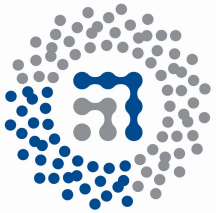

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Zientzia eta Teknologia Fakultatea
Facultad de Ciencia y Tecnología

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Universidad del País Vasco
Euskal Herriko Unibertsitatea

Magnetic Symmetry. Magnetic superspace groups

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TOPICAL REVIEW

Magnetic superspace groups and symmetry constraints in incommensurate magnetic phases

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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. We analyze in detail the relation between the description using superspace symmetry

Symmetry-Based Computational Tools for Magnetic Crystallography

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

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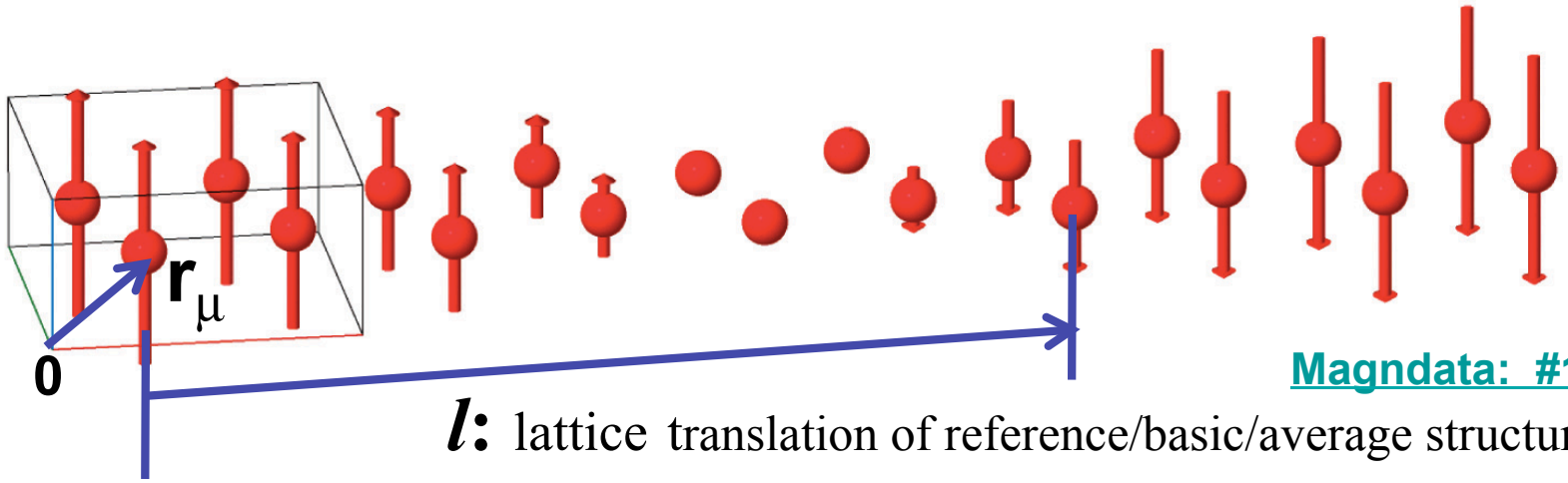
Keywords: magnetic structures database; *MAGNDATA*; incommensurate magnetic structures; magnetic superspace groups; Bilbao Crystallographic Server; superspace symmetry; irreducible representations.

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.

J. Appl. Cryst. (2016) 49, 1941-1956

Incommensurate modulated structures



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

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

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 $\mathbf{A}_\mu(x_4)$**

general anharmonic case

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

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

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

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

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

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

Description of an incommensurate modulated structure

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

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

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

modulation functions:

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

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

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

The superspace:

We can use the additional coordinate x4 of the modulations functions $A_\mu(x4)$ defining the modulation of the structure as an additional dimension and construct in this "superspace" a mathematical 4-dim lattice periodic "supercrystal" where the equation:

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

which defines the atomic values of the real crystal is equivalent to considering a certain section of this mathematical 4-dim construct.

The superspace concept is just a mathematical construct, which allows to interpret the equations characterizing incommensurate structures and 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: $\{ \{\mathbf{R}_i | \mathbf{t}_i , \tau_i\} , \{\mathbf{R'}_j | \mathbf{t}_j , \tau_j\} \}$

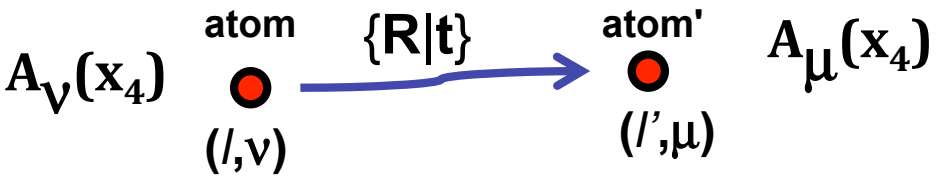
Incommensurate magnetic structures have an unambiguous magnetic point group symmetry

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

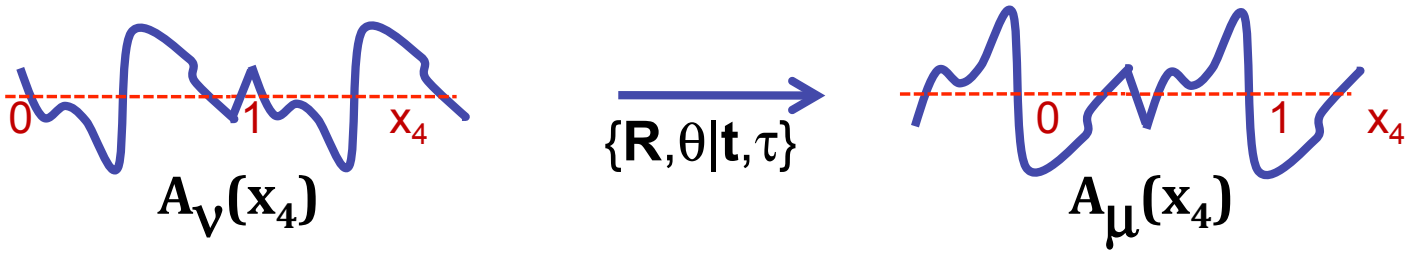
Symmetry relations between the modulation functions of different atoms in the basic unit cell due to a symmetry operation.

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:

$$\mathbf{M_\mu}(R_I x_4+\tau_o + \mathbf{H_R}.\mathbf{r_\nu}) = \theta \det(\mathbf{R})\mathbf{R} \,.\, \mathbf{M_\nu}(x_4)$$

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

If μ= ν ⟶ $\mathbf{M_\nu(x_4)}$ **symmetry constrained!**

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

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

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 also a translation $-\mathbf{k}.\mathbf{t}$ along x_4

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

$\mathbf{R_S}$ 4X4 matrix

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

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

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

ELSEVIER

Comptes Rendus Physique

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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

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

A recent review for the general case of several ncommensurate wave vectors

DOI: 10.1016/j.crhy.2019.07.004

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

superspace operation

$(-1|000,0)$: **-x1 –x2 –x3 –x4 +1**

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

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

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

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

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

Relation between the modulation of their magnetic moments

atom 2 atom 1

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

it chooses the origin along x4 on the inversion center

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

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

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

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

$\mathbf{M}^2(-x_4) = \mathbf{M}^1(x_4)$ Relation between the modulation of their magnetic moments

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

If atom 1= atom 2:

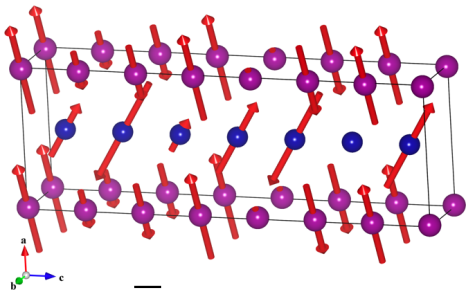
only cosine terms **all modulations In phase**

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

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

α= *x, y, z* **(collinear)**

A centrosymmetric incommensurate modulation



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

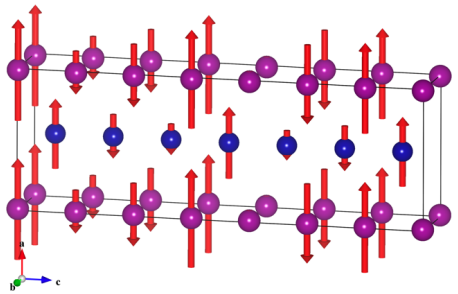
$\{1|0000\}$ **: x1 x2 x3 x4 +1**

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

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

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

A non-centrosymmetric incommensurate modulation



$P1\,1'(\alpha\beta\gamma)0s$

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

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

propagation vector:

***k*=(α,β,γ)**

Translation into FullProf k-vector parameters:

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

Superspace

atom v at cell L:

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

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

FullProf

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

Translation into FullProf k-vector parameters:

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

Superspace

atom v at cell L:

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

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

FullProf

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

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**

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

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

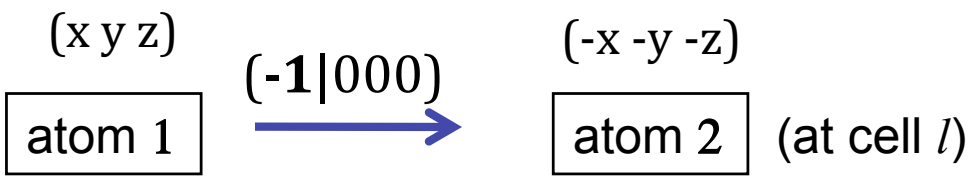
t must be such that μ atom is in zero cell !

Symmetry relations between the atomic modulations if described with FullProf parameterization

Example: inversion

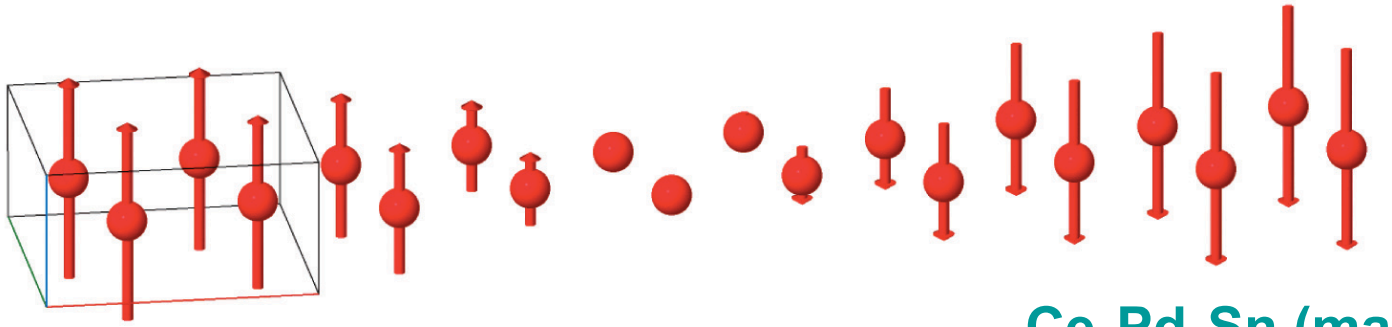
superspace operation

(-1|000,0): -x1 –x2 –x3 –x4 +1



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

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



Ce_2Pd_2Sn (magndata #1.1.9)

magCIF file

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_cell_length_b                    7.7620(5)
_cell_length_c                    3.9300(10)
_cell_angle_alpha                 90
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_cell_angle_gamma                 90

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3 -x1+1/2,x2+1/2,-x3,-x4+1/2,+1
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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_space_group_symop_magn_ssg_centering.algebraic
1 x1,x2,x3,x4,+1
2 x1,x2,x3,x4+1/2,-1
```

(1'| 0 0 0 ½)

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Sn1 Sn 0 0 0 1


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_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
```

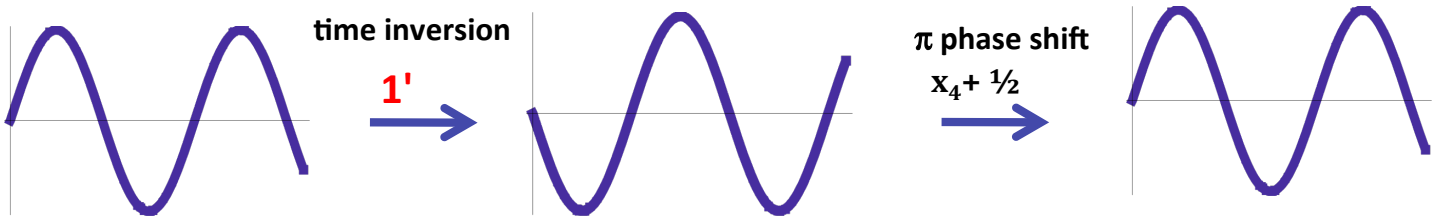
average moment cero (symmetry forced)

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) : $A_\mu(x_4+ ½) = 1' A_\mu(x_4)$

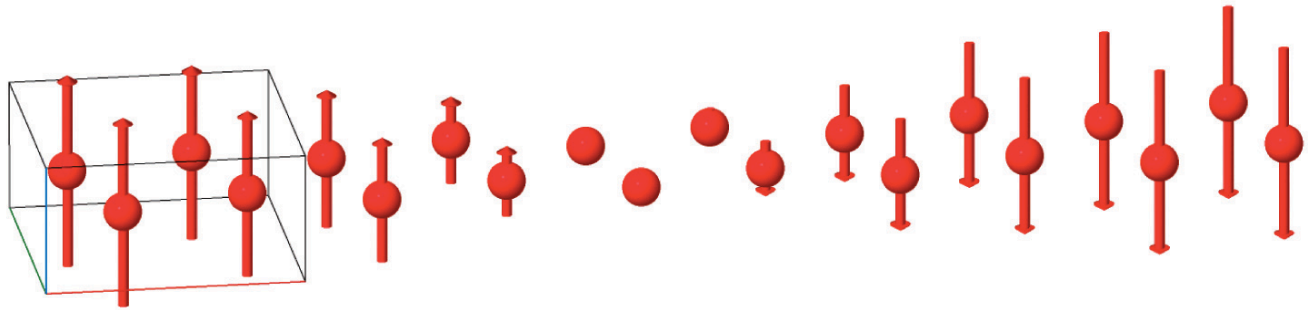
modulation of magnetic moments: $M_\mu(x_4+ ½) = - M_\mu(x_4)$ — odd-harmonics : 1k, 3k ,5k …

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)

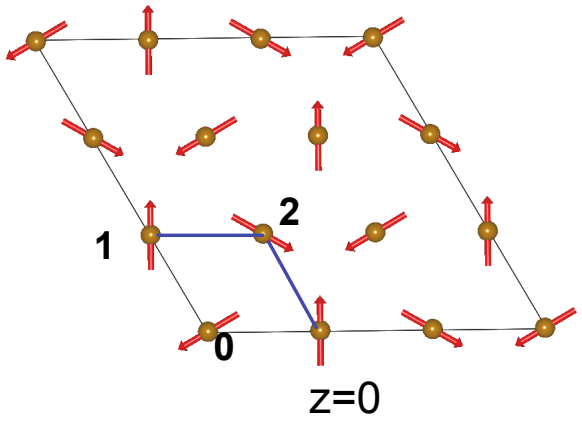
superspace symmetry constraint: 2 parameters
(same amplitude for the 4 atoms, but atoms related by inversion are not in phase but with opposite phases)

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	$M_z$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

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:



magndata 1.1.2

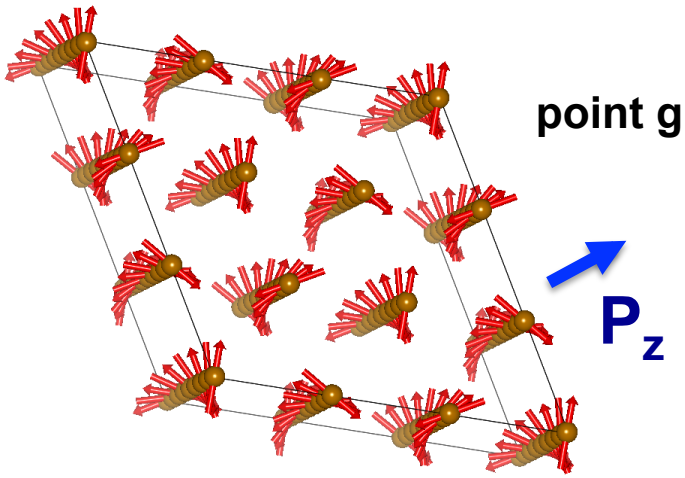
P-3 → **P31'(1/3 1/3 γ) ts** $\gamma \approx 0.458$

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

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

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

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



point group: 31'

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

magndata 1.1.33

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 }

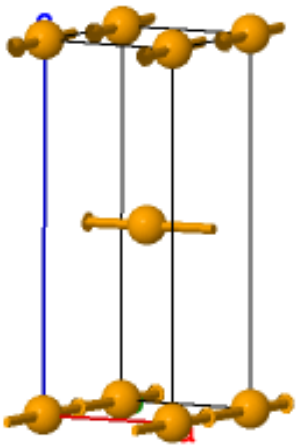
$$\mathbf{M}_\mu(R_I x_4+\tau_o + \mathbf{H}_R.\mathbf{r}_\nu) = \theta \det(\mathbf{R})\mathbf{R}\,.\,\mathbf{M}_\nu(x_4)$$

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

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

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

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



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

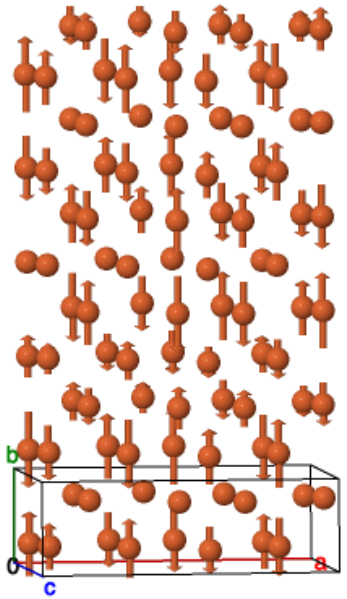
$M_{z\,sin1} = M_{z\,cos1} = 0$

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

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

$CaFe_4AS_3$ 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** β≈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

$$\mathbf{M}_{\mu}(-\mathbf{x}_4) = -\,\mathbf{m}_{010}\,.\,\mathbf{M}_{\mu}(\mathbf{x}_4)$$

Mx,Mz : Sin

My: Cos

Magnetic moment modulation parameters of symmetry independent atoms

Wave vector 1

in phase

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)

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

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

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

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 $\boldsymbol{H} = \boldsymbol{H}.\boldsymbol{R}_s$

Systematic Absence (Extinction rules)

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

Extinction rules: ("trivial" cases)

{1'| 0 0 0 0 }

(non-magnetic structures)

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

no condition

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

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)

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

Extinction rules:

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

k=(α,0,0) $\quad F_M(h00m) = e^{i\pi(h+m)}\ 2_x\ F_M(h00m) \rightarrow$ h+m= odd $\boldsymbol{F}_M$=(0,Fy,Fz)

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

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

$$F(H) = e^{i2\pi \mathbf{H}.\mathbf{t}_s} F(H.\ R_S)$$

$$F_M(H) = e^{i2\pi \mathbf{H}.\mathbf{t}_s}\, \theta\, det(R)\, \mathbf{R}.F_M(H.\ R_S).$$

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

X-centerings: avoiding complex descriptions of the modulations

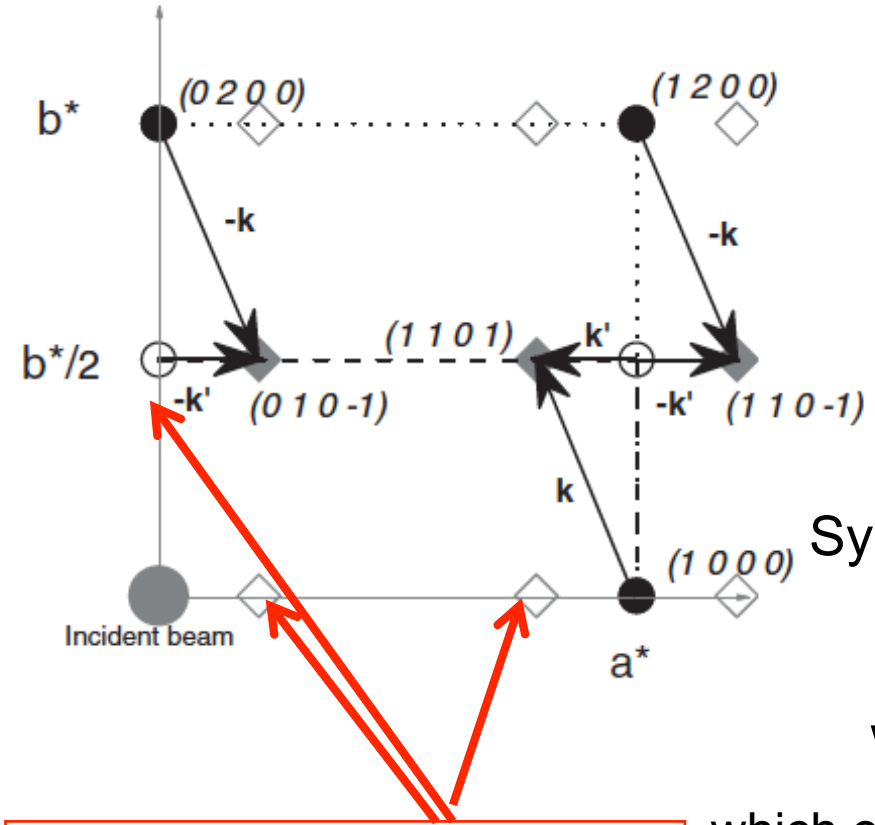
$$\mathbf{M}_\mu(R_I x_4+\tau_o + \mathbf{H}_R.\mathbf{r}_\nu) = \theta \det(\mathbf{R})\mathbf{R}\,.\,\mathbf{M}_\nu(x_4)$$

$\mathbf{H}_R \neq 0$

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):

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

Acta Cryst. (1980). A **36**, 399–408

Symmetry of Incommensurate Crystal Phases. I. Commensurate Basic Structures

BY A. JANNER AND T. JANSSEN

9. Magnetic superspace groups

As shown by Overhauser (1962, 1968), the ground state of an electron gas in a crystal does not necessarily have a uniform spin and charge distribution, but may show charge-density waves (CDW) and/or spin-density waves (SDW). We have already seen that CDW's may lead to an incommensurate crystal phase. The same can occur in magnetic crystals through SDW's. Actually, incommensurability was discovered first in

10. Magnetic superspace-group symmetry of Cr

Our analysis is based on those of Tsunoda, Mori, Kunitomi, Teraoka & Kanamori (1974), Eagen & Werner (1975) and Pynn, Press & Shapiro (1976). For

In the AF_2 phase **S**(**k**) is parallel to the z axis and left invariant [according to (72)] by $(4_z, 1)$ and $(m_x, 1)'$. Again, if the phase relation (84) holds, then it is also left invariant by $(m_z, \bar{1})$. In this case the magnetic superspace group for the AF_2 phase is

$$M_{AF_2} = P^{I_p 4/m m' m'}_{b1 \quad \bar{1} \; 1 \; 1}. \qquad (86)$$

Magnetic superspace groups were proposed from the very "beginning"

IUCr Ewald Prize to Janner and Janssen

Netherlands, have been awarded the tenth Ewald Prize, 'for the development of superspace crystallography and its application to the analysis of aperiodic crystals'. The award will be presented on August 5, 2014, at the opening ceremony of the IUCr congress in Montreal, Canada.

Aperiodic crystals are well ordered materials that lack translational lattice periodicity. One of the most famous examples of an aperiodic crystal is calaverite, a gold telluride mineral discovered in the gold mines of California. At the beginning of the 1900's, mineralogists had noticed that the morphology of calaverite's crystal faces did not follow the accepted empirical rule of crystal growth (Haüy's law of rational indices). The diffraction patterns of calaverite also departed from those of a perfect crystal, then defined as an ordered and periodic arrangement of atoms in space. De Wolff linked these spots to the absence of lattice periodicity in Na_2CO_3 crystals. He described these crystals as 'incommensurately modulated structures' - they are superimpositions of basic periodic structures, with a symmetry that can be described by a three-dimensional space group. Janner and Janssen, who were investigating the relationship between symmetry and physical properties in condensed matter, began collaboration with de Wolff. Together they conceived and developed the 'super space' theory, publishing the first complete list of (3+1)-dimensional super space groups in 1981. De Wolff, Janner and Janssen shared the 1998 Gregori Aminoff Prize awarded by the Royal Swedish Academy of Sciences.

T. W. J. M. (Ted) Janssen.

Aloysio Janner.

Janner and Janssen have dedicated more than thirty years to expanding the theoretical treatment of aperiodic crystals. They laid the groundwork for the development of methods to solve and refine the structure of aperiodic crystals, with applications from condensed matter physics to structural biology. Their superspace formalism also applies to the analysis of quasicrystals, a specific class of aperiodic crystals, described in 1982 by Schechtman who won the 2011 Nobel Prize in Chemistry for the discovery. The award of the Ewald Prize to Janner and Janssen highlights the tremendous impact that their work has had on the development of crystallography.

Superspace symmetry became rapidly the most efficient approach (software developed!) for the characterization of incommensurate modulated non-magnetic structures and is nowadays routinarily used

But in general the community dedicated to the analysis of magnetic structures remained aside from superspace groups until the last decade…

Why?

Representation analysis had been taken as a "superior" alternative to magnetic symmetry groups, and it included incommensurate cases

Acta Cryst. (1968). A**24**, 217

Representation Analysis of Magnetic Structures

BY E. F. BERTAUT

Abstract:

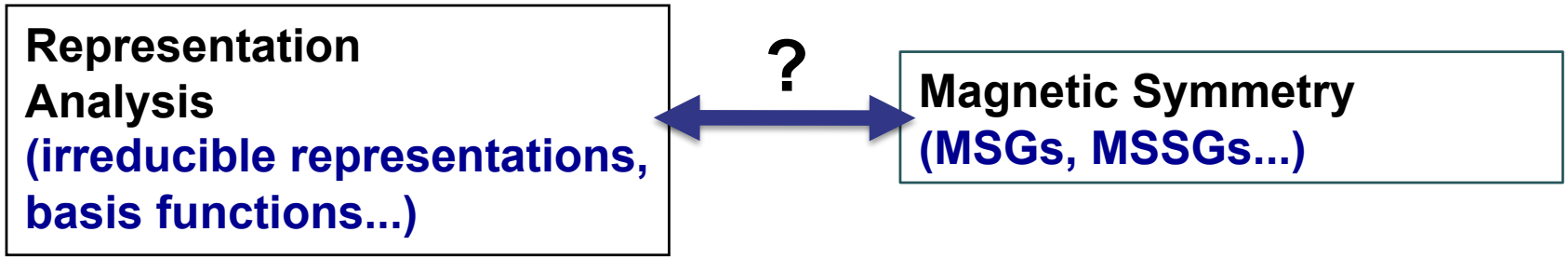
In the analysis of spin structures a 'natural' point of view looks for the set of symmetry operations which leave the magnetic structure invariant and has led to the development of magnetic or Shubnikov groups. A second point of view presented here simply asks for the transformation properties of a magnetic structure under the classical symmetry operations of the 230 conventional space groups and allows one to assign irreducible representations of the actual space group to all known magnetic structures. The superiority of representation theory over symmetry invariance under Shubnikov groups is already demonstrated by the fact proven here that the only invariant magnetic structures describable by magnetic groups belong to real one-dimensional representations of the 230 space groups. Representation theory on the other hand is richer because the number of representations is infinite, *i.e.* it can deal not only with magnetic structures belonging to one-dimensional real representations, but also with those belonging to one-dimensional complex and even to two-dimensional and three-dimensional representations associated with any **k** vector in or on the first Brillouin zone.

We generate from the transformation matrices of the spins a representation Γ of the space group

It includes incommensurate magnetic structures…

Representation analysis vs magnetic symmetry

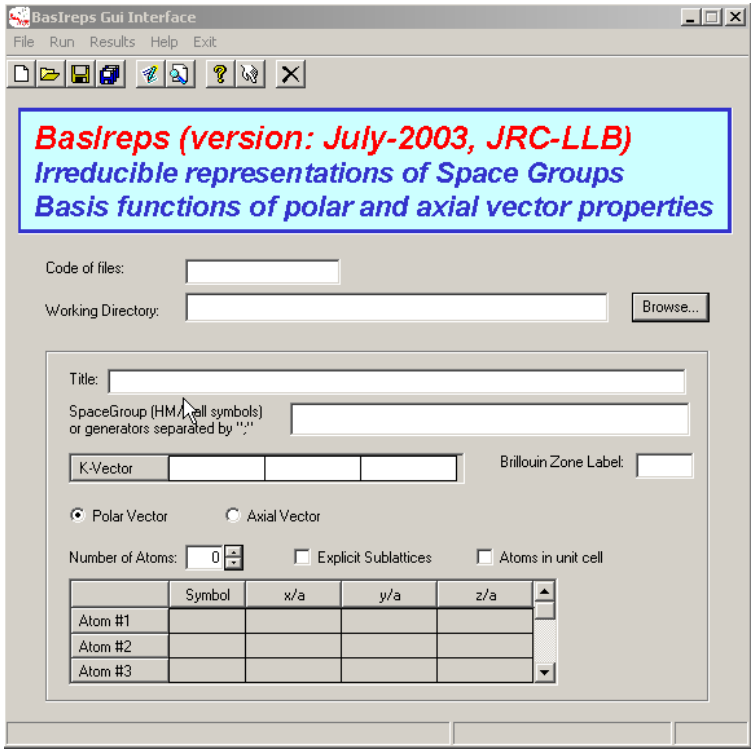
Commensurate magnetic structures:



They are not equivalent: in general several MSGs or MSSGs may be possible for the same irrep.

But computer tools for applying magnetic superspace groups were not developed until 2009-2010…

Computer programs for representation analysis were soon available:



from J. Rodriguez-Carvajal

SARA*h* Representational Analysis -
Performs the calculations of Representational Analysis. These allow the determination of atomic displacements or magnetic structures that can accompany a second-order phase transition. Output files includes a tailored summary with cut-and-paste tables written in LaTeX. (Win9x, 2000, Vista and Windows 7) [1]

from A.S. Wills

Once the representation approach became the most used method of analysis, most magnetic structures were determined and reported without the assignment of a space (or superspace) group symmetry,

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:**

$$M(\mu,\boldsymbol{l}) = \sum_{i=1,\ldots,N} S_i(\boldsymbol{k})\sigma_i(\mu)e^{-i\,2\,\pi\boldsymbol{k}.(\boldsymbol{l}+\boldsymbol{r}_\mu)} + S_i(-\boldsymbol{k})\sigma_i^*(\mu)e^{i\,2\,\pi\boldsymbol{k}.(\boldsymbol{l}+\boldsymbol{r}_\mu)}$$

Generalized invariance equation:

phase shift

N-dim small irrep

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

(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)

$\mathbf{T}[(\mathbf{R},\theta|\mathbf{t})]$: 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.

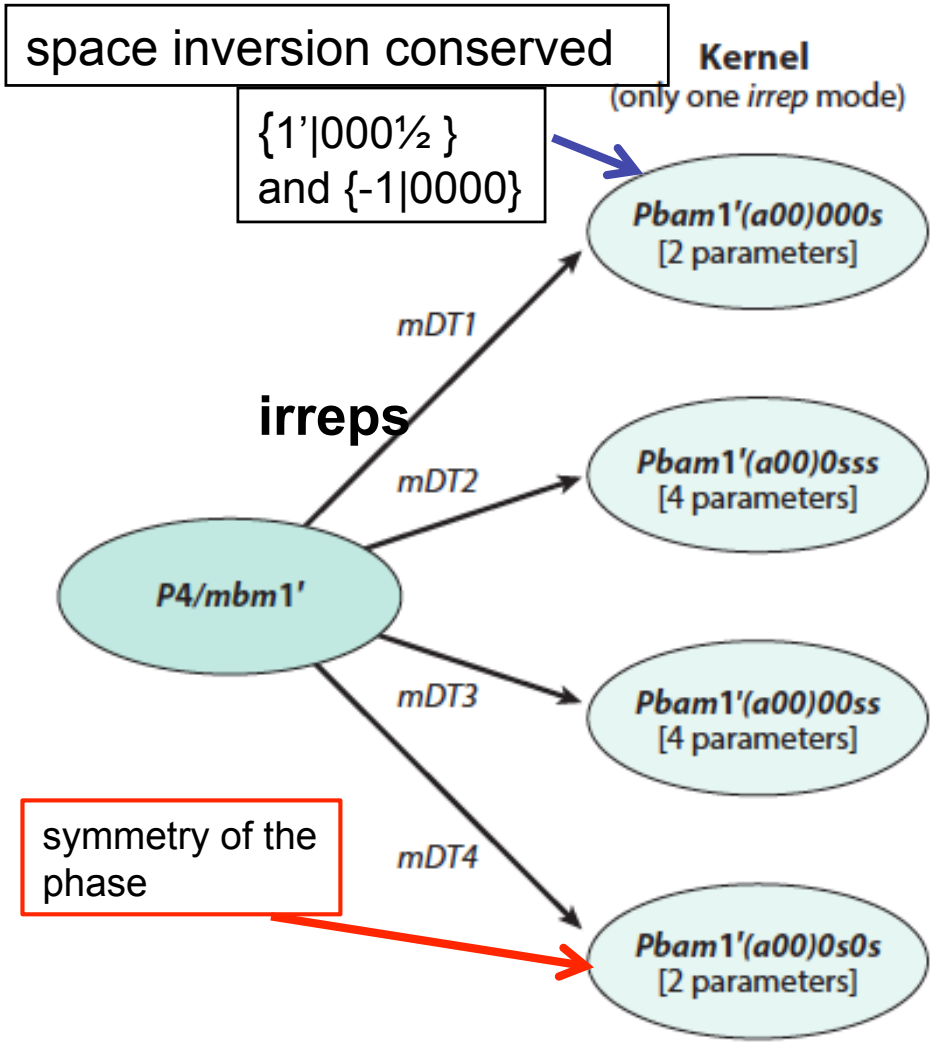
N =1 **one to one correspondance irrep – superspace group**

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:

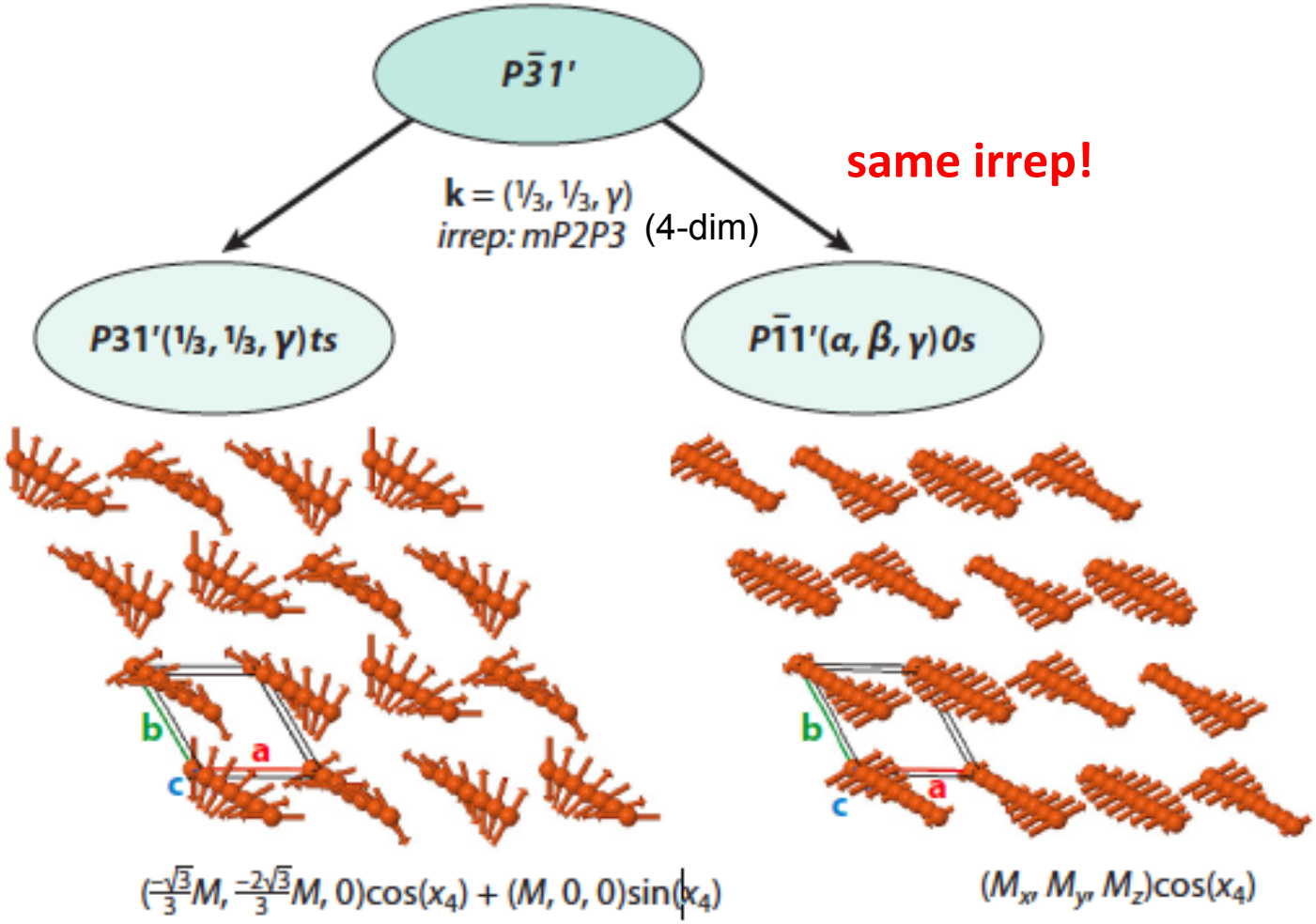
N >1

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

N-dim

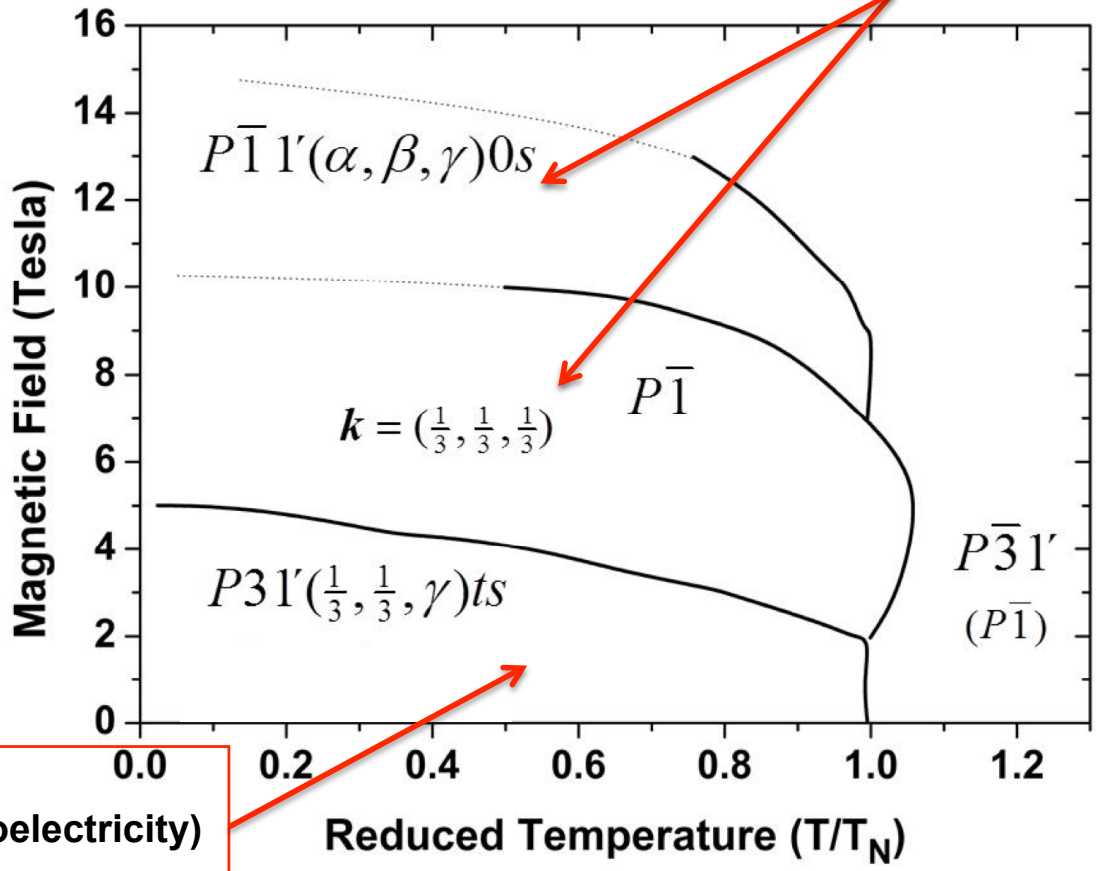
One irrep with N>1 ➔ several possible superspace groups

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

Polar symmetry: induced (improper ferroelectricity) Multiferroic phase

Phase diagram after Kenzelmann et al.

PRL 2007

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 http://jana.fzu.cz/ V. Petricek, Prague
Department of Structure Analysis
Cukrovarnicka 10
16253 Praha 6
Czech Republic

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

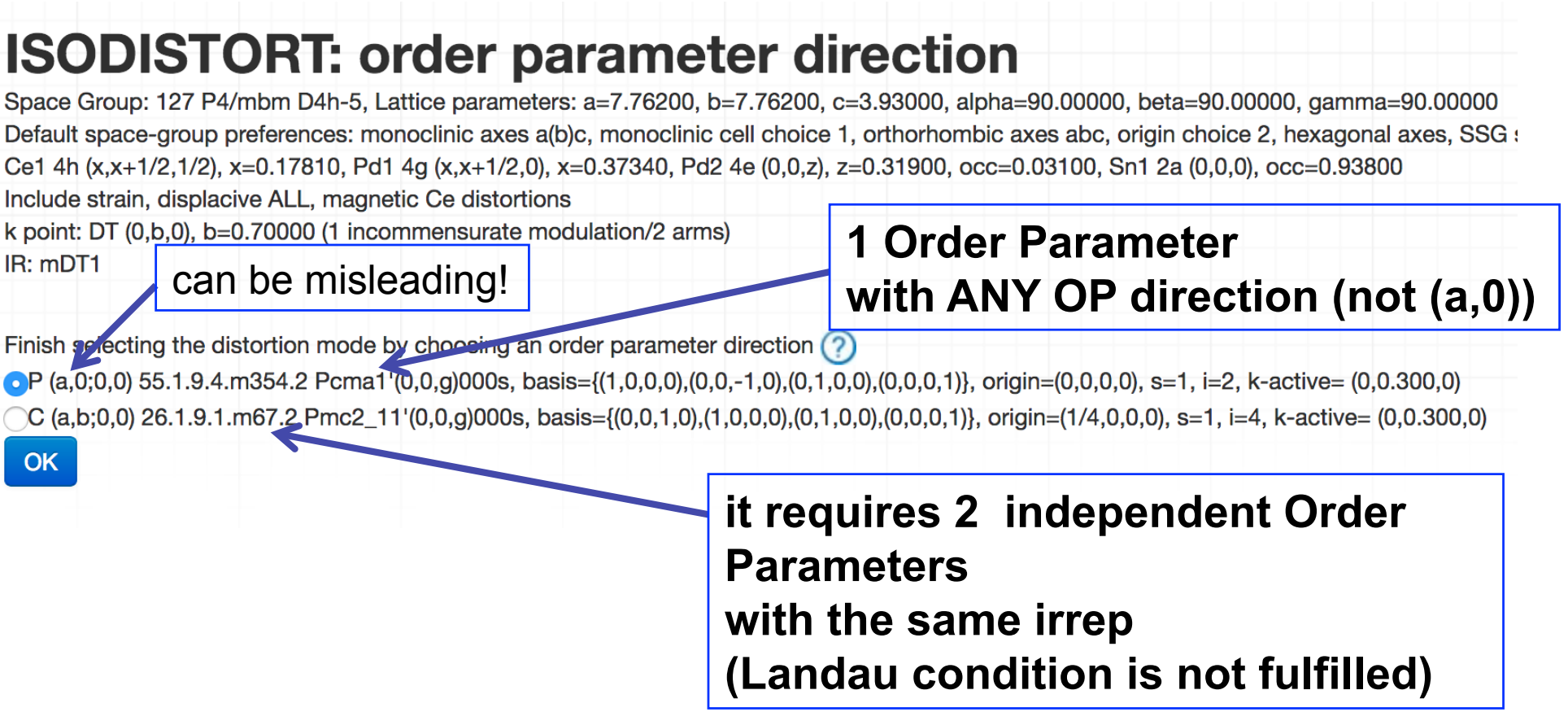
CRYSTALLOGRAPHIC COMPUTING SYSTEM FOR STANDARD AND MODULATED STRUCTURES

Vaclav Petricek, Michal Dusek & Lukas Palatinus

News

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

Beware when interpreting ISODISTORT output:



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

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
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MAGNEXT: Magnetic Systematic Absences

tinction rules for
any Shubnikov magnetic

e obtained introducing the
for this purpose at the
pted form of the structure

a set of generators in any

patible with a set of

r 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!

Magnetic Symmetry and Applications	
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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

Superspace magnetic symmetry tools and applications in the BCS :

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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

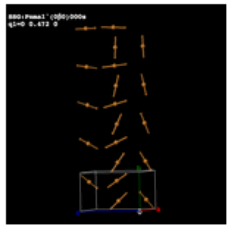
View Full Database

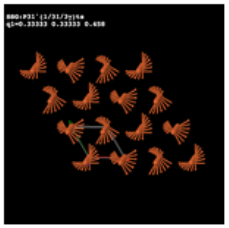
Element search (separate with space or comma): AND ○ OR Search

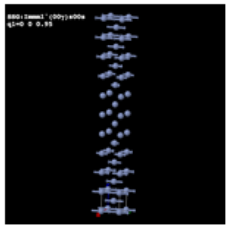
Enter the label of the structure: Submit

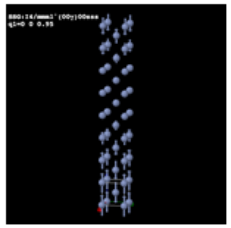
INCOMMENSURATE STRUCTURES

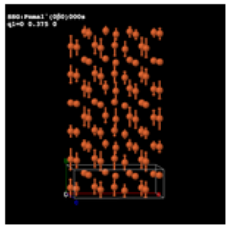
One propagation vector

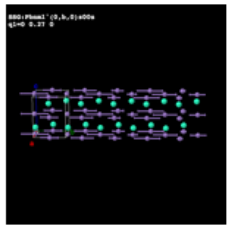

1.1.1 Cs_2CuCl_4


1.1.2 $RbFe(MoO_4)_2$

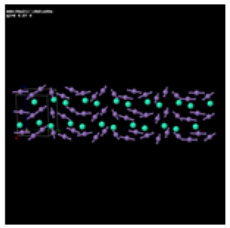

1.1.3 Cr

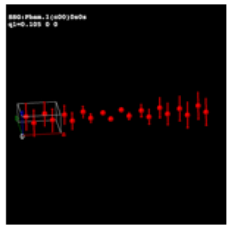

1.1.4 Cr

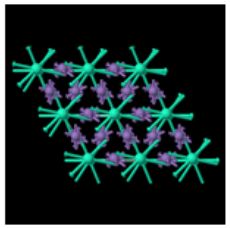

1.1.5 $CaFe_4As_3$

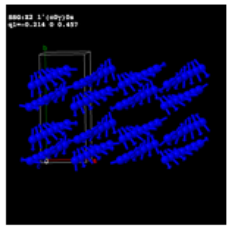

1.1.6 $TbMnO_3$

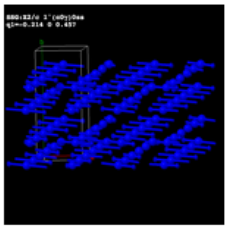

1.1.7 $TbMnO_3$

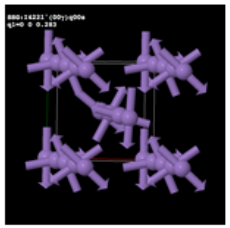

1.1.8 $TbMnO_3$

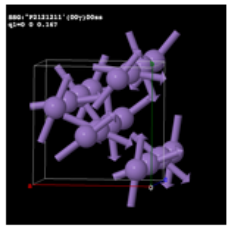

1.1.9 Ce_2Pd_2Sn

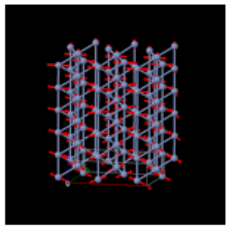

1.1.10 $DyMn_6Ge_6$


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.*

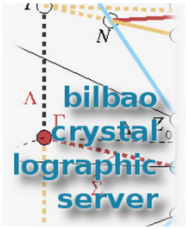
- *Representation analysis of magnetic structures is NOT in general equivalent to the use of magnetic symmetry (i.e. to give an irrep is not equivalent to give the magnetic space (superspace) group of the system)*

- *The best approach in incommensurate structures: to combine magnetic symmetry and representation analysis*

FCT/ZTF

bilbao crystallographic server

UPV EHU



Crystallography Online: Workshop on the use of the structural and magnetic tools of the Bilbao Crystallographic Server
September 2021, Leioa (Spain)

Forthcoming schools and workshops

News:

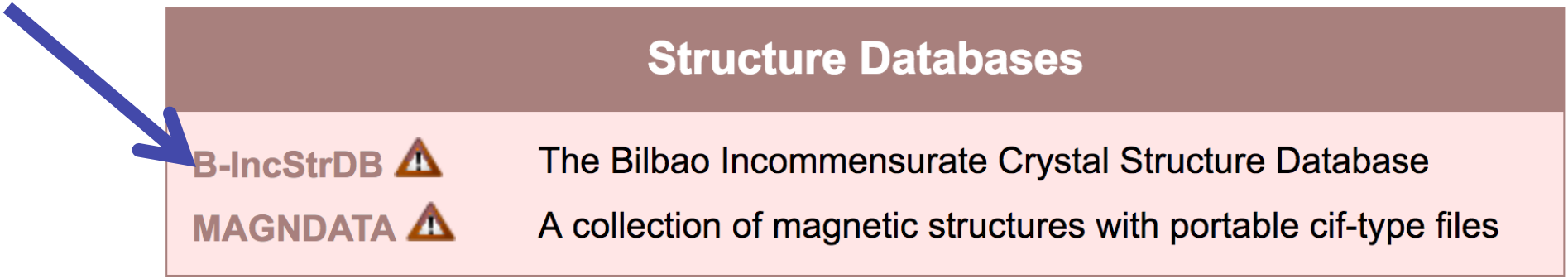
- **New Article in Nature**
  10/2020: Xu *et al.* "High-throughput calculations of magnetic topological materials" *Nature* (2020) **586**, 702-707.
- New programs: **MBANDREP**, **COREPRESENTATIONS**, **COREPRESENTATIONS PG**, **MCOMPREL**, **MSITESYM**, **MKVEC**, **Check Topological Magnetic Mat**
  10/2020: new tools in the sections "Magnetic Symmetry and Applications" and "Representations and Applications". **More info**

- Space-group symmetry
- Magnetic Symmetry and Applications
- Group-Subgroup Relations of Space Groups
- Representations and Applications
- Solid State Theory Applications
- Structure Utilities
- Topological Quantum Chemistry
- Subperiodic Groups: Layer, Rod and Frieze Groups
- Structure Databases
- Raman and Hyper-Raman scattering
- Point-group symmetry

Quick access to some tables

- Space Groups
- Plane Groups
- Layer Groups
- Rod Groups
- Frieze Groups
- 2D Point Groups
- 3D Point Groups
- Magnetic Space Groups

Databases



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).

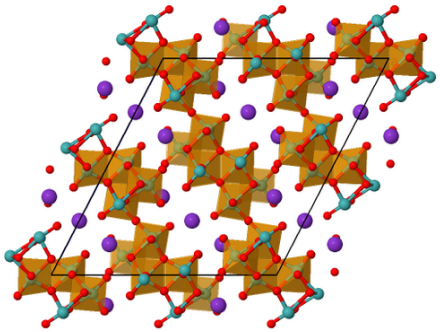
Explore the database ›

B-IncStrDB: The Bilbao Incommensurate Crystal Structure Database :

Author name | = | Search | + | Search | ?

Order by: Date: first submitted

Search results: 255



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

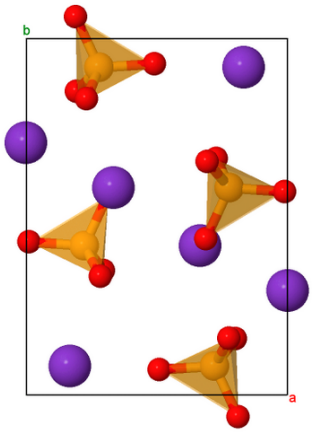
View entry | Download CIF | Open in JSmol

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:** 472EPJIsw



Incommensurately Modulated Structure of K_2SeO_4

View entry | Download CIF | Open in JSmol

Authors:
Yamada, N.; Ikeda, T.

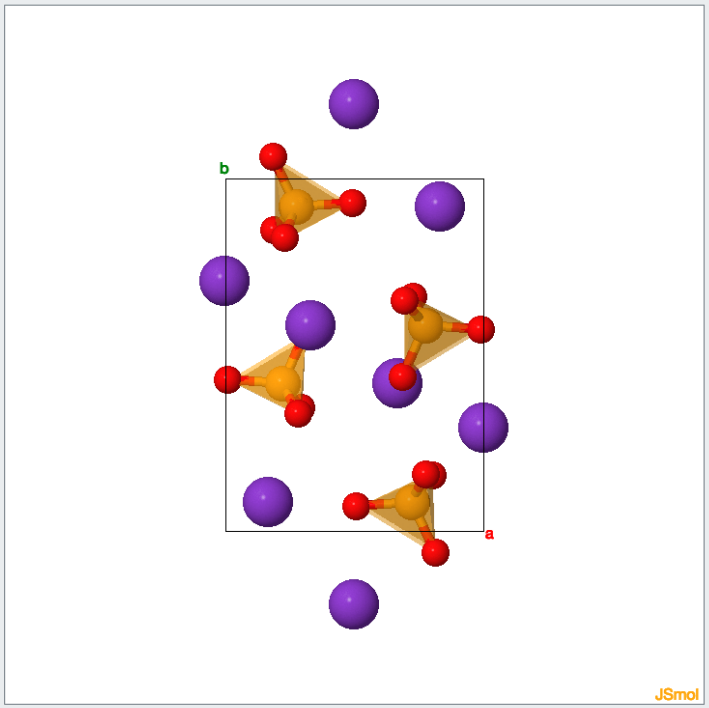
Journal:
J. Phys. Soc. Jpn. **53** 2555-2564 (1984)

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

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

3D Visualization of modulated structures with JSmol

Structure code: 492E3r0gG



View Along Axis...

Unit Cell Info

All / Modulated Atoms

Show element/label/Hide

Larger Smaller *Atoms*

Modulation On/Off

Modulation scale

Larger Smaller

Vectors 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

Jmol help Jmol console About the applet Reload initial model