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Magnetic Symmetry. 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 Fisica de la Materia Condensada, Facultad de Ciencia y Tecnología, Universidad del País Vasco, UPV/EHU, Apartado 644, E-48080 Bilbao, Spain
[2] Centro de Fisica 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

Symmetry-Based Computational Tools for Magnetic Crystallography

J.M. Perez-Mato,[1] S.V. Gallego,[1] E.S. Tasci,[2] L. Elcoro,[1] G. de la Flor,[1] and M.I. Aroyo[1]

[1]Departamento de Física de la Materia Condensada, Facultad de Ciencia y Tecnología, Universidad del País Vasco, UPV/EHU, 48080 Bilbao, Spain; email: jm.perez-mato@ehu.es

[2]Department of Physics Engineering, Hacettepe University, 06800 Ankara, Turkey

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MAGNDATA: towards a database of magnetic structures. II. The incommensurate case

Samuel V. Gallego,[a] J. Manuel Perez-Mato,[a*] Luis Elcoro,[a] Emre S. Tasci,[b] Robert M. Hanson,[c] Mois I. Aroyo[a] and Gotzon Madariaga[a]

[a]Departamento de Fisica de la Materia Condensada, Facultad de Ciencia y Tecnología, Universidad del País Vasco (UPV/EHU), Apartado 644, Bilbao 48080, Spain, [b]Department of Physics Engineering, Hacettepe University, Ankara 06800, Turkey, and [c]Department of Chemistry, St Olaf College, Northfield, MN 55057, USA. *Correspondence e-mail: jm.perez-mato@ehu.es

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A free web page under the name *MAGNDATA*, which provides detailed quantitative information on more than 400 published magnetic structures, has been made available at the Bilbao Crystallographic Server (http://www.cryst.ehu.es). It includes both commensurate and incommensurate structures. In the first article in this series, the information available on commensurate magnetic structures was presented [Gallego, Perez-Mato, Elcoro, Tasci, Hanson, Momma, Aroyo & Madariaga (2016). *J. Appl. Cryst.* **49**, 1750–1776]. In this second article, the subset of the database devoted to incommensurate magnetic structures is discussed. These structures are described using magnetic superspace groups, *i.e.* a direct extension of the non-magnetic superspace groups, which is the standard approach in the description of aperiodic crystals. The use of magnetic superspace symmetry ensures a robust and unambiguous description of both atomic positions and magnetic moments within a common unique formalism.

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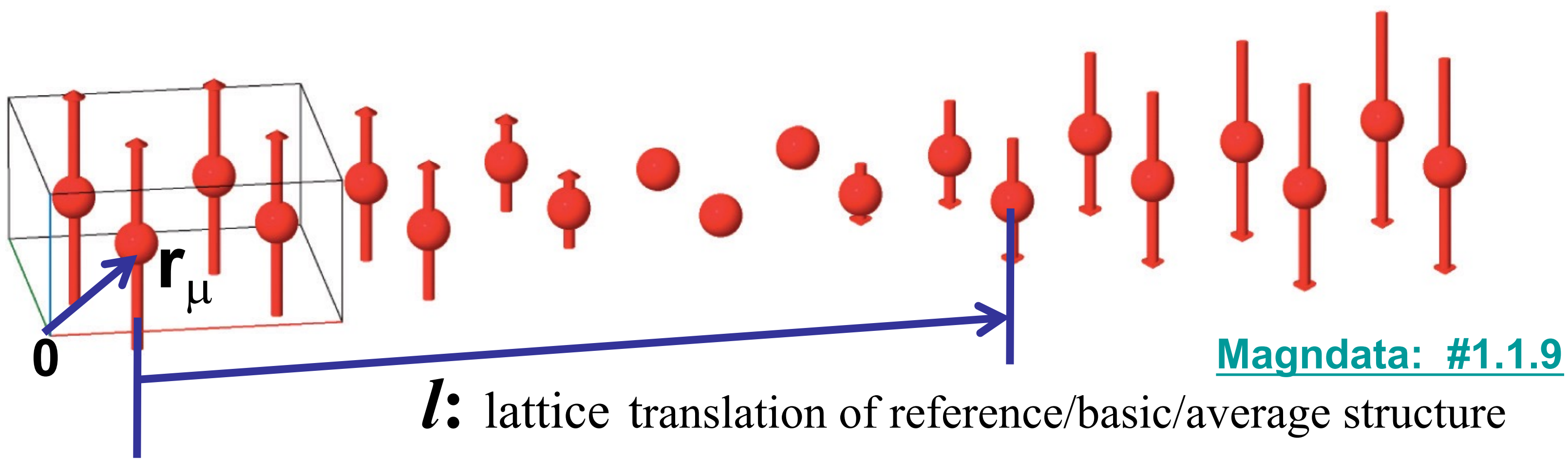
Incommensurate modulated structures



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

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

if k is incommensurate k.l (mod. 1) takes ANY VALUE at some lattice vector *l*

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** $A_{\mu}(x_4)$

general anharmonic case

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

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

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

$$\mathbf{A}(x_4) = \mathbf{A}(x_4 + 1)$$

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

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:

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

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

fourth coordinate in superspace – period 1

k = incommensurate propagation vector

example: 1.1.9

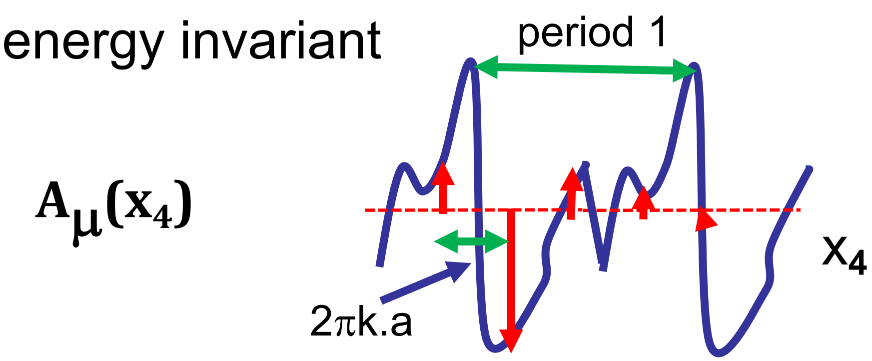
A global shift of the modulation functions along x_4 keeps the energy invariant

The superspace:

X4 – additional "dimension"

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

x4 - phase shift is energy invariant



k-incommensurate: all values of the periodic function are realized at some unit cell

The superspace concept is just a mathematical construct, their symmetry as analogous to those of ordinary crystallography for a structure with lattice periodicity, but in a (3+1)-dim mathematical space.

BUT this superspace concept is just a help! Essential are only the equations!, and these can be derived without the need of a 4-dim superspace.

MAGNETIC SYMMETRY IN COMMENSURATE CRYSTALS:
MAGNETIC SPACE GROUPS OR SHUBNIKOV GROUPS

A symmetry operation fullfills:

- the operation belongs to the set of transformations that keep 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 $\{ \{\mathbf{R}_i , \theta | \mathbf{t}_i\}\}$ θ= +1 without time reversal
θ= -1 with time reversal

SYMMETRY OF INCOMMENSURATE PHASES

Phase shift of the whole modulation: energy invariant!

Symmetry operations in 1-k incommensurate crystals:

sym. operations: space group operations

+ phase shifts of the modulation

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

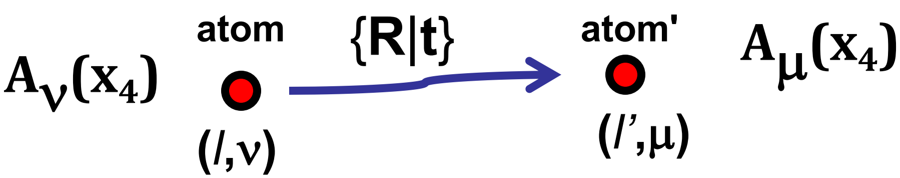
Incommensurate magnetic structures have an unambiguous magnetic point group symmetry

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

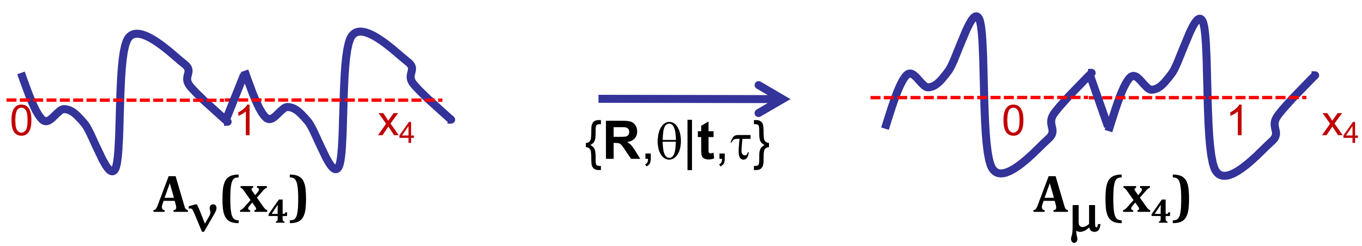
Symmetry relations between the modulation functions of different atoms in the basic unit cell due to a symmetry operation.

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

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



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:



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 constrained!**

Symmetry relations between the modulation functions of different atoms in the basic unit cell due to the symmetry operation $\{\mathbf{R},\theta|\mathbf{t},\tau\}$:

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

R_I, τ_o , $\mathbf{H}_R$ defined by $\{\mathbf{R},\theta|\mathbf{t},\tau\}$: $\quad \boldsymbol{k}.\boldsymbol{R} = R_I\, \boldsymbol{k} + \boldsymbol{H}_R \qquad R_I$ =+1 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 also a translation $-\mathbf{k}.\mathbf{t}$ along x_4

Example and notation of operation with $\mathbf{H}_R \neq 0$:

$$\boldsymbol{k} = (\alpha\ ,\ \tfrac{1}{2},\ 0) \xrightarrow{m_y} \boldsymbol{k}' = (\alpha\ ,\ -\tfrac{1}{2},\ 0) = \boldsymbol{k} + (0,\ -1,\ 0)$$

$\{m'_y|1/2\ 1/2\ 0\ 1/2\}$ $\qquad R_I$ =+1 $\quad \mathbf{H}_R = (0,\ -1,\ 0)$

R_S 4X4 matrix

$$\left(\begin{array}{ccc|c} & \mathbf{R}\ (3\times3) & & \begin{matrix}0\\0\\0\end{matrix} \\ \hline H_{Rx} & H_{Ry} & H_{Rz} & R_i \end{array}\right)\begin{pmatrix}x_1\\x_2\\x_3\\ \hline x_4\end{pmatrix} + \begin{pmatrix}t_1\\t_2\\t_3\\ \hline \tau_o\end{pmatrix} = \left(\begin{array}{ccc|c} 1 & 0 & 0 & 0\\ 0 & -1 & 0 & 0\\ 0 & 0 & 1 & 0\\ \hline 0 & -1 & 0 & 1\end{array}\right)\begin{pmatrix}x_1\\x_2\\x_3\\ \hline x_4\end{pmatrix} + \begin{pmatrix}1/2\\1/2\\0\\ \hline 1/2\end{pmatrix} = x1+1/2,-x2+1/2,x3,-x2+x4,-1$$

notation used
for symmetry operations

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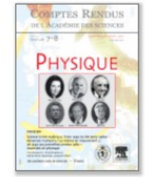

Science in the making 2: From 1940 to the early 1980s / *La science en mouvement 2 : de 1940 aux premières années 1980*

Magnetic structures

Structures magnétiques

A review for the general case of several ncommensurate wave vectors

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Juan Rodríguez-Carvajal [a], Jacques Villain [b]

8. Superspace approach to invariance symmetry of crystal structures and spin configurations

8.1. Concept of superspace

The basic concepts related with incommensurate crystal structures and their symmetry description using superspace groups can be found in references [81], [82], [83], [84], [85], [86], [87]. The case of magnetic superspace groups has been treated exhaustively in reference [88] and here we will follow some of their explanations and generalise some expressions for multiple propagation vectors.

The concept of superspace comes from the consideration that all Bragg spots observed in a modulated structure can be indexed using a series of modulation (propagation) vectors $\mathbf{q}_p$ with $p = 1, 2, \ldots, d$. The scattering vector for a Bragg spot (diffraction vector) can be written as:

$$\mathbf{h} = h_1\mathbf{a}_1^* + h_2\mathbf{a}_2^* + h_3\mathbf{a}_3^* + \sum_{p=1}^{d} m_p\mathbf{q}_p \tag{41}$$

The extra integer indices m_p correspond to the harmonics of the modulation

Symmetry relations between the atomic modulations

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

Example: inversion

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

atom 1 → atom 2

superspace operation

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

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

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

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

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

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

Relation between the modulation of their magnetic moments

it chooses the origin along x4 on the inversion center

atom 2 atom 1

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

Symmetry relations between the atomic modulations

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

Example: inversion

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

superspace operation

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

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

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

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

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

$$\boxed{\mathbf{M}^2(-x_4) = \mathbf{M}^1(x_4)}$$

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)**

Translation into FullProf k-vector parameters:

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

Superspace

atom v at cell L:

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

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

FullProf

$$\boxed{2S_{\boldsymbol{k}}^{\nu}\, e^{i2\pi \boldsymbol{k} \cdot \boldsymbol{r}_{\nu}} = \boldsymbol{M}_{\cos 1}^{\nu} + i\, \boldsymbol{M}_{\sin 1}^{\nu}}$$

Translation into FullProf k-vector parameters:

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

Superspace

atom v at cell L:

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

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

FullProf

$$\boxed{2\boldsymbol{S}_{\boldsymbol{k}}^{\nu} e^{i2\pi \boldsymbol{k} \cdot \boldsymbol{r}_{\nu}} = \boldsymbol{M}_{\cos 1}^{\nu} + i\, \boldsymbol{M}_{\sin 1}^{\nu}}$$

Symmetry relation for the FullProf parameters:

$\{\mathbf{R},\theta|\mathbf{t},\tau\}$: $(l,\nu) \longrightarrow (l,\mu)$ **same cell: t must be a specific one**

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

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

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

Symmetry relations between the atomic modulations if described with FullProf parameterization

Example: inversion

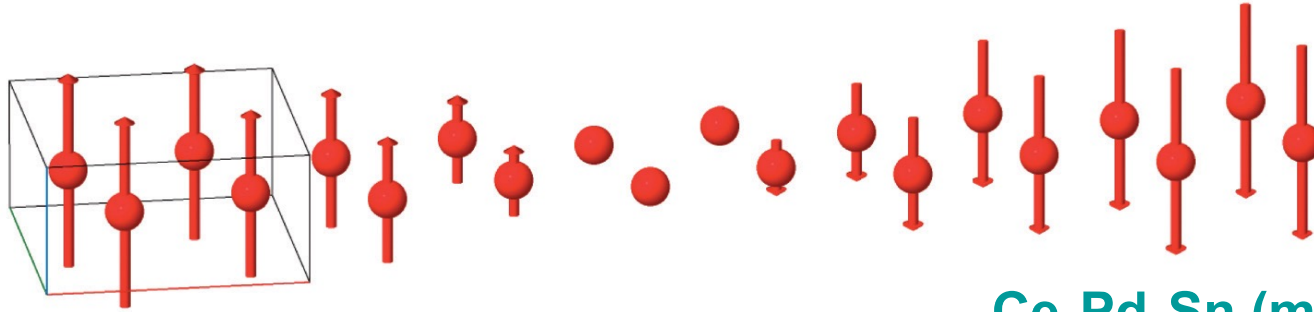
superspace operation

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

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

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

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



Ce_2Pd_2Sn (magndata #1.1.9)

magCIF file

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4 x1+1/2,-x2+1/2,-x3,x4+1/2,+1
5 -x1,-x2,-x3,-x4,+1
6 x1,x2,-x3,x4,+1
7 x1+1/2,-x2+1/2,x3,x4+1/2,+1
8 -x1+1/2,x2+1/2,x3,-x4+1/2,+1

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2 x1,x2,x3,x4+1/2,-1
```

(1' | 0 0 0 ½)

```
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Pd1 Pd 0.37340(10) 0.8734 0 1
Sn1 Sn 0 0 0 1

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_atom_site_moment_Fourier_param.sin
_atom_site_moment_Fourier_param.cos_symmform
_atom_site_moment_Fourier_param.sin_symmform
Ce1 x 1 0 0 0 0
Ce1 y 1 0 0 0 0
Ce1 z 1 1.70(5) 0 mzc1 mzs1
```

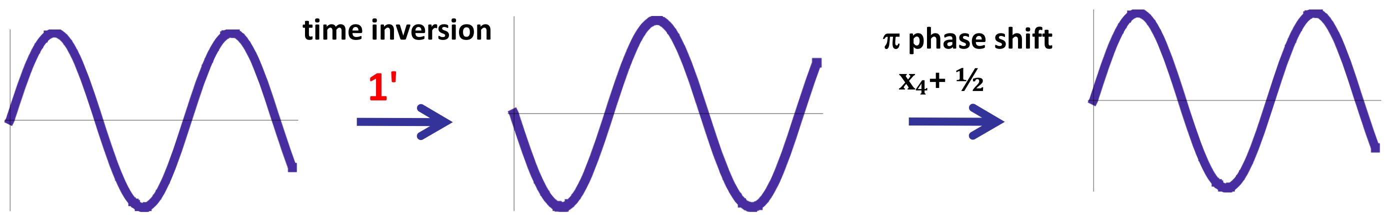
average moment cero (symmetry forced)

moment along z (symmetry forced)

A simple but <u>very important general</u> "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)

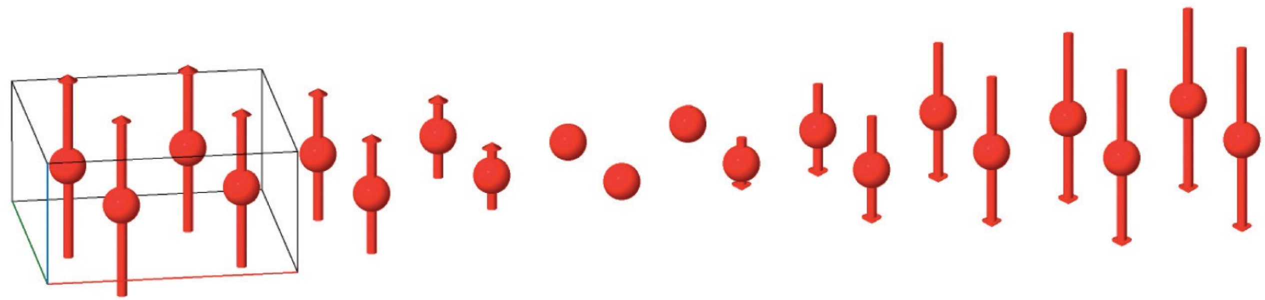
Consequences of (1'| 0 0 0 ½) : $\boxed{A_\mu(x_4 + ½) = 1' A_\mu(x_4)}$

modulation of magnetic moments	$M_\mu(x_4 + ½) = - M_\mu(x_4)$	odd-harmonics : 1k, 3k ,5k ...
modulation of atomic displac.	$u_\mu(x_4 + ½) = u_\mu(x_4)$	even-harmonics : 2k, 4k ...

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)

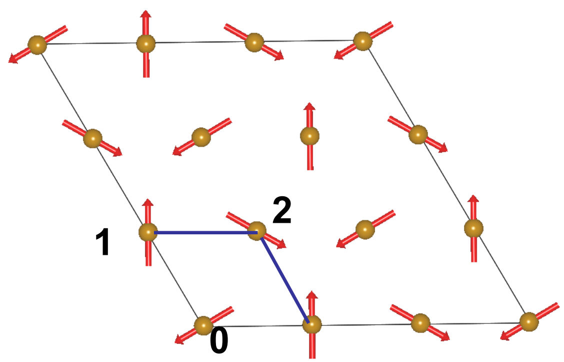
superspace symmetry constraint: 2 parameters
(same amplitude for the 4 atoms, but atoms related by
inversion are not in phase but with opposite phases)

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	$M_z\cos 1$	0.0	0.0	1.70000	0	0	$M_z\sin 1$	0.0	0.0	0.0
2	0	0	$M_z\cos 1$	0.0	0.0	1.70000	0	0	$-M_z\sin 1$	0.0	0.0	0.0
3	0	0	$M_z\cos 1$	0.0	0.0	1.70000	0	0	$-M_z\sin 1$	0.0	0.0	0.0
4	0	0	$M_z\cos 1$	0.0	0.0	1.70000	0	0	$M_z\sin 1$	0.0	0.0	0.0

Mulferroic $RbFe(MoO_4)_2$:

Superspace group: P31'(1/3 1/3 γ) ts
or P31'(1/3 1/3 γ) -ts

A "120º spin arrangement" and a spiral modulation is forced by the superspace group:



z=0

magndata 1.1.2

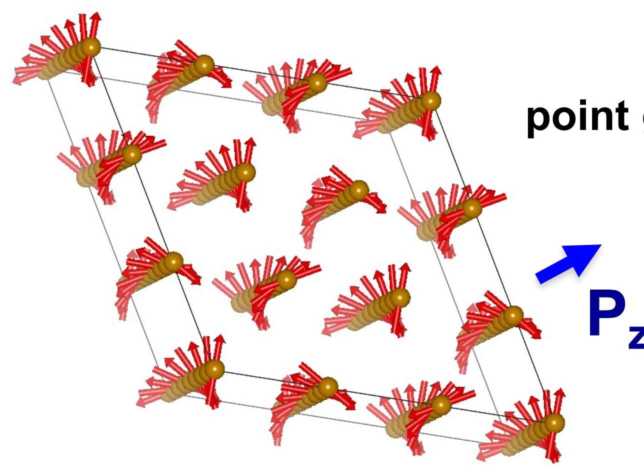
P-3 $\longrightarrow$ **P31'(1/3 1/3 γ) ts** $\gamma \approx 0.458$

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

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



point group: 31'

perspective

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

magndata 1.1.33

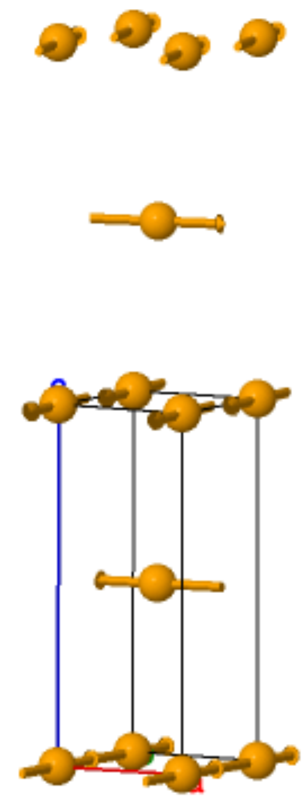
$\boldsymbol{k}$ =(0 0 0.52) Parent space group: I4mm

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



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

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

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

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

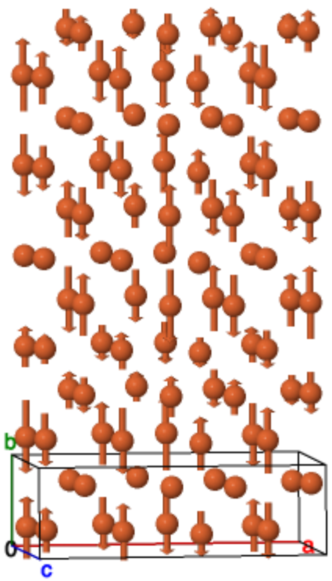
$$\boxed{\mathbf{M_{z\,sin1} = M_{z\,cos1} = 0}}$$

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

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

$CaFe_4AS_3$ magndata 1.1.5 **Superspace group: Pnma1'(0 β 0)000s**

The MSSG symmetry forces that modulations of independent atoms must be in phase



Pnma ⟶ **Pnma1'(0 β 0)000s** $\beta \approx 0.375$

Average atomic positions of symmetry independent atoms

Label	Atom type	x	y	z	Multiplicity
Fe1	Fe	0.02100(15)	0.25	0.31350(19)	4
Fe2	Fe	0.06677(16)	0.25	0.53727(18)	4
Fe3	Fe	0.30580(17)	0.25	0.12471(18)	4
Fe4	Fe	0.31841(17)	0.25	0.72371(18)	4

$\{\mathbf{m}_{010}|0\ 1/2\ 0\ 0\}$: x1,-x2+1/2,x3,-x4,+1

it fixes the global phase

$$\mathbf{M}_{\mu}(-x_4) = -\,\mathbf{m}_{010}\,.\,\mathbf{M}_{\mu}(x_4)$$

Mx,Mz : Sin

My: Cos

Magnetic moment modulation parameters of symmetry independent atoms

in phase

Wave vector 1

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
Fe1	0	$M_y\cos1$	0	0.0	2.14	0.0	$M_x\sin1$	0	$M_z\sin1$	0.0	0.0	0.0
Fe2	0	$M_y\cos1$	0	0.0	1.55	0.0	$M_x\sin1$	0	$M_z\sin1$	0.0	0.0	0.0
Fe3	0	$M_y\cos1$	0	0.0	-1.83	0.0	$M_x\sin1$	0	$M_z\sin1$	0.0	0.0	0.0
Fe4	0	$M_y\cos1$	0	0.0	1.94	0.0	$M_x\sin1$	0	$M_z\sin1$	0.0	0.0	0.0

Diffraction symmetry (non-polarized)

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

Magnetic diffraction at diffraction vector *H* is proportional to the squared modulus of the component of F_M(*H*) perpendicular to *H*

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(***H.R***$_s$)=Intensity(***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(***H.R***$_s$)=Intensity(***H***)

axial vector

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

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

point-group symmetry in the diffraction diagram

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

Systematic Absence (Extinction rules)

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

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)

$$\boldsymbol{H} = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^* + mk$$

Extinction rules:

{2_x| 1/2 0 0 1/2 } $F(h00m) = e^{i\pi(h+m)} F(h00m)$ → **absent h+m= odd**

k=(α,0,0) $F_M(h00m) = e^{i\pi(h+m)} 2_x . F_M(h00m)$ → 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**

$$F(\boldsymbol{H}) = e^{i2\pi \boldsymbol{H}.\boldsymbol{t}_s} F(\boldsymbol{H}.\boldsymbol{R}_S)$$

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

MAGNEXT provides systematic absences of magnetic diffraction for any (3+1) MSSG

X-centerings: avoiding complex descriptions of the modulations

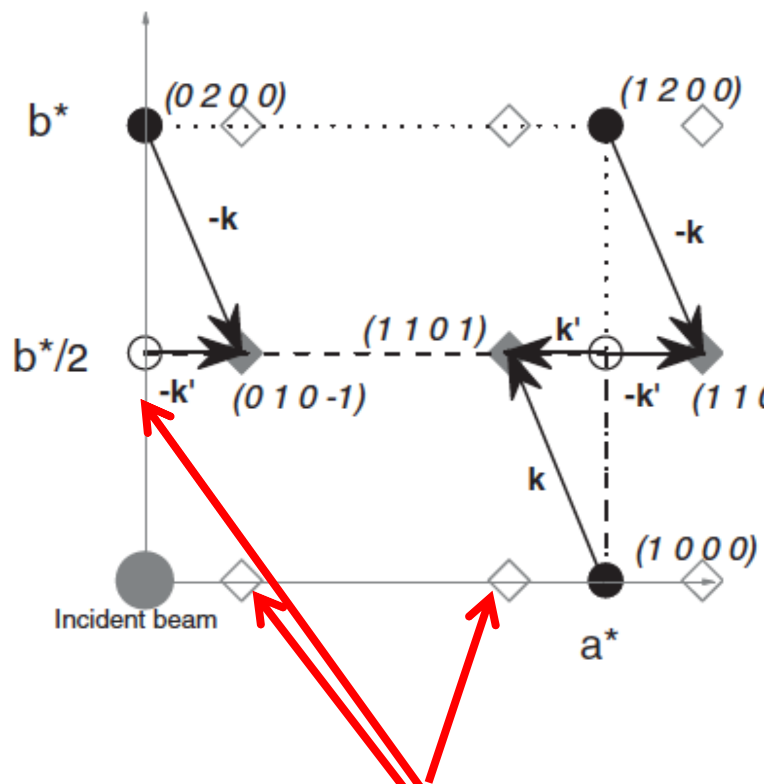
$$\boxed{\mathbf{M}_{\mu}(R_I x_4+\tau_o + \mathbf{H}_R.\mathbf{r}_{\nu}) = \theta \det(\mathbf{R})\mathbf{R}\,.\,\mathbf{M}_{\nu}(x_4)}$$

$\mathbf{H}_R \neq 0$

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

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)**

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

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

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

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

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

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

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

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

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:**

Generalized invariance equation:

phase shift

N-dim small irrep

$(\mathbf{R},\theta|\mathbf{t},\tau)$ belongs to superspace group if : $\begin{pmatrix} \mathbf{1}e^{i2\pi\tau} & 0 \\ 0 & \mathbf{1}\,e^{-i2\pi\tau} \end{pmatrix} T[(\mathbf{R},\theta|\mathbf{t})] \begin{pmatrix} \mathbf{S}(k) \\ \mathbf{S}(-k) \end{pmatrix} = \begin{pmatrix} \mathbf{S}(k) \\ \mathbf{S}(-k) \end{pmatrix}$

(R|t) is an operation of the grey paramagnetic space group that either keeps k invariant or transforms it into -k

Additional term in an incommensurate phase

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

$T[(\mathbf{R},\theta|\mathbf{t})]$: 2N x 2N matrices

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

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

If the small irrep is 1-dim: only one global complex amplitude S(k) for the spin wave, and a shift of this phase can always be included in the symmetry operation.

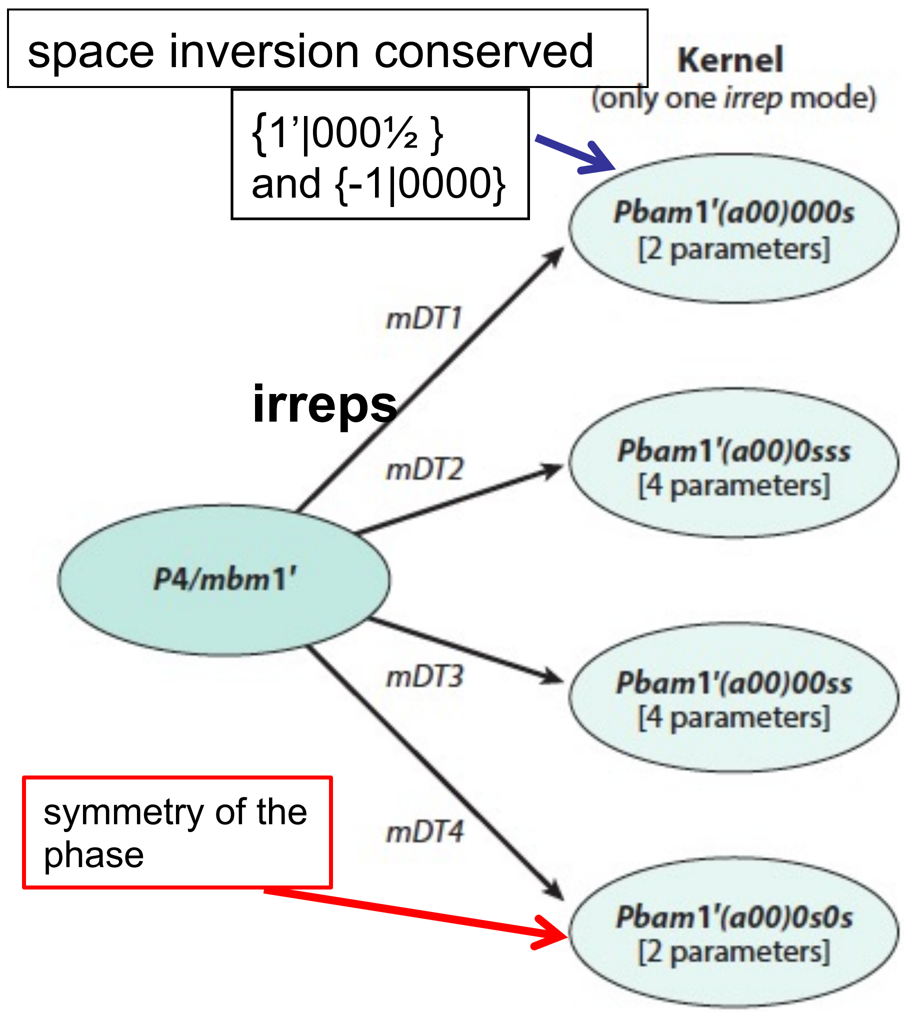
N =1	**one to one correspondance irrep – superspace group**

But including operations changing *k* into –*k* !

Ce_2Pd_2Sn magndata 1.1.9 **space inversion is maintained !**

superspace group: Pbam1'(α00)0s0s parent space group: P4/mbm

k= (α,0,0)



Superspace magnetic symmetry produced by an irrep magnetic mode:

Generalized invariance equation:

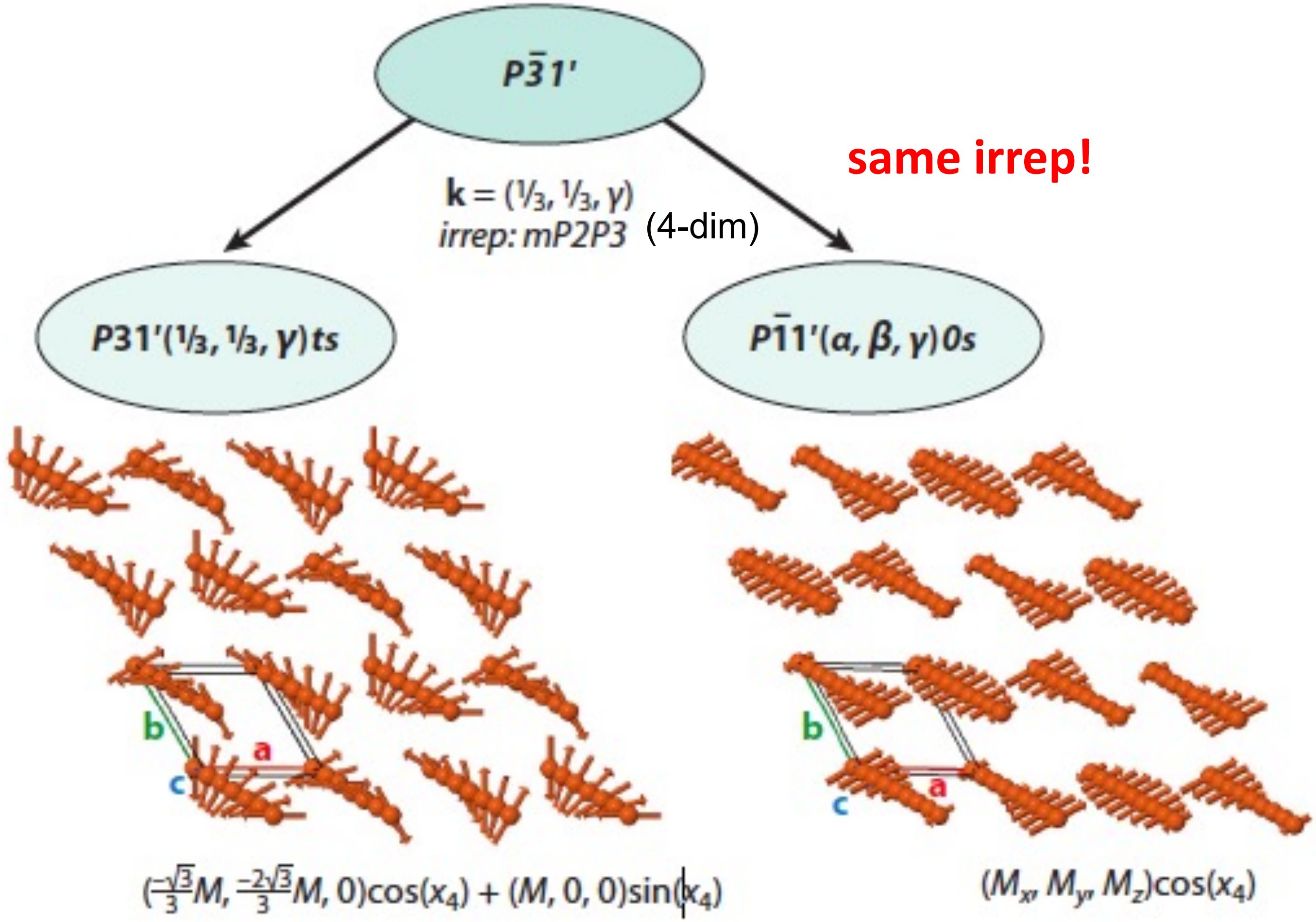
$\boxed{N > 1}$

$\boxed{\text{N-dim}}$

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

One irrep with N>1 ➔ several possible superspace groups

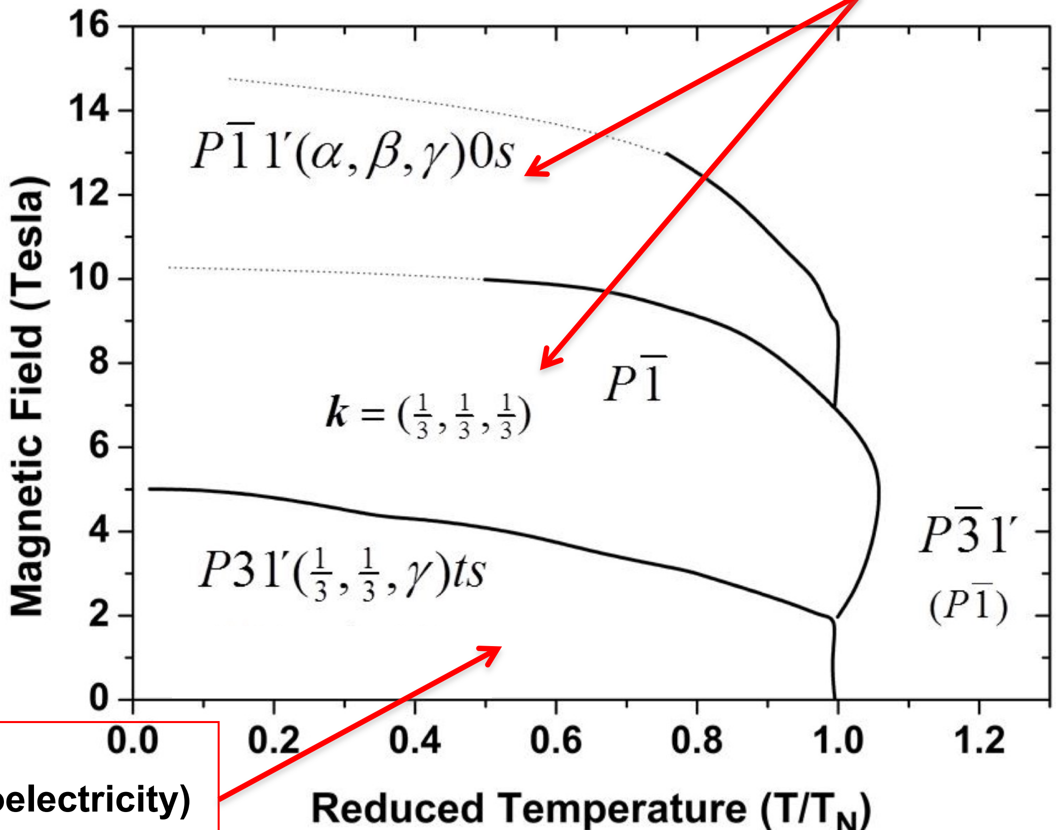
Another example: two possible higher alternative superspace symmetries for the same irrep.



$RbFe(MoO_4)_2$: 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

Programs that determine the epikernels and kernel of any irrep, and produce magnetic structural models complying with them, using MSSGs

Program for mode analysis:

ISODISTORT http://stokes.byu.edu/iso/isotropy.php Stokes & Campbell, Provo

Version 6.1.8, November 2014

Harold T. Stokes. Branton J. Campbell, and Dorian M. Hatch, Department of Physics and Astronomy, Brigham Young University, Provo, Utah, 84602, USA, stokesh@byu.edu

Description: ISODISTORT is a tool for exploring the structural distortion modes of crystalline materials. It provides a user-friendly interface to many of the algorithms used by the **Isotropy Software Suite**, allowing one to generate and explore distortion modes induced by irreducible representations of the parent space-group symmetry. It also provides a Java applet for visualizing and interactively manipulating the free parameters associated with these modes.

Help, **Tutorials**, **Version History**

NOTICE: Version 6.1 is a major new release. We appreciate your bug reports -- please send relevant input files along with the html page showing the failed output.

Legacy copy of ISODISTORT version 5.6.1, August 2013

Begin by entering the structure of parent phase: ?

Get started quickly with a cubic perovskite parent.

Import parent structure from a CIF structure file: OK Browse… No file selected.

Both programs also support incommensurate cases, deriving epikernels and kernel of the irreps in the form of MSSGs, and corresponding magnetic models

Program for structure refinement:

JANA

Institute of Physics
Department of Structure Analysis
Cukrovarnicka 10
16253 Praha 6
Czech Republic

http://jana.fzu.cz/ V. Petricek, Prague

Academy of Sciences | Institute of Physics
Dept of Structure Analysis | Laboratory of Crystallography
ECA-SIG#3 | Contact Us

CRYSTALLOGRAPHIC COMPUTING SYSTEM FOR STANDARD AND MODULATED STRUCTURES

Vaclav Petricek, Michal Dusek & Lukas Palatinus

News

January 24, 2015 APERIODIC2015: abstract submission, deadline 30 April

Beware when interpreting ISODISTORT output:

ISODISTORT: order parameter direction

Space Group: 127 P4/mbm D4h-5, Lattice parameters: a=7.76200, b=7.76200, c=3.93000, alpha=90.00000, beta=90.00000, gamma=90.00000

Default space-group preferences: monoclinic axes a(b)c, monoclinic cell choice 1, orthorhombic axes abc, origin choice 2, hexagonal axes, SSG :

Ce1 4h (x,x+1/2,1/2), x=0.17810, Pd1 4g (x,x+1/2,0), x=0.37340, Pd2 4e (0,0,z), z=0.31900, occ=0.03100, Sn1 2a (0,0,0), occ=0.93800

Include strain, displacive ALL, magnetic Ce distortions

k point: DT (0,b,0), b=0.70000 (1 incommensurate modulation/2 arms)

IR: mDT1

can be misleading!

1 Order Parameter
with ANY OP direction (not (a,0))

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

- P (a,0;0,0) 55.1.9.4.m354.2 Pcma1'(0,0,g)000s, basis={(1,0,0,0),(0,0,-1,0),(0,1,0,0),(0,0,0,1)}, origin=(0,0,0,0), s=1, i=2, k-active= (0,0.300,0)
- C (a,b;0,0) 26.1.9.1.m67.2 Pmc2_11'(0,0,g)000s, basis={(0,0,1,0),(1,0,0,0),(0,1,0,0),(0,0,0,1)}, origin=(1/4,0,0,0), s=1, i=4, k-active= (0,0.300,0)

OK

it requires 2 independent Order Parameters
with the same irrep
(Landau condition is not fulfilled)

Superspace magnetic symmetry tools and applications in the BCS :

Magnetic Symmetry and Applications	
MGENPOS	General Positions of Magnetic Space Groups
MWYCKPOS	Wyckoff Positions of Magnetic Space Groups
MKVEC	The k-vector types and Brillouin zones of Magnetic Space Groups
IDENTIFY MAGNETIC GROUP	Identification of a Magnetic Space Group from a set of generators in an arbitrary setting
BNS2OG	Transformation of symmetry operations between BNS and OG settings
mCIF2PCR	Transformation from mCIF to PCR format (FullProf).
MPOINT	Magnetic Point Group Tables
MAGNEXT	Extinction Rules of Magnetic Space Groups
MAXMAGN	Maximal magnetic space groups for a given space group and a propagation vector
MAGMODELIZE	Magnetic structure models for any given magnetic symmetry
STRCONVERT	Convert & Edit Structure Data (supports the CIF, mCIF, VESTA, VASP formats -- with magnetic information where available)
k-SUBGROUPSMAG	Magnetic subgroups consistent with some given propagation vector(s) or a supercell
MAGNDATA	A collection of magnetic structures with portable cif-type files
MVISUALIZE	3D Visualization of magnetic structures with Jmol
MTENSOR	Symmetry-adapted form of crystal tensors in magnetic phases
MAGNETIC REP.	Decomposition of the magnetic representation into irreps
Get_mirreps	Irreps and order parameters in a paramagnetic space group- magnetic subgroup phase transition

MAGNEXT: Magnetic diffraction systematic absences

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MAGNEXT: Magnetic Systematic Absences

tinction rules for
any Shubnikov magnetic

pe obtained introducing the
l for this purpose at the
pted form of the structure

/ a set of generators in any

patible with a set of

or a superspace group

Option A: Systematic absences for a magnetic space group in standard settings

Magnetic Space Group number: Please, enter the label of group or choose it

Standard/Default Setting

Other interfaces for alternative uses MAGNEXT are:

- **Option B:** For systematic absences for a magnetic space group **in any setting**, click here
- **Option C:** For a list of magnetic space groups **compatible with a given set of systematic absences**, click here
- For systematic absences for ***magnetic superspace groups*** click here

also for incommensurate magnetic structures from the input of its superspace group operations

MTENSOR: Symmetry-adapted form of crystal tensors properties of magnetic crystals. Only the magnetic point group is relevant!

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MTENSOR

Magnetoelectric tensor:

Group 6/m' (#23.4.85)

α^T_{ij}	j		
i	1	2	3
1	α^T_{11}	α^T_{12}	0
2	$-\alpha^T_{12}$	α^T_{11}	0
3	0	0	α^T_{33}

Number of independent coefficients: 3

Group 622 (#24.1.87)

α^T_{ij}	j		
i	1	2	3
1	α^T_{11}	0	0
2	0	α^T_{11}	0
3	0	0	α^T_{33}

Number of independent coefficients: 2

Group 62'2' (#24.4.90)

α^T_{ij}	j		
i	1	2	3
1	0	α^T_{12}	0
2	$-\alpha^T_{12}$	0	0
3	0	0	0

Number of independent coefficients: 1

Group 6mm (#25.1.91)

α^T_{ij}	j		
i	1	2	3
1	0	α^T_{12}	0
2	$-\alpha^T_{12}$	0	0
3	0	0	0

Number of independent coefficients: 1

Group 6m'm' (#25.4.94)

α^T_{ij}	j		
i	1	2	3
1	α^T_{11}	0	0
2	0	α^T_{11}	0
3	0	0	α^T_{33}

Number of independent coefficients: 2

Group -6'm'2 (#26.3.97)

α^T_{ij}	j		
i	1	2	3
1	α^T_{11}	0	0
2	0	α^T_{11}	0
3	0	0	α^T_{33}

Number of independent coefficients: 2

Group -6'm2' (#26.4.98)

α^T_{ij}	j		
i	1	2	3
1	0	α^T_{12}	0
2	$-\alpha^T_{12}$	0	0
3	0	0	0

Number of independent coefficients: 1

Group 6/m'mm (#27.3.102)

α^T_{ij}	j		
i	1	2	3
1	0	α^T_{12}	0
2	$-\alpha^T_{12}$	0	0
3	0	0	0

Number of independent coefficients: 1

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MAGNDATA: Database with CIF files of magnetic structures both commensurate and incommensurate, using MSGs and MSSGs

MAGNDATA: A Collection of magnetic structures with portable cif-type files

Log in

> 140 incommensurate magnetic structures

MAGNDATA: A collection of magnetic structures with portable cif-type files

A database of more than 300 published commensurate and incommensurate magnetic structures can be found here. The structures are described using magnetic symmetry (Shubnikov magnetic space groups) in the BNS

View Full Database

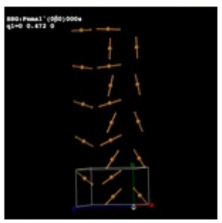
Element search (separate with space or comma):

AND OR Search

Enter the label of the structure: Submit

INCOMMENSURATE STRUCTURES

One propagation vector



1.1.1 Cs_2CuCl_4

1.1.2 $RbFe(MoO_4)_2$

1.1.3 Cr

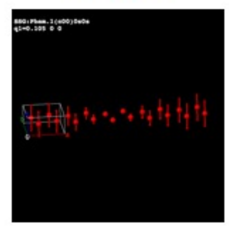
1.1.4 Cr

1.1.5 $CaFe_4As_3$

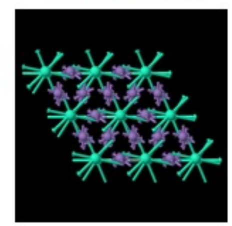
1.1.6 $TbMnO_3$

1.1.7 $TbMnO_3$

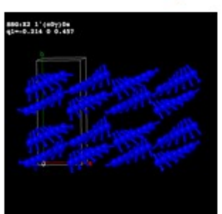
1.1.8 $TbMnO_3$



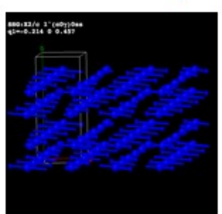
1.1.9 Ce_2Pd_2Sn



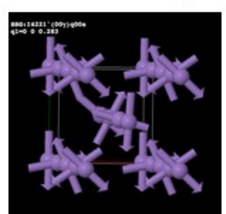
1.1.10 $DyMn_6Ge_6$



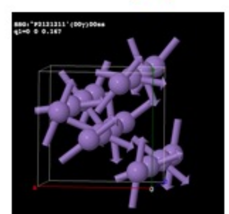
1.1.11 $MnWO_4$



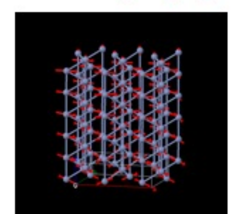
1.1.12 $MnWO_4$



1.1.13 $MnAu_2$



1.1.14 MnGe



1.1.15 $CaCr_2O_4$

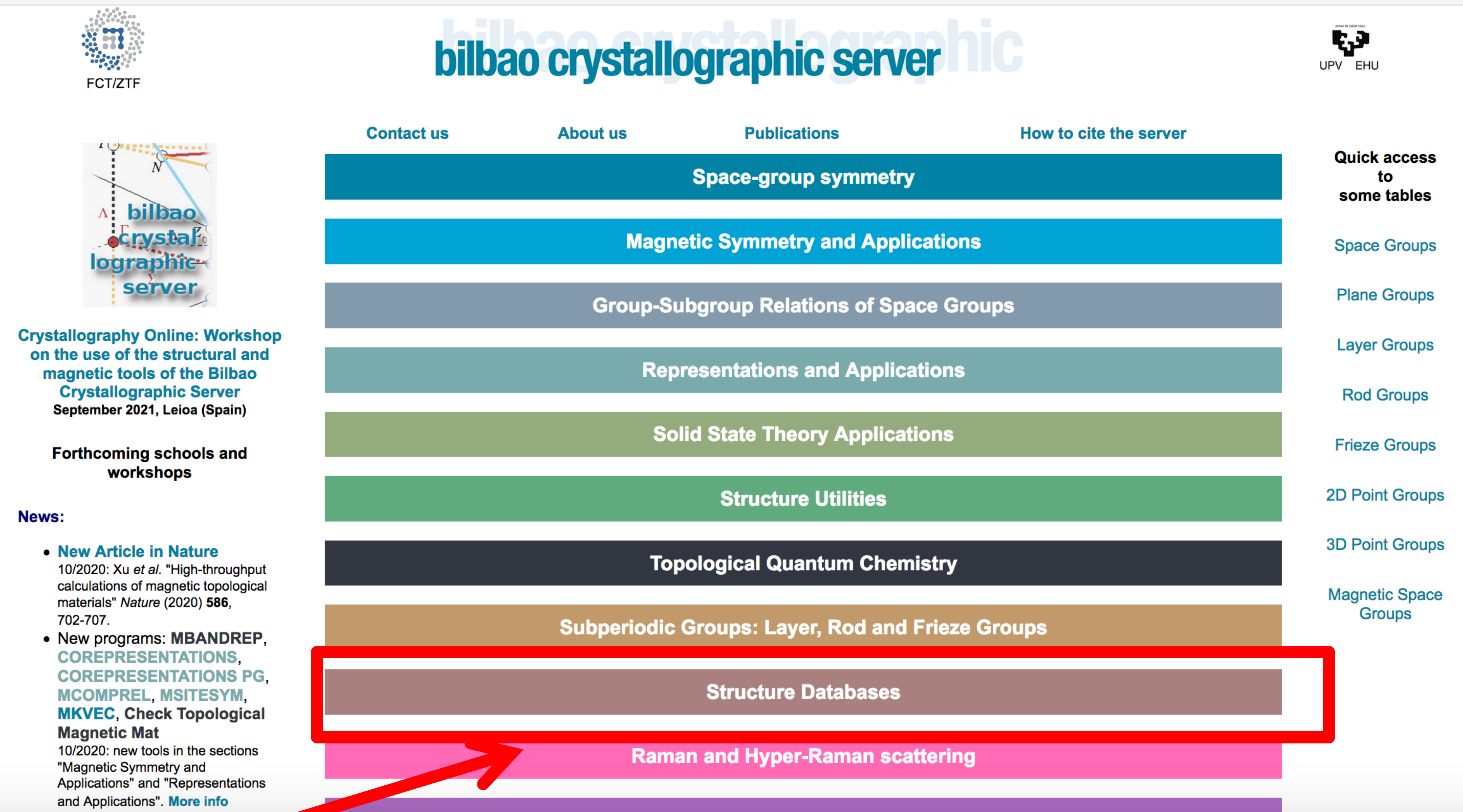
Conclusions:

- ***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 in general 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 in incommensurate structures: to combine magnetic symmetry and representation analysis***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September 2021, Leioa (Spain)
Forthcoming schools and workshops
News:
New Article in Nature
10/2020: Xu et al. "High-throughput calculations of magnetic topological materials" Nature (2020) 586, 702-707.
New programs: MBANDREP, COREPRESENTATIONS, COREPRESENTATIONS PG, MCOMPREL, MSITESYM, MKVEC, Check Topological Magnetic Mat
10/2020: new tools in the sections "Magnetic Symmetry and Applications" and "Representations and Applications". More info

Databases

Structure Databases

B-IncStrDB ⚠	The Bilbao Incommensurate Crystal Structure Database
MAGNDATA ⚠	A collection of magnetic structures with portable cif-type files

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Fully Upgraded version!

The Bilbao Incommensurate Structures Database

B-IncStrDB

This database is dedicated to incommensurate modulated and composite structures.

Commensurate structures described in the superspace formalism are also included.

The database currently hosts 255 entries (of which 44 are composites).

Explore the database ›

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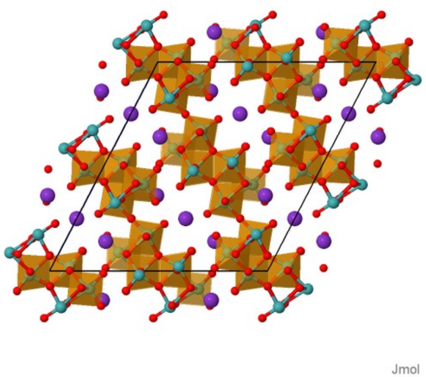
Order by: Date: first submitted

Search results: 255



The incommensurately modulated structure of the blue bronzes $K_{0.3}MoO_3$ and $Rb_{0.3}MoO_3$

Authors:
Schutte, W.J.; de Boer, J.L.

Journal:
Acta Cryst. B 49 579-591 (1993)

DOI:
https://doi.org/10.1107/S0108768192006578

Entry date: 2010-11-08 **B-IncStrDB ID:** 472EPJlsw

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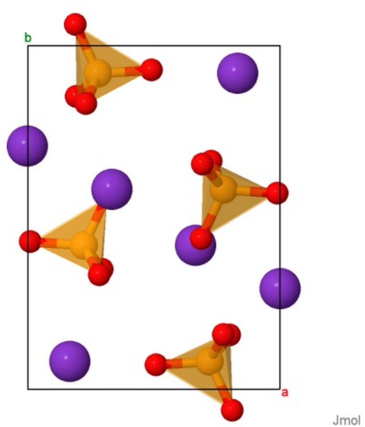

Incommensurately Modulated Structure of K_2SeO_4

Authors:
Yamada, N.; Ikeda, T.

Journal:
J. Phys. Soc. Jpn. 53 2555-2564 (1984)

DOI:
https://doi.org/10.1143/JPSJ.53.2555

Entry date: 2010-11-08 **B-IncStrDB ID:** 492E3r0gG

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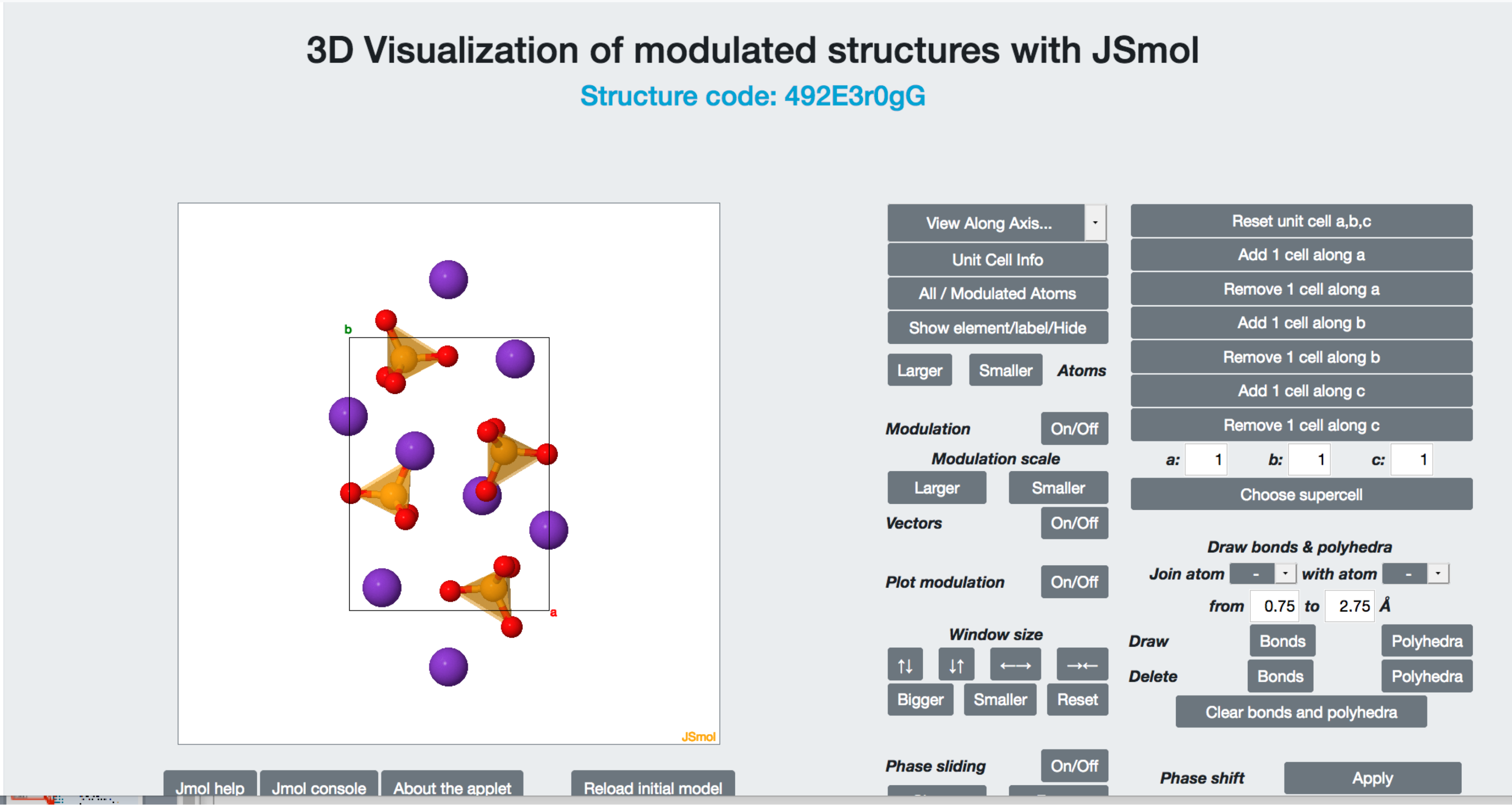
3D Visualization of modulated structures with JSmol
Structure code: 492E3r0gG
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On/Off
Plot modulation
On/Off
Window size
Bigger
Smaller
Reset
Phase sliding
On/Off
Reset unit cell a,b,c
Add 1 cell along a
Remove 1 cell along a
Add 1 cell along b
Remove 1 cell along b
Add 1 cell along c
Remove 1 cell along c
a: 1
b: 1
c: 1
Choose supercell
Draw bonds & polyhedra
Join atom - with atom -
from 0.75 to 2.75 Å
Draw Bonds Polyhedra
Delete Bonds Polyhedra
Clear bonds and polyhedra
Phase shift
Apply