H) = F(H)$$

no condition

$$F_M(H) = e^{i2\pi H.t_s} \theta\, det(R) R.F_M(H.R_s), \rightarrow F_M(H) = -F_M(H)$$

zero!

{1'| 0 0 0 1/2 }

(all 1k magn.structures)

$$F(H) = e^{i\pi m} F(H)$$

absent m= odd

$$F_M(H) = -e^{i\pi m} F_M(H)$$

absent m= even

Systematic absences or extinction rules coming from superspace symmetry operations:

To derive them for any MSSG: program MAGNEXT

Diffraction symmetry (non-polarized)

$$\boldsymbol{H} = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^* + m\mathbf{k} \quad = \quad (h,k,l,m)$$

Extinction rules:

{2_x| 1/2 0 0 1/2 }

k=(α,0,0)

$$F(h00m) = e^{i\pi(h+m)} F(h00m) \rightarrow$$

absent h+m= odd

$$F_M(h00m) = e^{i\pi(h+m)} 2_x . F_M(h00m) \rightarrow$$

h+m= odd $\boldsymbol{F}_M$=(0,Fy,Fz)

h+m= even $\boldsymbol{F}_M$=(Fx,0,0) // $\boldsymbol{H}$

Magnetic diffraction: **absent h+m= even**

{2_z| 0 0 0 0 }

k=(0,0,γ)

$$F_M(00lm) = 2_z . F_M(00lm), \rightarrow$$

$\boldsymbol{F}_M$=(0,0,Fz) // $\boldsymbol{H}$

absent all (0,0,*l*,*m*)

Use MAGNEXT …

Conclusions:

- Properties of magnetic phases are constrained by their magnetic symmetry: a magnetic space group (if commensurate) or superspace group (if incommensurate)

- Whatever method one has employed to determine a magnetic structure, the final model should include its magnetic symmetry.

- Representation analysis of magnetic structures is NOT equivalent to the use of magnetic symmetry (i.e. to give an irrep is not equivalent to give the magnetic space (superspace) group of the system)

- The best approach: to combine both representation analysis and magnetic symmetry

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