Introduction to Magnetic space groups (Shubnikov groups)

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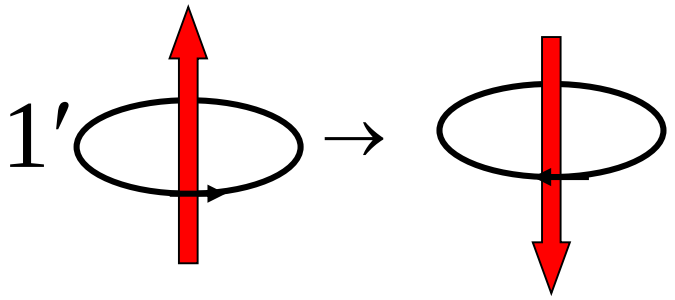
Magnetic moments as axial vectors

The magnetic moment (shortly called "spin") of an atom can be considered as an "axial vector". It may be associated to a "current loop". The behaviour of elementary current loops under symmetry operators can be deduced from the behaviour of the "velocity" vector that is a "polar" vector.

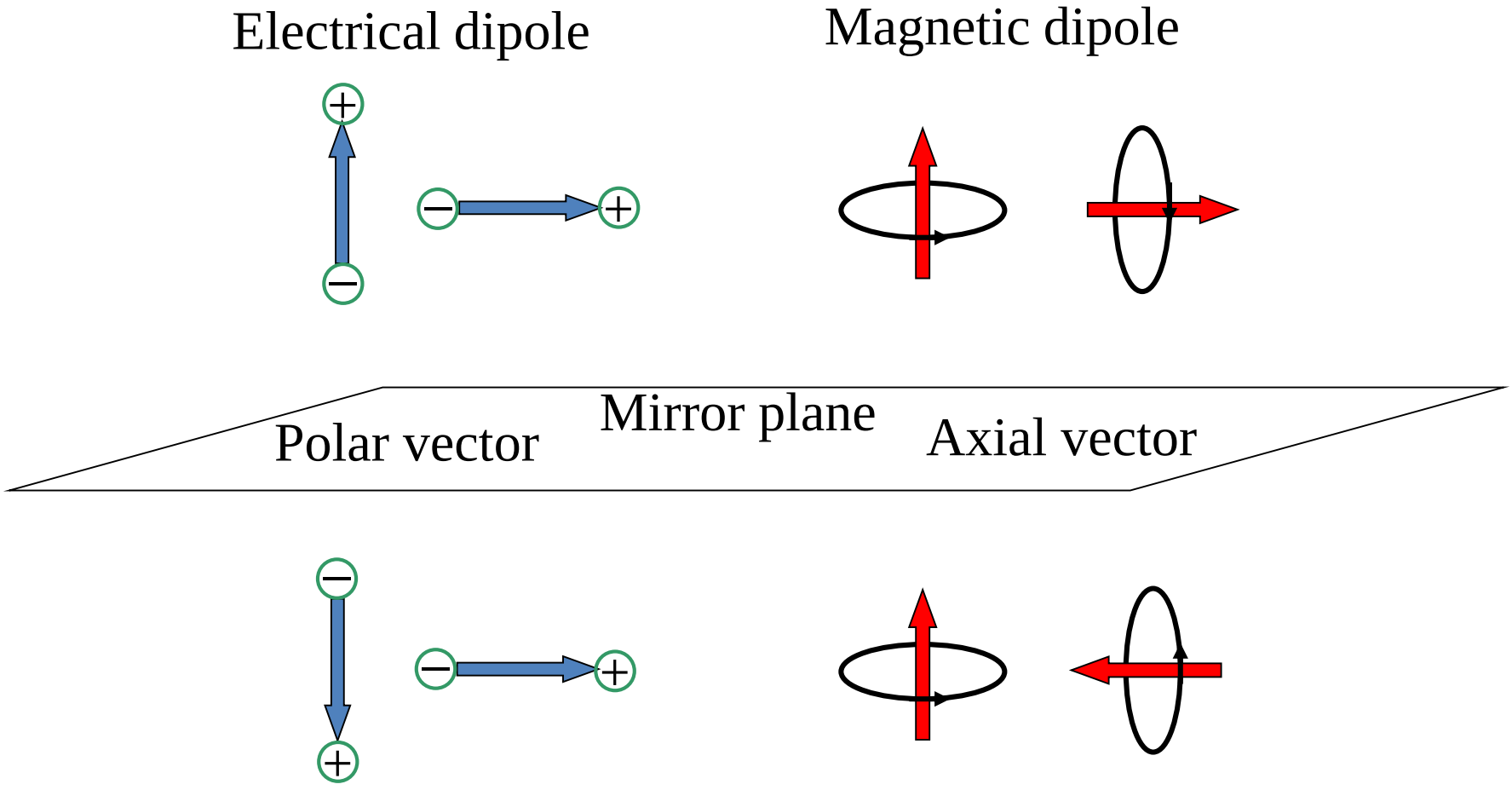
Time reversal = spin reversal

(change the sense of the current)



A new operator can be introduced and noted as 1′, it flips the magnetic moment. This operator is called "spin reversal" operator or classical "time reversal" operator

Magnetic moments as axial vectors



$$\mathbf{m}_j' = g\,\mathbf{m}_j = \det(h)\,\delta h\,\mathbf{m}_j$$

Shubnikov Magnetic Space Groups

The group $\mathbf{R} = \{1, 1'\}$ is called the time/spin reversal group Magnetic point and space groups can be obtained as outer direct product of point and space groups with $\mathbf{R}$. The operators of a magnetic group are called "primed" if they result from the combination of the crystallographic operator with the element $1'$ of $\mathbf{R}$. Those combined with 1 are called "unprimed"

A general operator $g = \{h|\mathbf{t}_h+\mathbf{n}\}$ acting on an atom $\mathbf{r}_j$ in the cell at the origin (zero-cell) having a magnetic moment $\mathbf{m}_j$ is transformed as follows:

$$\mathbf{r}_j' = g\,\mathbf{r}_j = \{h\,|\,\mathbf{t}_h + \mathbf{n}\}\mathbf{r}_j = h\mathbf{r}_j + \mathbf{t}_h + \mathbf{n} = \mathbf{r}_i + \mathbf{a}_{gj}$$

$$\mathbf{m}_j' = g\,\mathbf{m}_j = \det(h)\,\delta h\,\mathbf{m}_j$$

The "signature" is $\delta = 1$ for unprimed elements
and $\delta = -1$ for primed elements

Shubnikov Magnetic Space Groups

The position of an arbitrary atom in the crystal described by a magnetic space group can be deduced using the following formula:

Atom positions in a crystal:

$$\mathbf{R}_{ljs} = \mathbf{R}_l + \mathbf{r}_{js} = \mathbf{R}_l + \{h \mid \mathbf{t}_h\}_s \mathbf{r}_j = l_1\mathbf{a}+l_2\mathbf{b}+l_3\mathbf{c} + \{h \mid \mathbf{t}_h\}_s (x_j\mathbf{a}+y_j\mathbf{b}+z_j\mathbf{c})$$

$$\mathbf{R}_{ljs} = \begin{pmatrix}\mathbf{a} & \mathbf{b} & \mathbf{c}\end{pmatrix}\begin{pmatrix} l_1 \\ l_2 \\ l_3 \end{pmatrix} + \begin{pmatrix}\mathbf{a} & \mathbf{b} & \mathbf{c}\end{pmatrix}\begin{pmatrix} h^s_{11} & h^s_{12} & h^s_{13} \\ h^s_{21} & h^s_{22} & h^s_{23} \\ h^s_{31} & h^s_{32} & h^s_{33} \end{pmatrix}\begin{pmatrix} x_j \\ y_j \\ z_j \end{pmatrix} + \begin{pmatrix}\mathbf{a} & \mathbf{b} & \mathbf{c}\end{pmatrix}\begin{pmatrix} t^s_1 \\ t^s_3 \\ t^s_3 \end{pmatrix}$$

$$\mathbf{R}_{ljs} = \begin{pmatrix}\mathbf{a} & \mathbf{b} & \mathbf{c}\end{pmatrix}\left\{\begin{pmatrix} l_1 + t^s_1 \\ l_2 + t^s_2 \\ l_3 + t^s_3 \end{pmatrix} + \begin{pmatrix} h^s_{11} & h^s_{12} & h^s_{13} \\ h^s_{21} & h^s_{22} & h^s_{23} \\ h^s_{31} & h^s_{32} & h^s_{33} \end{pmatrix}\begin{pmatrix} x_j \\ y_j \\ z_j \end{pmatrix}\right\}$$

l : index of a direct lattice point (origin of an arbitrary unit cell)
j : index for a Wyckoff site (orbit)
s: index of a sublattice of the j site

For a primitive basis the indices l_i are integers. For a centred cell they can also be rational numbers. In general, the fractional coordinates giving the atom positions in the asymmetric unit are real numbers.

Shubnikov Magnetic Space Groups

The magnetic moment of an arbitrary magnetic atom in the crystal can be deduced

Magnetic moment of atoms in a crystal with a commensurate magnetic structure:

$$\mathbf{m}_{ljs} = \mathbf{m}_{js} \quad (\textit{the magnetic unit cell is used}\,!)$$

$$\mathbf{m}_{ljs} = \det(h)\delta\begin{pmatrix}\mathbf{e}_x & \mathbf{e}_y & \mathbf{e}_z\end{pmatrix}\begin{pmatrix}h^s_{11} & h^s_{12} & h^s_{13}\\ h^s_{21} & h^s_{22} & h^s_{23}\\ h^s_{31} & h^s_{32} & h^s_{33}\end{pmatrix}\begin{pmatrix}m_{xj}\\ m_{yj}\\ m_{zj}\end{pmatrix}$$

$\det(h)$: determinant of the matrix corresponding to the operator $g=\{h|\mathbf{t}_h\}$
δ : signature of the operator g, $\delta=1$ when g **is not associated** with time reversal, and $\delta=-1$ when g **is associated** with time reversal: g is primed.

Example from ITC: Space groups

International Tables of Crystallography (Volume A).
Example: group number 46, *Ima*2

Can be interpreted as a "representation" of the symmetry operations

Site symmetry and positions of space group *Ima*2

			(0, 0, 0)+	(½, ½, ½)+		
8	*c*	1	(1) *x*, *y*, *z*	(2) -*x*, -*y*, *z*	(3) *x*+½, -*y*, *z*	(4) -*x*+½, *y*, *z*
4	*b*	*m* . .	¼, *y*, *z*		¼, -*y*, *z*	
4	*a*	. . 2	0, 0, *z*		½, 0, *z*	

T- coset representatives

Symmetry operations

For (0, 0, 0)+ set

(1) 1 (2) 2 0, 0, *z* (3) *a* *x*, 0, *z* (4) *m* ¼, y, z

For (½ , ½ , ½)+ set

(1) *t*(½ , ½ , ½) (2) 2(0,0, ½) ¼,¼,*z* (3) *c* *x*, ¼,*z* (4) *n*(0, ½ , ½) 0, y, z

Maximal non-isomorphic subgroups of *Ima*2

I [2] *I* 1 1 2 (*C* 2) (1; 2)+
[2] *I* 1 *a* 1 (*C c*) (1; 3)+
[2] *I m* 1 1 (*C m*) (1; 4)+

IIa [2] *P m a* 2 1; 2; 3; 4
[2] *P n c* 2 1; 2; (3; 4) + (½ , ½ , ½)
[2] *P n a* 2_1 1; 3; (2; 4) + (½ , ½ , ½)
[2] *P m c* 2_1 1; 4; (2; 3) + (½ , ½ , ½)

IIb *none*

Magnetic space groups

Whatever crystallographic magnetic group, **M**, can be obtained as a subgroup of the outer direct product of **R** by the crystallographic group **G**: $\mathbf{M} \subset \mathbf{G} \otimes \mathbf{R}$.

The group **G** is always a magnetic group ("colourless")
Paramagnetic ("grey") groups are of the form: $\mathbf{P}=\mathbf{G}+\mathbf{G}1'$.

Nontrivial groups ("black-white" groups)
Constructive lemma: *the magnetic groups derived from the crystallographic group* **G** *can be constructed considering the index 2 subgroups* **H** *of* **G** *as constituting the "unprimed" elements and the rest of operators,* $\mathbf{G} - \mathbf{H}$, *those that are multiplied by the time reversal operator.*

The magnetic group is then related to the subgroup $\mathbf{H} \subset \mathbf{G}$ (of index 2) by the expression: $\mathbf{M} = \mathbf{H} + (\mathbf{G} - \mathbf{H})\, 1'$.

This is valid for all kind of groups: point groups, translation groups and space groups. This is a consequence of "primed" x "primed" = "unprimed"

Example: construction of magnetic point groups

ITA: maximal subgroups and minimal super-groups of point groups

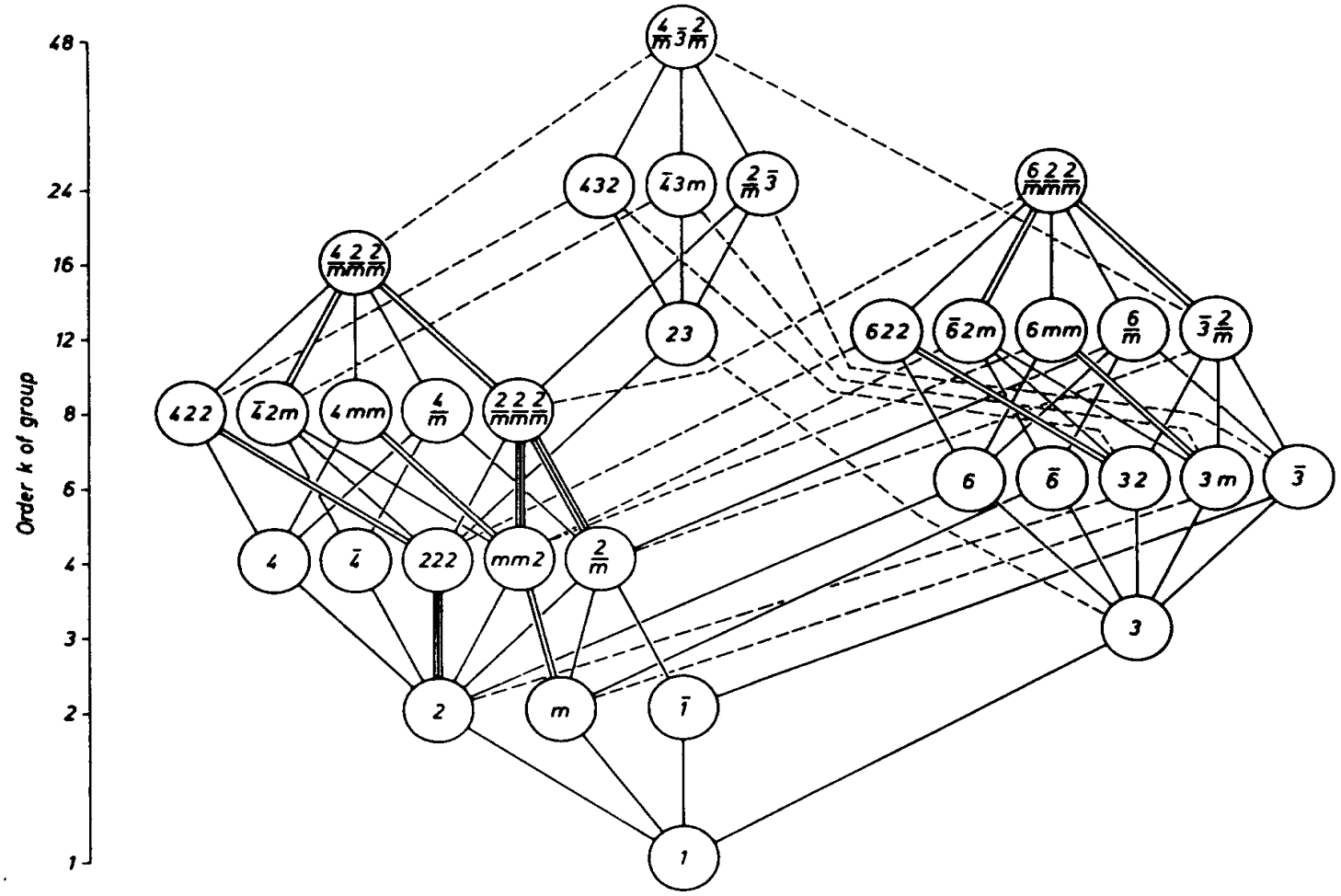


Fig. 10.3.2. Maximal subgroups and minimal supergroups of the three-dimensional crystallographic point groups. Solid lines indicate maximal normal subgroups; double or triple solid lines mean that there are two or three maximal normal subgroups with the same symbol. Dashed lines refer to sets of maximal conjugate subgroups. The group orders are given on the left. Full Hermann–Mauguin symbols are used.

Example: construction of magnetic point groups

It is easy to apply the constructive lemma to the crystallographic point groups and deduce that we have **32** trivial magnetic point groups (identical to the 32 crystallographic point groups), **32** paramagnetic groups, and **<3+3>+ (5)+(13+5)+ [5]+ [13+8]+3=58** black-white point groups.

This is obtained by counting the number of lines connecting groups with subgroups of index 2 in the previous figure.

The symbols <>, (), [] surrounding the figures refers to cubic, hexagonal-trigonal and tetragonal-orthorhombic groups; the absence of parenthesis for the last figure refers to monoclinic-triclinic point groups.

Example: magnetic point groups from 4/m

Consider the point group **G**=4/*m* of order 8. Its subgroups of index 2 are $\mathbf{H}_1$=4, $\mathbf{H}_2$= and $\mathbf{H}_3$=2/m. There are then four magnetic point groups derived from **G**, they have the following elements:

$$\mathbf{G} = 4/m = \{1, 4_z^+, 2_z, 4_z^-, \bar{1}, m_z, \overline{4_z^+}, \overline{4_z^-}\}$$

$$\mathbf{H}_1 = 4 = \{1, 4_z^+, 2_z, 4_z^-\}$$

$$\mathbf{H}_2 = \bar{4} = \{1, \overline{4_z^+}, 2_z, \overline{4_z^-}\}$$

$$\mathbf{H}_3 = 2/m = \{1, 2_z, \bar{1}, m_z\}$$

$$\mathbf{M}_0 = \mathbf{G} = 4/m$$

$$\mathbf{M}_1 = \mathbf{H}_1 + (\mathbf{G} - \mathbf{H}_1)1' = \{1, 4_z^+, 2_z, 4_z^-, \bar{1}', m_z', \overline{4_z^+}', \overline{4_z^-}'\} = 4/m'$$

$$\mathbf{M}_2 = \mathbf{H}_2 + (\mathbf{G} - \mathbf{H}_2)1' = \{1, 4_z^+', 2_z, 4_z^-', \bar{1}', m_z', \overline{4_z^+}, \overline{4_z^-}\} = 4'/m'$$

$$\mathbf{M}_3 = \mathbf{H}_3 + (\mathbf{G} - \mathbf{H}_3)1' = \{1, 4_z^+', 2_z, 4_z^-', \bar{1}, m_z, \overline{4_z^+}', \overline{4_z^-}'\} = 4'/m$$

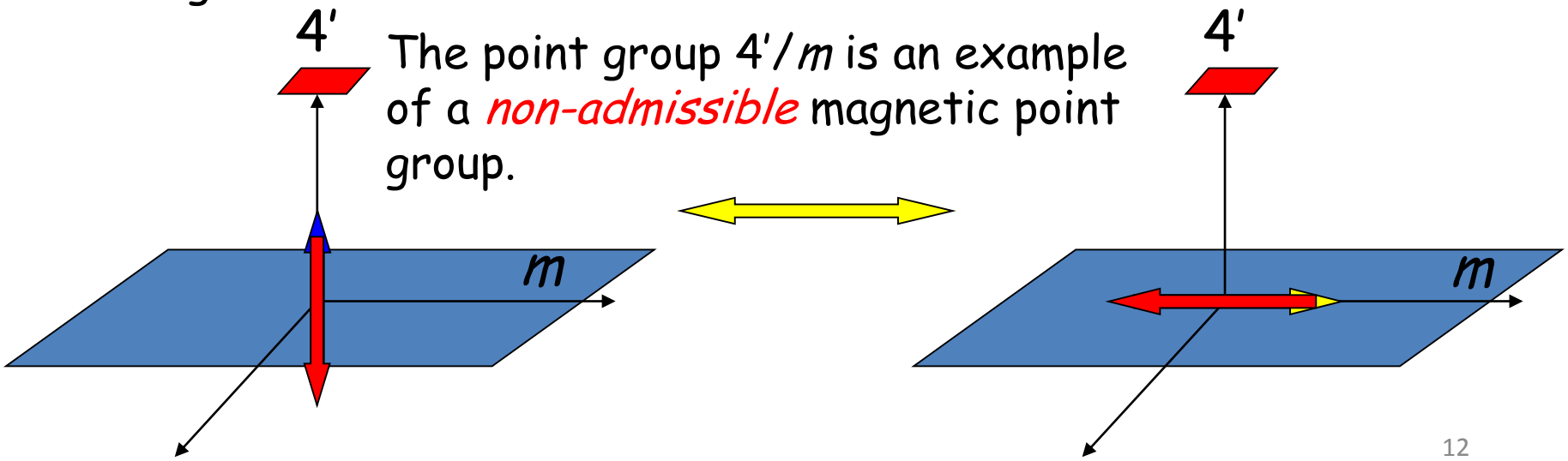
Admissible point groups

In magnetically ordered systems, the magnetic point group of a magnetic atom cannot be one of the paramagnetic groups. Moreover many of the colourless and black-white magnetic point groups cannot be realized in ordered system.

Let us consider the magnetic point group **M**3=4′/*m*.

Action of 4′ when the spin is along its axis

Action of *m* when the spin is within it



The point group 4′/*m* is an example of a *non-admissible* magnetic point group.

Admissible point groups

Admissible magnetic point groups					Admissible spin direction	
1					Any direction	[1]
2′	2′/*m*′	*m*′*m*2′			Perpendicular to the 2-fold axis	[3]
m′					Any direction within the plane	[1]
m					Perpendicular to the plane	[1]
m′*m*′*m*					Perpendicular to the unprimed plane	[1]
2′2′2					Along the unprimed axis	[1]
2	2/*m*	*m*′*m*′2			Along the 2-fold axis	[3]
4		4/*m*	42′2′		Along the four-fold axis	[3]
4*m*′*m*′		2*m*′		4/*mm*′*m*′	Along the four-fold axis	[3]
3		32′	3*m*′	*m*′	Along the three-fold axis	[4]
6		6/*m*	62′2′		Along the six-fold axis	[3]
6*m*′*m*′		*m*′2′		6/*mm*′*m*′	Along the six-fold axis	[3]

27 admissible magnetic point groups!

Magnetic Lattices

For primitive Bravais lattices integer linear combinations of the three vectors $\{\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3\}$ generate the whole lattice:

$$\mathbf{T}_P = \{\mathbf{t} \mid \mathbf{t} = l_1\,\mathbf{a}_1 + l_2\,\mathbf{a}_2 + l_3\,\mathbf{a}_3,\ l_i \in \mathbb{Z}\}$$

If we consider centred lattices the whole group is generated not only by the integer linear combinations of the basis vector representing the conventional cell but by adding centring vectors $\mathbf{t}_{cn}$ (n=1… m):

$$\mathbf{T}_C = \{\mathbf{t} \mid \mathbf{t} = l_1\,\mathbf{a}_1 + l_2\,\mathbf{a}_2 + l_3\,\mathbf{a}_3 + n_1\,\mathbf{t}_{c1} + n_2\,\mathbf{t}_{c2} + \ldots n_{cm}\,\mathbf{t}_{cm};\ \ l_i \in \mathbb{Z},\ n_i \in \{0,1\}\}$$

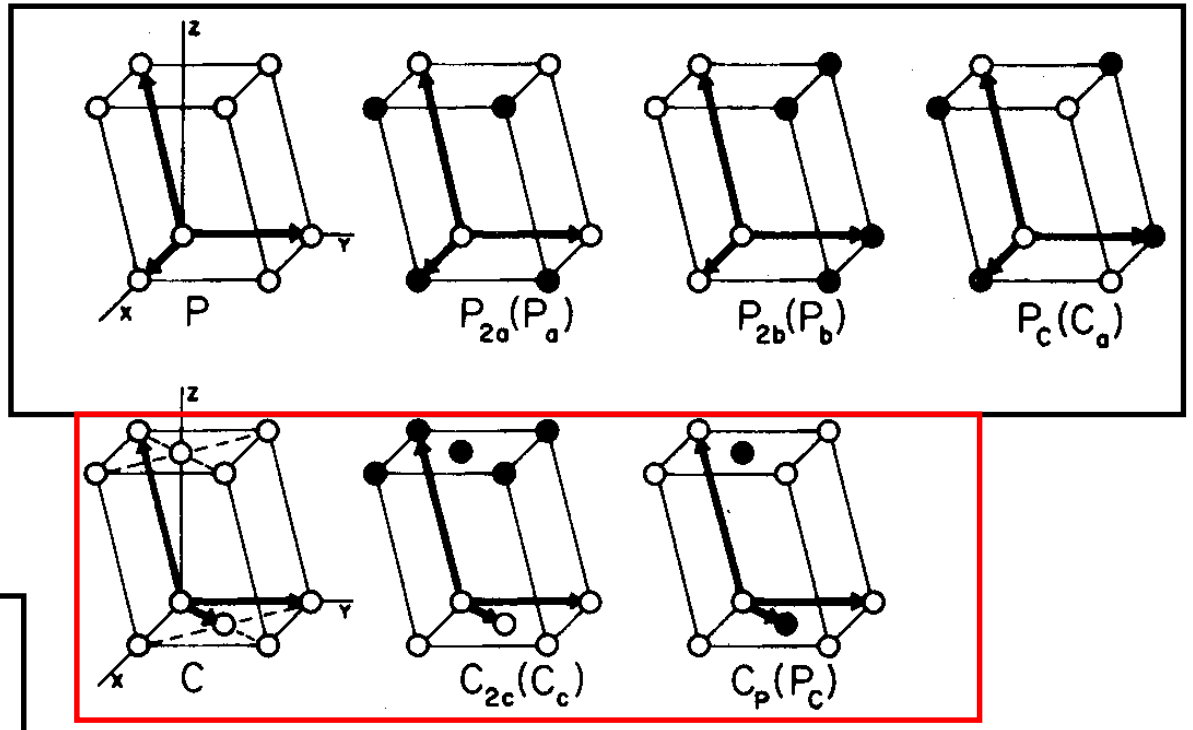
The centring vectors have rational components when referred to the conventional basis: $\mathbf{t}_{ci} = q_{1i}\,\mathbf{a}_1 + q_{2i}\,\mathbf{a}_2 + q_{3i}\,\mathbf{a}_3$ $(q_i \in \mathbb{Q})$

A subgroup, of index 2, of the translation group can be obtained just by suppressing half the translations, for instance if we take $l_1 = 2n$ we obtain a lattice **L** that is described with a unit cell with $\mathbf{a}_1' = 2\mathbf{a}_1$.

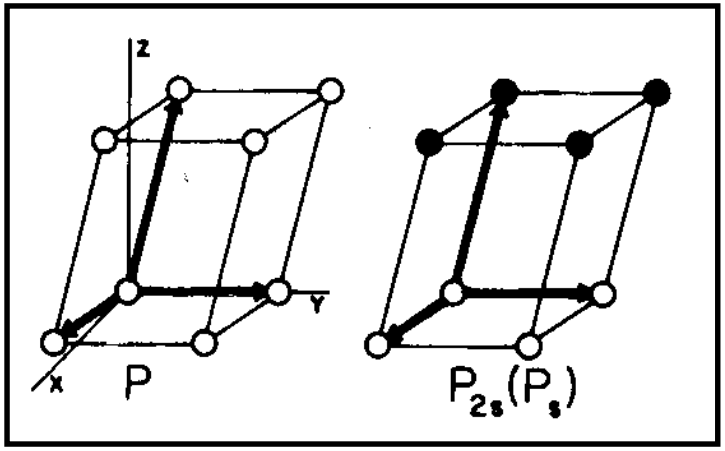
This lattice is generates a subgroup of index 2 of **T** ($\mathbf{L} \subset \mathbf{T}$, [i]=n(**T**)/ n(**L**)=2), the lost translations (**T**-**L**) can be associated with time reversal for constructing the magnetic lattice: $\mathbf{M_L} = \mathbf{L} + (\mathbf{T}\text{-}\mathbf{L})1'$.

Magnetic Lattices

Open circles: Translations
Black circles: Anti-translations (primed)



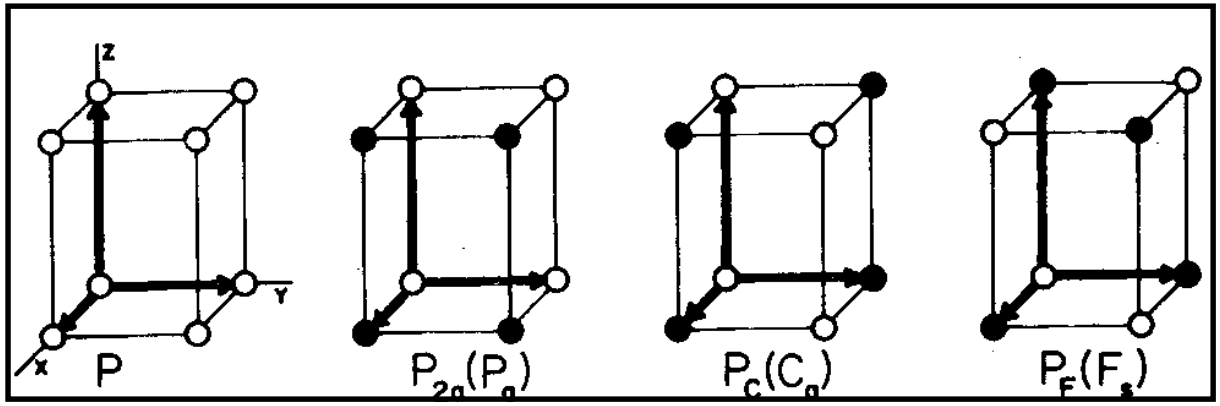
Magnetic Lattices of the **Triclinic System**

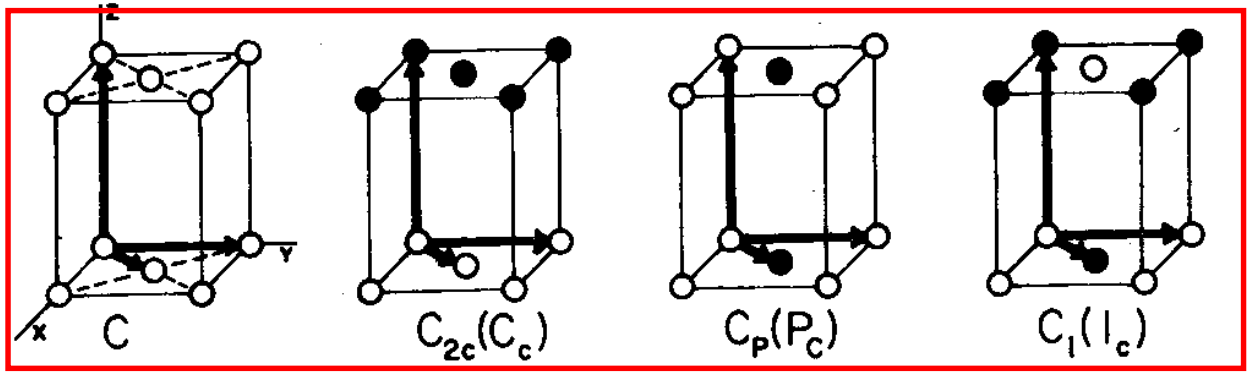


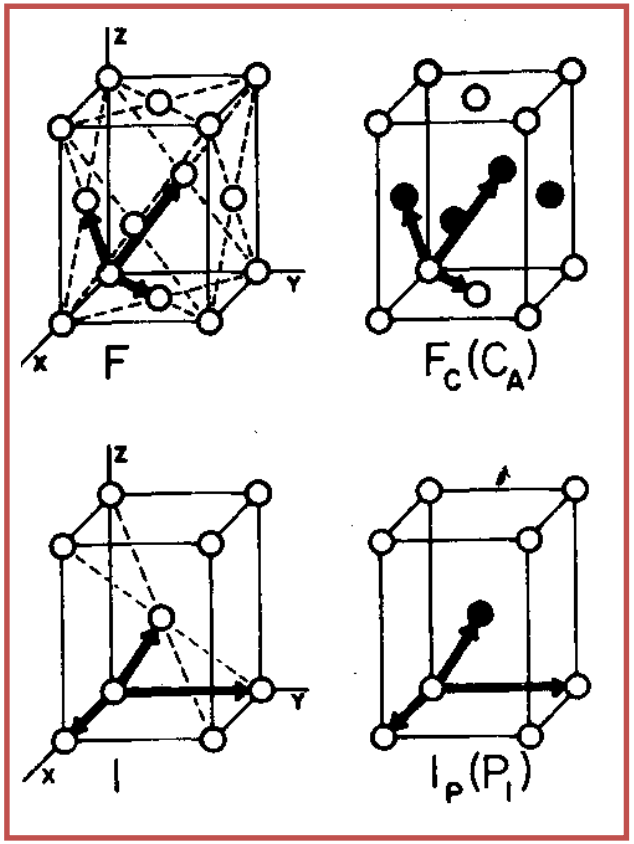
Magnetic Lattices of the **Monoclinic System**

Magnetic Lattices

Magnetic Lattices of the **Orthorhombic System**

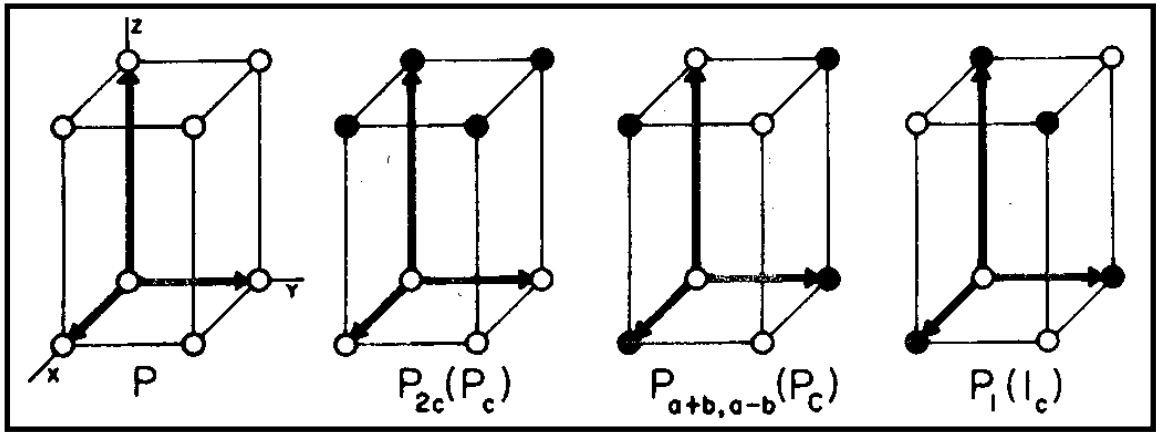


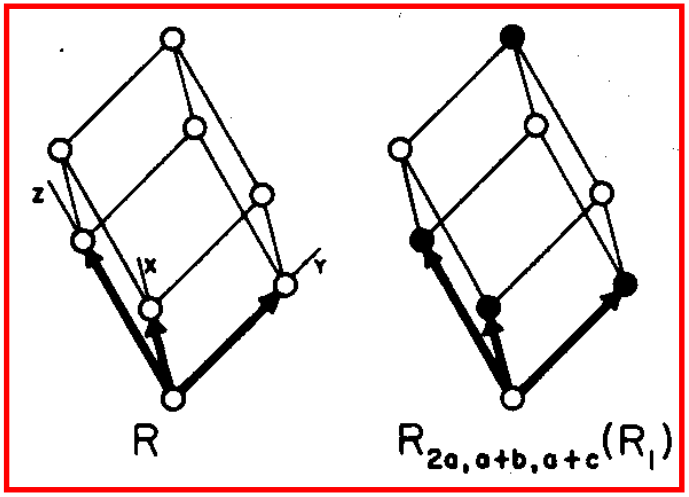


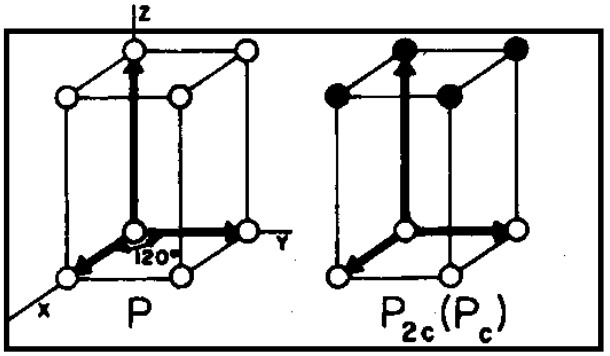


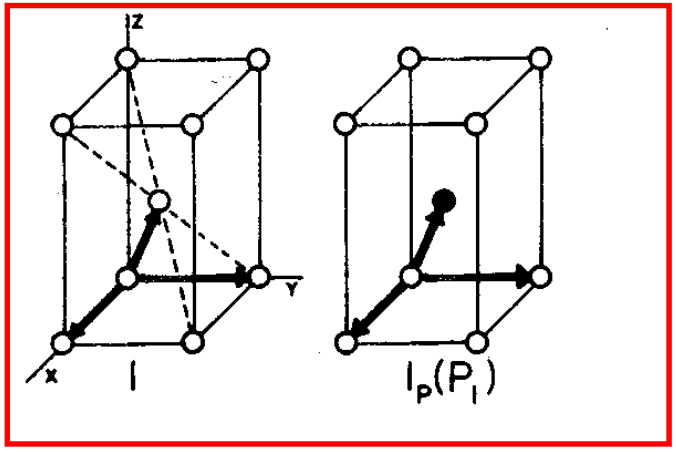
Magnetic Lattices

Magnetic Lattices of the **Tetragonal System**





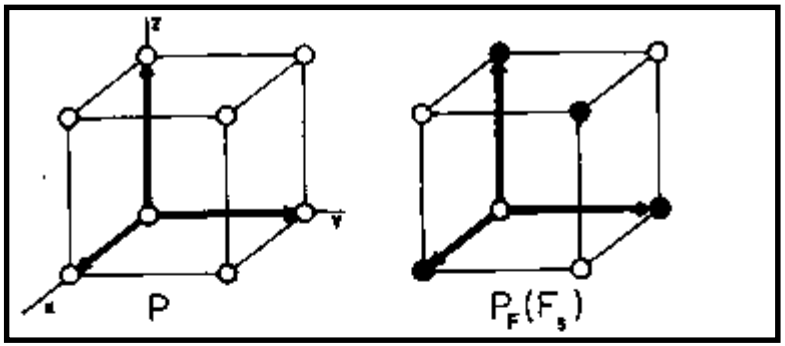


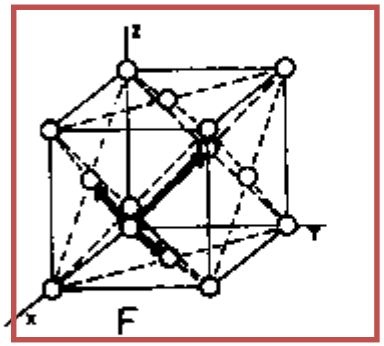


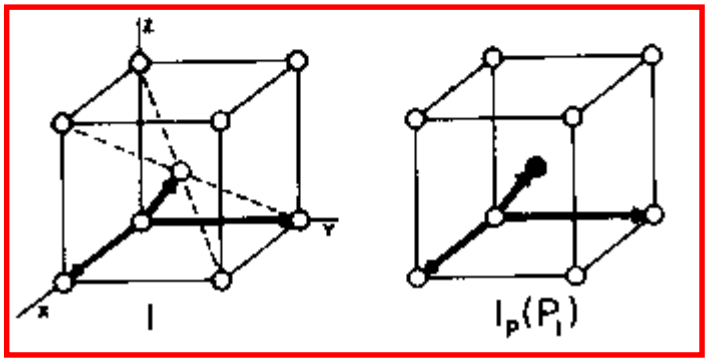
Magnetic Lattices of the **Hexagonal** and **Trigonal Systems**

Magnetic Lattices

Magnetic Lattices of the **Cubic System**







Shubnikov Groups: Magnetic Space Groups

The same procedure points groups and Bravais lattices can be applied to space groups. One obtains a total of **1651** types of Shubnikov groups.

T1: **230** are of the form $\mathbf{M_0=G}$ ("monochrome", "colourless" groups),
T2: **230** of the form $\mathbf{P=G+G}1'$ ("paramagnetic" or "grey" groups)

1191 of the form $\mathbf{M= H + (G - H)}1'$ ("black-white", BW, groups).

T3: Among the BW group there are **674** in which the subgroup $\mathbf{H} \subset \mathbf{G}$ is an equi-translation group: $\mathbf{H}$ has the same translation group as $\mathbf{G}$ (first kind, BW1).

T4: The rest of black-white groups, **517**, are equi-class group (second kind, BW2). In this last family the translation subgroup contains "anti-translations" (pure translations associated with the spin reversal operator).

Shubnikov Groups: Magnetic Space Groups

There are two notations to denote the magnetic space groups: the Opechowsky-Guccione (OG) and the Belov-Neronova-Smirnova (BNS) notations. They differ in the notation for the magnetic lattices and for the **BW2** groups. In the BNS notations the primed elements do not appear in the symbol of the group, they can be deduced from the magnetic lattice type.

In the **BW1** groups (**type 3**) the subgroup of translations is the same as that of the space group of which they derive, so the spin reversal operator is not associated with translations: the magnetic unit cell is the same as the crystallographic cell.

In the **BW2** groups (**type 4**) there are some translations associated with spin reversal, so that the "magnetic primitive cell" is bigger than the crystal primitive cell.

Shubnikov Groups: Example using ITA

The magnetic space groups can be constructed using the International Tables of Crystallography (Volume A).
Example: group number 46, I*ma*2

Site symmetry and positions of space group *Ima*2

			(0, 0, 0)+ (½, ½, ½)+		
8 *c*	1	(1) *x*, *y*, *z*	(2) -*x*, -*y*, *z*	(3) *x*+½, -*y*, *z*	(4) -*x*+½, *y*, *z*
4 *b*	*m* . .	¼, *y*, *z*	¼, -*y*, *z*		
4 *a*	. . 2	0, 0, *z*	½, 0, *z*		

Symmetry operations

For (0, 0, 0)+ set

(1) 1 (2) 2 0,0,*z* (3) *a* *x*,0,*z* (4) *m* ¼, y,z

For (½ , ½ , ½)+ set

(1) *t*(½ , ½ , ½) (2) 2(0,0, ½) ¼,¼,*z* (3) *c* *x*, ¼,*z* (4) *n*(0, ½ , ½) 0, y, z

Maximal non-isomorphic subgroups of *Ima*2

I [2] *I* 1 1 2 (*C* 2) (1; 2)+
[2] *I* 1 *a* 1 (*C c*) (1; 3)+
[2] *I m* 1 1 (*C m*) (1; 4)+

IIa [2] *P m a* 2 1; 2; 3; 4
[2] *P n c* 2 1; 2; (3; 4) + (½ , ½ , ½)
[2] *P n a* 2_1 1; 3; (2; 4) + (½ , ½ , ½)
[2] *P m c* 2_1 1; 4; (2; 3) + (½ , ½ , ½)

IIb *none*

Shubnikov Groups: Example using ITA

The groups **I** correspond to the *translationengleiche* of *t*-subgroups and the groups **II** to the *klassengleiche* or *k*-subgroups that are also subdivided in order to distinguish those having the same conventional cell (**IIa**) from those having a multiple cell (**IIb**). The division I and II correspond to the BW1 and BW2 respectively.

Applying the formula $\mathbf{M} = \mathbf{H} + (\mathbf{G} - \mathbf{H})\,1'$ we obtain:

Colourless trivial magnetic group: $\mathbf{M}_0 = I\,m\,a\,2 = \{1, 2_z, a_y, m_x\}\mathbf{T}$

For simplicity we remove the translation group and use only the coset representatives.

I

$\mathbf{M}_1 = I\,1\,1\,2 \;+(\mathrm{I\ m\ a\ 2} - I\,1\,1\,2\,)1' = \{1, 2_z\}+\{ a_y, m_x\}1' = I\,m'\,a'\,2$

$\mathbf{M}_2 = I\,1\,a\,1 \;+(\mathrm{I\ m\ a\ 2} - I\,1\,a\,1\,)1' = \{1, a_y\}+\{ 2_z, m_x\}1' = I\,m'\,a\,2'$

$\mathbf{M}_3 = I\,m\,1\,1 \;+(\mathrm{I\ m\ a\ 2} - I\,m\,1\,1)1' = \{1, m_x\}+\{2_z, a_y\}1' = I\,m\,a'\,2'$

For the BW2 groups, the translation subgroup is that formed by integer linear combinations of conventional cell parameters. The centring translations $\mathbf{t}_c=(½, ½, ½)$ become anti-translations, so the magnetic lattice contains the following set of translations and anti-translations

$$\mathbf{L} = \{\mathbf{t} \mid \mathbf{t} = l_1\,\mathbf{a}_1 + l_2\,\mathbf{a}_2 + l_3\,\mathbf{a}_3;\ \ l_i \in \mathbb{Z}\}$$

$$\mathbf{L}' = (\mathbf{T}\text{-}\mathbf{L})1' = \{\mathbf{t}' \mid \mathbf{t}' = l_1\,\mathbf{a}_1 + l_2\,\mathbf{a}_2 + l_3\,\mathbf{a}_3 + \mathbf{t}_c;\ \ l_i \in \mathbb{Z}\}$$

Shubnikov Groups: Example using ITA

IIa We write below the BW2 groups using the data of the ITA and show the BNS and the OG notation. It is clearly seen that the BNS notation correspond directly to the subgroups written in ITA by putting the lattice symbol P_I for stating that an original body centred lattice becomes primitive and the centring translations become anti-translations. None of the generators appearing in the symbol is primed. This is a characteristic of the BNS notation for all BW2 groups.

On the contrary the OG conserves the original HM symbol changing the lattice type to I_P and using primed generators when they appear. From the information given in the decomposition of the magnetic group in terms of translations and anti-translations one can derive easily the BNS (makes reference to the coset representatives with respect to **L**) or the OG notation (makes reference to the coset representatives with respect to **L**′).

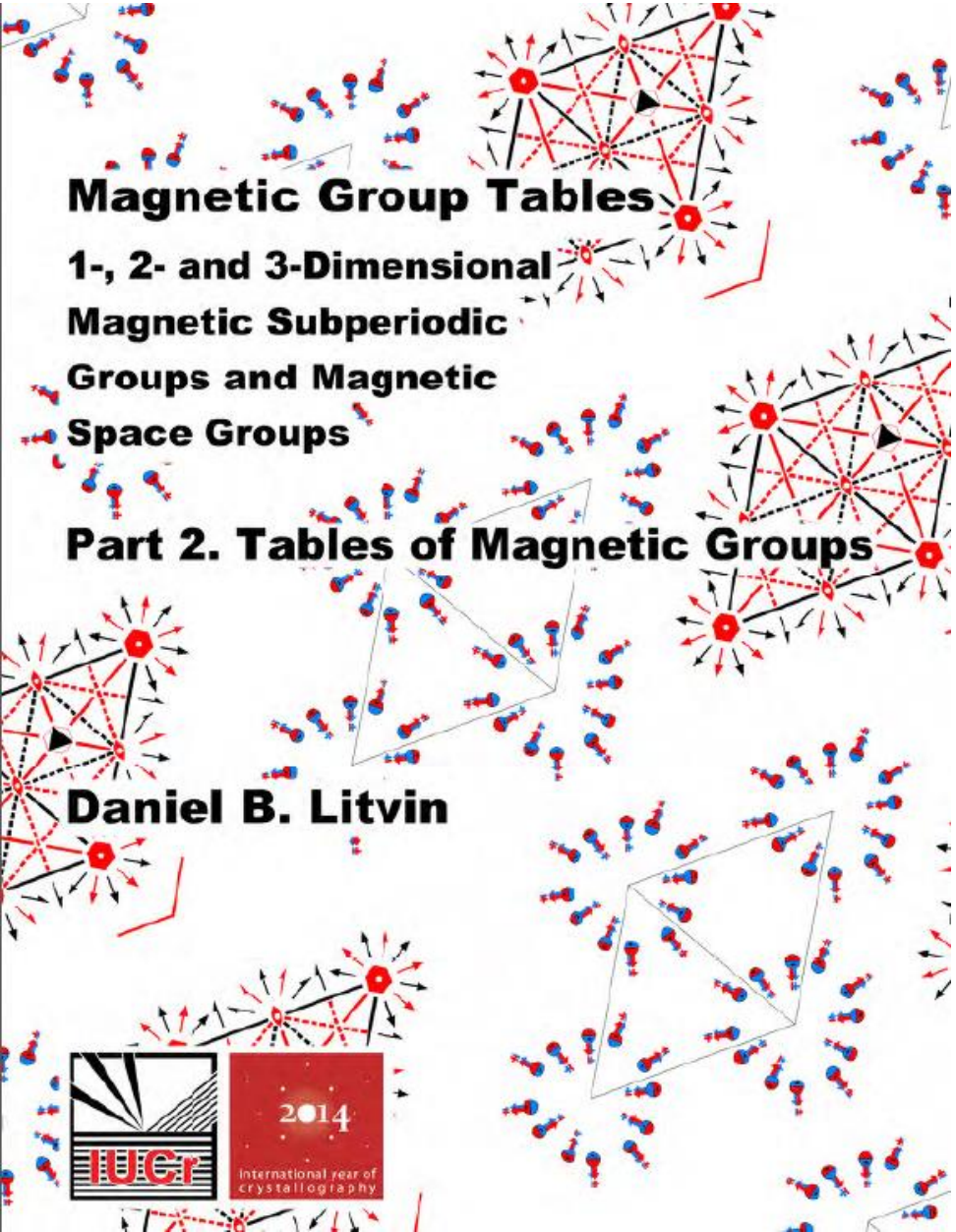
ITA	Notations:	BNS	OG
[2] $P\,m\,a\,2$	$\mathbf{M}_4 = \{1, 2_z, a_y, m_x\}\mathbf{L} + \{1, 2_{1z}, c_y, n_x\}\mathbf{L}'$	$= P_I\,m\,a\,2$	$I_P\,m\,a\,2$
[2] $P\,n\,c\,2$	$\mathbf{M}_5 = \{1, 2_z, c_y, n_x\}\mathbf{L} + \{1, 2_{1z}, a_y, m_x\}\mathbf{L}'$	$= P_I\,n\,c\,2$	$I_P\,m'\,a'\,2$
[2] $P\,n\,a\,2_1$	$\mathbf{M}_6 = \{1, a_y, 2_{1z}, n_x\}\mathbf{L} + \{1, 2_z, c_y, m_x\}\mathbf{L}'$	$= P_I\,n\,a\,2_1$	$I_P\,m'\,a\,2'$
[2] $P\,m\,c\,2_1$	$\mathbf{M}_7 = \{1, m_x, 2_{1z}, c_y\}\mathbf{L} + \{1, 2_z, a_y, n_x\}\mathbf{L}'$	$= P_I\,m\,c\,2_1$	$I_P\,m\,a'\,2'$

Magnetic Structure Description and Determination

2001: Daniel B. Litvin provides for the first time the full description of all Shubnikov (Magnetic Space) Groups. Acta Cryst. **A57**, 729-730

http://www.bk.psu.edu/faculty/litvin/home.html

Magnetic Structure Description and Determination



We are concerned here with the tables of Magnetic Groups, but many other papers from D.B. Litvin can be downloaded from its personal page at

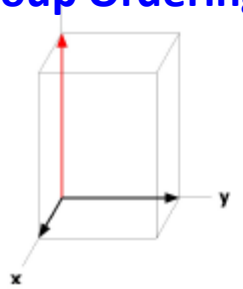
http://www.bk.psu.edu/faculty/litvin/

The first part is a comprehensive introduction to the tables and the second part contain each individual Magnetic Space Group item with Wyckoff positions and diagrams

Magnetic Structure Description and Determination

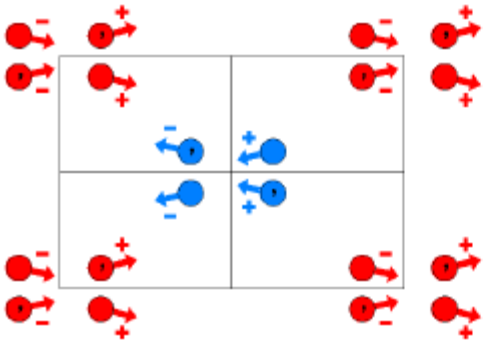
Group Ordering Number (BNS): 548, BNS: 62.450, OG: 59.9.486

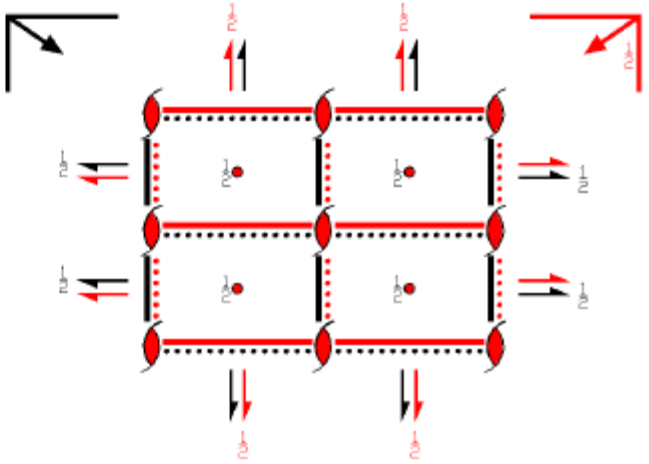
OG: $P_{2c}m'mm$
BNS: $P_a nma$



P_{2c} m'mn	mmm1'	Orthorhombic
59.9.486	$P_{2c}2_1/m'2_1'/m2'/n$	

OG-BNS transformation: (1/2,1/2,1/2; c,-b,2a)





Origin at m'm2'/n at 1/4,1/4,0 from $\bar{1}'$

Asymmetric unit $0 \le x \le 1/2$; $0 \le y \le 1/2$; $0 \le z \le 1/2$

Symmetry Operations

For (0,0,0) + set

(1) 1 (1|0,0,0)	(2) 2' 0,0,z (2_z|0,0,0)'	(3) 2' (0,1/2,0) 1/4,y,0 (2_y|1/2,1/2,0)'	(4) 2 (1/2,0,0) x,1/4,0 (2_x|1/2,1/2,0)
(5) $\bar{1}'$ 1/4,1/4,0 ($\bar{1}$|1/2,1/2,0)'	(6) n (1/2,1/2,0) x,y,0 (m_z|1/2,1/2,0)	(7) m x,0,z (m_y|0,0,0)	(8) m' 0,y,z (m_x|0,0,0)'

For (0,0,1)' + set

(1) t' (0,0,1) (1|0,0,1)'	(2) 2 (0,0,1) 0,0,z (2_z|0,0,1)	(3) 2 (0,1/2,0) 1/4,y,1/2 (2_y|1/2,1/2,1)	(4) 2' (1/2,0,0) x,1/4,1/2 (2_x|1/2,1/2,1)'
(5) $\bar{1}$ 1/4,1/4,1/2 ($\bar{1}$|1/2,1/2,1)	(6) n' (1/2,1/2,0) x,y,1/2 (m_z|1/2,1/2,1)'	(7) c' (0,0,1) x,0,z (m_y|0,0,1)'	(8) c (0,0,1) 0,y,z (m_x|0,0,1)

Magnetic Structure Description and Determination

Continued	59.9.486	P_{2c} m'mn

Only recently the magnetic space groups have been made available in a computer database

Magnetic Space Groups
Compiled by Harold T. Stokes and Branton J. Campbell
Brigham Young University, Provo, Utah, USA
June 2010

These data are based on data from:
Daniel Litvin, **Magnetic Space Group Types**,
Acta Cryst. **A57** (2001) 729-730.
http://www.bk.psu.edu/faculty/litvin/Download.html

Symmetry of Special Projections

Along [0,0,1] c2mm1'	Along [1,0,0] p2mg	Along [0,1,0] p2mg1'
a* = a b* = b	a* = b b* = c	a* = -a b* = c
Origin at 0,0,z	Origin at x,1/4,0	Origin at 1/4,y,0

Shubnikov Groups: Computing tools

NEUTRONS FOR SCIENCE®

ISOTROPY Software Suite

Harold T. Stokes, Dorian M. Hatch, and Branton J. Campbell, Department of Physics and Astronomy, Brigham Young University, Provo, Utah 84606, USA, stokesh@byu.edu

Description: The ISOTROPY software suite is a collection of software which applies group theoretical methods to the analysis of phase transitions in crystalline solids.
How to cite: ISOTROPY Software Suite, iso.byu.edu.

References and Resources

Isotropy subgroups and distortions

- ISODISTORT: Explore and visualize distortions of crystalline structures. Possible distortions include atomic displacements, atomic ordering, strain, and magnetic moments.
- ISOSUBGROUP: Coming soon!
- ISOTROPY: Interactive program using command lines to explore isotropy subgroups and their associated distortions.
- SMODES: Find the displacement modes in a crystal which brings the dynamical matrix to block-diagonal form, with the smallest possible blocks.
- FROZSL: Calculate phonon frequencies and displacement modes using the method of frozen phonons.

Space groups and irreducible representations

- ISOCIF: Create or modify CIF files.
- FINDSYM: Identify the space group of a crystal, given the positions of the atoms in a unit cell.
- **New!** ISO-IR: Tables of Irreducible Representations. The 2011 version of IR matrices.
- ISO-MAG: Tables of magnetic space groups, both in human-readable and computer-readable forms.

Superspace Groups

- ISO(3+d)D: (3+d)-Dimensional Superspace Groups for d=1,2,3
- ISO(3+1)D: Isotropy Subgroups for Incommensurately Modulated Distortions in Crystalline Solids: A Complete List for One-Dimensional Modulations
- FINDSSG: Identify the superspace group symmetry given a list of symmetry operators.
- TRANSFORMSSG: Transform a superspace group to a new setting.

Phase Transitions

- COPL: Find a complete list of order parameters for a phase transition, given the space-group symmetries of the parent and subgroup phases.
- INVARIANTS: Generate invariant polynomials of the components of order parameters.
- COMSUBS: Find common subgroups of two structures in a reconstructive phase transition

Linux

- ISOTROPY Software Suite for Linux: includes ISOTROPY, FINDSYM, SMODES, COMSUBS.

Shubnikov Groups: Computing tools

FCT/ZTF

bilbao crystallographic server

UPV EHU

[The crystallographic site at the Condensed Matter Physics Dept. of the University of the Basque Country]

[Space Groups] [Layer Groups] [Rod Groups] [Frieze Groups] [Wyckoff Sets]

IYCr2014

2014: International Year of Crystallography

NEW!

Satellite workshop of the 2014 IUCr Congress:

Role of Magnetic Symmetry in the Description and Determination of Magnetic Structures.
Hamilton, Canada
14-16 August 2014

Sections

- Retrieval Tools
- Magnetic Symmetry and Applications
- Group-Subgroup

Space Groups Retrieval Tools

GENPOS	Generators and General Positions of Space Groups
WYCKPOS	Wyckoff Positions of Space Groups
HKLCOND	Reflection conditions of Space Groups
MAXSUB	Maximal Subgroups of Space Groups
SERIES	Series of Maximal Isomorphic Subgroups of Space Groups
WYCKSETS	Equivalent Sets of Wyckoff Positions
NORMALIZER	Normalizers of Space Groups
KVEC	The k-vector types and Brillouin zones of Space Groups
SYMMETRY OPERATIONS	Geometric interpretation of matrix column representations of symmetry operations

Magnetic Symmetry and Applications

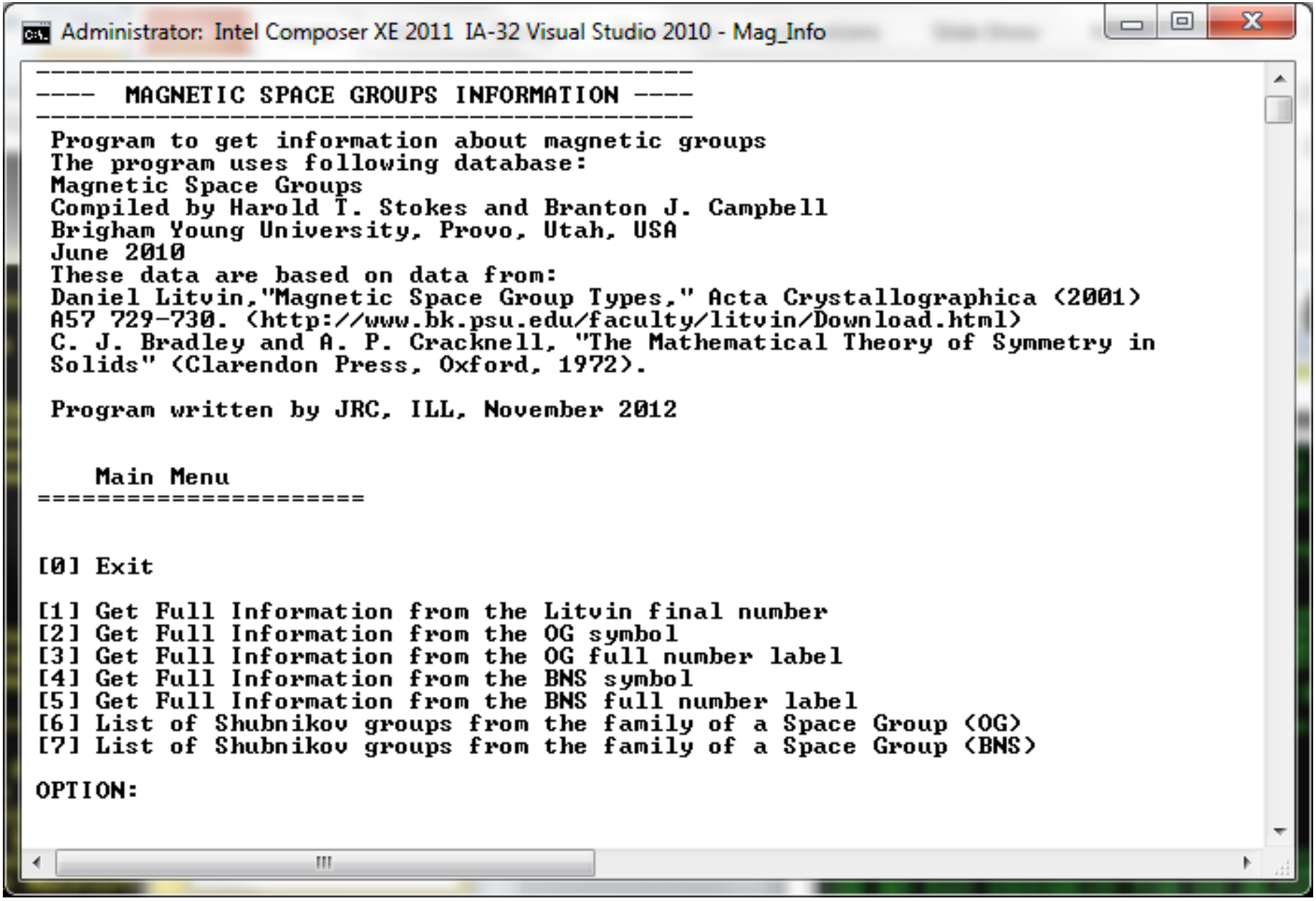
MGENPOS	General Positions of Magnetic Space Groups
MWYCKPOS	Wyckoff Positions of Magnetic Space Groups
MAGNEXT	Extinction Rules of Magnetic Space Groups
MAXMAGN ⚠	Maximal magnetic space groups for a given space group and a propagation vector

Shubnikov Groups: Computing tools

The program **Mag_Info** has been included, as a console application, for obtaining information about magnetic space groups. In the near future this program will be extended with a GUI and a wizard to create PCR files for magnetic structures using Shubnikov groups in whatever setting.

The program reads the database 'magnetic_data.txt' compiled by Harold T. Stokes and Branton J. Campbell (Brigham Young University, Provo, Utah, USA) based on data from: Daniel Litvin,"Magnetic Space Group Types", Acta Cryst **A57** (2001) 729.
http://www.bk.psu.edu/faculty/litvin/Download.html

Shubnikov Groups: Computing tools



Opechowski-Guccione Description

Number of OG operators: 32

# 1: (1|0,0,0)	# 2: (2yz|0,0,0)	# 3: (2-xz|0,0,0)	# 4: (4y|0,0,0)
# 5: (4x-1|0,0,0)	# 6: (2-yz|0,0,0)	# 7: (2xz|0,0,0)	# 8: (4x|0,0,0)
# 9: (-1|0,0,0)	# 10: (myz|0,0,0)	# 11: (m-xz|0,0,0)	# 12: (-4y|0,0,0)
# 13: (-4x-1|0,0,0)	# 14: (m-yz|0,0,0)	# 15: (mxz|0,0,0)	# 16: (-4x|0,0,0)
# 17: (1|1,0,0)'	# 18: (2yz|1,0,0)'	# 19: (2-xz|1,0,0)'	# 20: (4y|1,0,0)'
# 21: (4x-1|1,0,0)'	# 22: (2-yz|1,0,0)'	# 23: (2xz|1,0,0)'	# 24: (4x|1,0,0)'
# 25: (-1|1,0,0)'	# 26: (myz|1,0,0)'	# 27: (m-xz|1,0,0)'	# 28: (-4y|1,0,0)'
# 29: (-4x-1|1,0,0)'	# 30: (m-yz|1,0,0)'	# 31: (mxz|1,0,0)'	# 32: (-4x|1,0,0)'

Number of OG lattice translations: 3

# 1: (1,-1,0)	# 2: (1, 1,0)	# 3: (0,0, 1)

Number of OG Wyckoff positions: 21

Wyckoff site # 1: 32 32u

# 1: (x,y,z;u,v,w)	# 2: (-y,x,z;-v,u,w)	# 3: (y,-x,z;v,-u,w)
# 4: (x,-y,-z;u,-v,-w)	# 5: (-x,y,-z;-u,v,-w)	# 6: (-x,-y,z;-u,-v,w)
# 7: (y,x,-z;v,u,-w)	# 8: (-y,-x,-z;-v,-u,-w)	# 9: (-x,-y,-z;u,v,w)
# 10: (y,-x,-z;-v,u,w)	# 11: (-y,x,-z;v,-u,w)	# 12: (-x,y,z;u,-v,-w)
# 13: (x,-y,z;-u,v,-w)	# 14: (x,y,-z;-u,-v,w)	# 15: (-y,-x,z;v,u,-w)
# 16: (y,x,z;-v,-u,-w)	# 17: (x+1,y,z;-u,-v,-w)	# 18: (-y+1,x,z;v,-u,-w)
# 19: (y+1,-x,z;-v,u,-w)	# 20: (x+1,-y,-z;-u,v,w)	# 21: (-x+1,y,-z;u,-v,w)
# 22: (-x+1,-y,z;u,v,-w)	# 23: (y+1,x,-z;-v,-u,w)	# 24: (-y+1,-x,-z;v,u,w)
# 25: (-x+1,-y,-z;-u,-v,-w)	# 26: (y+1,-x,-z;v,-u,-w)	# 27: (-y+1,x,-z;-v,u,-w)
# 28: (-x+1,y,z;-u,v,w)	# 29: (x+1,-y,z;u,-v,w)	# 30: (x+1,y,-z;u,v,-w)
# 31: (-y+1,-x,z;-v,-u,w)	# 32: (y+1,x,z;v,u,w)	

Wyckoff site # 2: 16 16t

# 1: (x,x+1/2,z;u,u,w)	# 2: (-x-1/2,x,z;-u,u,w)	# 3: (x+1/2,-x,z;u,-u,w)
# 4: (x-1/2,-x,-z;u,-u,-w)	# 5: (-x+1/2,x,-z;-u,u,-w)	# 6: (-x,-x-1/2,z;-u,-u,w)
# 7: (x,x-1/2,-z;u,u,-w)	# 8: (-x,-x+1/2,-z;-u,-u,-w)	# 9: (-x,-x-1/2,-z;u,u,w)
# 10: (x+1/2,-x,-z;-u,u,w)	# 11: (-x-1/2,x,-z;u,-u,w)	# 12: (-x+1/2,x,z;u,-u,-w)
# 13: (x-1/2,-x,z;-u,u,-w)	# 14: (x,x+1/2,-z;-u,-u,w)	# 15: (-x,-x+1/2,z;u,u,-w)
# 16: (x,x-1/2,z;-u,-u,-w)		

Wyckoff site # 3: 16 16s

# 1: (x,x,z;u,-u,0)	# 2: (-x,x,z;u,u,0)	# 3: (x,-x,z;-u,-u,0)
# 4: (x,-x,-z;u,u,0)	# 5: (-x,x,-z;-u,-u,0)	# 6: (-x,-x,z;-u,u,0)
# 7: (x,x,-z;-u,u,0)	# 8: (-x,-x,-z;u,-u,0)	# 9: (x+1,x,z;-u,u,0)
# 10: (-x+1,x,z;-u,-u,0)	# 11: (x+1,-x,z;u,u,0)	# 12: (x+1,-x,-z;-u,-u,0)
# 13: (-x+1,x,-z;u,u,0)	# 14: (-x+1,-x,z;u,-u,0)	# 15: (x+1,x,-z;u,-u,0)
# 16: (-x+1,-x,-z;-u,u,0)		

Wyckoff site # 4: 16 16r

# 1: (0,y,z;u,0,0)	# 2: (-y,0,z;0,u,0)	# 3: (y,0,z;0,-u,0)
# 4: (0,-y,-z;u,0,0)	# 5: (0,y,-z;-u,0,0)	# 6: (0,-y,z;-u,0,0)
# 7: (y,0,-z;0,u,0)	# 8: (-y,0,-z;0,-u,0)	# 9: (1,y,z;-u,0,0)
# 10: (-y+1,0,z;0,-u,0)	# 11: (y+1,0,z;0,u,0)	# 12: (1,-y,-z;-u,0,0)
# 13: (1,y,-z;u,0,0)	# 14: (1,-y,z;u,0,0)	# 15: (y+1,0,-z;0,-u,0)
# 16: (-y+1,0,-z;0,u,0)		

Wyckoff site # 5: 16 16q

# 1: (x,y,1/2;0,0,w)	# 2: (-y,x,1/2;0,0,w)	# 3: (y,-x,1/2;0,0,w)
# 4: (x,-y,-1/2;0,0,-w)	# 5: (-x,y,-1/2;0,0,-w)	# 6: (-x,-y,1/2;0,0,w)
# 7: (y,x,-1/2;0,0,-w)	# 8: (-y,-x,-1/2;0,0,-w)	# 9: (x+1,y,1/2;0,0,-w)
# 10: (-y+1,x,1/2;0,0,-w)	# 11: (y+1,-x,1/2;0,0,-w)	# 12: (x+1,-y,-1/2;0,0,w)
# 13: (-x+1,y,-1/2;0,0,w)	# 14: (-x+1,-y,1/2;0,0,-w)	# 15: (y+1,x,-1/2;0,0,w)
# 16: (-y+1,-x,-1/2;0,0,w)		

Wyckoff site # 6: 16 16p

# 1: (x,y,0;0,0,w)	# 2: (-y,x,0;0,0,w)	# 3: (y,-x,0;0,0,w)
# 4: (x,-y,0;0,0,-w)	# 5: (-x,y,0;0,0,-w)	# 6: (-x,-y,0;0,0,w)
# 7: (y,x,0;0,0,-w)	# 8: (-y,-x,0;0,0,-w)	# 9: (x+1,y,0;0,0,-w)
# 10: (-y+1,x,0;0,0,-w)	# 11: (y+1,-x,0;0,0,-w)	# 12: (x+1,-y,0;0,0,w)
# 13: (-x+1,y,0;0,0,w)	# 14: (-x+1,-y,0;0,0,-w)	# 15: (y+1,x,0;0,0,w)
# 16: (-y+1,-x,0;0,0,w)		

Programs for symmetry analysis

The irreducible representations of space groups can be obtained consulting tables or using computer programs for calculating them.

The basis functions of the irreducible representations depend on the particular problem to be treated and they have to be calculated by using projection operator formula. A series of programs allow these kind of calculations to be done. Doing that by hand may be quite tedious and prone to errors.

Concerning magnetic structures three programs are of current use: **BasIreps** (J. Rodríguez-Carvajal), **SARAh** (Andrew Wills) and **MODY** (Wiesława Sikora). One can use also **BCS** (Perez-Mato et al.) or **ISODISTORT** (B.Campbell and H. Stokes)

Programs for symmetry analysis

A series of computing tools for crystallography including magnetic structures are available at Bilbao Crystallographic Server

bilbao crystallographic server

[The crystallographic site at the Condensed Matter Physics Dept. of the University of the Basque Country]

[Space Groups] [Layer Groups] [Rod Groups] [Frieze Groups] [Wyckoff Sets]

IYCr2014
2014: International Year of Crystallography

NEW!

Satellite workshop of the 2014 IUCr Congress:

Role of Magnetic Symmetry in the Description and Determination of Magnetic Structures.
Hamilton, Canada
14-16 August 2014

Space Groups Retrieval Tools

GENPOS	Generators and General Positions of Space Groups
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MAXSUB	Maximal Subgroups of Space Groups
SERIES	Series of Maximal Isomorphic Subgroups of Space Groups
WYCKSETS	Equivalent Sets of Wyckoff Positions
NORMALIZER	Normalizers of Space Groups
KVEC	The k-vector types and Brillouin zones of Space Groups
SYMMETRY OPERATIONS	Geometric interpretation of matrix column representations of symmetry operations
IDENTIFY GROUP	Identification of a Space Group from a set of generators in an arbitrary setting

Programs for symmetry analysis

Magnetic Symmetry and Applications	
MGENPOS	General Positions of Magnetic Space Groups
MWYCKPOS	Wyckoff Positions of Magnetic Space Groups
MAGNEXT	Extinction Rules of Magnetic Space Groups
IDENTIFY MAGNETIC GROUP ⚠	Identification of a Magnetic Space Group from a set of generators in an arbitrary setting
MAXMAGN ⚠	Maximal magnetic space groups for a given a propagation vector and resulting magnetic structural models
k-SUBGROUPSMAG ⚠	Magnetic subgroups consistent with some given propagation vector(s) or a supercell
MAGNDATA ⚠	A collection of magnetic structures with transportable cif-type files

Structure Utilities	
CELLTRAN	Transform Unit Cells
STRAIN	Strain Tensor Calculation
WPASSIGN	Assignment of Wyckoff Positions
TRANSTRU	Transform structures.
SETSTRU ⚠	Alternative Settings for a given Crystal Structure
EQUIVSTRU	Equivalent Descriptions for a given Crystal Structure
STRCONVERT	Convert & Edit Structure Data (supports the CIF, mCIF, VESTA, VASP formats -- with magnetic information where available)
VISUALIZE	Visualize structures using Jmol
COMPSTRU ⚠	Comparison of Crystal Structures with the same Symmetry
STRUCTURE RELATIONS ⚠	Evaluation of structure relationships [transformation matrix] between group-subgroup related phases
PSEUDOLATTICE	Pseudosymmetry of a lattice and compatible supergroups

Programs for symmetry analysis

ISOTROPY Software Suite

Harold T. Stokes, Dorian M. Hatch, and Branton J. Campbell, Department of Physics and Astronomy, Brigham Young University, Provo, Utah 84606, USA, stokesh@byu.edu

Description: The ISOTROPY software suite is a collection of software which applies group theoretical methods to the analysis of phase transitions in crystalline solids.
How to cite: ISOTROPY Software Suite, iso.byu.edu.

A huge amount of work on symmetry has been developed by Harold Stokes, Dorian Hatch and Branton Campbell.
Stokes developed ISOTROPY and many algorithms for working with space groups and representations. Together with the programs they have made available databases to be used by external software

- FINDSYM: Identify t
- New! ISO-IR: Table
- ISO-MAG: Tables of

Superspace Gro

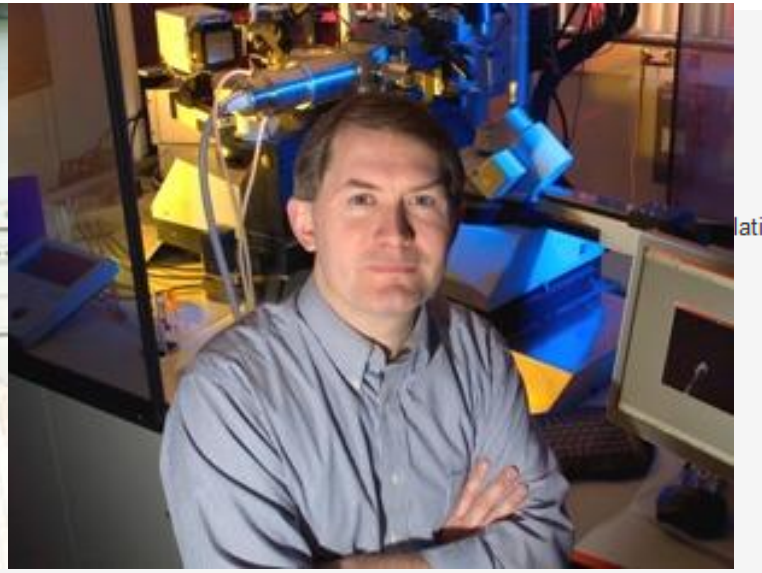
- ISO(3+d)D: (3+d)-Di
- ISO(3+1)D: Isotropy
- FINDSSG: Identify t
- TRANSFORMSSG:

Phase Transitio

- COPL: Find a comp
- INVARIANTS: Gene
- COMSUBS: Find co

Linux

- ISOTROPY Softwa



lations

New facilities for Magnetic Structures in FullProf

- **FullProf** is now able to produce a magnetic CIF file (extension mCIF) for conmmensurate magnetic structures described in the magnetic cell. This mCIF file can be directly read by **FP_Studio** and also by the program **VESTA**.

The program converts the user-description of the magnetic structure, using the crystal cell and propagation vector and MSYM operators or basis functions, to the magnetic cell with all the magnetic atoms inside that cell.

This mCIF file may be used to determine the Shubnikov group of the used model thanks to the program ISOCIF that can be executed via the Web at http://stokes.byu.edu/iso/isocif.php

New facilities for Magnetic Structures in FullProf

A new option for reading symmetry operators for magnetic structures in **FullProf** has been implemented.
These operators are for commensurate structures and the mix in some sense SYMM and MSYM operators.
The value **Isy=2** is used to inform the program that this kind of operator will be provided. Four forms are recognized by **FullProf**, examples of these operators for are given below:

```
1->   SHUB    x+1/2,-y,z   -u,v,-w
2->   SHUB    x+1/2,-y,z   -mx,my,-mz   +1
3->   SHUB    x+1/2,-y,z   +1
4->   SHUB    x+1/2,-y,z,+1
```

The three operator are identical (the +1 indicated that time reversal is not associated to the operator, a -1 indicates the opposite situation). The keyword SHUB is not strictly needed, it may be replaced by any word or number but it cannot be omitted.

New facilities for Magnetic Structures in FullProf

The complete list of symmetry operators corresponding to a particular setting of any magnetic space group may be obtained through the **Bilbao Crystallographic Server** using the programs **MAXMAGN** or **STRCONVERT**.

A console program converting mCIF files (as produced by the **Bilbao Crystallographic Server** or by **ISOCIF**) to PCR files has been included in the new **FullProf Suite**.
The console program is called **mCIF_to_PCR** and will be extended with a GUI in the near future.
Presently the provided PCR file is adequate for a simulation and the user should change by hand the parameters.

New facilities for Magnetic Structures

Structure Data Converter & Editor

Symmetry

Space Group # : 1 (P1)

Title: New Structure

Lattice Parameters

a: 4 Å b: 4 Å c: 4 Å

α 90 ° β: 90 ° γ: 90 °

Short Definition:

Source DOI:

Update Structure

Symmetry Operations [Show/Hide]

Atomic Positions & Displacements

Switch to the treatment of the vectors as: Magnetic Moments P1 (#1.1) -- Type I Go!

	Label	Element	x	y	z	Occ.	Δ_x	Δ_y	Δ_z
☐	X1	X	0.00000	0.00000	0.00000	1.00000	0.00000	0.00000	0.00000

Add atoms more. || Remove selected atoms || Change the selected atoms' symbol to

Select the atoms with the symbol: || Select all atoms || Unselect all atoms

Longest Arrow size: 1.000 [for VESTA format export: Å *(Default: min(a,b,c)/4)]*
[for Jmol visualize: a proportional coefficient]

Export to BCS format | Export to VESTA format (displacement)

Export to Standard CIF format | Export to MCIF format (displacement)

Export to VASP format | Transform the structure to P1 setting

Remove the magnetic information | Re-order the sites | Visualize (displacement)

Find Symmetry Tolerance: 0.01
[via FINDSYM by Stokes & Campell]

Superspace Symmetry

Pim de Wolff (1919–1998), Delft Institute of Technology, The Nederland

The introduction of superspace approach was a breakthrough that allowed to treat “aperiodic crystals” diffraction data

Superspace Symmetry

Seminal papers on superspace approach

Wolff, P. M. de (1974). *Acta Cryst.* A**30**, 777-785.

Wolff, P. M. de (1977). *Acta Cryst.* A**33**, 493-497.

Wolff, P. M. de, Janssen, T. & Janner, A. (1981). *Acta Cryst.* A**37**, 625-636.

Superspace Symmetry

research perspectives

Acta Crystallographica Section B
Structural Science, Crystal Engineering and Materials

ISSN 2052-5206

Aperiodic crystals and superspace concepts

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Received 12 June 2014
Accepted 24 June 2014

For several decades the lattice periodicity of crystals, as shown by Laue, was considered to be their essential property. In the early sixties of the last century compounds were found which for many reasons should be called crystals, but were not lattice periodic. This opened the field of aperiodic crystals. An overview of this development is given. Many materials of this kind were found, sometimes with very interesting properties. In the beginning the development was slow, but the number of structures of this type increased enormously. In the meantime hundreds of scientists have contributed to this field using a multi-disciplinary approach.

Awarded with the tenth Ewald Prize for "the development of superspace crystallography and its application to the analysis of aperiodic crystals" (Montreal 2014)

Superspace and Representations

PHYSICAL REVIEW B VOLUME 30, NUMBER 3 1 AUGUST 1984

Superspace groups and Landau theory. A physical approach to superspace symmetry in incommensurate structures

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(Received 19 December 1983)

Magnetic space and superspace groups, representation analysis: competing or friendly concepts?

Acta Cryst **A66**, 649 (2010)

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Magnetic superspace groups

Journal of Physics: Condensed Matter **24**, 163201 (2012)

IOP PUBLISHING JOURNAL OF PHYSICS: CONDENSED MATTER

J. Phys.: Condens. Matter **24** (2012) 163201 (20pp) doi:10.1088/0953-8984/24/16/163201

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]

The future of Magnetic Crystallography is clearly an unified approach of symmetry invariance and representations

Superspace operations

$$\mathbf{r}_{l\mu} = \boldsymbol{l} + \mathbf{r}_{\mu} \qquad x_4 = \mathbf{k}\mathbf{r}_{l\mu}$$

$$\mathbf{M}_{\mu}(x_4) = \mathbf{M}_{\mu,0} + \sum_{n}[\mathbf{M}_{\mu,ns}\sin(2\pi n x_4) + \mathbf{M}_{\mu,nc}\cos(2\pi n x_4)]$$

$$(\boldsymbol{R}, \theta \,|\, \mathbf{t}) \in \Omega_b \qquad \theta = -1(time\ reversal)\ \theta = 1(otherwise)$$

The application of $(\boldsymbol{R}, \theta \,|\, \mathbf{t})$ operation to the modulated structure change the structure to another one with the modulation functions changed by a translation in the fourth coordinate

$$\mathbf{M}'_{\mu} = \mathbf{M}_{\mu}(x_4 + \tau)$$

The original structure can be recovered by a translation in the internal space and one can introduce a symmetry operator

$$(\boldsymbol{R}, \theta \,|\, \mathbf{t}, \tau)$$

Superspace operations

If $(\boldsymbol{R},\theta\,|\,\mathbf{t},\tau)$ belongs to the (3+1)-dim superspace group of an incommensurate magnetic phase, the action of **R** on its propagation vector **k** necessarily transforms this vector into a vector equivalent to either **k** (R_I = +1) or **-k** (R_I = -1).

$$\mathbf{k}\cdot\boldsymbol{R}=R_I\mathbf{k}+\mathbf{H}_{\boldsymbol{R}}$$

$\mathbf{H}_{\boldsymbol{R}}$ is a reciprocal lattice vector of the basic structure and is different of zero only if **k** contains a commensurate component.

If in the basic structure $(\boldsymbol{R}\,|\,\mathbf{t})\mathbf{r}_\nu=\mathbf{r}_\mu+\boldsymbol{l}$ their atomic modulation functions are not independent and should verify

$$\mathbf{M}_\mu(R_I x_4+\tau_0+\mathbf{H}_{\boldsymbol{R}}\mathbf{r}_\nu)=\theta\det(\boldsymbol{R})\boldsymbol{R}\mathbf{M}_\nu(x_4)$$

$$\mathbf{u}_\mu(R_I x_4+\tau_0+\mathbf{H}_{\boldsymbol{R}}\mathbf{r}_\nu)=\boldsymbol{R}\mathbf{u}_\nu(x_4)$$

$$\tau_0=\tau+\mathbf{kt}$$

Superspace operations

The operators of the **magnetic superspace groups** are the same a those of **superspace groups** just extended with the time inversion label θ

The operators of the form: $(\boldsymbol{1}, +1 \,|\, \mathbf{t}, -\mathbf{k}\,\mathbf{t})$ constitute the lattice of the (3+1)-dim superspace group

The basic lattice translations are:

$$(\boldsymbol{1}, +1 \,|\, 100, -k_x), (\boldsymbol{1}, +1 \,|\, 010, -k_y), (\boldsymbol{1}, +1 \,|\, 001, -k_z), (\boldsymbol{1}, +1 \,|\, 000, 1)$$

Using the above basis the we can define 3+1 symmetry operators of the form:

$$(\boldsymbol{R}, \theta \,|\, \mathbf{t}, \tau) \;\rightarrow\; (\boldsymbol{R}_S, \theta \,|\, \mathbf{t}_S) \quad \mathbf{t} = (t_1, t_2, t_3) \quad \tau_0 = \tau + \mathbf{k}\mathbf{t}$$

$$\boldsymbol{R}_S = \begin{pmatrix} R_{11} & R_{12} & R_{13} & 0 \\ R_{21} & R_{22} & R_{23} & 0 \\ R_{31} & R_{32} & R_{33} & 0 \\ H_{R1} & H_{R2} & H_{R3} & R_I \end{pmatrix} \qquad \mathbf{t}_S = (t_1, t_2, t_3, \tau_0)$$

Superspace operations

Simplified Seitz symbols for 3+1 symmetry operators

$$(\boldsymbol{R},\theta\,|\,\mathbf{t},\tau) \;\rightarrow\; (\boldsymbol{R}_S,\theta\,|\,\mathbf{t}_S) \quad \mathbf{t}_S=(t_1,t_2,t_3,\tau_0) \quad \tau_0=\tau+\mathbf{kt}$$

$$(\boldsymbol{R},\theta\,|\,\mathbf{t},\tau) \;\rightarrow\{\boldsymbol{R},\theta\,|\,t_1t_2t_3\tau_0\}\rightarrow\{\boldsymbol{R}\,|\,t_1t_2t_3\tau_0\}\;or\;\{\boldsymbol{R}'\,|\,t_1t_2t_3\tau_0\}$$

$$(\boldsymbol{R},\theta\,|\,00\frac{1}{2},\frac{1}{2}-\frac{1}{2}\gamma)\rightarrow\{\boldsymbol{R},\theta\,|\,00\frac{1}{2}\frac{1}{2}\} \quad with\;\mathbf{k}=\gamma\mathbf{c}^*$$

Simple example

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

$\{1\,\vert\,0000\}$	$x_1,x_2,x_3,x_4,+1$
$\{\bar{1}\,\vert\,0000\}$	$-x_1,-x_2,-x_3,-x_4,+1$
$\{1'\,\vert\,0001/2\}$	$x_1,x_2,x_3,x_4+1/2,-1$
$\{\bar{1}'\,\vert\,0001/2\}$	$-x_1,-x_2,-x_3,-x_4+1/2,-1$

Magnetic Structure Factor

Simplified magnetic structure factor in the superspace description with the notation used in **JANA-2006**

$$\mathbf{r}_{l\mu} = \boldsymbol{l} + \mathbf{r}_{\mu} \qquad x_4 = \mathbf{k}\mathbf{r}_{l\mu}$$

$$\mathbf{M}_{\mu}(x_4) = \mathbf{M}_{\mu,0} + \sum_{n}[\mathbf{M}_{\mu,ns}\sin(2\pi n x_4) + \mathbf{M}_{\mu,nc}\cos(2\pi n x_4)]$$

$$\mathbf{F}_{mag}(\mathbf{H} \pm m\mathbf{k}) = p\sum_{\mu=1}^{n} f_{\mu}(|\mathbf{H} \pm m\mathbf{k}|)T(\mathbf{H} \pm m\mathbf{k})\frac{\mathbf{M}_{\mu,mc} \pm i\mathbf{M}_{\mu,ms}}{2}exp\{2\pi i\mathbf{H}\mathbf{r}_{\mu}\}$$

Magnetic Structure Factor

Simplified magnetic structure factor in the description used in **FullProf** (with notations adapted to those used in superspace approach)

$$\mathbf{M}_{l\mu} = \sum_{\{\mathbf{k}\}} \mathbf{S}_{\mathbf{k}\mu}\, exp\{-2\pi\, i\mathbf{k}\boldsymbol{l}\} = \sum_{\{\mathbf{k}\}} \mathbf{M}_{\mathbf{k}\mu}\, exp\{-2\pi\, i\mathbf{k}\mathbf{r}_{l\mu}\}$$

$$\mathbf{S}_{\mathbf{k}\mu} = \frac{1}{2}(\mathbf{R}_{\mathbf{k}\mu} + i\mathbf{I}_{\mathbf{k}\mu})\exp\{-2\pi i\phi_{\mathbf{k}}\} = \frac{1}{2}(\mathbf{M}_{\mathbf{k}\mu,c} + i\mathbf{M}_{\mathbf{k}\mu,s})\exp\{-2\pi i\mathbf{k}\mathbf{r}_{\mu}\}$$

$$\mathbf{M}(\mathbf{h}) = p\sum_{\mu=1}^{n} f_{\mu}(h)T_{\mu}\mathbf{S}_{\mathbf{k}\mu}exp\{2\pi i(\mathbf{H}+\mathbf{k})\mathbf{r}_{\mu}\}$$

$$\mathbf{M}(\mathbf{h}) = \frac{1}{2}\, p\sum_{\mu=1}^{n} f_{\mu}(h)T_{\mu}(\mathbf{M}_{\mathbf{k}\mu,c} + i\mathbf{M}_{\mathbf{k}\mu,s})exp\{2\pi i\mathbf{H}\mathbf{r}_{\mu}\}$$

Thank you for your attention!