Representation Theory in Magnetic Structure Analysis

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Outline

1: Summary of Group Representation Theory

2: Basis functions of a representation

3: Representations of the Translation Group

4: Representations of Space Groups: little group and the star of k

5: Representations Analysis for Magnetic Structures

6: BasIreps a program for getting irreps and basis vectors of the little group

SUMMARY OF GROUP REPRESENTATION THEORY

A representation of a group is a set of matrices satisfying the same operation rules as the group elements

$$\Gamma = \{\Gamma(g) \mid g \in G\}, \quad \Gamma(g_1 g_2) = \Gamma(g_1)\Gamma(g_2)$$

Under the ordinary matrix product the given set constitutes an isomorphic group (preserves the multiplication table).

A similarity transformation applied to all matrices provides an equivalent representation (the matrix U is generally unitary: $U^{-1} = U^{\dagger}$).

$$\Gamma(g) = U\,\Gamma(g)\,U^{-1} \{with\ g \in G\}$$

A particular group has an infinite number of representations of arbitrary dimensions. The most important representations are called “Irreducible Representations” (Irreps). An arbitrary representation may be reduced to “block-diagonal form” by an appropriate similarity transformation. Those representations that cannot be reduced are the Irreps.

Group theory: Irreducible representations

Given the representation Γ={Γ(*e*), Γ(*a*), Γ(*b*)…} of the group **G**={*e*, *a*, *b*,…}, if we are able to find a similarity transformation *U* converting all matrices to the same block-diagonal form, we obtain an equivalent representation that can be decomposed as follows:

$$\Gamma(g) = U\,\Gamma(g)\,U^{-1}\left\{with\ g \in G\right\} \Rightarrow \Gamma = U\,\Gamma\,U^{-1}$$

$$\Gamma(g) = \begin{pmatrix} A_{11} & A_{12} & 0 & 0 & 0 & 0 & 0 \\ A_{21} & A_{22} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & B_{11} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & B_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{11} & C_{12} & C_{13} \\ 0 & 0 & 0 & 0 & C_{21} & C_{22} & C_{23} \\ 0 & 0 & 0 & 0 & C_{31} & C_{32} & C_{33} \end{pmatrix} = A(g) \oplus 2B(g) \oplus C(g)$$

Irreducible representations

Γ^1 ={A(*e*), A(*a*), A(*b*),…}

Γ^2 = {B(*e*), B(*a*), B(*b*),…}

Γ^3 = {C(*e*), C(*a*), C(*b*),…}

In general:

$$\Gamma = \sum_{\oplus\nu} n_\nu \Gamma^\nu = n_1\Gamma^1 \oplus n_2\Gamma^2 ... \oplus n_m\Gamma^m$$

Formulas of the group representation theory

We shall note the different irreducible representations with the index ν and a symbol Γ that may be used also for matrices. The dimension of the representation Γ_ν is l_ν. The characters of a representation (traces of the matrices) will be represented as $\chi^\nu(g)$

The great orthogonality theorem:

$$\sum_{g\in G}\Gamma^{\nu}_{ij}(g)\Gamma^{*\mu}_{lm}(g)=\frac{n(G)}{l_\nu}\,\delta_{il}\,\delta_{jm}\,\delta_{\mu\nu}$$

Particularized for the characters:

$$\sum_{g\in G}\chi^{\nu}(g)\chi^{*\mu}(g)=n(G)\,\delta_{\mu\nu}$$

Decomposition of a representation in Irreps:

$$\Gamma=\sum_{\oplus\nu}n_\nu\Gamma_\nu, \qquad n_\nu=\frac{1}{n(G)}\sum_{g\in G}\chi(g)\chi^{*\nu}(g)$$

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Basis functions of a representation

The elements of the symmetry groups act on position vectors. For each particular problem we can select a set of physically relevant variables φ_i $\{i = 1, 2, \ldots p\}$ spanning a working functional space **W**. These functions constitute a basis of the **W** space.

The action of the operator associated to a symmetry operator when applied to a function of position vectors is defined by the expression:

$$O(g)\varphi(\mathbf{r}) = \varphi(g^{-1}\mathbf{r}) \equiv \varphi'(\mathbf{r})$$

When using the functions φ_i $(\mathbf{r})$, the action of the operator $O(g)$ gives rise to a linear combination, defining a representation of the group G:

$$O(g)\varphi_j(\mathbf{r}) = \varphi'(\mathbf{r}) = \sum_i \Gamma_{ij}(g)\varphi_i(\mathbf{r})$$

Basis functions of irreducible representations

If we take another basis ψ related to the initial one by a unitary transformation we may get the matrices of the Γ representation in block-diagonal form.

$$\psi_j(\mathbf{r}) = \sum_i U_{ij}\varphi_i(\mathbf{r})$$

The system of p ψ-functions splits in subsystems defining irreducible subspaces of the working space **W**. If we take one of these subspaces (labelled ν), the action of the operator $O(g)$ on the basis functions is:

$$O(g)\psi_j(\mathbf{r}) = \sum_{i=1}^{l_\nu}\Gamma_{ij}^{\nu}(g)\psi_i(\mathbf{r})$$

Here the functions are restricted to those of the subspace ν

Basis functions of irreps: Projection Operators

Projection operators

There is a way for obtaining the basis functions of the *irreps* for the particular physical problem by applying the following projection operator formula:

$$\psi_i^\nu = P^\nu \varphi = \frac{1}{n(G)} \sum_{g \in G} \Gamma_{i[j]}^{*\nu}(g)\, O(g)\, \varphi \qquad (i = 1, \ldots l_\nu)$$

The result of the above operation is zero or a basis function of the corresponding *irrep*. The index [*j*] is fixed, taking different values provide new basis functions or zero.

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Representations of the Translation Group (1)

Representations of the translation group

The translation group is Abelian so the *irreps* are all *one-dimensional*. Considering the properties of the translation operators and the Born-Von Karman periodic boundary conditions the representation matrix (a single number equal to its character) is given by the expression:

$$O(\mathbf{t}) = O(l_1\mathbf{a}_1 + l_2\mathbf{a}_2 + l_3\mathbf{a}_3) = O(\mathbf{a}_1)^{l_1} O(\mathbf{a}_2)^{l_2} O(\mathbf{a}_3)^{l_3}$$

$$O(\mathbf{a}_j)^{N_j+1} = O(\mathbf{a}_j)$$

$$O(\mathbf{t}) \to \exp\left\{2\pi i\left(\frac{p_1 l_1}{N_1} + \frac{p_2 l_2}{N_2} + \frac{p_3 l_3}{N_3}\right)\right\}, \qquad 0 \le p_i \in Z \le N_i - 1$$

$$N = N_1 \times N_2 \times N_3$$

$$\mathbf{k} = \left(\frac{p_1}{N_1}, \frac{p_2}{N_2}, \frac{p_3}{N_3}\right) = \frac{p_1}{N_1}\mathbf{b}_1 + \frac{p_2}{N_2}\mathbf{b}_2 + \frac{p_3}{N_3}\mathbf{b}_3$$

Representations of the Translation Group (2)

The matrix of the representation **k** corresponding to the translation **t** is then:

$$\Gamma^{\mathbf{k}}(\mathbf{t}) = \exp\left\{2\pi i\left(\frac{p_1 l_1}{N_1} + \frac{p_2 l_2}{N_2} + \frac{p_3 l_3}{N_3}\right)\right\} = \exp\{2\pi i\,\mathbf{k}\,\mathbf{t}\}$$

Where the **k** vectors in reciprocal space are restricted to the first Brillouin Zone. It is clear that adding a reciprocal lattice vector **H** to **k**, does not change the matrix, so the vectors **k**'=**H**+**k** and **k** are equivalent.

The basis functions of the group of translations must satisfy the equation:

$$O(\mathbf{t})\psi^{\mathbf{k}}(\mathbf{r}) = \Gamma^{\mathbf{k}}(\mathbf{t})\psi^{\mathbf{k}}(\mathbf{r}) = \exp\{2\pi i\,\mathbf{k}\,\mathbf{t}\}\psi^{\mathbf{k}}(\mathbf{r})$$

The most general form for the functions $\psi^{\mathbf{k}}(\mathbf{r})$ are the Bloch functions:

$$\psi^{\mathbf{k}}(\mathbf{r}) = u_{\mathbf{k}}(\mathbf{r})\exp\{-2\pi i\,\mathbf{kr}\},\ with\ u_{\mathbf{k}}(\mathbf{r}\pm\mathbf{t}) = u_{\mathbf{k}}(\mathbf{r})$$

This is easily verified by applying the rules or the action of operators on functions

$$O(\mathbf{t})\psi^{\mathbf{k}}(\mathbf{r}) = \psi^{\mathbf{k}}(\mathbf{r}-\mathbf{t}) = u_{\mathbf{k}}(\mathbf{r}-\mathbf{t})\exp\{-2\pi i\,\mathbf{k}(\mathbf{r}-\mathbf{t})\} =$$

$$= \exp\{2\pi i\,\mathbf{kt}\}\,u_{\mathbf{k}}(\mathbf{r})\exp\{-2\pi i\,\mathbf{k}\,\mathbf{r}\} = \exp\{2\pi i\,\mathbf{kt}\}\psi^{\mathbf{k}}(\mathbf{r})$$

The k-vector Types of Group 10 [*P*2/*m*]

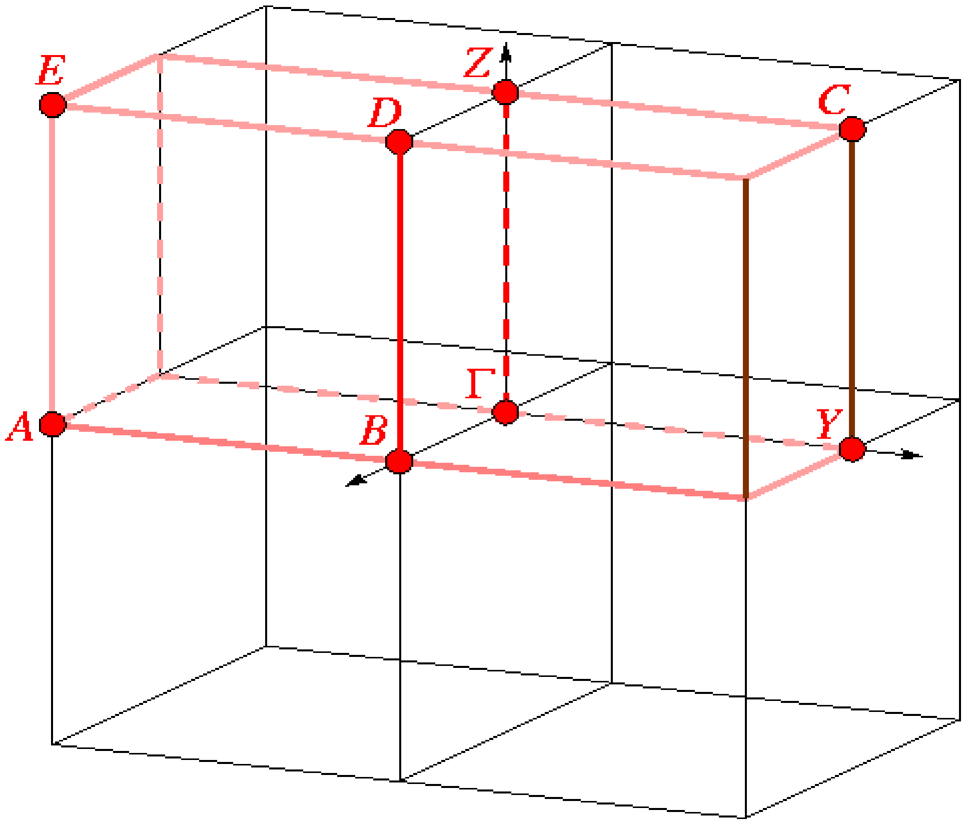
Brillouin zone

(Diagram for arithmetic crystal class 2/mP)

P112/m (P2/m)-C_{2h}^1 (10), P112$_1$/m (P2$_1$/m)-C_{2h}^2 (11), P112/a (P2/c)-C_{2h}^4 (13), P112$_1$/a (P2$_1$/c)-C_{2h}^5 (14)

Reciprocal-space group (P112/m)*, No. 10

The table with the k vectors.



In the Bilbao Crystallographic Server one can find pictures of the Brillouin Zones (BZ) for the different space groups and sizes of unit cell parameters.
The labelling of each special points in the BZ are also given and serve for labelling the irreducible representations

The k-vector Types of Group 71 [*Immm*]

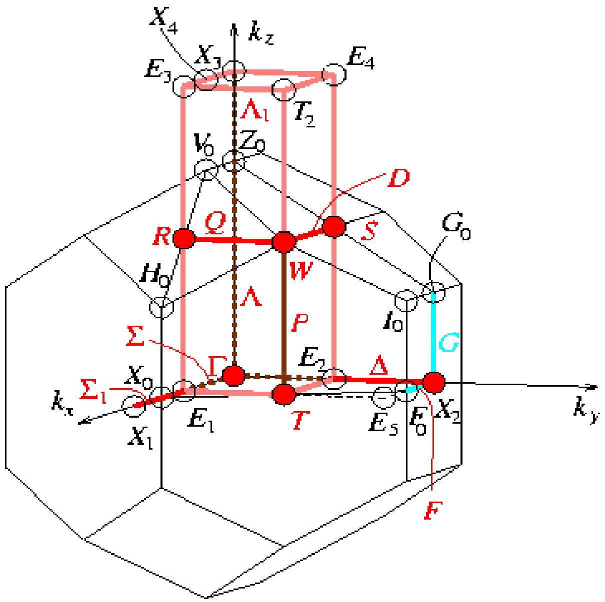
Brillouin zone

(Diagram for arithmetic crystal class mmmI)

(b>a>c or b>c>a) Immm-D_{2h}^{25} (71) to Imma-D_{2h}^{28} (74)

Reciprocal-space group (Fmmm)*, No.69 : $b^*<a^*<c^*$ or $b^*<c^*<a^*$

The table with the k vectors.



The k-vector Types of Group 71 [*Immm*]

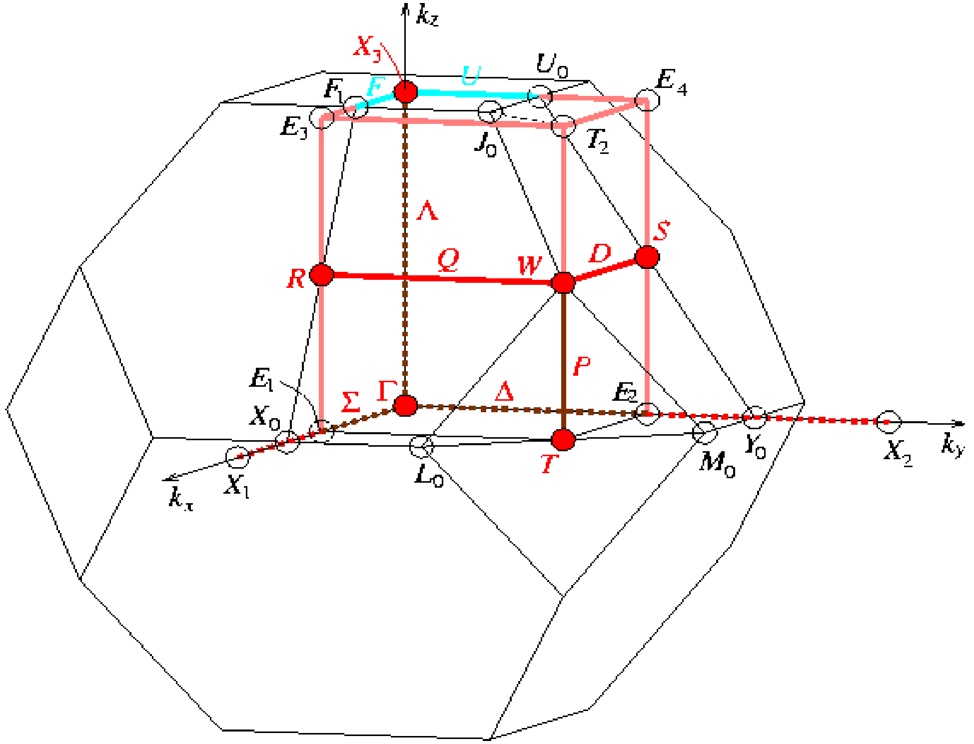
Brillouin zone

(Diagram for arithmetic crystal class mmmI)

(c>b>a or c>a>b) Immm-D_{2h}^{25} (71) to Imma-D_{2h}^{28} (74)

Reciprocal-space group (Fmmm)*, No.69 : $c^*<b^*<a^*$ or $c^*<a^*<b^*$

The table with the k vectors.



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The basis functions of the representations of Space Groups

For constructing the representations of the space groups it is important to start with the basis functions. Let us see how the Bloch functions behave under the action of a general element of the space group $g=\{h|\mathbf{t}_h\}$

$$O(g)\psi^{\mathbf{k}}(\mathbf{r})=\{h\,|\,\mathbf{t}_h\}\psi^{\mathbf{k}}(\mathbf{r})=\psi'(\mathbf{r})$$

To determine the form of the functions $\psi'(\mathbf{r})$ one can see that they should also be Bloch functions with a different **k**-label

$$O(\mathbf{t})\psi'(\mathbf{r})=\{1\,|\,\mathbf{t}\}\psi'(\mathbf{r})=\{1\,|\,\mathbf{t}\}\{h\,|\,\mathbf{t}_h\}\psi^{\mathbf{k}}(\mathbf{r})=\{h\,|\,\mathbf{t}_h\}\{1\,|\,h^{-1}\mathbf{t}\}\psi^{\mathbf{k}}(\mathbf{r})=$$

$$=\{h\,|\,\mathbf{t}_h\}\exp\{2\pi i\,\mathbf{k}\,h^{-1}\mathbf{t}\}\psi^{\mathbf{k}}(\mathbf{r})=\exp\{2\pi i\,\mathbf{k}\,h^{-1}\mathbf{t}\}\{h\,|\,\mathbf{t}_h\}\psi^{\mathbf{k}}(\mathbf{r})=$$

$$=\exp\{2\pi i\;h\mathbf{k}\;\mathbf{t}\}\psi'(\mathbf{r})$$

So that: $O(g)\psi^{\mathbf{k}}(\mathbf{r})=\{h\,|\,\mathbf{t}_h\}\psi^{\mathbf{k}}(\mathbf{r})=\psi^{h\mathbf{k}}(\mathbf{r})$

The Bloch functions also serve as basis functions but the representations are no longer one-dimensional because the Bloch functions whose wave vectors are related by the rotational part of $g\in\mathbf{G}$ belong to a same subspace.

THE STAR OF THE VECTOR K AND THE LITTLE GROUP

The set of non-equivalent **k** vectors obtained by applying the rotational part of the symmetry operators of the space group constitute the so called "star of **k**"

$$\{\mathbf{k}\} = \{\mathbf{k}_1, h_1\mathbf{k}_1, h_2\mathbf{k}_1, h_3\mathbf{k}_1, \ldots\} = \{\mathbf{k}_1, \mathbf{k}_2, \ldots \mathbf{k}_{l_k}\}$$

The $\mathbf{k}_i$ vectors are called the arms of the star. The number l_k is less or equal to the order of the point group $n(\mathbf{G}_0)$

The set of elements $g \in \mathbf{G}$ leaving the **k** vector invariant, or equal to an equivalent vector, form the group $\mathbf{G}_\mathbf{k}$. Called the group of the wave vector (or propagation vector group) or the "little group". It is always a subgroup of **G**. The whole space/point group (little co-group) can be decomposed into cosets of the propagation vector group:

$$\mathbf{G} = \mathbf{G}_\mathbf{k} + g_2\mathbf{G}_\mathbf{k} + \ldots = \sum_{L=1}^{l_k} g_L \mathbf{G}_\mathbf{k} \qquad \mathbf{k}_L = g_L \mathbf{k}$$

$$\mathbf{G}_0 = \mathbf{G}_{0\mathbf{k}} + h_2\mathbf{G}_{0\mathbf{k}} + \ldots = \sum_{L=1}^{l_k} h_L \mathbf{G}_{0\mathbf{k}} \qquad \mathbf{k}_L = h_L \mathbf{k}$$

The representations of G_K and G

We need to know the *irreps* of $\mathbf{G_k}$, $\Gamma^{\mathbf{k}\nu}$, only for the coset representatives (with respect to the translation group) of $\mathbf{G_k}$

$$\mathbf{G_k} = 1\mathbf{T} + g_2\mathbf{T} + g_3\mathbf{T} + \ldots + g_n\mathbf{T}$$

For a general element of $\mathbf{G_k}$ we have:

$$\Gamma^{\mathbf{k}\nu}(g) = \Gamma^{\mathbf{k}\nu}(\{h|\mathbf{t}_h + \mathbf{t}\}) = \Gamma^{\mathbf{k}\nu}(\{1|\mathbf{t}\}\{h|\mathbf{t}_h\}) = \Gamma^{\mathbf{k}\nu}(\{1|\mathbf{t}\})\ \Gamma^{\mathbf{k}\nu}(\{h|\mathbf{t}_h\})$$

$$\Gamma^{\mathbf{k}\nu}(\{h|\mathbf{t}_h + \mathbf{t}\}) = e^{2\pi i\mathbf{k}\,\mathbf{t}}\ \Gamma^{\mathbf{k}\nu}(\{h|\mathbf{t}_h\})$$

The matrices $\Gamma^{\mathbf{k}\nu}$ can be easily calculated from the projective (or *loaded*) representations that are tabulated in the Kovalev book

$$\Gamma^{\mathbf{k}\nu}(g) = \Gamma^{\mathbf{k}\nu}(\{h|\mathbf{t}_h\}) = \Gamma^{\nu}_{proj}(h)\, e^{2\pi i\mathbf{k}\,\mathbf{t}_h}$$

Alternatively they can be calculated using special algorithms (Zak's method)

THE REPRESENTATIONS OF G_K AND G

Let us note the irreducible representations of $\mathbf{G_k}$ as $\Gamma^{\mathbf{k}\nu}$ of dimensionality l_ν .

The basis functions should be of the form: $\psi_i^{\mathbf{k}\nu}(\mathbf{r})=u_{\mathbf{k}i}^{\nu}(\mathbf{r})\exp(-2\pi i\mathbf{kr})$ $(i=1,\ldots l_\nu)$

Under the action of the elements of $\mathbf{G_k}$ the functions transform into each other with the same **k**-vector.

Using the elements of **G** not belonging to $\mathbf{G_k}$ one generates other sets of basis functions: $\psi_i^{\mathbf{k}_1\nu}(\mathbf{r})$; $\psi_i^{\mathbf{k}_2\nu}(\mathbf{r})$; … $\psi_i^{\mathbf{k}_{l_k}\nu}(\mathbf{r})$ that constitute the basis functions of the representations of the total space group.

THE REPRESENTATIONS OF G_K AND G

These representations are labelled by the star of the **k** vector as: $\Gamma^{\{\mathbf{k}\}\nu}$ and are of dimensionality $l_\nu \times l_k$. Each irreducible "small representation" induces an irreducible representation of the total space group. The matrices of the *irreps* are obtained from the small representations of $G_{\mathbf{k}}$. The *induction formula* is:

$$\Gamma^{\{\mathbf{k}\}\nu}_{Li,Mj}(g) = \Gamma^{\mathbf{k}\nu}_{ij}(g_L^{-1} g\, g_M)\,\delta_{g_L^{-1} g\, g_M \in \mathbf{G_k}}$$

The δ symbol is 1 if the subscript condition is true, otherwise is zero

Where the indices *L* and *M* have values runs between 1 and l_k (number of star arms). The indices *i* and *j* run from 1 to dim($\boldsymbol{\Gamma}^{\mathbf{k}\nu}$).

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2: BASIS FUNCTIONS OF A REPRESENTATION

3: REPRESENTATIONS OF THE TRANSLATION GROUP

4: REPRESENTATIONS OF SPACE GROUPS: LITTLE GROUP AND THE STAR OF K

5: REPRESENTATIONS ANALYSIS FOR MAGNETIC STRUCTURES

6: BASIREPS A PROGRAM FOR GETTING IRREPS AND BASIS VECTORS OF THE LITTLE GROUP

Representations Analysis for Magnetic Structures

A reducible representation of the propagation vector group can be constructed by selecting the atoms of a Wyckoff position and applying the symmetry operators to both positions and axial vectors (spins).

This gives rise to the so called Magnetic Representation of dimension: $3n_a$ (being n_a the number of atoms in the primitive cell)

This representation can be decomposed in Irreps and the number of times a particular *Irrep*, Γ^{ν}, is included can be easily calculated

$$\Gamma_{Mag} = \Gamma_{Perm} \otimes \Gamma_{Axial} = \sum_{\oplus \nu} n_{\nu} \, \Gamma^{\nu}$$

$\boxed{\text{The basis functions, for each } \textit{Irrep} \text{ and each sublattice of a Wyckoff site, can be calculated by using the projection operator formula. The basis functions are constant vectors of the form (1,0,0), (0.5, 1,0) … with components referred to the crystallographic unitary frame: } \{\mathbf{a}/a, \mathbf{b}/b, \mathbf{c}/c\} \text{ attached to each sublattice.}}$

The working space for symmetry analysis of magnetic structures: magnetic representation

One can generate a reducible representation of $\mathbf{G_k}$ by considering the complex working space spanned by all the components of $\mathbf{S}_{\mathbf{k}js}$. Each vector has three complex components.

As the atoms belonging to different sites do not mix under symmetry operators, we can treat separately the different sites. The index j is then fixed and the index s varies from 1 to p_j. Being p_j the number of sublattices generated by the site j.

Case α=y and s

The working complex space for site j has dimension $n_j=3\times p_j$ is then spanned by unit vectors $\{\boldsymbol{\varepsilon}^{\mathbf{k}j}{}_{\alpha s}\}$($\alpha$ = 1, 2, 3 –or x, y, z and s = 1… p_j,) represented as column vectors (with a single index n) with zeroes everywhere except for $n=\alpha+3(s-1)$. The n_j vectors refers to the zero-cell.

$$\boldsymbol{\varepsilon}^{\mathbf{k}j}_{ys} = \begin{array}{c}\left(\begin{array}{c}0\\0\\\vdots\\0\\0\\1\\0\\\vdots\\\vdots\\\vdots\\0\\0\end{array}\right)\end{array}\begin{array}{c}x,1\\y,1\\\vdots\\z,s-1\\x,s\\y,s\\z,s\\\vdots\\\vdots\\\vdots\\y,p_j\\z,p_j\end{array}$$

NEUTRONS FOR SOCIETY

THE WORKING SPACE FOR SYMMETRY ANALYSIS OF MAGNETIC STRUCTURES: MAGNETIC REPRESENTATION

One can extend the basis vectors to the whole crystal by using the Bloch propagation then forming column vectors of $n_j \times N$ dimensions:

$$\boldsymbol{\varphi}^{\mathbf{k}j}_{\alpha s} = \sum_{\oplus l} \boldsymbol{\varepsilon}^{\mathbf{k}j}_{\alpha s} \exp(-2\pi i \mathbf{k} \mathbf{R}_l)$$

If one applies the symmetry operators of $\mathbf{G_k}$ to the vectors $\{\boldsymbol{\varepsilon}^{\mathbf{k}j}{}_{\alpha s}\}$, taking into account that they are axial vectors, we obtain another vector (after correcting for the Bloch phase factor if the operator moves the atom outside the reference zero-cell) of the same basis. The matrices $\Gamma^{\mathbf{k}j}{}_{\alpha s, \beta q}(g)$ of dimension $n_j \times n_j = 3p_j \times 3p_j$ corresponding to the different operators constitute what is called the "Magnetic Representation" for the site j and propagation vector $\mathbf{k}$.

The Magnetic Representation

The vectors $\{\boldsymbol{\varepsilon}^j_{\alpha s}\}$ are formed by direct sums (juxtaposition) of normal 3D vectors $\mathbf{u}^j_{\alpha s}$. Applying a symmetry operator to the vector position and the unit spin associated to the atom *js* along the α-axis, changes the index *js* to *jq* and reorient the spin according to the nature of the operator $g=\{h|\mathbf{t}_h\}$ for axial vectors.

$$g\mathbf{r}_s^j = h\mathbf{r}_s^j + \mathbf{t}_h = \mathbf{r}_q^j + \mathbf{a}_{gs}^j ; \quad gs \rightarrow (q, \mathbf{a}_{gs}^j)$$

$$(g\mathbf{u}_{\alpha s}^j)_\beta = \det(h) \sum_n h_{\beta n} (\mathbf{u}_{\alpha s}^j)_n = \det(h) \sum_n h_{\beta n} \delta_{n,\alpha} = \det(h) h_{\beta\alpha}$$

$$O(g)\boldsymbol{\varepsilon}_{\alpha s}^{\mathbf{k}j} = \sum_{\beta q} \Gamma_{\beta q,\alpha s}^{\mathbf{k}j}(g)\, \boldsymbol{\varepsilon}_{\beta q}^{\mathbf{k}j} = \sum_{\beta q} e^{2\pi i \mathbf{k}\,\mathbf{a}_{gs}^j} \det(h) h_{\beta\alpha} \delta_{s,gq}^j \boldsymbol{\varepsilon}_{\beta q}^{\mathbf{k}j}$$

Matrices of the magnetic representation

$$\Gamma_{Mag} \rightarrow \Gamma_{\beta q,\alpha s}^{\mathbf{k}j}(g) = e^{2\pi i \mathbf{k}\,\mathbf{a}_{gs}^j} \det(h) h_{\beta\alpha} \delta_{q,gs}^j$$

The magnetic representation as direct product of permutation and axial representations

An inspection to the explicit expression for the magnetic representation for the propagation vector **k**, the Wyckoff position *j*, with sublattices indexed by (*s*, *q*), shows that it may be considered as the direct product of the permutation representation, of dimension $p_j \times p_j$ and explicit matrices:

$$\Gamma_{Perm} \to P_{qs}^{\mathbf{k}j}(g) = e^{2\pi i \mathbf{k}\,\mathbf{a}_{gs}^{j}}\,\delta_{q,gs}^{j}$$

Permutation representation

by the axial (or in general "vector") representation, of dimension 3, constituted by the rotational part of the $\mathbf{G_k}$ operators multiplied by -1 when the operator $g=\{h|\mathbf{t}_h\}$ corresponds to an improper rotation.

$$\Gamma_{Axial} \to V_{\beta\alpha}(g) = \det(h)h_{\beta\alpha}$$

Axial representation

$$\Gamma_{Mag} \to \Gamma_{\beta q,\alpha s}^{\mathbf{k}j}(g) = e^{2\pi i \mathbf{k}\,\mathbf{a}_{gs}^{j}} \det(h)h_{\beta\alpha}\delta_{q,gs}^{j}$$

Magnetic representation

Basis Functions of the *Irreps* of G_K

The magnetic representation, hereafter called Γ_M irrespective of the indices, can be decomposed in irreducible representations of $\mathbf{G_k}$.

We can calculate a priori the number of possible basis functions of the Irreps of $\mathbf{G_k}$ describing the possible magnetic structures.
This number is equal to the number of times the representation Γ^ν is contained in Γ_M times the dimension of Γ^ν. The projection operators provide the explicit expression of the basis vectors of the *irreps* of $\mathbf{G_k}$

$$\boldsymbol{\psi}_\lambda^{\mathbf{k}\nu}(j) = \frac{1}{n(\mathbf{G_{0k}})} \sum_{g \in \mathbf{G_{0k}}} \Gamma^{*\nu}_{\lambda[\mu]}(g)\, O(g)\, \boldsymbol{\varepsilon}_{\alpha s}^{\mathbf{k}j} \qquad (\lambda = 1, \ldots l_\nu)$$

$$\boldsymbol{\psi}_\lambda^{\mathbf{k}\nu}(j) = \frac{1}{n(\mathbf{G_{0k}})} \sum_{g \in \mathbf{G_{0k}}} \Gamma^{*\nu}_{\lambda[\mu]}(g) \sum_{\beta q} \exp(2\pi i\, \mathbf{k}\, \mathbf{a}_{gs}^{j}) \det(h) h_{\beta\alpha} \delta^{j}_{s,gq} \boldsymbol{\varepsilon}_{\beta q}^{\mathbf{k}j}$$

Basis Functions of the *Irreps* of G_K

It is convenient to use, instead of the basis vectors for the whole set of magnetic atoms in the primitive cell, the so called *atomic components* of the basis vectors, which are normal 3D constant vectors attached to individual atoms:

$$\psi_{\lambda}^{\mathbf{k}\nu}(j) = \sum_{\oplus, s=1,\dots p_j} \mathbf{S}_{\lambda}^{\mathbf{k}\nu}(js)$$

The explicit expression for the atomic components of the basis functions is:

$$\mathbf{S}_{\lambda}^{\mathbf{k}\nu}(js) \propto \sum_{g \in \mathbf{G_{0k}}} \Gamma_{\lambda[\mu]}^{*\nu}(g)\, \mathrm{e}^{2\pi i \mathbf{k}\, \mathbf{a}_{gs}^{j}} \det(h) \delta_{s,g[q]}^{j} \begin{pmatrix} h_{1\alpha} \\ h_{2\alpha} \\ h_{3\alpha} \end{pmatrix}$$

Going beyond G_K: representations of the whole space Group

Up to now we have considered only the *irreps* of the little group. In some cases we can add more constraints considering the representations of the whole space group (or the extended little group). This is a way of connecting split orbits (j and j') due, for instance, to the fact that the operator transforming **k** into –**k** is lost in $\mathbf{G_k}$.

$$\mathbf{G} = \mathbf{G_k} + g_2\mathbf{G_k} + \ldots g_{l_k}\mathbf{G_k} = \sum_{L=1}^{l_k} g_L \mathbf{G_k} = \sum_{L=1}^{l_k} \{h_L \mid \mathbf{t}_{h_L}\}\mathbf{G_k} \qquad \mathbf{k}_L = h_L\mathbf{k}$$

$$Star\ of\ \mathbf{k}:\ \{\mathbf{k}\}=\{\mathbf{k},\ h_2\mathbf{k},\ h_3\mathbf{k},\ \ldots\ h_{l_k}\mathbf{k}\}=\{\mathbf{k}_1,\ \mathbf{k}_2,\ \mathbf{k}_3,\ \ldots\ \mathbf{k}_{l_k}\}$$

The little groups $\mathbf{G}_{\mathbf{k}L}$ are conjugate groups to $\mathbf{G_k}$

$$\mathbf{G}_{\mathbf{k}_L} = g_L \mathbf{G_k} g_L^{-1} \qquad g_L \mathbf{r}_s^j = h_L \mathbf{r}_s^j + \mathbf{t}_{h_L} = \mathbf{r}_q^{j'} + \mathbf{a}_{g_L s}^j$$

$$\boldsymbol{\Gamma}^{\mathbf{k}_L \nu}(g) = \boldsymbol{\Gamma}^{\mathbf{k}\nu}(g_L g g_L^{-1}) \qquad \boldsymbol{\Psi}_\lambda^{\mathbf{k}_L \nu} = O(g_L)\boldsymbol{\Psi}_\lambda^{\mathbf{k}\nu} \qquad (\lambda = 1,\ldots l_\nu)$$

Going beyond G_K: The extended little group

The extended little group $\mathbf{G_{k,-k}}$ corresponds to a part of the full space group in which we add to the little group $\mathbf{G_k}$ the operators transforming **k** into –**k** when –**k is not** in $\mathbf{G_k}$.

Suppose that the operator g_{-k} that does not belong to $\mathbf{G_k}$, transform **k** into –**k**, then the little group is

$$\mathbf{G_{k,-k}} = \mathbf{G_k} + g_{-k}\mathbf{G_k}$$

The representation of the extended little group has dimension $2\dim(\Gamma^{\mathbf{k}\nu})$ and the expression for all elements is a particular case of the general induction formula

$$\Gamma^{\{\mathbf{k,-k}\}\nu}_{Li,Mj}(g) = \Gamma^{\mathbf{k}\nu}_{ij}(g_L^{-1} g\, g_M)\,\delta_{g_L^{-1} g\, g_M \in \mathbf{G_k}}$$

Where the indices L and M have values 1, 2 and g_1=identity and g_2= g_{-k}. The indices i and j run from 1 to $\dim(\Gamma^{\mathbf{k}\nu})$.

Representations of dimensions higher than 1

When the dimension of the irreps is higher than 1, the list of possible basis vectors may be quite high (sum over λ below)

$$\mathbf{S}_{\mathbf{k}js} = \sum_{n\lambda} C^{\nu}_{n\lambda} \mathbf{S}^{\mathbf{k}\ \nu}_{n\lambda}(js)$$

In order to properly select the appropriate basis vectors, and the possible symmetries derived from the representation, the concept of isotropy subgroups and the order parameter direction is of capital importance.

The abstract space in which the matrices of the representation act is formed by vectors **η** of the same dimension. An isotropy subgroup is formed by the operators that leave invariant a particular order parameter vector

$$I^{\nu}_{\boldsymbol{\eta}}(G) = \{\, g \in G \mid \Gamma^{\nu}(g)\boldsymbol{\eta} = \boldsymbol{\eta} \,\}$$

The systematic study of the isotropy subgroups is not implemented in BasIreps, but you can use the ISOTROPY software suite to do the work.

OUTLINE

1: SUMMARY OF GROUP REPRESENTATION THEORY

2: BASIS FUNCTIONS OF A REPRESENTATION

3: REPRESENTATIONS OF THE TRANSLATION GROUP

4: REPRESENTATIONS OF SPACE GROUPS: LITTLE GROUP AND THE STAR OF K

5: REPRESENTATIONS ANALYSIS FOR MAGNETIC STRUCTURES

6: BASIREPS A PROGRAM FOR GETTING IRREPS AND BASIS VECTORS OF THE LITTLE GROUP

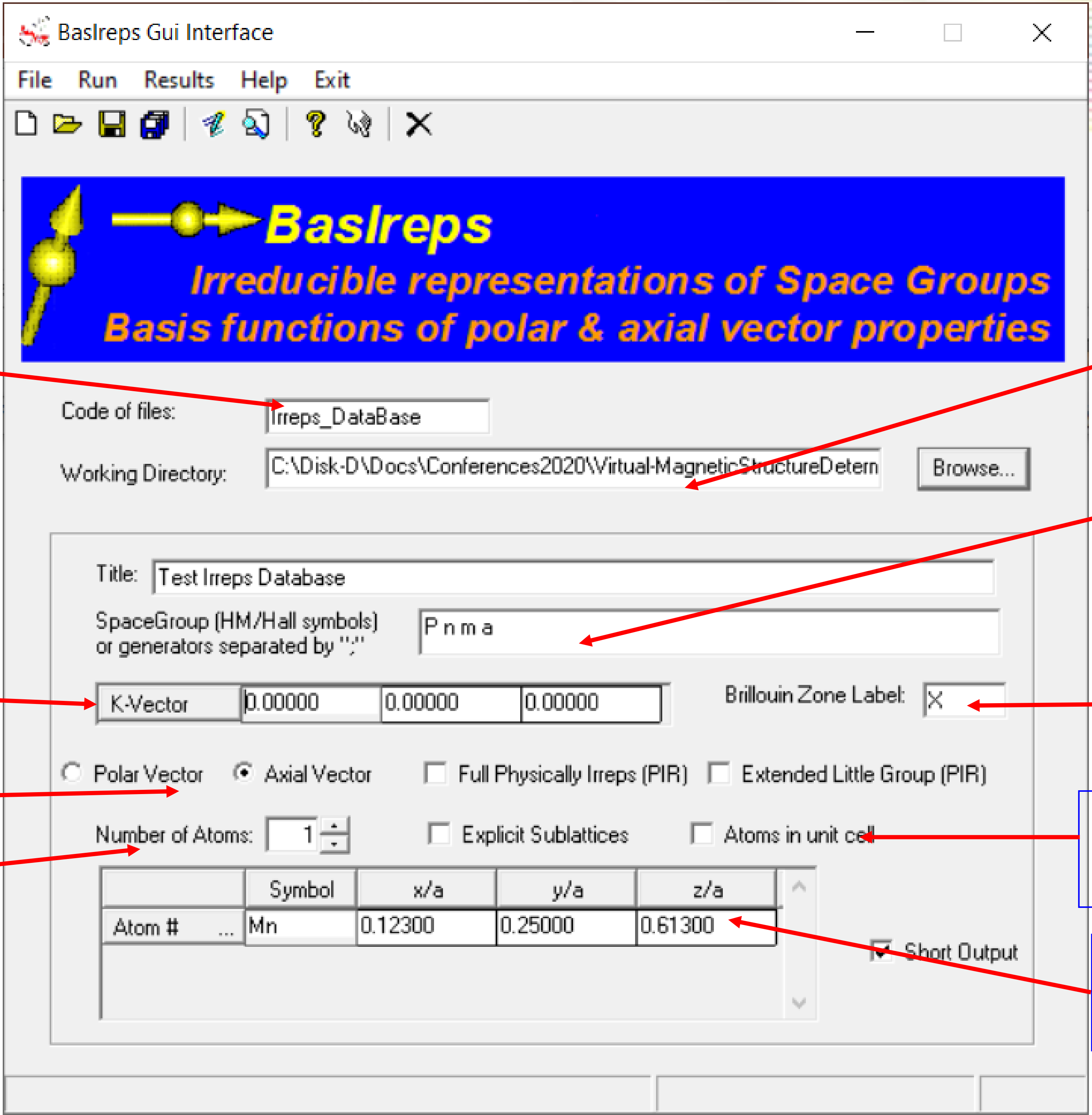
Code of files

Title

k-vector

Axial/polar

Number of atoms



Working directory

Space group symbol or generators

Brillouin Zone label

Atoms in Unit Cell

Atom positions

SOURCE

NEUTRONS FOR SOCIETY

```
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=> Number of generators of space group:   3

GEN(1): -x+1/2,-y,z+1/2
GEN(2): -x,y+1/2,-z
GEN(3): -x,-y,-z

 TRANSLATIONAL COSET REPRESENTATIVES OF SPACE GROUP: P n m a

 Num          Symmetry-Element                     Eqv. Positions
-----------------------------------------------------------------
(  1)   1                                          x,y,z
(  2)   2 (0,0,1/2) 1/4,0,z                        -x+1/2,-y,z+1/2
(  3)   2 (0,1/2,0) 0,y,0                          -x,y+1/2,-z
(  4)   2 (1/2,0,0) x,1/4,1/4                      x-1/2,-y+1/2,-z-1/2
(  5)   -1 0,0,0                                   -x,-y,-z
(  6)   a x,y,1/4                                  x-1/2,y,-z-1/2
(  7)   m x,1/4,z                                  x,-y-1/2,z
(  8)   n (0,1/2,1/2) 1/4,y,z                      -x+1/2,y-1/2,z+1/2

=> The lattice symbol is oP


 The conventional k-vector is
    0.00000     0.00000     0.00000

THE GENERATORS OF THE LITTLE GROUP OF BRILLOUIN ZONE POINT  X

The little group can be generated from the following 3 elements:-

 => GENk(1): -x+1/2,-y,z+1/2
 => GENk(2): -x,y+1/2,-z
 => GENk(3): -x,-y,-z

REPRESENTATIVE ELEMENTS OF THE LITTLE GROUP OF BRILLOUIN ZONE POINT  X

 Operator of Gk Number( 1): x,y,z
 Operator of Gk Number( 2): -x+1/2,-y,z+1/2
 Operator of Gk Number( 3): -x,y+1/2,-z
 Operator of Gk Number( 4): x-1/2,-y+1/2,-z-1/2
 Operator of Gk Number( 5): -x,-y,-z
 Operator of Gk Number( 6): x-1/2,y,-z-1/2
 Operator of Gk Number( 7): x,-y-1/2,z
 Operator of Gk Number( 8): -x+1/2,y-1/2,z+1/2

-----------------------------------------------------------
=> Number of elements of G_k:    8
=> Number of irreducible representations of G_k:    8
=> Dimensions of Ir(reps):   1  1  1  1  1  1  1  1

Line:1  Col:1     NUM  INS
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```
BasIreps Text Editor - [C:\Disk-D\Docs\Conferences2020\Virtual-MagneticStructureDetermination\Talks\Irreps_DataBase.bsr]
File  Edit  Search
=> Number of elements of G_k:    8
=> Number of irreducible representations of G_k:    8
=> Dimensions of Ir(reps):   1  1  1  1  1  1  1  1


   =====================================================================
   Writing of Irreps matrices in symbolic form:  Module:Phase (fractions of 2pi)
   Numeric values of symbols a,b,c,d, ... are given at the end of the table
   =====================================================================

  In this section the translations associated to Seitz symbols are simplified as
     1/2  1/3  2/3  1/4  3/4  1/6  5/6  1/8  3/8  5/8  7/8
      p    q    r    s    t    u    v    w    x    y    z

   The rotational part of Seitz symbols contains information about the orientation as
  defined in Kovalev. The international symbols may be truncated (for format reasons) in
  the table below. The complete international symbols can be found in the previous list.
   Symmetry elements are reduced to the standard form (positive translations < 1)
   The matrices of IRreps have been multiplied by the appropriate phase factor

-------------------------------------------------------------------------------------------
 Ireps          Symmetry operators ->
   v               1            2 (0,0,1/2) 1/4,0,z   2 (0,1/2,0) 0,y,0   2 (1/2,0,0) x,1/4,1/4   -1 0,0,0      a x,y,1/4
   v            {1|000}         {2_00z|p0p}           {2_0y0|0p0}          {2_x00|ppp}             {-1|000}      {m_xy0|p0p}
   v            Symm( 1)        Symm( 2)              Symm( 3)             Symm( 4)                Symm( 5)      Symm( 6)
-------------------------------------------------------------------------------------------

IRrep( 1):         1               1                     1                    1                      1              1

IRrep( 2):         1               1                     1                    1                     -1             -1

IRrep( 3):         1               1                    -1                   -1                      1              1

IRrep( 4):         1               1                    -1                   -1                     -1             -1

IRrep( 5):         1              -1                     1                   -1                      1             -1

IRrep( 6):         1              -1                     1                   -1                     -1              1

IRrep( 7):         1              -1                    -1                    1                      1             -1

IRrep( 8):         1              -1                    -1                    1                     -1              1

Line:1  Col:1     NUM  INS
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This is to be done in a live presentation!