Magnetic structure determination from the combined use of representation analysis and magnetic crystallographic symmetry

Vladimir Pomjakushin

Laboratory for Neutron Scattering and Imaging, LNS, Paul Scherrer Institute

Plan

- Introduction to Representational & magnetic symmetry ways of description

Plan

- Introduction to Representational & magnetic symmetry ways of description
- Morden trends in magnetic structure determination from neutron diffraction ND. Advantages of the combined use of Representation Analysis RA and magnetic subgroups: Shubnikov or 3D+1

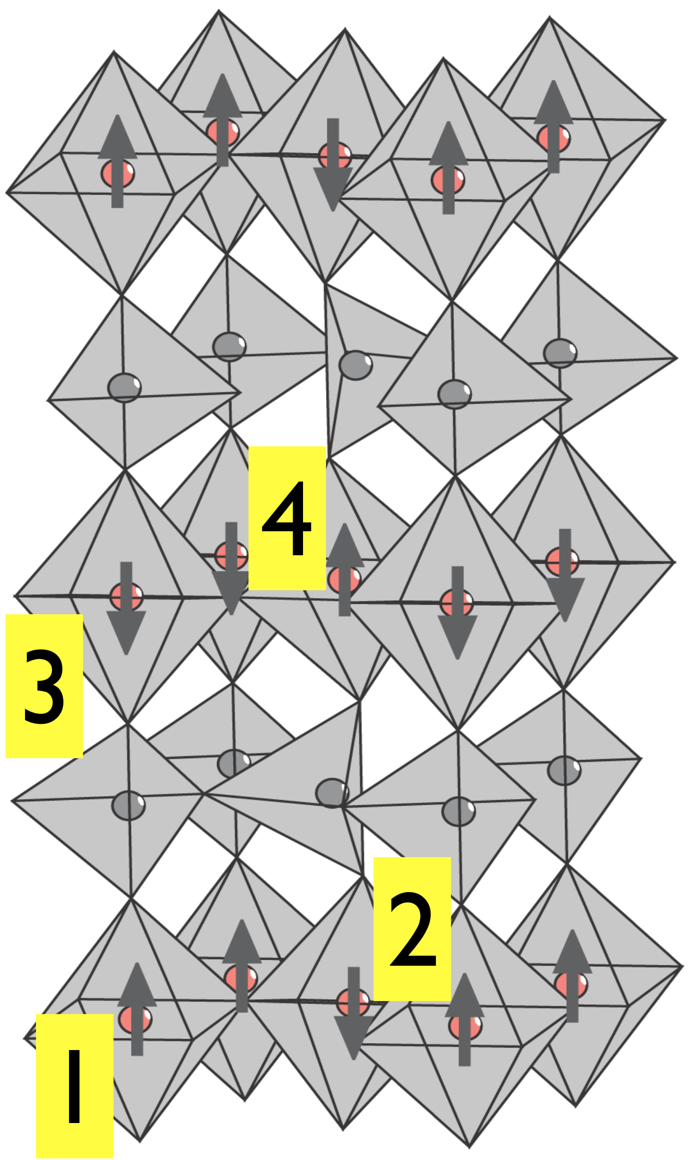
Plan

- Introduction to Representational & magnetic symmetry ways of description
- Morden trends in magnetic structure determination from neutron diffraction ND. Advantages of the combined use of Representation Analysis RA and magnetic subgroups: Shubnikov or 3D+1
- Examples: multiferroic $TmMnO_3$, pyrochlore $Tm_2Mn_2O_5$

Two ways of description of magnetic structures

Magnetic structure is an axial vector function $\mathbf{S}(\mathbf{r})$ defined on the discreet system of points (atoms), e.g. $\mathbf{S}(\mathbf{r}) = \mathbf{s}(\mathbf{r}_1) \oplus \mathbf{s}(\mathbf{r}_2) \oplus \mathbf{s}(\mathbf{r}_3) \oplus \mathbf{s}(\mathbf{r}_4)$

Crystal with space group *G*

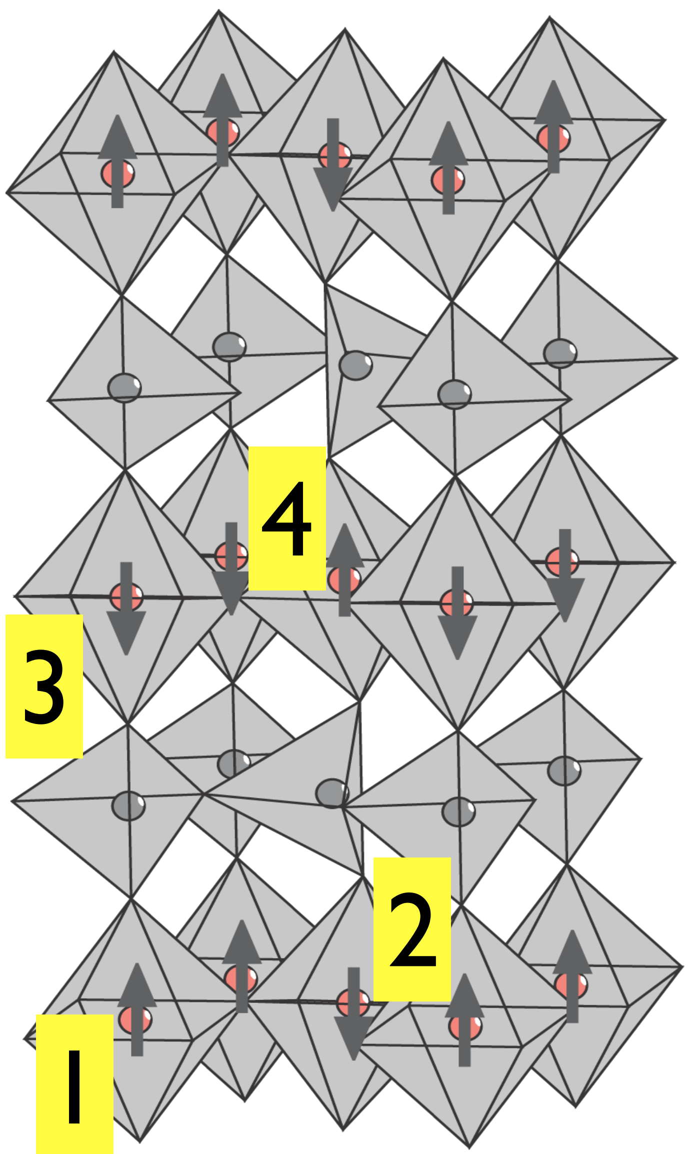


1. How to make $\mathbf{S}(\mathbf{r})$ invariant? Find (new) symmetry elements.
   $g_{new}\,\mathbf{S}(\mathbf{r}) = \mathbf{S}(\mathbf{r})$ to itself, where $g_{new} \in G_{sh}$ subgroup of PG paramagnetic space group: PG=$G\otimes 1'$, where 1'=spin/time reversal, G (parent space group).

Two ways of description of magnetic structures

Magnetic structure is an axial vector function $\mathbf{S}(\mathbf{r})$ defined on the discreet system of points (atoms), e.g. $\mathbf{S}(\mathbf{r}) = \mathbf{s}(\mathbf{r}_1) \oplus \mathbf{s}(\mathbf{r}_2) \oplus \mathbf{s}(\mathbf{r}_3) \oplus \mathbf{s}(\mathbf{r}_4)$

Crystal with space group *G*



1. How to make $\mathbf{S}(\mathbf{r})$ invariant? Find (new) symmetry elements.
   $g_{new}\,\mathbf{S}(\mathbf{r}) = \mathbf{S}(\mathbf{r})$ to itself, where $g_{new} \in G_{sh}$ subgroup of PG paramagnetic space group: PG=$G\otimes 1'$, where 1'=spin/time reversal, G (parent space group).

   or

2. How should $\mathbf{S}(\mathbf{r})$ be transformed under elements of G ?
   $g\mathbf{S}(\mathbf{r}) = \mathbf{S}^{new}{}_{g}(\mathbf{r})$ to different functions for each $g \in G$

Two ways of description of magnetic structures

1. How to make **S**(**r**) invariant?
   g**S**(**r**) = **S**(**r**) to itself, where g ∈ subgroup of PSG paramagnetic space group: PSG=SG⊗1', where 1'=spin/time reversal, SG (parent space group).
2. How should **S**(**r**) be transformed?
   g**S**(**r**) = $\mathbf{S}^{new}{}_{g}(\mathbf{r})$ to different functions for each g ∈ SG

1. **Magnetic or Shubnikov groups MSG.** Historically the first way of description (Landau , Lifshitz 1951). **S**(**r**) invariant under the Shubnikov subgroup G_{sh} of G⊗1' (1'=spin/time reversal). Identifying those symmetry elements that leave S(r) invariant. The MSG symbol looks similar to SG one, e.g. *I4/m'*

Two ways of description of magnetic structures

1. How to make **S**(**r**) invariant?
   g**S**(**r**) = **S**(**r**) to itself, where g ∈ subgroup of PSG paramagnetic space group: PSG=SG⊗1', where 1'=spin/time reversal, SG (parent space group).
2. How should **S**(**r**) be transformed?
   g**S**(**r**) = $\mathbf{S}^{new}{}_g(\mathbf{r})$ to different functions for each g ∈ SG

MSG Example:

87.1.733	I4/m
87.2.734	I4/m1'
87.3.735	I4'/m
87.4.736	I4/m'
87.5.737	I4'/m'
87.6.738	I_P4/m
87.7.739	I_P4'/m
87.8.740	I_P4/m'
87.9.741	I_P4'/m'

1. **Magnetic or Shubnikov groups MSG.** Historically the first way of description (Landau , Lifshitz 1951). S(**r**) invariant under the Shubnikov subgroup G_{sh} of G⊗1' (1'=spin/time reversal). Identifying those symmetry elements that leave S(r) invariant. The MSG symbol looks similar to SG one, e.g. *I4/m'*

Two ways of description of magnetic structures

1. How to make **S**(**r**) invariant?
   g**S**(**r**) = **S**(**r**) to itself, where g ∈ subgroup of PSG paramagnetic space group: PSG=SG⊗1', where 1'=spin/time reversal, SG (parent space group).
2. How should **S**(**r**) be transformed?
   g**S**(**r**) = $\mathbf{S}^{new}{}_{g}(\mathbf{r})$ to different functions for each g ∈ SG

MSG Example:

87.1.733	I4/m
87.2.734	I4/m1'
87.3.735	I4'/m
87.4.736	I4/m'
87.5.737	I4'/m'
87.6.738	I_P4/m
87.7.739	I_P4'/m
87.8.740	I_P4/m'
87.9.741	I_P4'/m'

1. **Magnetic or Shubnikov groups MSG.** Historically the first way of description (Landau , Lifshitz 1951). S(**r**) invariant under the Shubnikov subgroup G_{sh} of G⊗1' (1'=spin/time reversal). Identifying those symmetry elements that leave S(r) invariant. The MSG symbol looks similar to SG one, e.g. *I4/m'*

vs.

2. Representation analysis. (Bertaut 1967) S(**r**) is transformed to $\mathbf{S}^{i}(\mathbf{r})$ under *g* ∈ G (parent space group) according to a single irreducible representation* τ_i of *G.* Identifying/classifying all the functions $\mathbf{S}^{i}(\mathbf{r})$ that appears under all symmetry operators of the same space group G

*each group element *g --> matrix τ(g)*

Two ways of description of magnetic structures

1. How to make $\mathbf{S}(\mathbf{r})$ invariant?
   $g\mathbf{S}(\mathbf{r}) = \mathbf{S}(\mathbf{r})$ to itself, where $g \in$ subgroup of PSG paramagnetic space group: PSG=SG⊗1', where 1'=spin/time reversal, SG (parent space group).
2. How should $\mathbf{S}(\mathbf{r})$ be transformed?
   $g\mathbf{S}(\mathbf{r}) = \mathbf{S}^{new}{}_g(\mathbf{r})$ to different functions for each $g \in$ SG

MSG Example:

87.1.733	I4/m
87.2.734	I4/m1'
87.3.735	I4'/m
87.4.736	I4/m'
87.5.737	I4'/m'
87.6.738	I_P4/m
87.7.739	I_P4'/m
87.8.740	I_P4/m'
87.9.741	I_P4'/m'

1. **Magnetic or Shubnikov groups MSG.** Historically the first way of description (Landau , Lifshitz 1951). S(**r**) invariant under the Shubnikov subgroup G_{sh} of G⊗1' (1'=spin/time reversal). Identifying those symmetry elements that leave S(r) invariant. The MSG symbol looks similar to SG one, e.g. *I4/m'*

vs.

2. Representation analysis. (Bertaut 1967) S(**r**) is transformed to $\mathbf{S}^i(\mathbf{r})$ under $g \in$ G (parent space group) according to a single irreducible representation* τ_i of *G.* Identifying/classifying all the functions $\mathbf{S}^i(\mathbf{r})$ that appears under all symmetry operators of the same space group G

irrep Example:

I4/m, k=0 has 8 1D irreps τ_1,... τ_8.

	h_1	h_{14}	h_4	h_{15}	h_{25}	h_{38}	h_{28}	h_{39}
τ,ψ	1	4_z^+	2_z	4_z^-	-1	-4_z^+	m_z	-4_z^-
τ_2	1	1	1	1	-1	-1	-1	-1
τ_3	1	i	-1	$-i$	1	i	-1	$-i$
τ_5	1	-1	1	-1	1	-1	1	-1
τ_7	1	$-i$	-1	i	1	$-i$	-1	i

*each group element *g --> matrix τ(g)*

Two ways of description of magnetic structures

1. How to make $\mathbf{S}(\mathbf{r})$ invariant?
   $g\mathbf{S}(\mathbf{r}) = \mathbf{S}(\mathbf{r})$ to itself, where $g \in$ subgroup of PSG paramagnetic space group: PSG=SG⊗1', where 1'=spin/time reversal, SG (parent space group).
2. How should $\mathbf{S}(\mathbf{r})$ be transformed?
   $g\mathbf{S}(\mathbf{r}) = \mathbf{S}^{new}{}_{g}(\mathbf{r})$ to different functions for each $g \in$ SG

MSG Example:

87.1.733	I4/m
87.2.734	I4/m1'
87.3.735	I4'/m
87.4.736	I4/m'
87.5.737	I4'/m'
87.6.738	I_P4/m
87.7.739	I_P4'/m
87.8.740	I_P4/m'
87.9.741	I_P4'/m'

1. **Magnetic or Shubnikov groups MSG.** Historically the first way of description (Landau , Lifshitz 1951). <u>S(**r**) invariant under the Shubnikov subgroup G_{sh} of G⊗1'</u> (1'=spin/time reversal). Identifying those symmetry elements that leave S(r) invariant. The MSG symbol looks similar to SG one, e.g. *I4/m'*

vs.

2. Representation analysis. (Bertaut 1967) <u>S(**r**) is transformed to $\mathbf{S}^{i}(\mathbf{r})$ under $g \in$ G (parent space group) according to a single irreducible representation* τ_i of *G*.</u> Identifying/classifying all the functions $\mathbf{S}^{i}(\mathbf{r})$ that appears under all symmetry operators of the same space group G

*each group element *g --> matrix τ(g)*

irrep Example:

I4/m, k=0 has 8 1D irreps τ_1,... τ_8.

	h_1	h_{14}	h_4	h_{15}	h_{25}	h_{38}	h_{28}	h_{39}
τ,ψ	1	4_z^+	2_z	4_z^-	-1	-4_z^+	m_z	-4_z^-
τ_2	1	1	1	1	-1	-1	-1	-1
τ_3	1	i	-1	$-i$	1	i	-1	$-i$
τ_5	1	-1	1	-1	1	-1	1	-1
τ_7	1	$-i$	-1	i	1	$-i$	-1	i

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

In 1960th-70th opposed

E. F. Bertaut, CNRS, Grenoble
Representation Analysis (RA)*

W. Opechovski, UBC, Vancouver
Shubnikov magnetic space groups

even until recent times RA was considered to be more powerful in neutron scattering community.*

---

* Yu.A. Izyumov, V. E. Naish well known papers (1978-), book:, *"Neutron diffraction of magnetic materials"*, New York [etc.]: Consultants Bureau, 1991.

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

In 1960th-70th opposed

E. F. Bertaut, CNRS, Grenoble
Representation Analysis (RA)*

W. Opechovski, UBC, Vancouver
Shubnikov magnetic space groups

even until recent times RA was considered to be more powerful in neutron scattering community.*

Currently > 2010-…

(Representation Analysis) and (Magnetic space groups) are complementary and **must** be used together to fully identify the magnetic symmetry.

---

* Yu.A. Izyumov, V. E. Naish well known papers (1978-), book:, *"Neutron diffraction of magnetic materials"*, New York [etc.]: Consultants Bureau, 1991.

“Old new” trends in magnetic structure determination from ND. **Currently there is solid understanding that both RA and Shubnikov magnetic symmetry should be used together.** Big progress in software tools during last 5 years in this way of analysis …

IUCr Commission on Magnetic Structures

http://magcryst.org

- In some cases this allows one **to find a hidden symmetry**, which is not evident from the representation analysis alone.

“Old new” trends in magnetic structure determination from ND. **Currently there is solid understanding that both RA and Shubnikov magnetic symmetry should be used together.** Big progress in software tools during last 5 years in this way of analysis …

IUCr Commission on Magnetic Structures

http://magcryst.org

- In some cases this allows one **to find a hidden symmetry**, which is not evident from the representation analysis alone.
- Regular practice for crystal structure transitions: This approach is routinely used by crystallographers in the analysis of crystal phase transition,
- Magnetic transitions: Usually, representation approach with a single arm and general direction of order parameter of propagation vector star. Possible high symmetry Shubnikov subgroups are lost.

IUCr Commission on Magnetic Structures

Home | Membership | Meetings | Reports | Resources | Contact | IUCr

IUCr Commission on Magnetic Structures

The Commission on Magnetic Structures (CMS) was established *ad interim* by the Executive Committee in January 2011 and confirmed at the Madrid General Assembly in August 2011. It's primary purpose is to facilitate research on the discovery and communication of magnetic structures in magnetically ordered materials; and its present focus is to cultivate a community consisting of interested participants from diverse fields of research, who can establish standards for defining and communicating the crystallographic details of magnetic structures. The scope of the Commission's consideration encompasses a broad range of magnetic structure types, including commensurate magnetic structures, modulated and otherwise aperiodic magnetic structures, low-dimensional magnetic structures, disordered magnetic structures, etc.

http://magcryst.org

IUCr Commission on Magnetic Structures

Home | Membership | Meetings | Reports | Resources | Contact | IUCr

IUCr Commission on Magnetic Structures

The Commission on Magnetic Structures (CMS) was established *ad interim* by the Executive Committee in January 2011 and confirmed at the Madrid General Assembly in August 2011. It's primary purpose is to facilitate

to establish standards for the description and dissemination of magnetic structures and their underlying symmetries and promote these standards within the IUCr and among other research communities that rely on magnetic structure information.

http://magcryst.org

IUCr Commission on Magnetic Structures

Home | Membership | Meetings | Reports | Resources | Contact | IUCr

IUCr Commission on Magnetic Structures

The Commission on Magnetic Structures (CMS) was established *ad interim* by the Executive Committee in January 2011 ar ... ... bly in August 2011. It's primary purpose is to f...

http://magcryst.org

Symmetry heavyweights:
Software tools for detailed symmetry analysis both RA and Shubnikov, superspace 3D+1

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,

http://stokes.byu.edu/iso/

Bilbao Crystallographic Server
http://www.cryst.ehu.es
University of the Basque Country

Membership

- **B. Campbell** (Chair, USA)
- A. Cornia (Italy)
- D. B. Litvin (USA)
- J.M. Perez-Mato (Spain)
- V. Petricek (Czech Republic)
- A. Pirogov (Russia)
- V. Pomjakushin (Switzerland)
- J. Rodriguez-Carvajal (France)
- T. Sato (Japan)
- W. Sikora (Poland)
- A.S. Wills (UK)

Consultants

- M.I. Aroyo (Spain)
- J. Brown (France)
- M.T. Fernandez-Diaz (France)
- H.T. Stokes (USA)

IUCr Congress SatelliteWorkshop (Hamilton, Canada) on the Role of Magnetic Symmetry in the Description & Determination of Magnetic Structures
http://magcryst.org
http://magcryst.org/meetings/cmsworkshop2014/program/

Downloadable Lecture Presentations on:
The use of magnetic space groups and superspace groups, and magnetic irreducible representations, to constrain general magnetic-structure models. New magnetic-symmetry resources and capabilities for solving/refining magnetic structures.

IUCr Commission on Magnetic Structures

Home | Membership | Meetings | Reports | Resources | Contact | IUCr

IUCr Commission on Magnetic Structures

The Commission on Magnetic Structures (CMS) was established *ad interim* by the Executive Committee in January 2011 ar ... bly in August 2011 . It's primary purpose is to f

http://magcryst.org

Symmetry heavyweights:
Software tools for detailed symmetry analysis both RA and Shubnikov, superspace 3D+1

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,

http://stokes.byu.edu/iso/

Bilbao Crystallographic Server

http://www.cryst.ehu.es

University of the Basque Country

Software tools for symmetry analysis and data fitting

Jana2006 http://jana.fzu.cz

Fullprof suite http://www.ill.eu/sites/fullprof/

MODY http://www.ftj.agh.edu.pl/~sikora/modyopis.htm

SARAh suite https://dl.dropboxusercontent.com/u/8933134/Website/Site/Software/Software.html

Membership

- **B. Campbell** (Chair, USA)
- A. Cornia (Italy)
- D. B. Litvin (USA)
- J.M. Perez-Mato (Spain)
- V. Petricek (Czech Republic)
- A. Pirogov (Russia)
- V. Pomjakushin (Switzerland)
- J. Rodriguez-Carvajal (France)
- T. Sato (Japan)
- W. Sikora (Poland)
- A.S. Wills (UK)

Consultants

- M.I. Aroyo (Spain)
- J. Brown (France)
- M.T. Fernandez-Diaz (France)
- H.T. Stokes (USA)

IUCr Congress SatelliteWorkshop (Hamilton, Canada) on the Role of Magnetic Symmetry in the Description & Determination of Magnetic Structures

http://magcryst.org

http://magcryst.org/meetings/cmsworkshop2014/program/

Downloadable Lecture Presentations on:
The use of magnetic space groups and superspace groups, and magnetic irreducible representations, to constrain general magnetic-structure models. New magnetic-symmetry resources and capabilities for solving/refining magnetic structures.

Representation* Analysis (RA). Propagation vector k formalism. Magnetic mode S_0 is specified in zeroth block of the cell == parent cell without centering translations

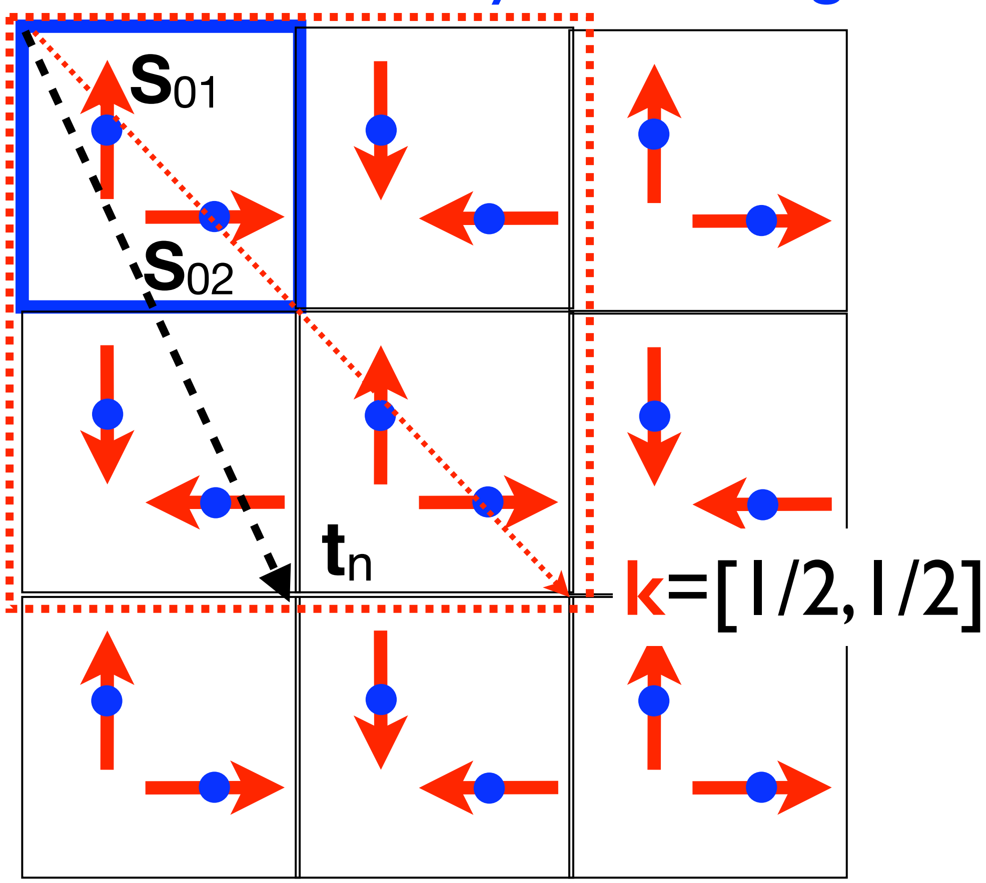
Magnetic moment
below a phase transition

$$\mathbf{S}(\mathbf{t}_n) = Re\left(C\mathbf{S}_0 e^{2\pi i \mathbf{t}_n \mathbf{k}}\right) \sim \cos(2\pi \mathbf{t}_n \mathbf{k} + \varphi)$$

amplitude or mixing coefficients

magnetic mode

0th cell with many atoms in general

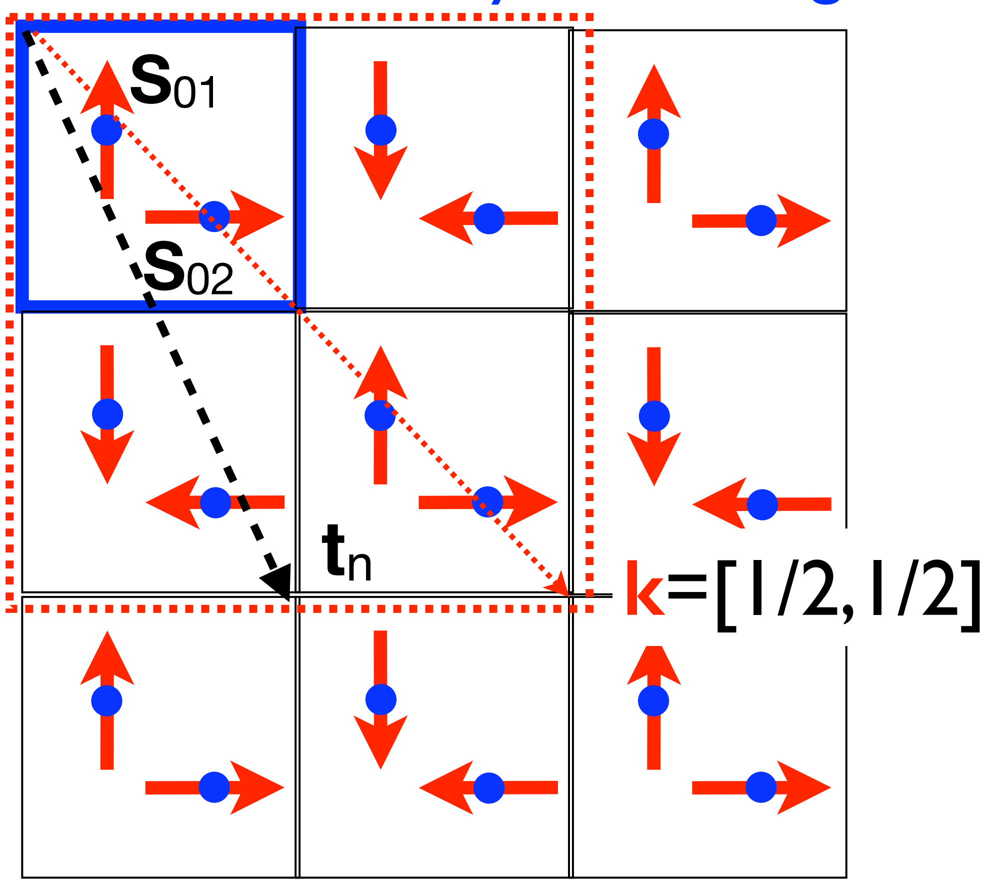


*irreducible representation irrep:
each group element *g* --> *matrix τ(g)* that
specifies the spin transformation under element *g*

Representation* Analysis (RA). Propagation vector k formalism. Magnetic mode S_0 is specified in zeroth block of the cell == parent cell without centering translations

Magnetic moment
below a phase transition

0th cell with many atoms in general



$$\mathbf{S}(\mathbf{t}_n) = Re\left(C\mathbf{S}_0 e^{2\pi i \mathbf{t}_n \mathbf{k}}\right) \sim \cos(2\pi \mathbf{t}_n \mathbf{k} + \varphi)$$

amplitude or mixing coefficients

magnetic mode

magnetic mode S_0 for chosen irrep* specifies magnetic configuration of all spins in zeroth cell $\longrightarrow$ $S_0 = \begin{pmatrix} s_{x1} \\ s_{y1} \\ s_{z1} \\ s_{x2} \\ s_{y2} \\ s_{z2} \\ \cdots \\ \cdots \\ \cdots \\ s_{xN} \\ s_{yN} \\ s_{zN} \end{pmatrix}$

*irreducible representation irrep:
each group element *g* --> *matrix τ(g)* that
specifies the spin transformation under element *g*

Representation* Analysis (RA). Propagation vector k formalism. Magnetic mode S_0 is specified in zeroth block of the cell == parent cell without centering translations

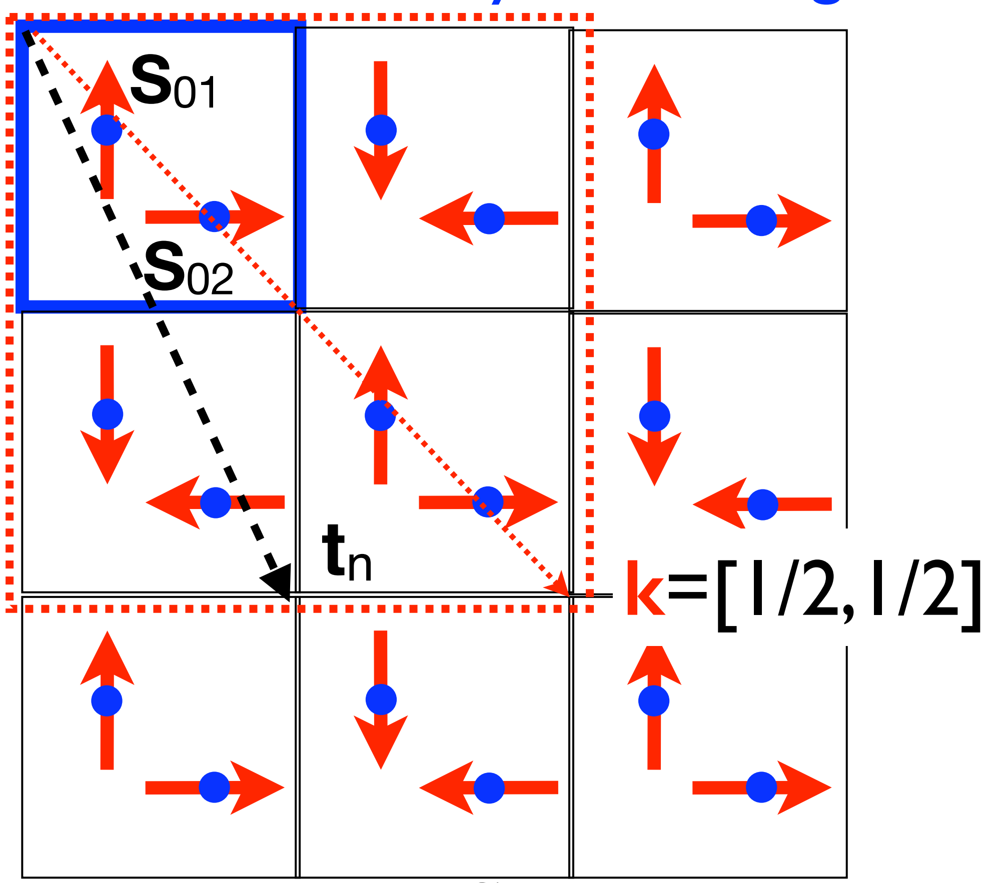
Magnetic moment below a phase transition

$$\mathbf{S}(\mathbf{t}_n) = Re\left(C\mathbf{S}_0 e^{2\pi i \mathbf{t}_n \mathbf{k}}\right) \sim \cos(2\pi \mathbf{t}_n \mathbf{k} + \varphi)$$

amplitude or mixing coefficients

magnetic mode

0th cell with many atoms in general



E.g., atom1 $\mathbf{S}_{01} = \mathbf{e}_y$

atom2 $\mathbf{S}_{02} = \mathbf{e}_x$

$$\mathbf{S}_1(\mathbf{t}_n) = C\mathbf{e}_y \cos(\pi(t_{nx} + t_{ny}))$$

$$\mathbf{S}_2(\mathbf{t}_n) = C\mathbf{e}_x \cos(\pi(t_{nx} + t_{ny}))$$

magnetic mode $\mathbf{S}_0$ for chosen irrep* specifies magnetic configuration of all spins in zeroth cell $\longrightarrow$

$$\mathbf{S}_0 = \begin{pmatrix} s_{x1} \\ s_{y1} \\ s_{z1} \\ s_{x2} \\ s_{y2} \\ s_{z2} \\ \cdots \\ \cdots \\ \cdots \\ s_{xN} \\ s_{yN} \\ s_{zN} \end{pmatrix}$$

Representation* Analysis (RA). Propagation vector k formalism. Magnetic mode S_0 is specified in zeroth block of the cell == parent cell without centering translations

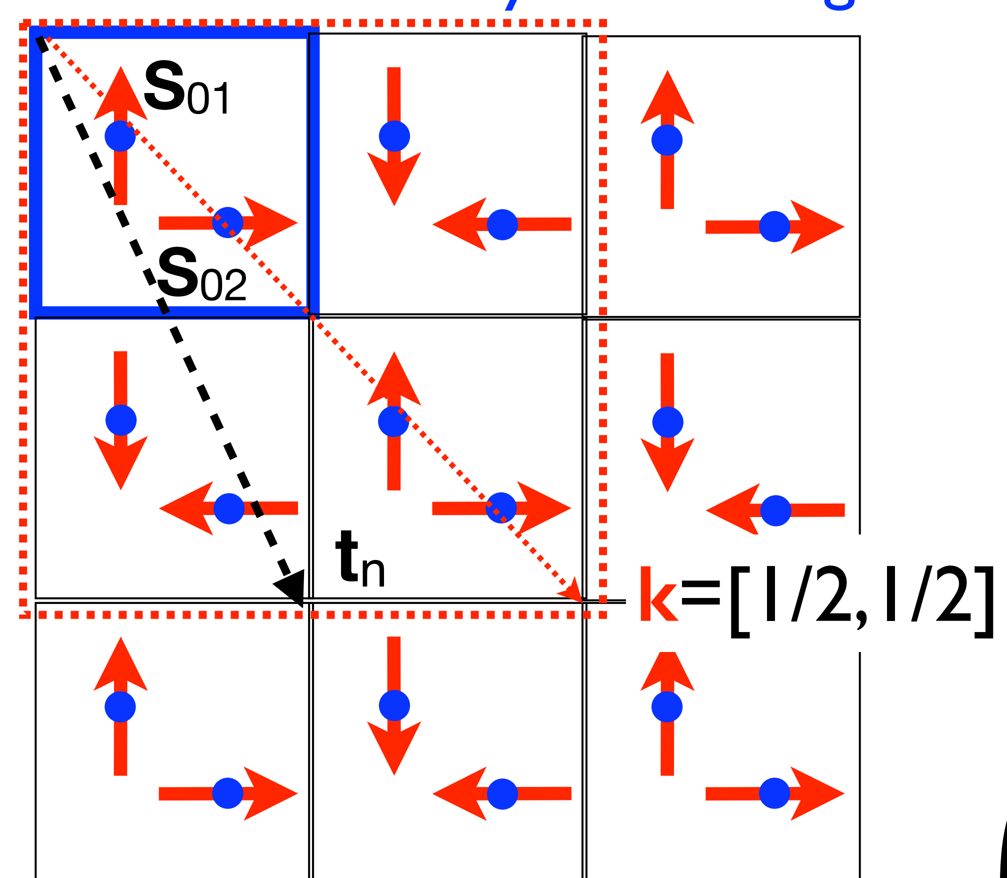
Magnetic moment below a phase transition

$$\mathbf{S}(\mathbf{t}_n) = Re\left(C\mathbf{S}_0 e^{2\pi i \mathbf{t}_n \mathbf{k}}\right) \quad \sim \cos(2\pi \mathbf{t}_n \mathbf{k} + \varphi)$$

amplitude or mixing coefficients

magnetic mode

0th cell with many atoms in general



magnetic mode $\mathbf{S}_0$ for chosen irrep* specifies magnetic configuration of all spins in zeroth cell

$$\mathbf{S}_0 = \begin{pmatrix} s_{x1} \\ s_{y1} \\ s_{z1} \\ s_{x2} \\ s_{y2} \\ s_{z2} \\ \cdots \\ \cdots \\ \cdots \\ s_{xN} \\ s_{yN} \\ s_{zN} \end{pmatrix}$$

E.g., atom1 $\mathbf{S}_{01} = \mathbf{e}_y$

atom2 $\mathbf{S}_{02} = \mathbf{e}_x$

$$\mathbf{S}_0 = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}$$

$$\mathbf{S}_1(\mathbf{t}_n) = C\mathbf{e}_y \cos(\pi(t_{nx} + t_{ny}))$$

$$\mathbf{S}_2(\mathbf{t}_n) = C\mathbf{e}_x \cos(\pi(t_{nx} + t_{ny}))$$

Representation* Analysis (RA). Propagation vector k formalism. Magnetic mode S_0 is specified in zeroth block of the cell == parent cell without centering translations

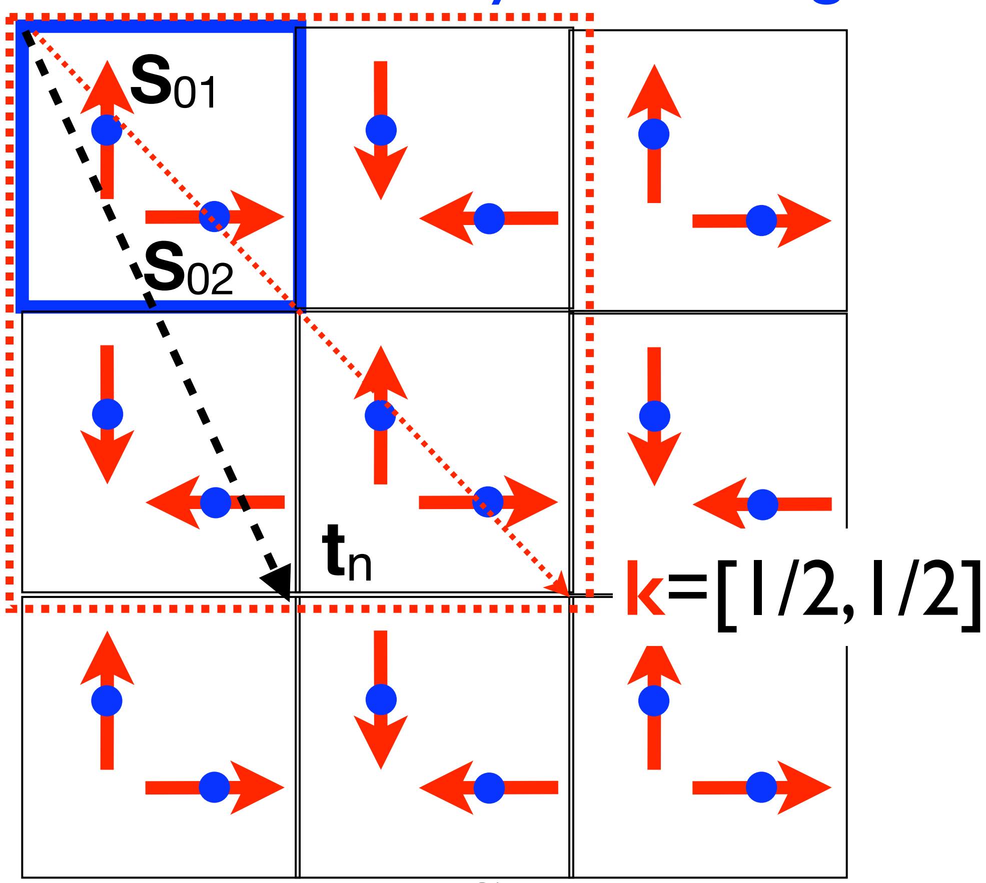
Magnetic moment below a phase transition

$$\mathbf{S}(\mathbf{t}_n) = Re\left(C\mathbf{S}_0 e^{2\pi i \mathbf{t}_n \mathbf{k}}\right) \sim \cos(2\pi \mathbf{t}_n \mathbf{k} + \varphi)$$

amplitude or mixing coefficients

magnetic mode

0th cell with many atoms in general



magnetic mode $\mathbf{S}_0$ for chosen irrep* specifies magnetic configuration of all spins in zeroth cell $\longrightarrow$

$$\mathbf{S}_0 = \begin{pmatrix} s_{x1} \\ s_{y1} \\ s_{z1} \\ s_{x2} \\ s_{y2} \\ s_{z2} \\ \cdots \\ \cdots \\ \cdots \\ s_{xN} \\ s_{yN} \\ s_{zN} \end{pmatrix}$$

$\mathbf{S}_0$ and $C = |C|e^{i\varphi}$ are complex quantities

$$s_{x1} = |s_{x1}|e^{i\phi_{x1}}\mathbf{e}_x$$
$$s_{y1} = |s_{y1}|e^{i\phi_{y1}}\mathbf{e}_y$$
$$\cdots$$
$$s_{zN} = |s_{zN}|e^{i\phi_{zN}}\mathbf{e}_z$$

E.g., atom1 $\mathbf{S}_{01} = \mathbf{e}_y$

atom2 $\mathbf{S}_{02} = \mathbf{e}_x$

$$\mathbf{S}_0 = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}$$

$$\mathbf{S}_1(\mathbf{t}_n) = C\mathbf{e}_y \cos(\pi(t_{nx} + t_{ny}))$$
$$\mathbf{S}_2(\mathbf{t}_n) = C\mathbf{e}_x \cos(\pi(t_{nx} + t_{ny}))$$

Representation* Analysis (RA). Propagation vector k formalism. Magnetic mode S_0 is specified in zeroth block of the cell == parent cell without centering translations

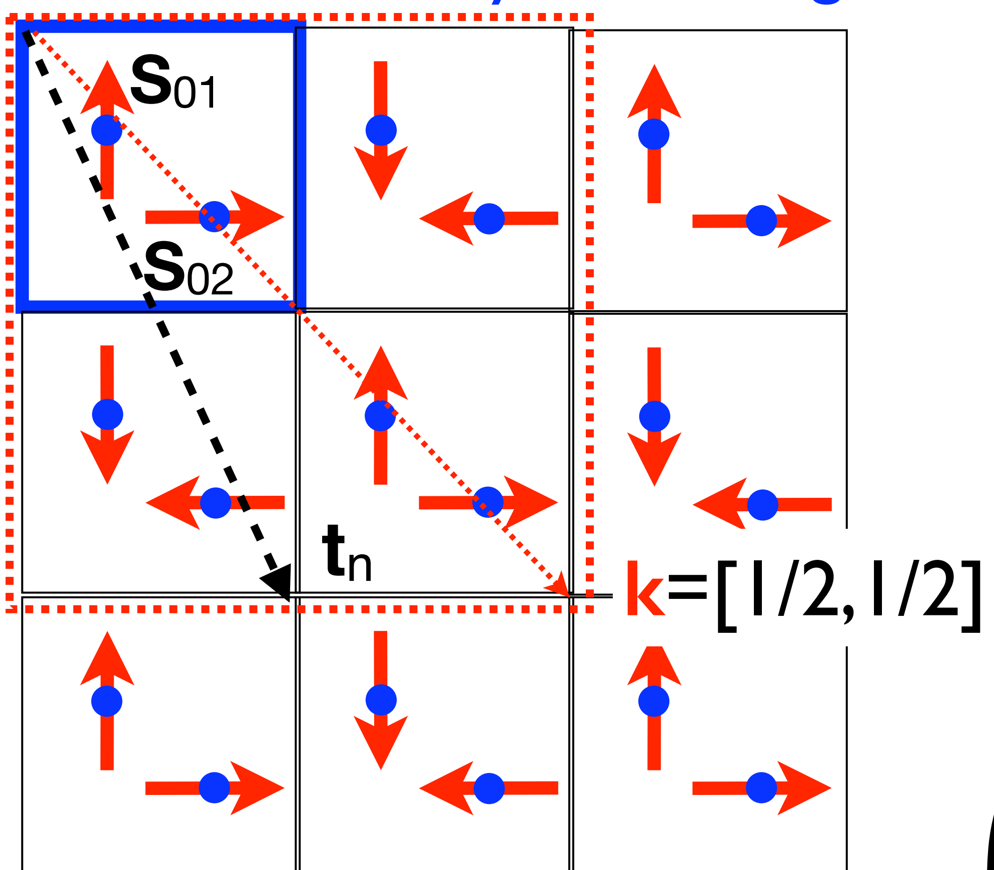
Magnetic moment below a phase transition

$$\mathbf{S}(\mathbf{t}_n) = Re\left(C\mathbf{S}_0 e^{2\pi i \mathbf{t}_n \mathbf{k}}\right) \quad \sim \cos(2\pi \mathbf{t}_n \mathbf{k} + \varphi)$$

amplitude or mixing coefficients

magnetic mode

0th cell with many atoms in general



magnetic mode $\mathbf{S}_0$ for chosen irrep* specifies magnetic configuration of all spins in zeroth cell $\longrightarrow$ $\mathbf{S}_0 = \begin{pmatrix} s_{x1} \\ s_{y1} \\ s_{z1} \\ s_{x2} \\ s_{y2} \\ s_{z2} \\ \cdots \\ \cdots \\ \cdots \\ s_{xN} \\ s_{yN} \\ s_{zN} \end{pmatrix}$

$\mathbf{S}_0$ and $C = |C|e^{i\varphi}$ are complex quantities

$$s_{x1} = |s_{x1}|e^{i\phi_{x1}}\mathbf{e}_x$$
$$s_{y1} = |s_{y1}|e^{i\phi_{y1}}\mathbf{e}_y$$
$$\ldots$$
$$s_{zN} = |s_{zN}|e^{i\phi_{zN}}\mathbf{e}_z$$

E.g., atom1 $\mathbf{S}_{01} = \mathbf{e}_y$

atom2 $\mathbf{S}_{02} = \mathbf{e}_x$ $\qquad \mathbf{S}_0 = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}$

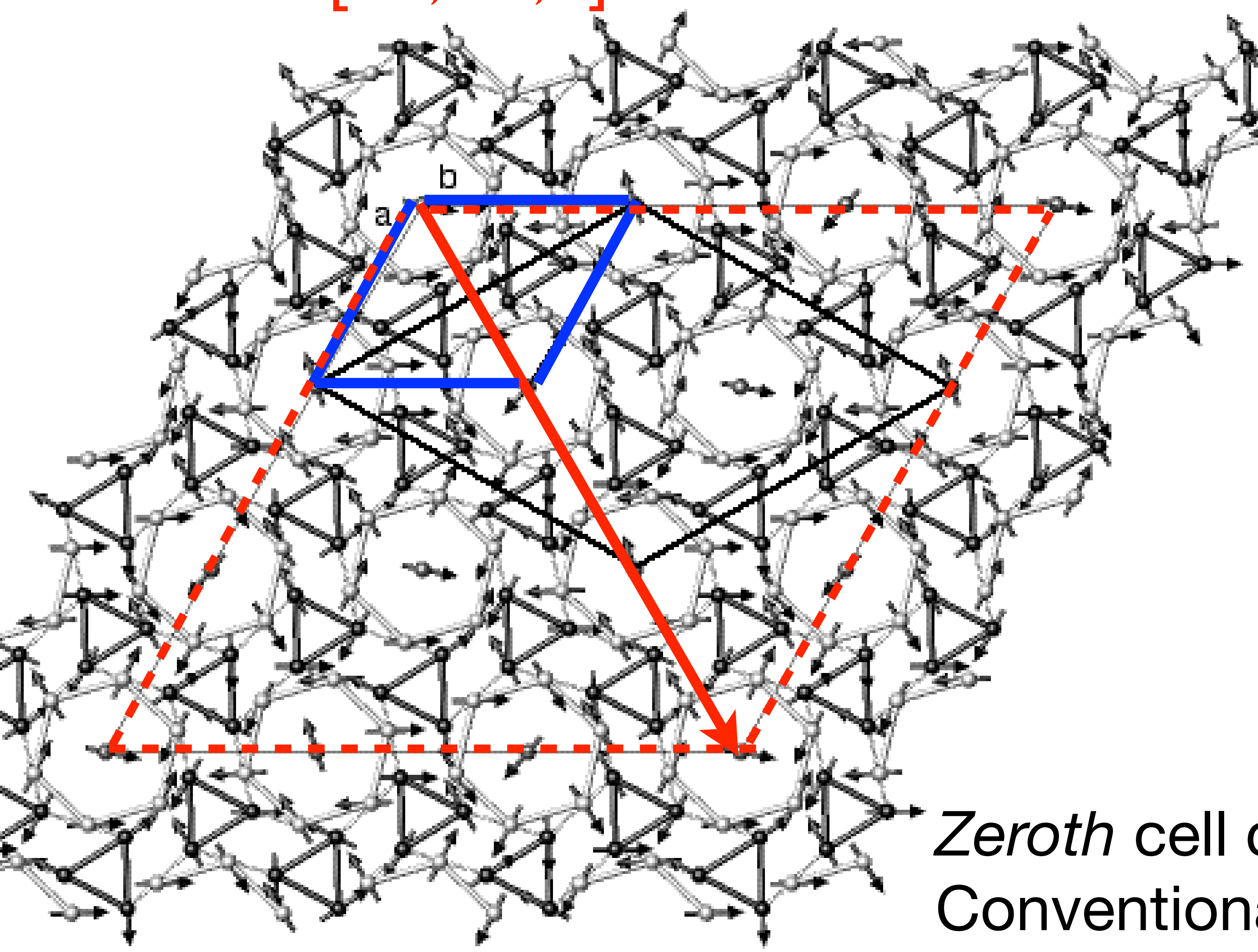
$$\mathbf{S}_1(\mathbf{t}_n) = C\mathbf{e}_y \cos(\pi(t_{nx} + t_{ny}))$$
$$\mathbf{S}_2(\mathbf{t}_n) = C\mathbf{e}_x \cos(\pi(t_{nx} + t_{ny}))$$

Example of complex magnetic structure

Antiferromagnetic (cycloidal spiral) three sub-lattice ordering in $Tb_{14}Au_{51}$

P6/m

k-vector=[1/3, 1/3, 0]



PHYSICAL REVIEW B 72, 134413 (2005)

Zeroth cell:
only 5 magnetic modes, i.e. 5 mixing coefficients C to find from experiment.

Zeroth cell contains 14 spins of Tb^{3+}
Conventional magnetic unit cell contains 126 spins of Tb^{3+}!!

what if several magnetic modes S_0 are possible in RA?

....

what if several magnetic modes S_0 are possible in RA?

Two commensurate cases when k="rational fraction"

1. multi-dimentional (nD) irreducible representation generates *nD* magnetic modes $\boldsymbol{S}_0{}^1$, $\boldsymbol{S}_0{}^2$, $\boldsymbol{S}_0{}^3$... $\boldsymbol{S}_0{}^{nD}$

$$\mathbf{S}(0) \sim \sum_{l=1}^{nD} C_l \mathbf{S}_0^l$$

....

what if several magnetic modes S_0 are possible in RA?

Two commensurate cases when k="rational fraction"

1. multi-dimentional (nD) irreducible representation generates *nD* magnetic modes $\boldsymbol{S}_0^1$, $\boldsymbol{S}_0^2$, $\boldsymbol{S}_0^3$... $\boldsymbol{S}_0^{nD}$

$$\mathbf{S}(0) \sim \sum_{l=1}^{nD} C_l \mathbf{S}_0^l$$

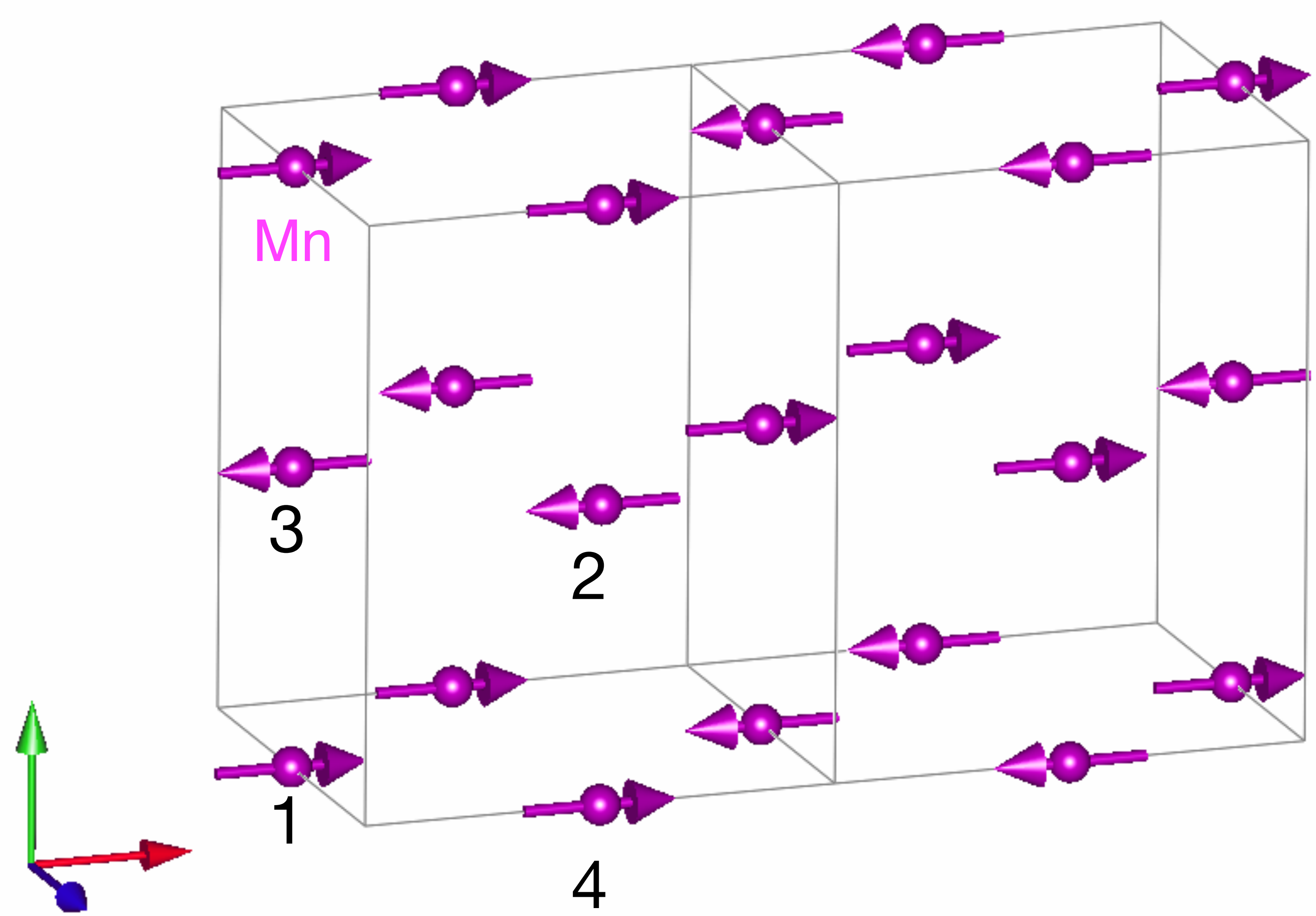
$$\boxed{\text{any relations between mixing coefficients } C_l \quad ?}$$

....

$TmMnO_3$
Two magnetic modes E_1 and E_2 along x.

Mn-position	(1) $0,0,\frac{1}{2}$	(2) $\frac{1}{2},\frac{1}{2},0$	(3) $0,\frac{1}{2},\frac{1}{2}$	(4) $\frac{1}{2},0,0$
$S_0^1 == E_1 =$	+1	+1	-1	-1
$S_0^2 == E_2 =$	+1	-1	-1	+1

Pnma k=[1/2,0,0], k20, *X*
irreps: two **2D** τ_1, τ_2
Mn mΓ: $\underline{3\tau_1} \oplus 3\tau_2$



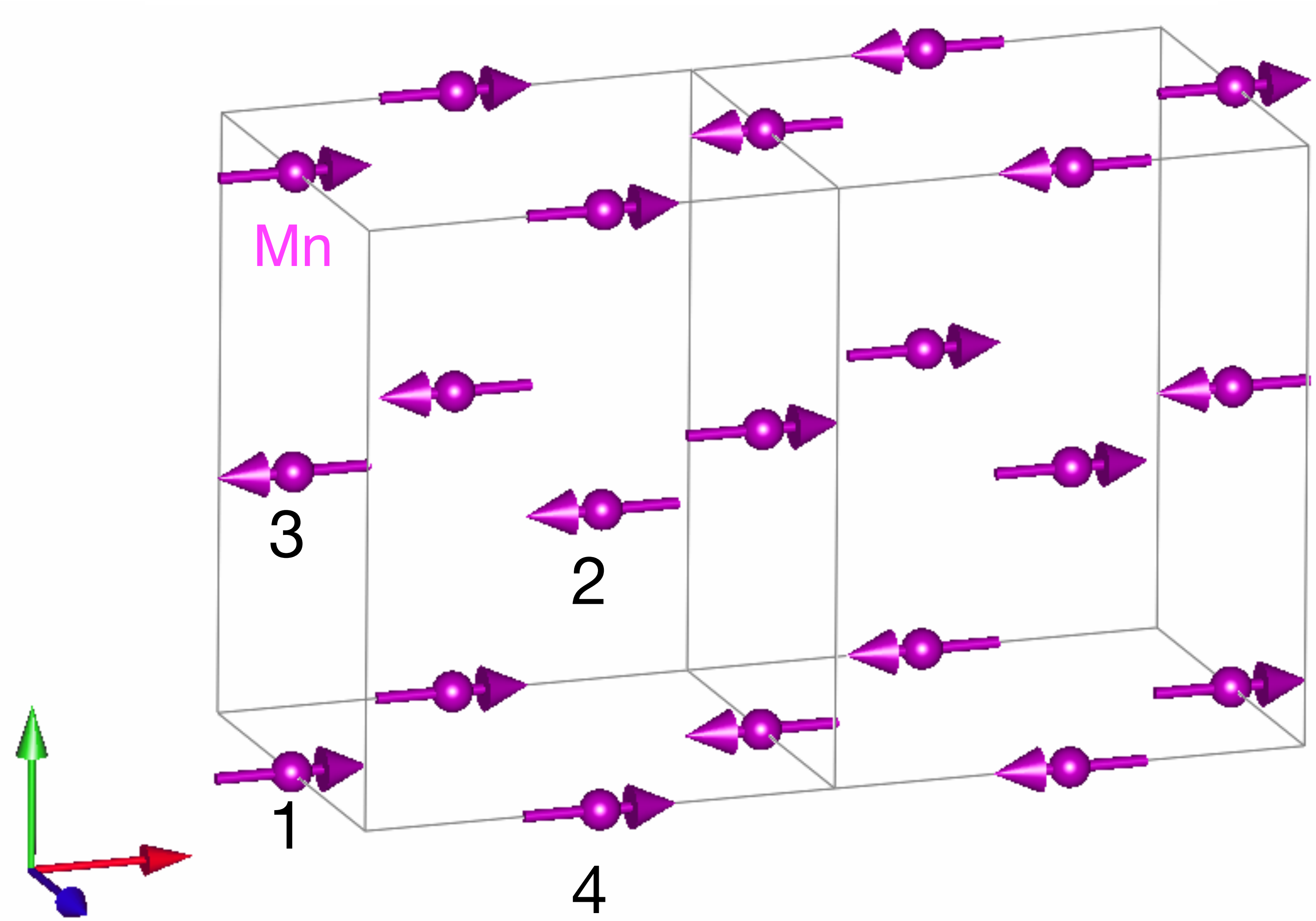
$TmMnO_3$
Two magnetic modes E_1 and E_2 along x.

Mn-position	(1) $0,0,\frac{1}{2}$	(2) $\frac{1}{2},\frac{1}{2},0$	(3) $0,\frac{1}{2},\frac{1}{2}$	(4) $\frac{1}{2},0,0$
$S_0^1 == E_1 =$	+1	+1	-1	-1
$S_0^2 == E_2 =$	+1	-1	-1	+1

Any linear combination, in general

$C_1E_1+C_2E_2$ =	C_1+C_2	C_1-C_2	$-C_1-C_2$	C_1+C_2
$(E_1+E_2)/2$ =	+1	0	-1	0
$(E_1-E_2)/2$ =	0	+1	0	-1

Pnma k=[1/2,0,0], k20, *X*
irreps: two **2D** τ_1, τ_2
Mn mΓ: $\underline{3\tau_1} \oplus 3\tau_2$



$TmMnO_3$
Two magnetic modes E_1 and E_2 along x.

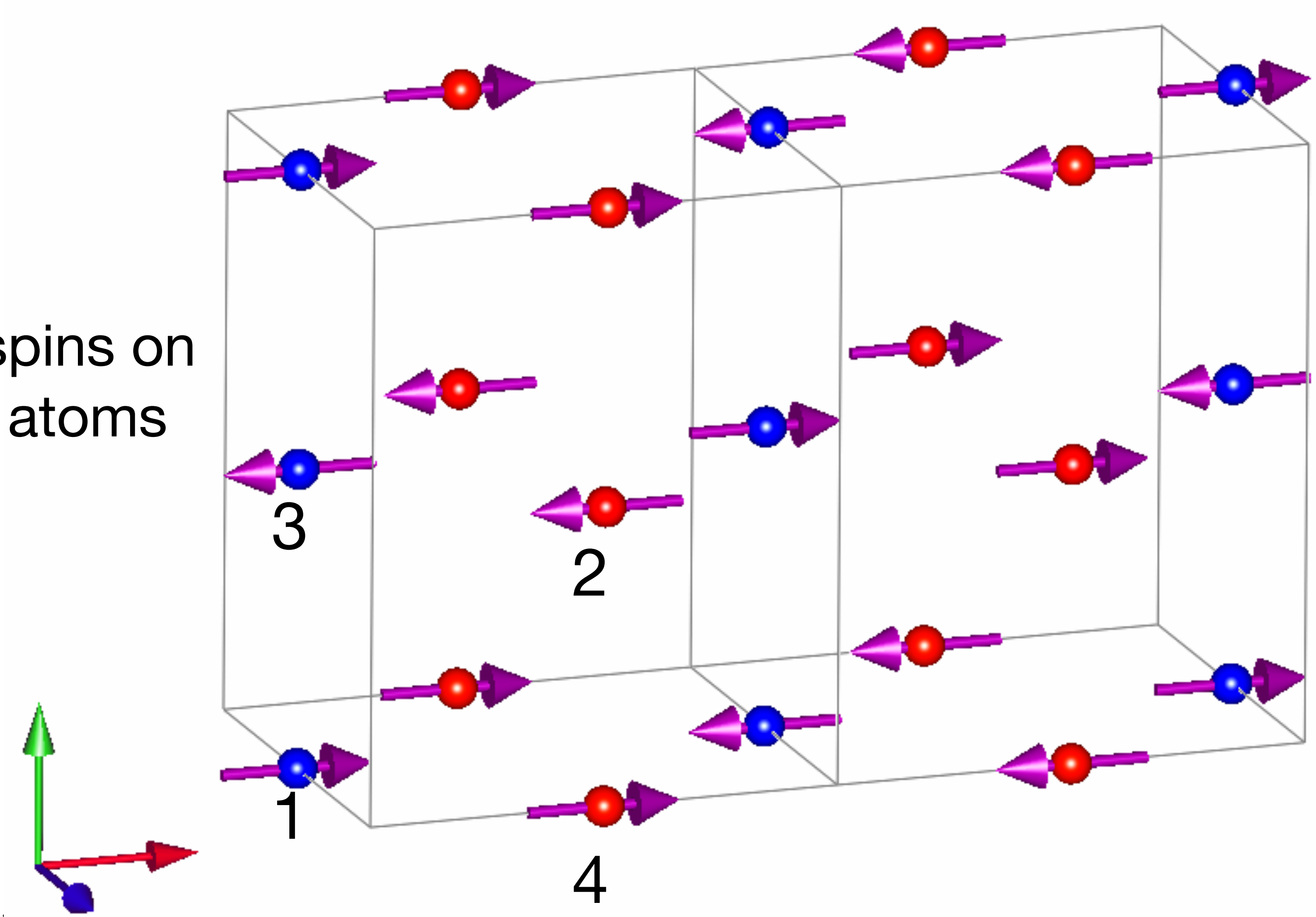
Mn-position	(1) $0,0,\frac{1}{2}$	(2) $\frac{1}{2},\frac{1}{2},0$	(3) $0,\frac{1}{2},\frac{1}{2}$	(4) $\frac{1}{2},0,0$
$S_0^1 == E_1 =$	+1	+1	-1	-1
$S_0^2 == E_2 =$	+1	-1	-1	+1

Any linear combination, in general

$C_1E_1+C_2E_2 =$	C_1+C_2	C_1-C_2	$-C_1-C_2$	C_1+C_2
$(E_1+E_2)/2 =$	+1	0	-1	0
$(E_1-E_2)/2 =$	0	+1	0	-1

Pnma k=[1/2,0,0], k20, *X*
irreps: two **2D** τ_1, τ_2
Mn mΓ: $\underline{3\tau_1} \oplus 3\tau_2$

independent spins on red and blue atoms



what if several magnetic modes S_0^1, S_0^2, S_0^3… are possible in RA?

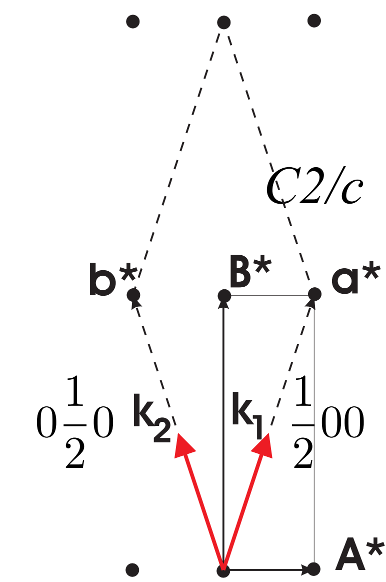
Two commensurate cases when k="rational fraction"

1. multi-dimentional (nD) irreducible representation generates *nD* magnetic modes S_0^1, S_0^2, S_0^3… S_0^{nD}

$$\mathbf{S}(0) \sim \sum_{l=1}^{nD} C_l \mathbf{S}_0^l$$

2. multi-*Arm*/multi-**k** structure (non-equivalent $\mathbf{k}_1$, $\mathbf{k}_2$, … $\mathbf{k}_m$). *nA* magnetic modes $\boldsymbol{S}_0^1$, $\boldsymbol{S}_0^2$, $\boldsymbol{S}_0^3$… $\boldsymbol{S}_0^{nA}$

RA: widespread unfavorable paradigm that one-**k** is enough…



Example of mutiarm, full star {$\mathbf{k}_1$,$\mathbf{k}_2$}: J. Phys.: Condens. Matter **26** 496002

any relations between mixing coefficients C_l ?

what if several magnetic modes S_0^1, S_0^2, S_0^3… are possible in RA?

Two commensurate cases when k=“rational fraction”

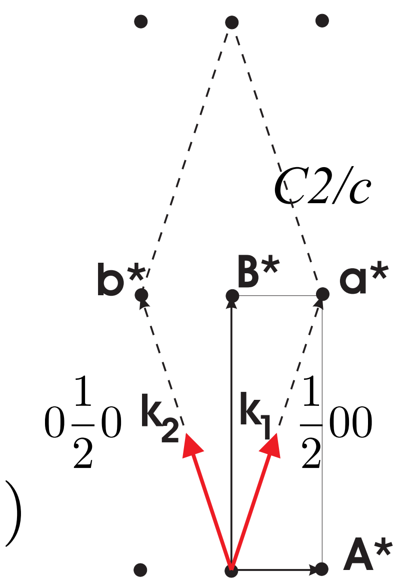
1. multi-dimentional (nD) irreducible representation generates *nD* magnetic modes $S_0{}^1$, $S_0{}^2$, $S_0{}^3$ … $S_0{}^{nD}$

$$\mathbf{S}(0) \sim \sum_{l=1}^{nD} C_l \mathbf{S}_0^l$$

2. multi-*Arm*/multi-**k** structure (non-equivalent $\mathbf{k}_1$, $\mathbf{k}_2$, … $\mathbf{k}_m$). *nA* magnetic modes $S_0{}^1$, $S_0{}^2$, $S_0{}^3$… $S_0{}^{nA}$

$$\mathbf{S}(\mathbf{t}_n) \sim \sum_{m=1}^{nA} C_m' \mathbf{S}_0^m \cos(2\pi \mathbf{k}_m \mathbf{t}_n + \varphi_m)$$

RA: widespread unfavorable paradigm that one-**k** is enough…



Example of mutiarm, full star {$\mathbf{k}_1$,$\mathbf{k}_2$}: J. Phys.: Condens. Matter **26** 496002

any relations between mixing coefficients C_l or C_m' ?

……………………………………………………………

what if several magnetic modes S_0^1, S_0^2, S_0^3... are possible in RA?

Two commensurate cases when k="rational fraction"

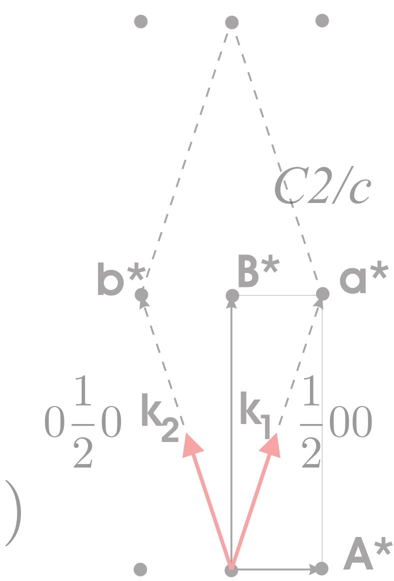
1. multi-dimentional (nD) irreducible representation generates *nD* magnetic modes $\boldsymbol{S_0}^1$, $\boldsymbol{S_0}^2$, $\boldsymbol{S_0}^3$ ... $\boldsymbol{S_0}^{nD}$

$$\mathbf{S}(0) \sim \sum_{l=1}^{nD} C_l \mathbf{S}_0^l$$

2. multi-*Arm*/multi-**k** structure (non-equivalent $\mathbf{k}_1$, $\mathbf{k}_2$, ... $\mathbf{k}_m$). *nA* magnetic modes $\boldsymbol{S_0}^1$, $\boldsymbol{S_0}^2$, $\boldsymbol{S_0}^3$ ... $\boldsymbol{S_0}^{nA}$

$$\mathbf{S}(\mathbf{t}_n) \sim \sum_{m=1}^{nA} C'_m \mathbf{S}_0^m \cos(2\pi \mathbf{k}_m \mathbf{t}_n + \varphi_m)$$

RA: widespread unfavorable paradigm that one-**k** is enough…



Example of mutiarm, full star {$\mathbf{k}_1$,$\mathbf{k}_2$}: J. Phys.: Condens. Matter **26** 496002

any relations between mixing coefficients C_l *or* C'_m ?

....

for incommensurate structures:

any constraints on mixing coefficients ?
1. between atoms unrelated by $\bar{1}$? 2. phases along x,y,z?

$$\mathbf{S}_0 = |C_x| e^{i\phi_x} \mathbf{e}_x + |C_y| \mathbf{e}_y, \phi_x = 0, \frac{\pi}{2}, ...?$$

amplitude modulation for $\phi_x = 0$,

cycloid or helix for e.g. $\phi_x = \frac{\pi}{2}$,...? $\{\mathbf{k}, -\mathbf{k}\}$

what if several magnetic modes S_0^1, S_0^2, S_0^3... are possible in RA?

Two commensurate cases when k="rational fraction"

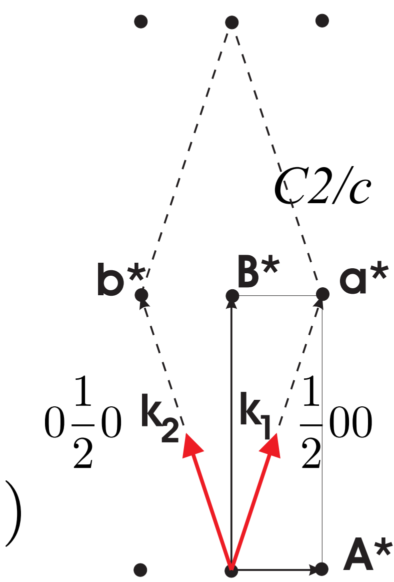
1. multi-dimentional (nD) irreducible representation generates *nD* magnetic modes $\boldsymbol{S}_0^1$, $\boldsymbol{S}_0^2$, $\boldsymbol{S}_0^3$... $\boldsymbol{S}_0^{nD}$

$$\mathbf{S}(0) \sim \sum_{l=1}^{nD} C_l \mathbf{S}_0^l$$

2. multi-*Arm*/multi-**k** structure (non-equivalent $\mathbf{k}_1$, $\mathbf{k}_2$, … $\mathbf{k}_m$). *nA* magnetic modes $\boldsymbol{S}_0^1$, $\boldsymbol{S}_0^2$, $\boldsymbol{S}_0^3$... $\boldsymbol{S}_0^{nA}$

$$\mathbf{S}(\mathbf{t}_n) \sim \sum_{m=1}^{nA} C'_m \mathbf{S}_0^m \cos(2\pi \mathbf{k}_m \mathbf{t}_n + \varphi_m)$$

RA: widespread unfavorable paradigm that one-**k** is enough…



Example of mutiarm, full star {$\mathbf{k}_1$,$\mathbf{k}_2$}: J. Phys.: Condens. Matter **26** 496002

any relations between mixing coefficients C_l or C'_m ?

No from RA alone…

Yes from magnetic symmetry!

for incommensurate structures:

any constraints on mixing coefficients ?
1. between atoms unrelated by $\bar{1}$? 2. phases along x,y,z?

$$\mathbf{S}_0 = |C_x|e^{i\phi_x}\mathbf{e}_x + |C_y|\mathbf{e}_y, \phi_x = 0, \frac{\pi}{2}, ...?$$

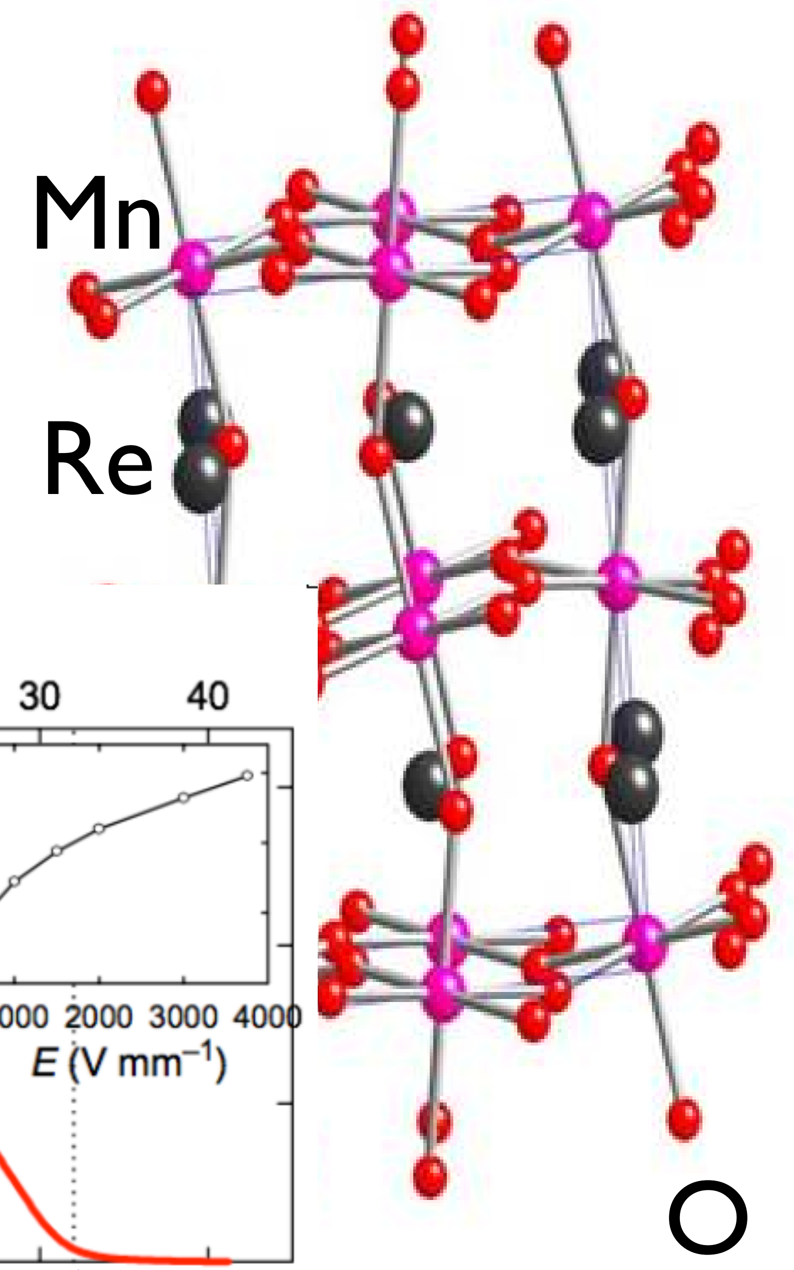
amplitude modulation for $\phi_x = 0$,

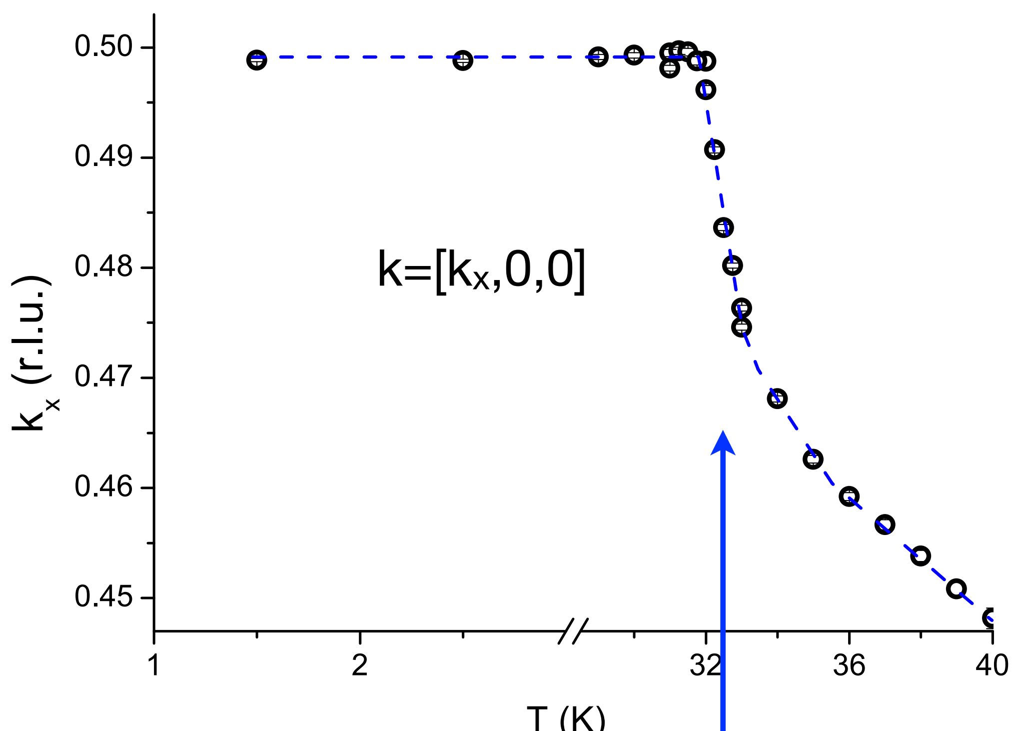
cycloid or helix for e.g. $\phi_x = \frac{\pi}{2}$,…?

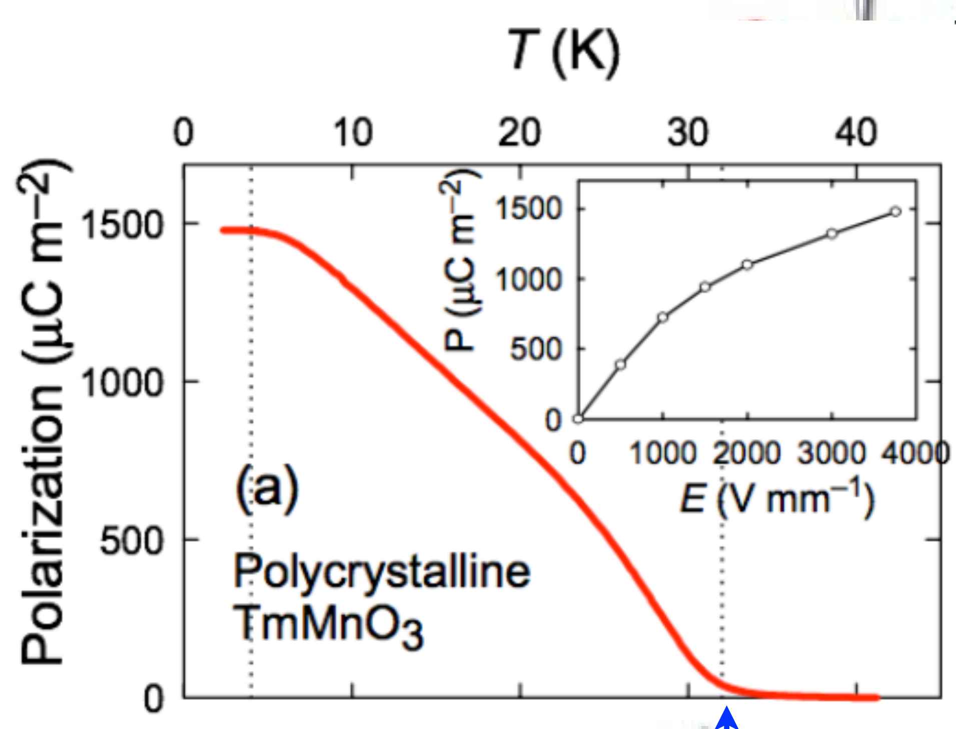
$\{\mathbf{k}, -\mathbf{k}\}$

Antiferromagnetic order in orthorhombic multiferroic $TmMnO_3$

1. one-arm two dimensional irrep **k**=[1/2,0,0]. Ferro-electric phase polar magnetic group P_bmn2_1
2. Constraints on basis functions vs. superspace for the incommensurate two arm **k**=[1/2±δ,0,0]. {**k**}={-**k**,+**k**}. Para-electric phase (3D+1) superspace magnetic group *Pmcn1'(00g)000s [Pnma, bca]*







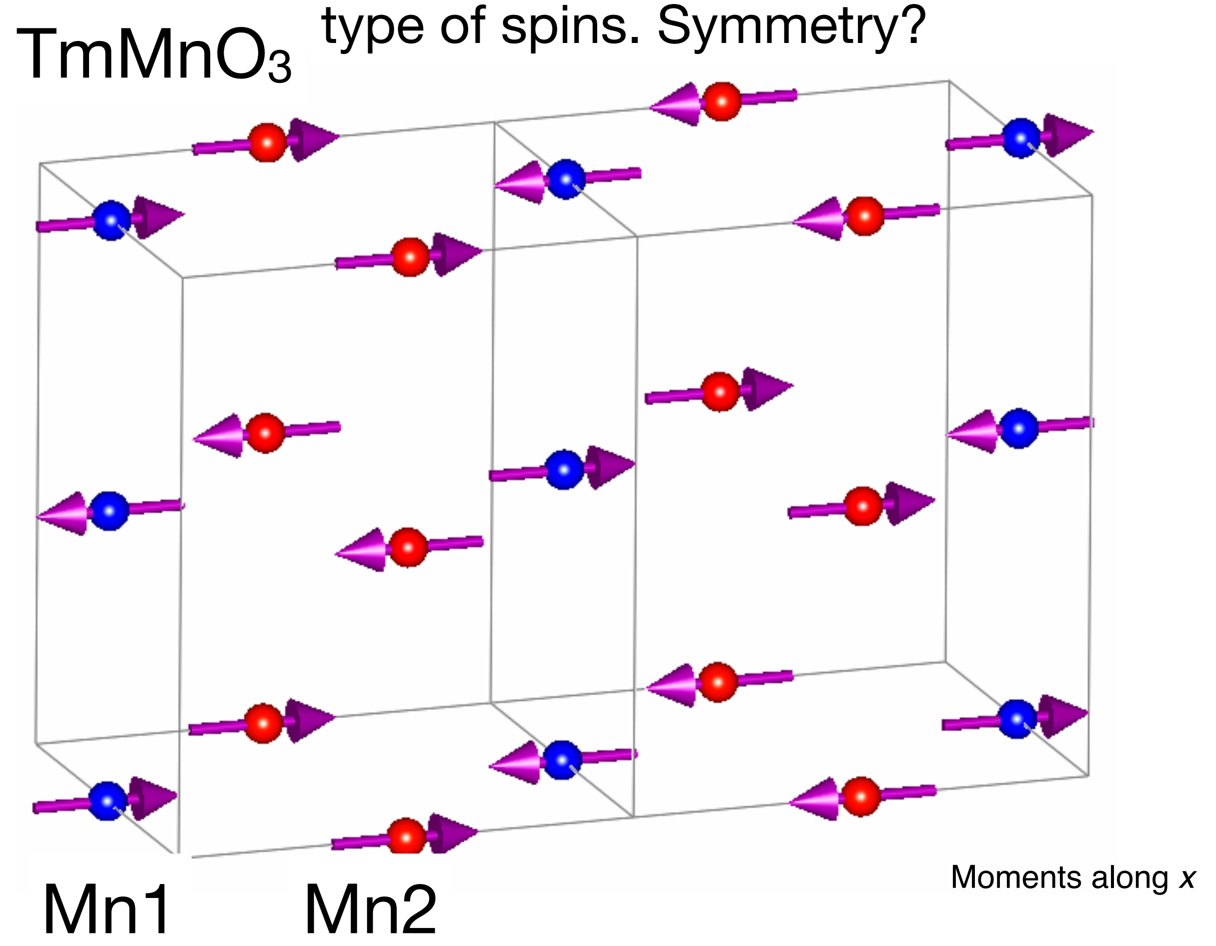
magnetic $T_{Néel}$ & electric: T_C

New Journal of Physics 11, 043019 (2009)

Symmetry analysis using both RA and magnetic subgroups

Pnma k=[1/2,0,0], *irrep*: **2D** mX1(τ_1)

RA with arbitrary mixing coefficients gives different spin sizes for the same type of spins. Symmetry?



Symmetry analysis using both RA and magnetic subgroups

Pnma k=[1/2,0,0], *irrep*: **2D** mX1(τ_1)

http://stokes.byu.edu/iso/

ISOTROPY Software Suite

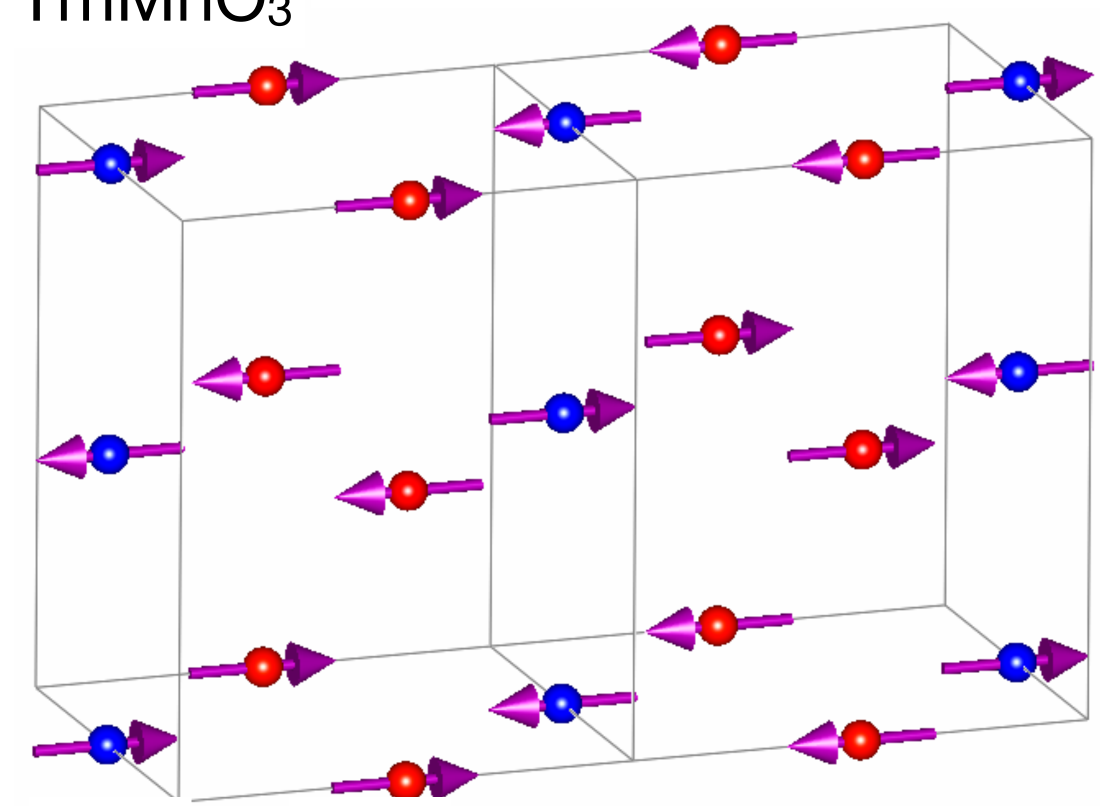
Harold T. Stokes, Dorian M. Hatch, and Branton J. Campbell, Department of Physics and Astronomy, Brigham Young University, Provo, Utah 84606, USA,

ISODISTORT

Version 6.1.8, November 2014
Harold T. Stokes. Branton J. Campbell, and Dorian M. Hatch,

RA with arbitrary mixing coefficients gives different spin sizes for the same type of spins. Symmetry?

$TmMnO_3$



Mn1 Mn2

Moments along *x*

Symmetry analysis using both RA and magnetic subgroups

Pnma k=[1/2,0,0], *irrep*: **2D** mX1(τ_1)

http://stokes.byu.edu/iso/

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,

ISODISTORT

Version 6.1.8, November 2014

Harold T. Stokes. Branton J. Campbell, and Dorian M. Hatch,

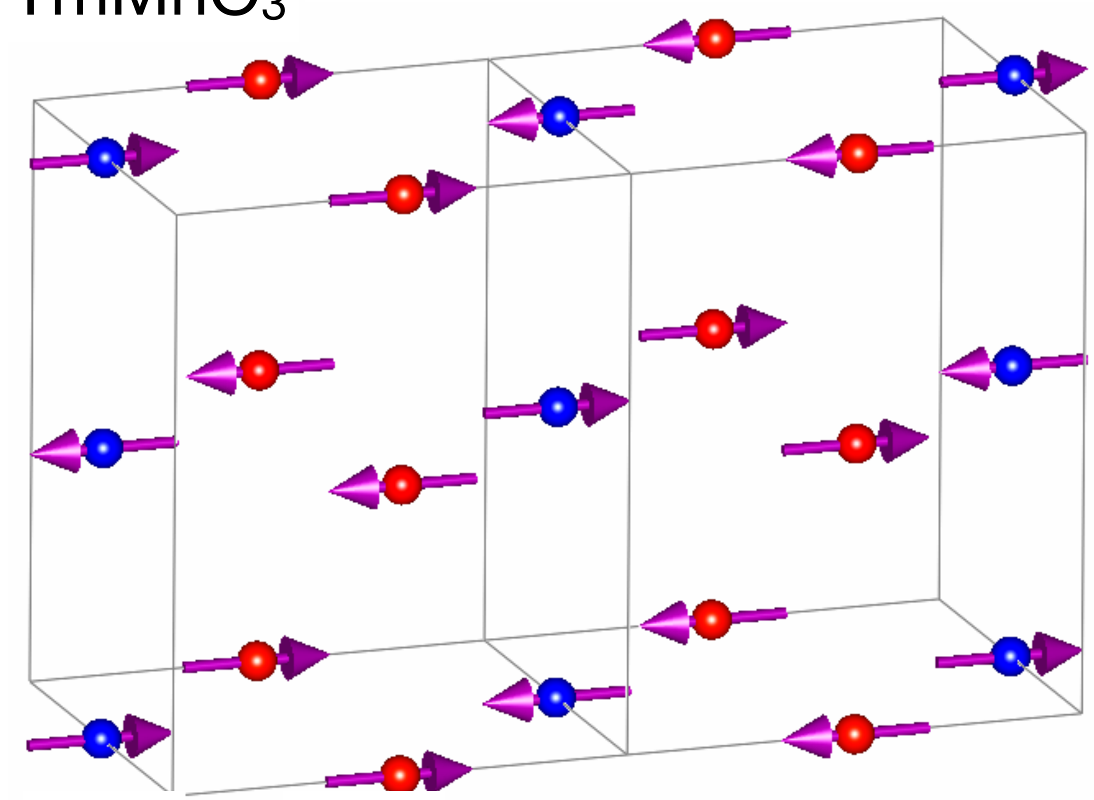
P1 (a,0) 11.55 P_a2_1/m, basis={(2,0,0),(0,1,0),(0,0,1)}, origin=(1/2,0,0), s=2, i=4, k-active= (1/2,0,0)
P3 (a,a) 31.129 P_bmn2_1, basis={(0,1,0),(2,0,0),(0,0,-1)}, origin=(3/4,1/4,0), s=2, i=4, k-active= (1/2,0,0)
C1 (a,b) 6.21 P_am, basis={(2,0,0),(0,1,0),(0,0,1)}, origin=(0,1/4,0), s=2, i=8, k-active= (1/2,0,0)

Order parameter direction

Magnetic Shubnikov Space group

RA with arbitrary mixing coefficients gives different spin sizes for the same type of spins. Symmetry?

$TmMnO_3$



Symmetry analysis using both RA and magnetic subgroups

Pnma k=[1/2,0,0], *irrep*: **2D** mX1(τ_1)

http://stokes.byu.edu/iso/

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,

ISODISTORT

Version 6.1.8, November 2014

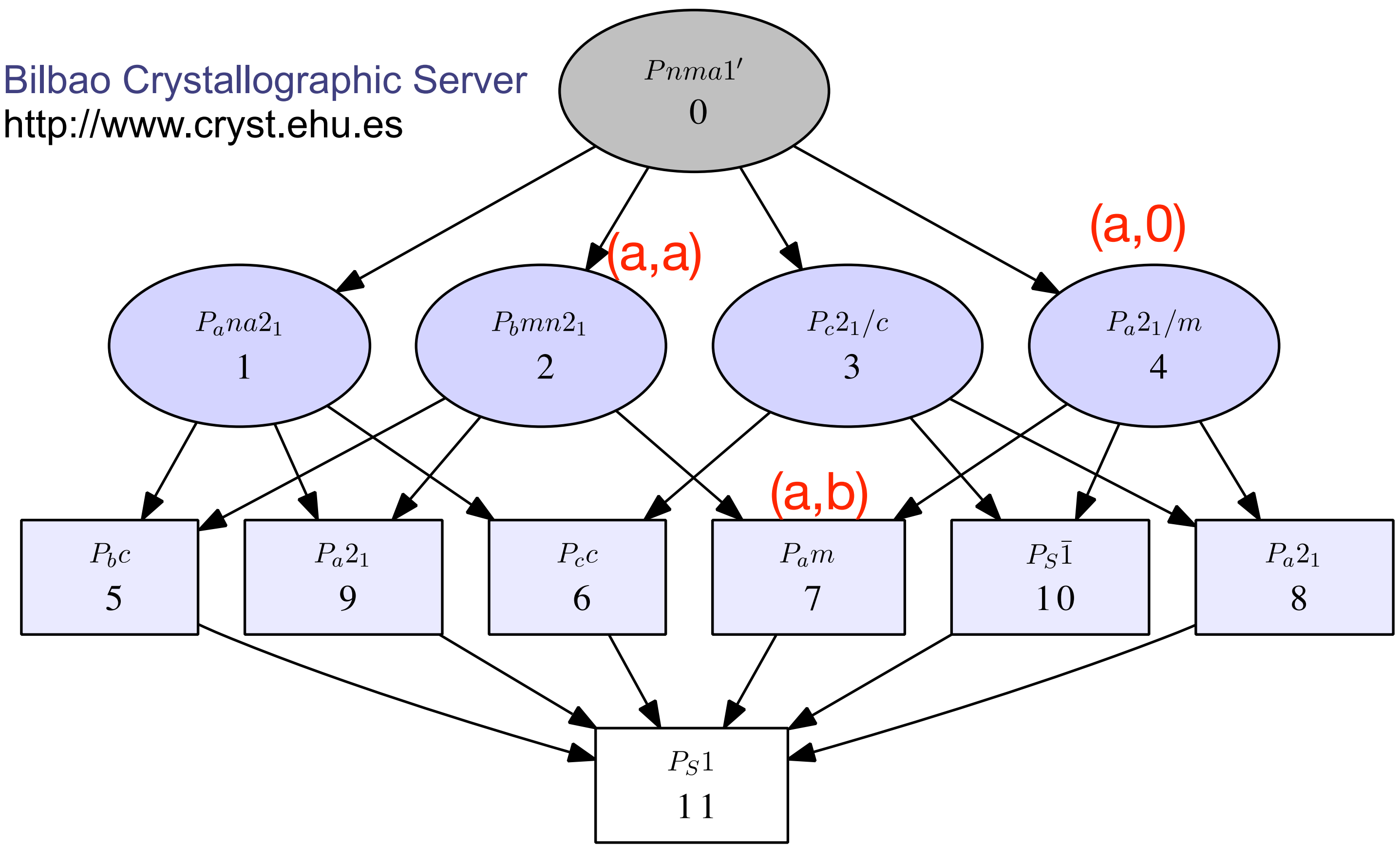
Harold T. Stokes. Branton J. Campbell, and Dorian M. Hatch,

P1 (a,0) 11.55 P_a2_1/m, basis={(2,0,0),(0,1,0),(0,0,1)}, origin=(1/2,0,0), s=2, i=4, k-active= (1/2,0,0)
P3 (a,a) 31.129 P_bmn2_1, basis={(0,1,0),(2,0,0),(0,0,-1)}, origin=(3/4,1/4,0), s=2, i=4, k-active= (1/2,0,0)
C1 (a,b) 6.21 P_am, basis={(2,0,0),(0,1,0),(0,0,1)}, origin=(0,1/4,0), s=2, i=8, k-active= (1/2,0,0)

Order parameter direction

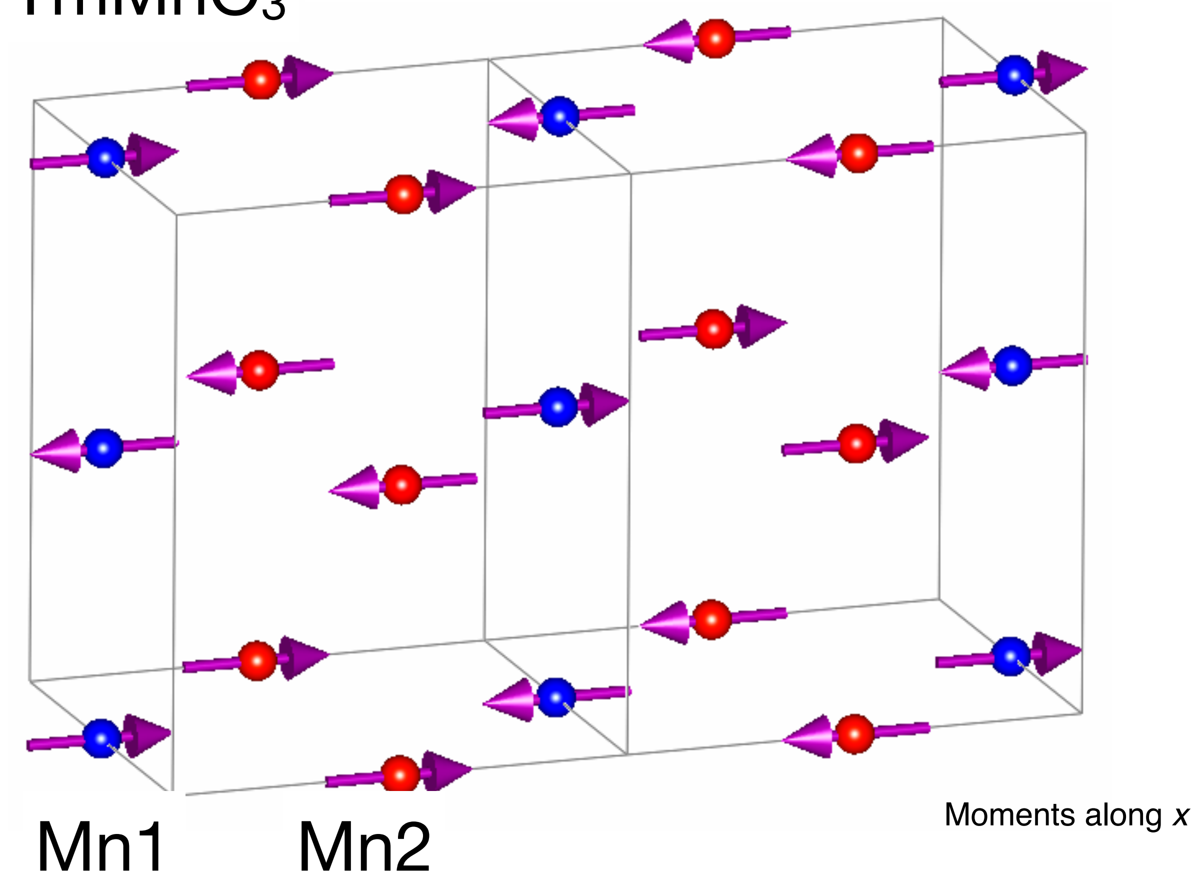
Magnetic Shubnikov Space group

Bilbao Crystallographic Server
http://www.cryst.ehu.es



RA with arbitrary mixing coefficients gives different spin sizes for the same type of spins. Symmetry?

$TmMnO_3$



Case 1: magnetic mode E1 -> most symmetric maximal subgroup of Pnma1'

Order parameter direction

Magnetic Shubnikov Space group

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

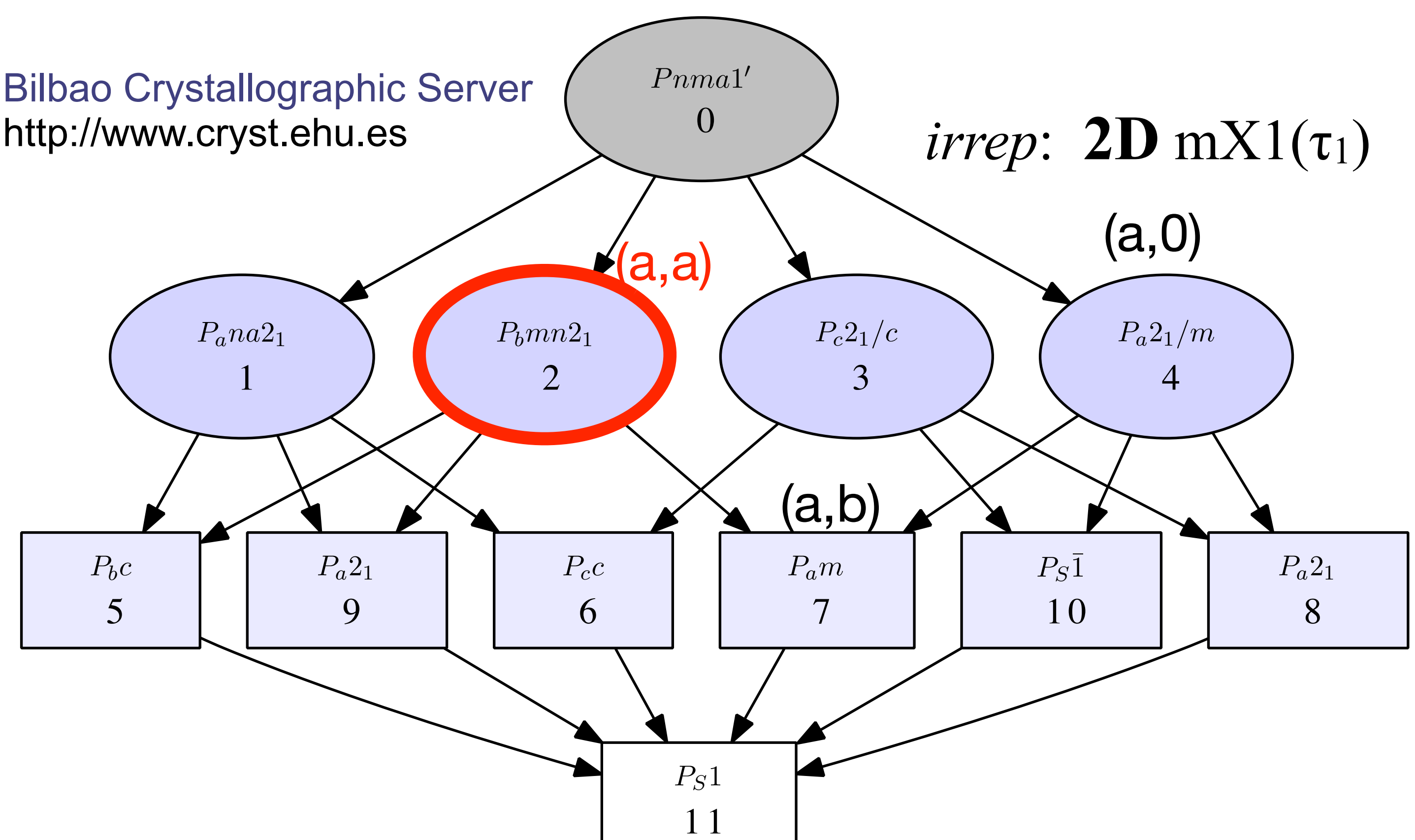
ISODISTORT

Version 6.1.8, November 2014
Harold T. Stokes. Branton J. Campbell, and Dorian M. Hatch,

Solution!

P1 (a,0) 11.55 P_a2_1/m, basis={(2,0,0),(0,1,0),(0,0,1)}, origin=(1/2,0,0), s=2, i=4, k-active= (1/2,0,0)
P3 (a,a) 31.129 P_bmn2_1, basis={(0,1,0),(2,0,0),(0,0,-1)}, origin=(3/4,1/4,0), s=2, i=4, k-active= (1/2,0,0)
C1 (a,b) 6.21 P_am, basis={(2,0,0),(0,1,0),(0,0,1)}, origin=(0,1/4,0), s=2, i=8, k-active= (1/2,0,0)

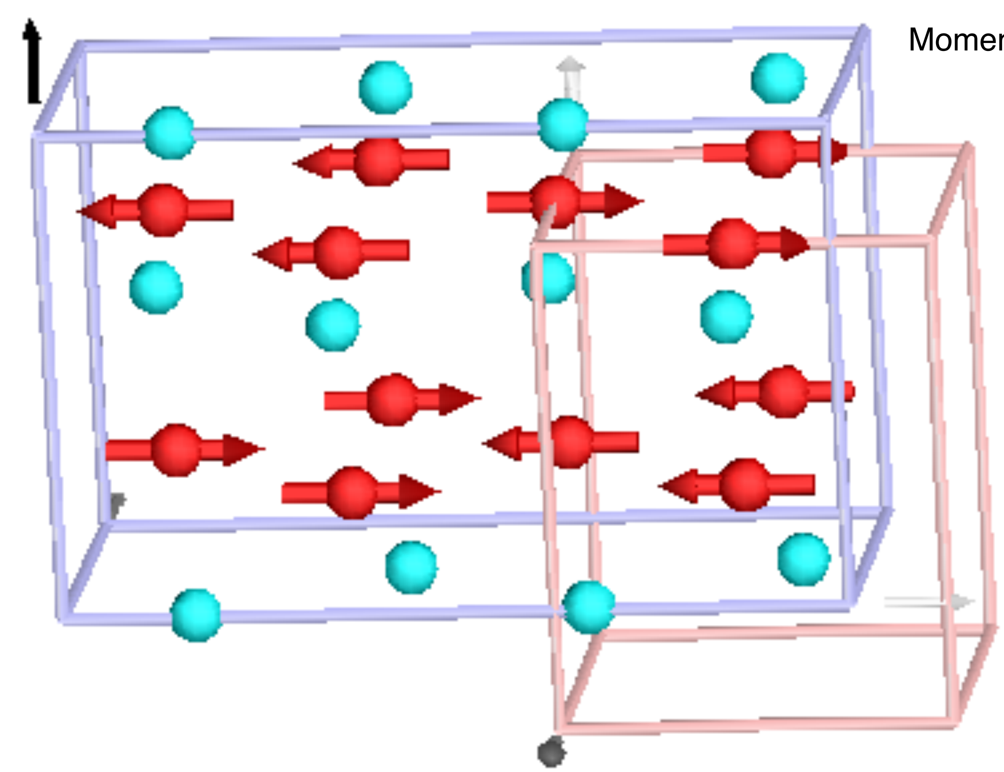
Bilbao Crystallographic Server
http://www.cryst.ehu.es



irrep: **2D** mX1(τ_1)

$TmMnO_3$

Moments along *x*



Case 1: magnetic mode E1 -> most symmetric maximal subgroup of Pnma1'

Order parameter direction

Magnetic Shubnikov Space group

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

ISODISTORT

Version 6.1.8, November 2014
Harold T. Stokes. Branton J. Campbell, and Dorian M. Hatch,

Solution!

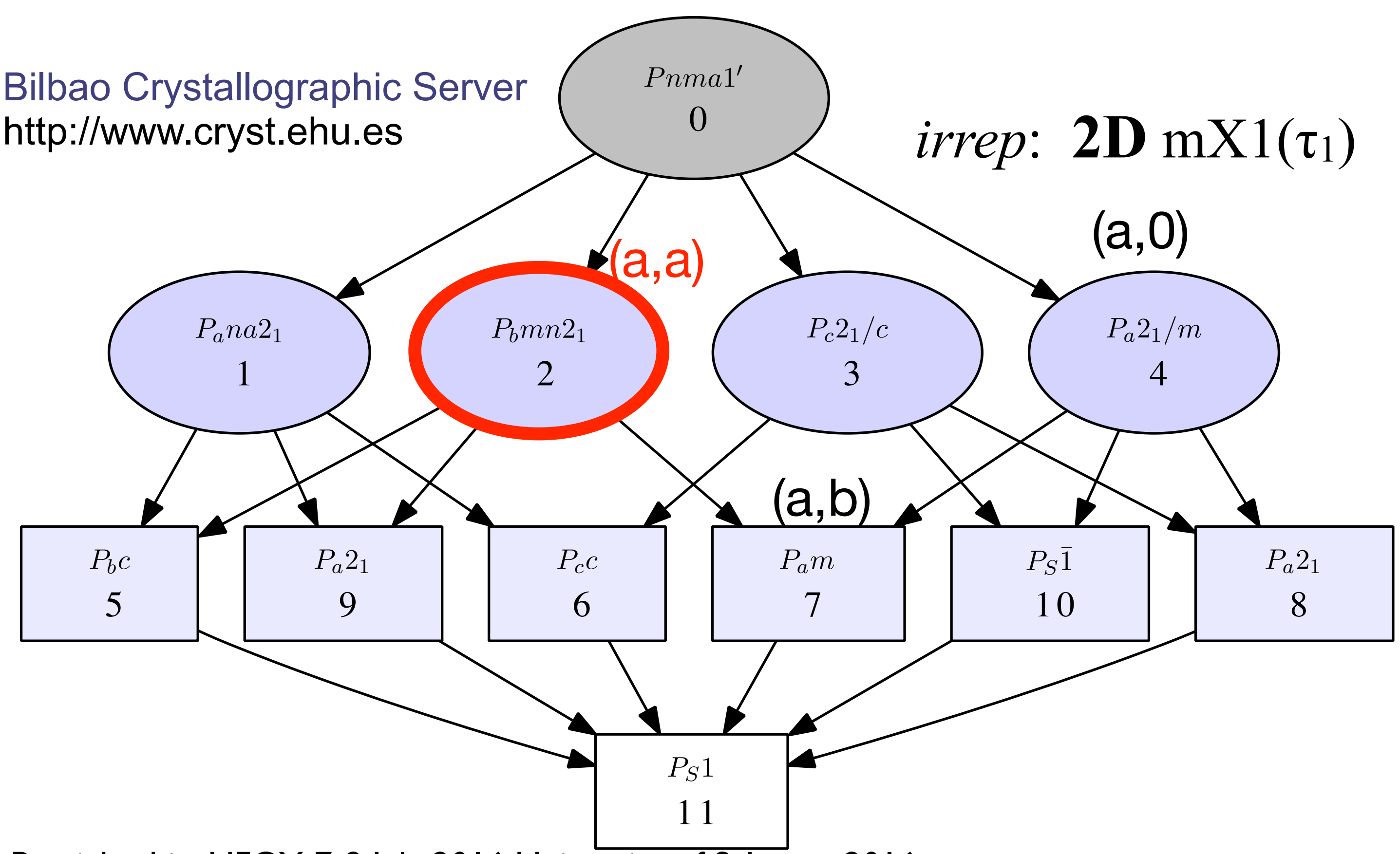
P1 (a,0) 11.55 P_a2_1/m, basis={(2,0,0),(0,1,0),(0,0,1)}, origin=(1/2,0,0), s=2, i=4, k-active= (1/2,0,0)
P3 (a,a) 31.129 P_bmn2_1, basis={(0,1,0),(2,0,0),(0,0,-1)}, origin=(3/4,1/4,0), s=2, i=4, k-active= (1/2,0,0)
C1 (a,b) 6.21 P_am, basis={(2,0,0),(0,1,0),(0,0,1)}, origin=(0,1/4,0), s=2, i=8, k-active= (1/2,0,0)

orthorhombic $Pmn2_1$

(1) 1 (2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},0,z$ (3) $2(0,\frac{1}{2},0)$ $0,y,0$ (4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},\frac{1}{4}$
(5) $\bar{1}$ $0,0,0$ (6) a $x,y,\frac{1}{4}$ (7) m $x,\frac{1}{4},z$ (8) $n(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4},y,z$

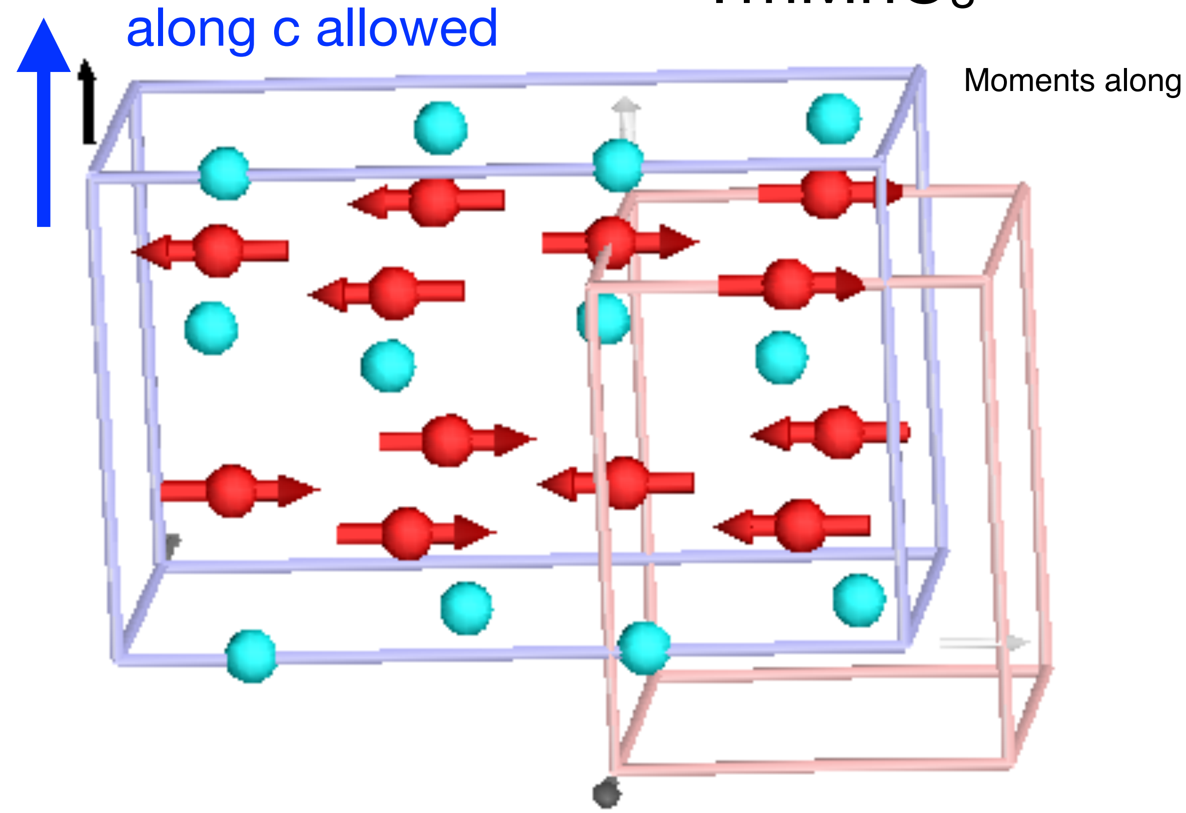
Bilbao Crystallographic Server
http://www.cryst.ehu.es

irrep: **2D** mX1(τ_1)



Electric polarisation along c allowed

$TmMnO_3$



Case 2: General solution in RA -> low symmetry non-maximal subgroup

Order parameter direction

Magnetic Shubnikov Space group

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

ISODISTORT

Version 6.1.8, November 2014
Harold T. Stokes. Branton J. Campbell, and Dorian M. Hatch,

P1 (a,0) 11.55 P_a2_1/m, basis={(2,0,0),(0,1,0),(0,0,1)}, origin=(1/2,0,0), s=2, i=4, k-active= (1/2,0,0)

P3 (a,a) 31.129 P_bmn2_1, basis={(0,1,0),(2,0,0),(0,0,-1)}, origin=(3/4,1/4,0), s=2, i=4, k-active= (1/2,0,0)

C1 (a,b) 6.21 P_am, basis={(2,0,0),(0,1,0),(0,0,1)}, origin=(0,1/4,0), s=2, i=8, k-active= (1/2,0,0)

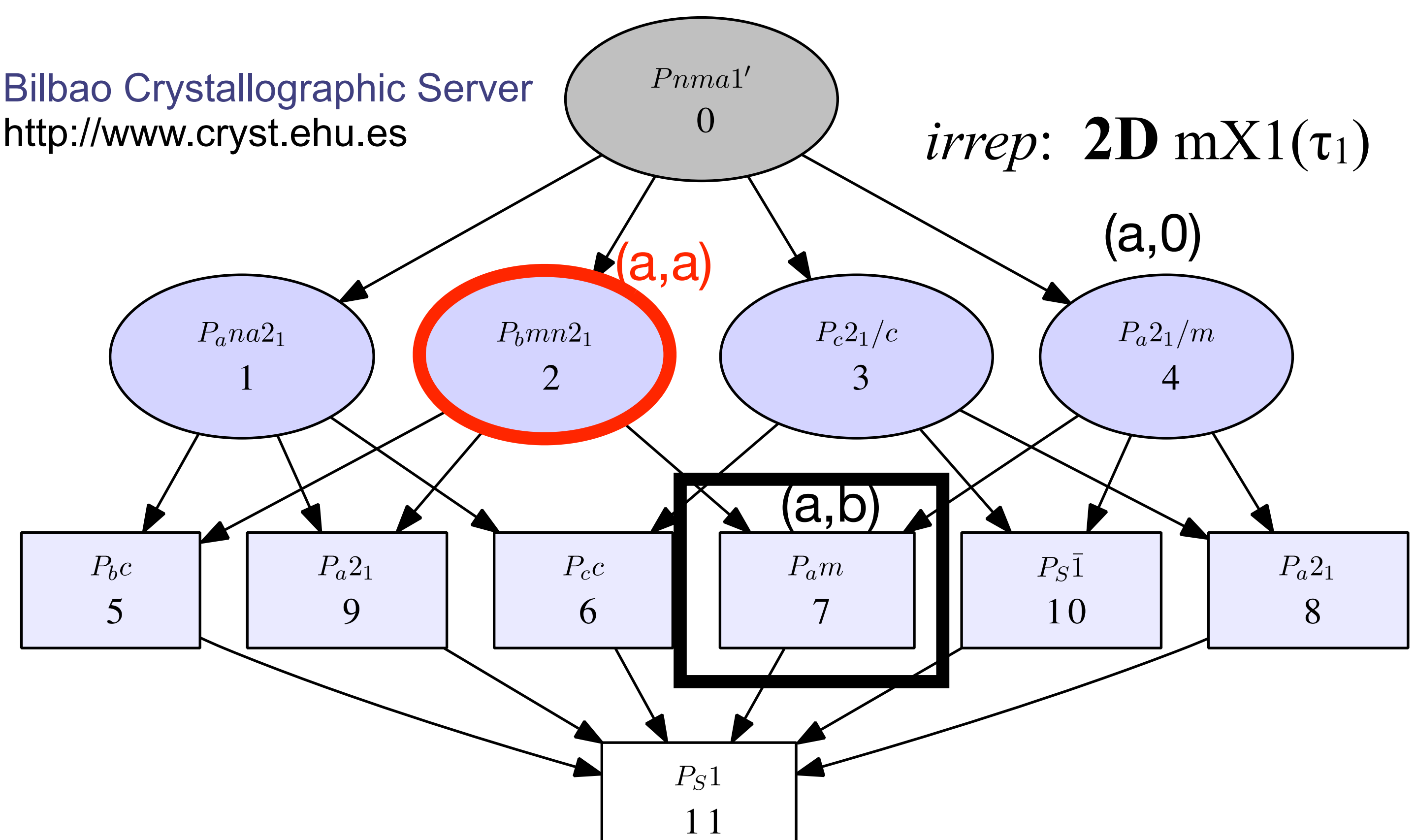
conventional general solution in RA: lowest symmetry for the given irrep

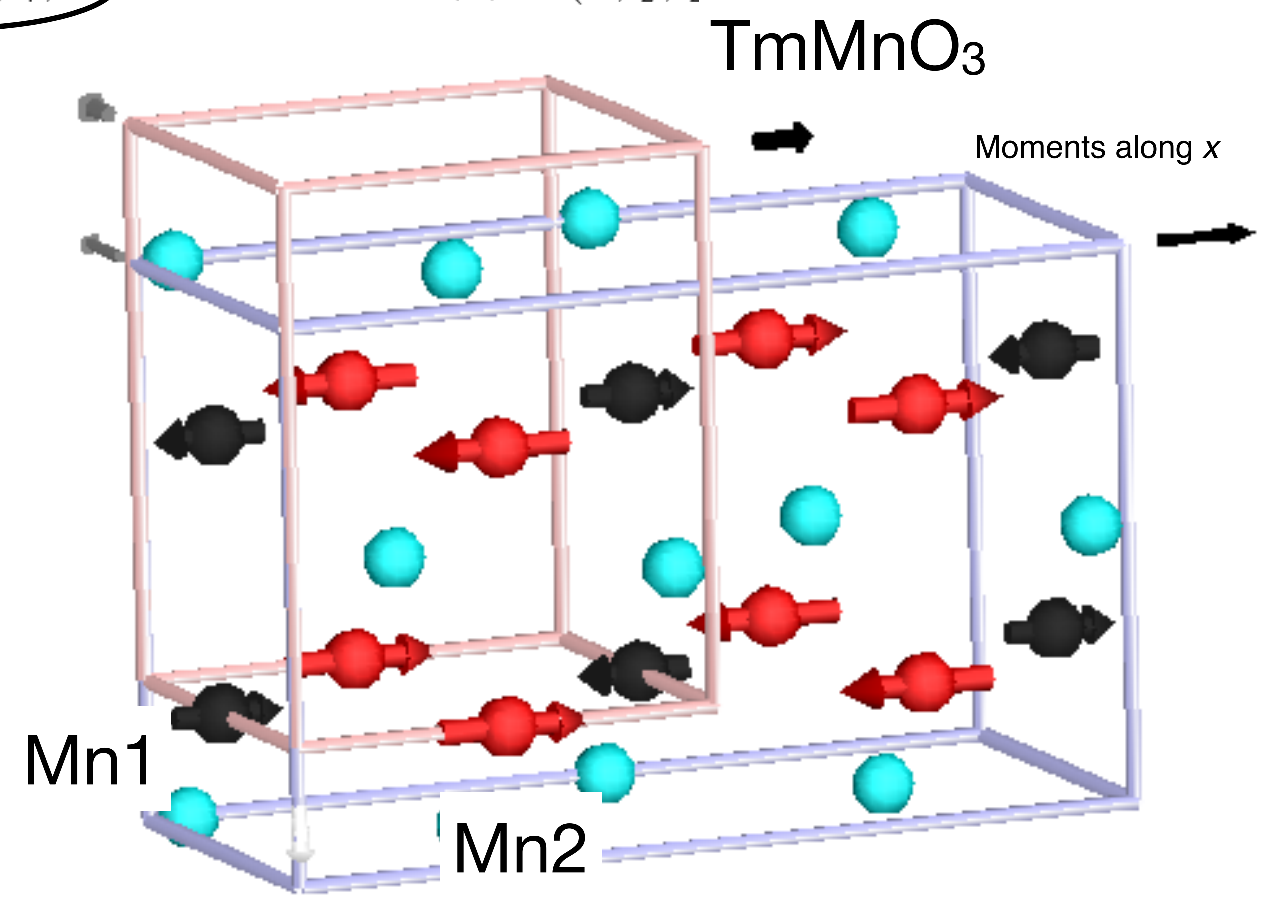
monoclinic Pm

(1) 1 (2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},0,z$ (3) $2(0,\frac{1}{2},0)$ $0,y,0$ (4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},\frac{1}{4}$

(5) $\bar{1}$ $0,0,0$ (6) a $x,y,\frac{1}{4}$ (7) m $x,\frac{1}{4},z$ (8) $n(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4},y,z$

Bilbao Crystallographic Server
http://www.cryst.ehu.es

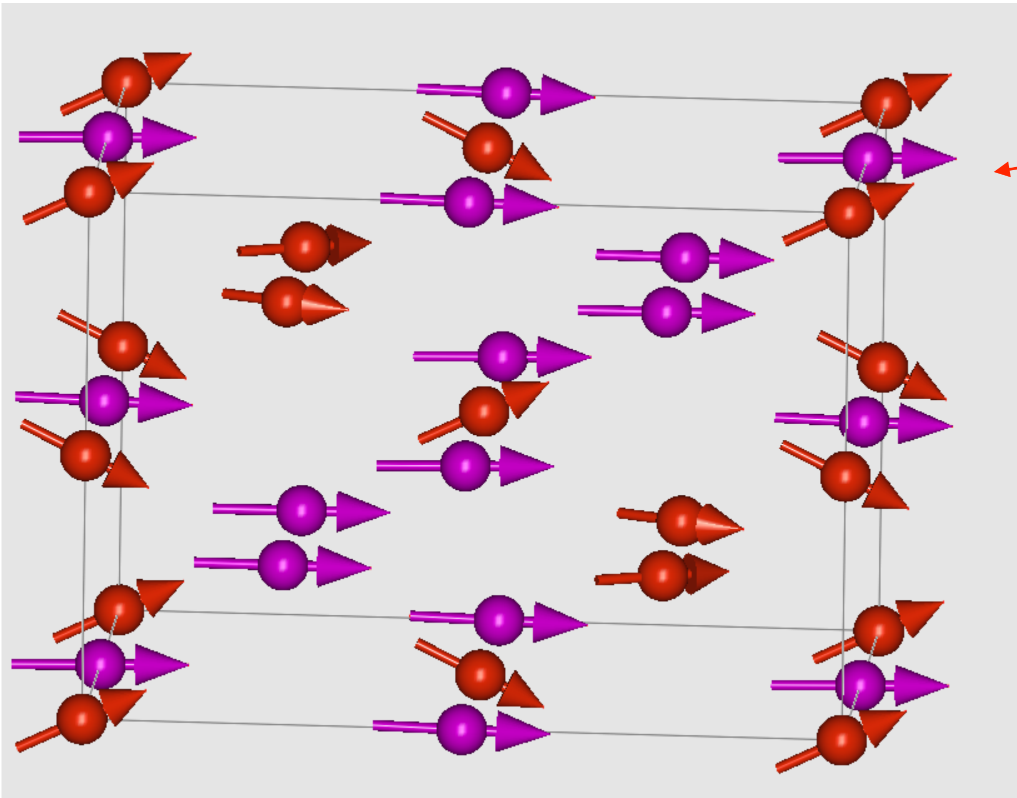


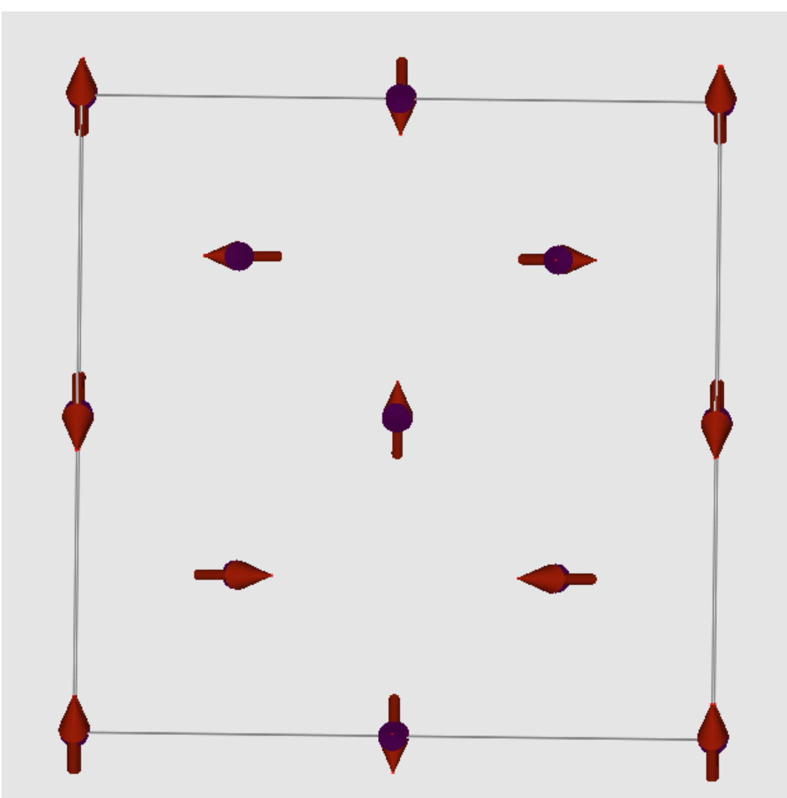


Magnetic structure of Pyrochlore $Tm_2Mn_2O_7$ at Γ-point k=0

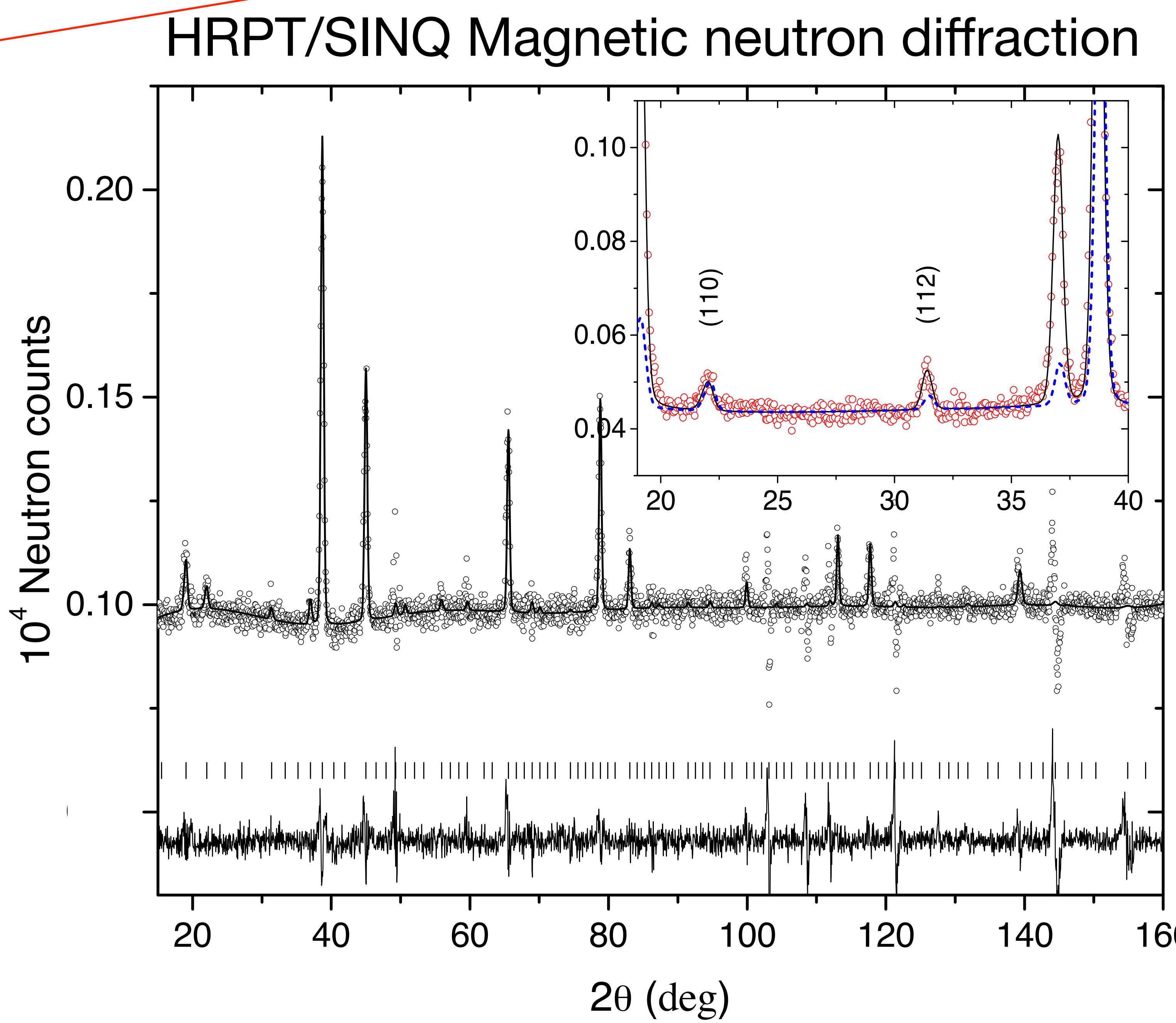
141.557 I4_1/am'd'

$$\Gamma_{\mathrm{mag}} = \Gamma_2^+(1D) \oplus \Gamma_3^+(2D) \oplus \Gamma_5^+(3D) \oplus \boxed{2\Gamma_4^+(3D)}$$





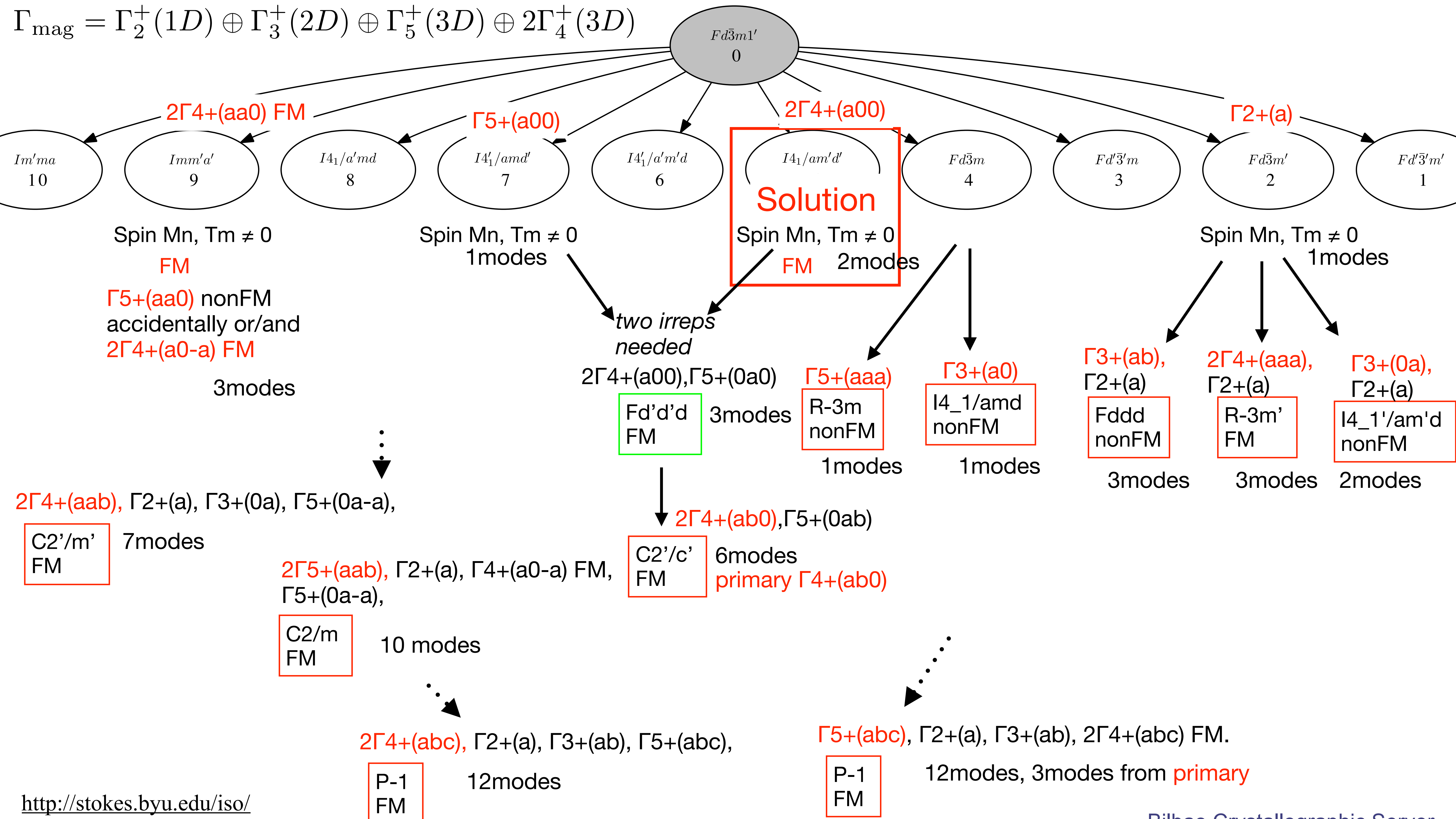
Inorg.Chem. 2015, 54, 9092-9097



Magnetic structure of Pyrochlore $Tm_2Mn_2O_7$ at Γ-point k=0

Maximal and non-maximal MG for the parent SG 227 (*Fd-3m*) at gamma point k = (0, 0, 0) generated by *one irrep* for 16d (1/2,1/2,1/2), 16c (0,0,0) position

$$\Gamma_{\rm mag} = \Gamma_2^+(1D) \oplus \Gamma_3^+(2D) \oplus \Gamma_5^+(3D) \oplus 2\Gamma_4^+(3D)$$



http://stokes.byu.edu/iso/

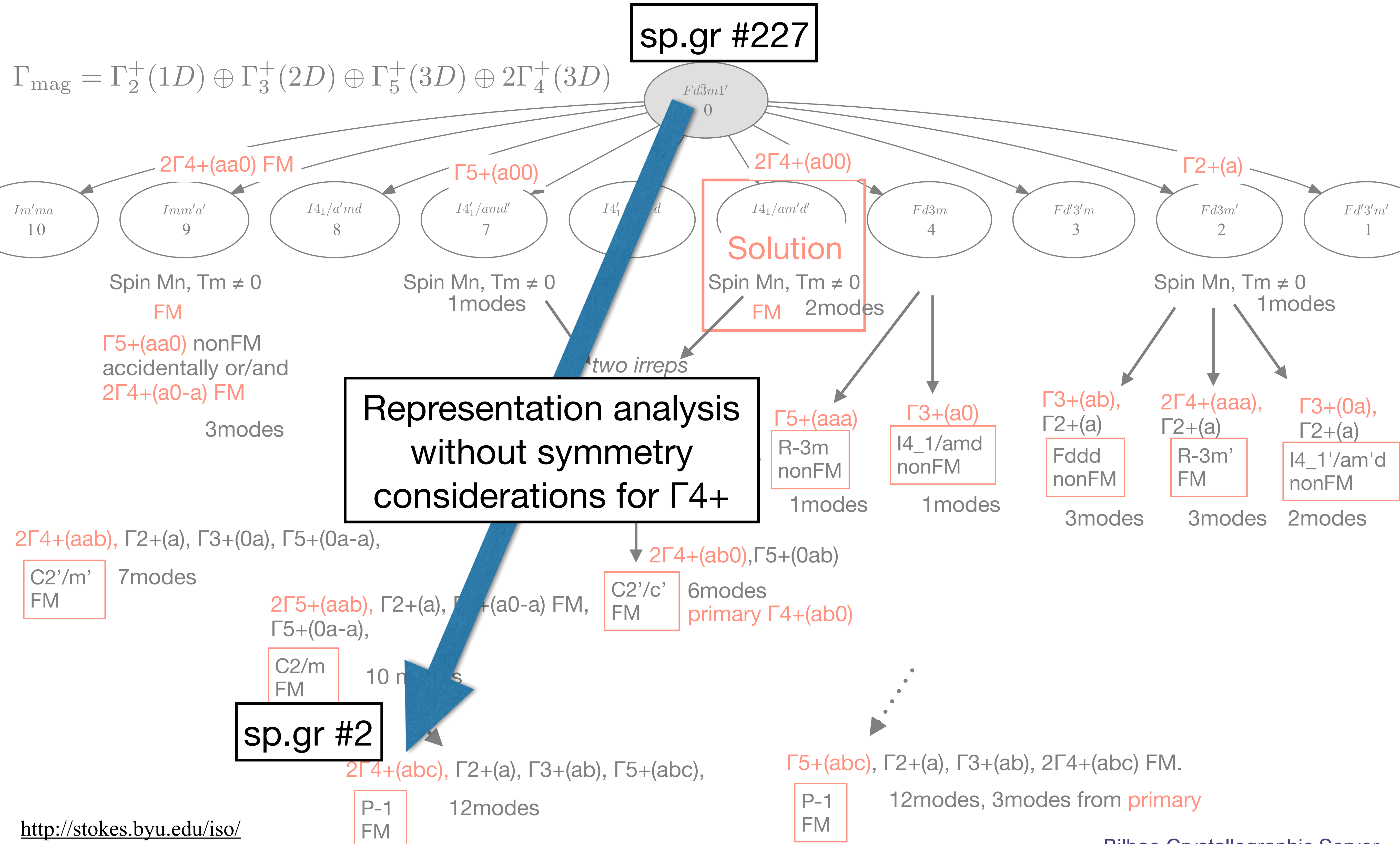
ISOTROPY Software Suite

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

Bilbao Crystallographic Server
http://www.cryst.ehu.es

Magnetic structure of Pyrochlore $Tm_2Mn_2O_7$ at Γ-point k=0

Maximal and non-maximal MG for the parent SG 227 (*Fd-3m*) at gamma point k = (0, 0, 0) generated by *one* irrep for 16d (1/2,1/2,1/2), 16c (0,0,0) position



http://stokes.byu.edu/iso/

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,

Bilbao Crystallographic Server
http://www.cryst.ehu.es

Relation of magnetic Shubnikov/superspace symmetry and representation analysis RA

Paramagnetic crystallographic space group (*PSG*)

Propagation vector of magnetic structure **k**

choose one irreducible representation (*irrep*) of *PSG*

magnetic symmetry

representation

Relation of magnetic Shubnikov/superspace symmetry and representation analysis RA

Paramagnetic crystallographic space group (*PSG*)

Propagation vector of magnetic structure **k**

choose one irreducible representation (*irrep*) of *PSG*

magnetic symmetry

representation

Construction of basis functions (normal modes)

<u>Constraints</u> on the mixing coefficients of basis function for >1D *irrep* and/or multi-arm star of **k**,

{-**k**,**k**} star for incommensurate.

Magnetic structure made from linear combination of normal modes.

Relation of magnetic Shubnikov/superspace symmetry and representation analysis RA

Paramagnetic crystallographic space group (*PSG*)

Propagation vector of magnetic structure **k**

choose one irreducible representation (*irrep*) of *PSG*

magnetic symmetry

representation

Construction of basis functions (normal modes)

Constraints ? the mixing coefficients of basis function for >1D *irrep* and/or multi-arm star of **k**,

{-**k**,**k**} star for incommensurate.

Magnetic structure made from linear combination of normal modes.

Relation of magnetic Shubnikov/superspace symmetry and representation analysis RA

Paramagnetic crystallographic space group (*PSG*)

Propagation vector of magnetic structure **k**

choose one irreducible representation (*irrep*) of *PSG*

magnetic symmetry

representation

is *irrep* real and 1D, and single arm {**k**}-star?

Yes

Shubnikov from *PSG*
Symop g that have *irrep*(*g*)=-1
are primed in Sh-group

Construction of basis functions (normal modes)

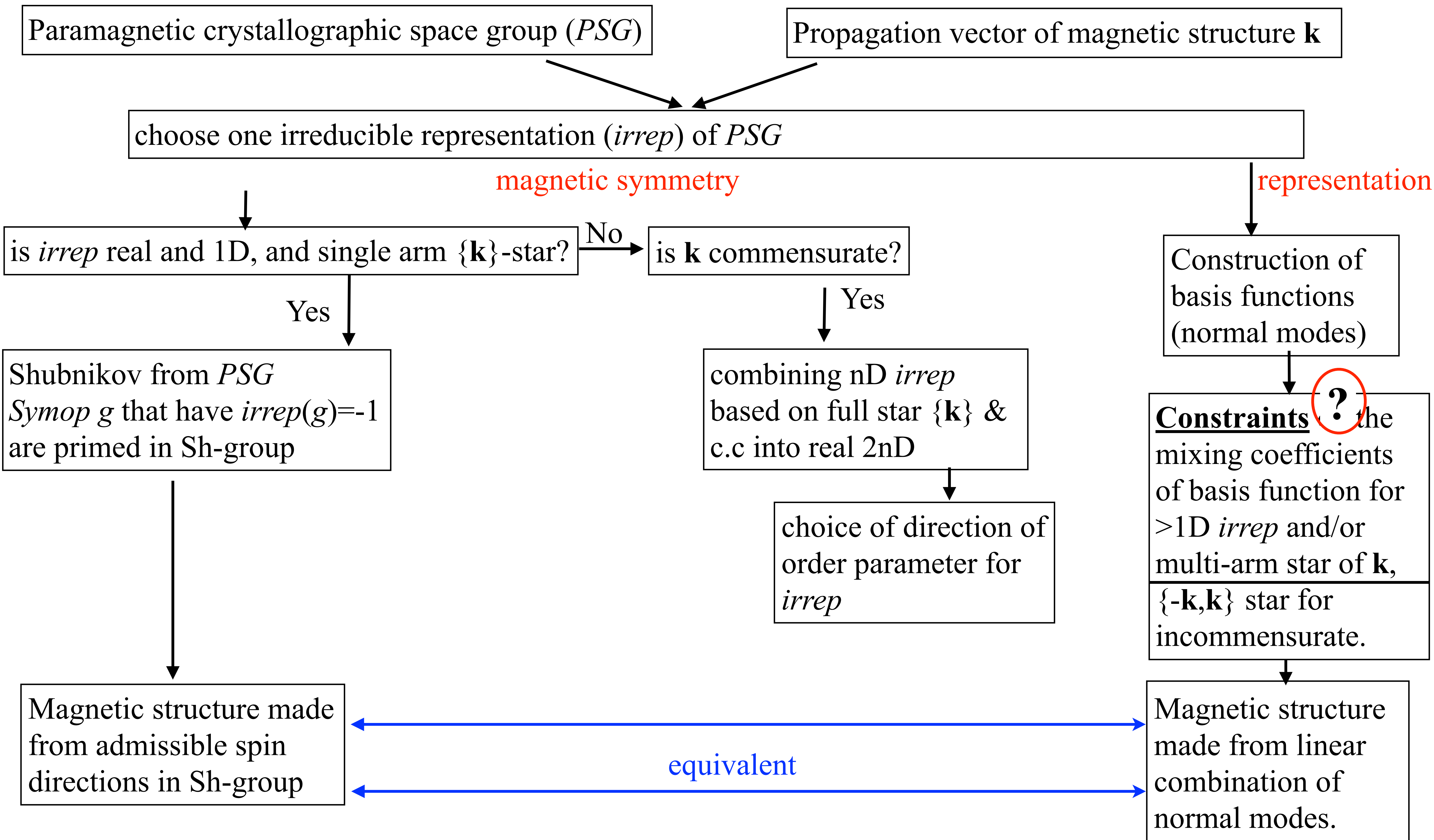
Constraints ? the mixing coefficients of basis function for >1D *irrep* and/or multi-arm star of **k**, {-**k**,**k**} star for incommensurate.

Magnetic structure made from admissible spin directions in Sh-group

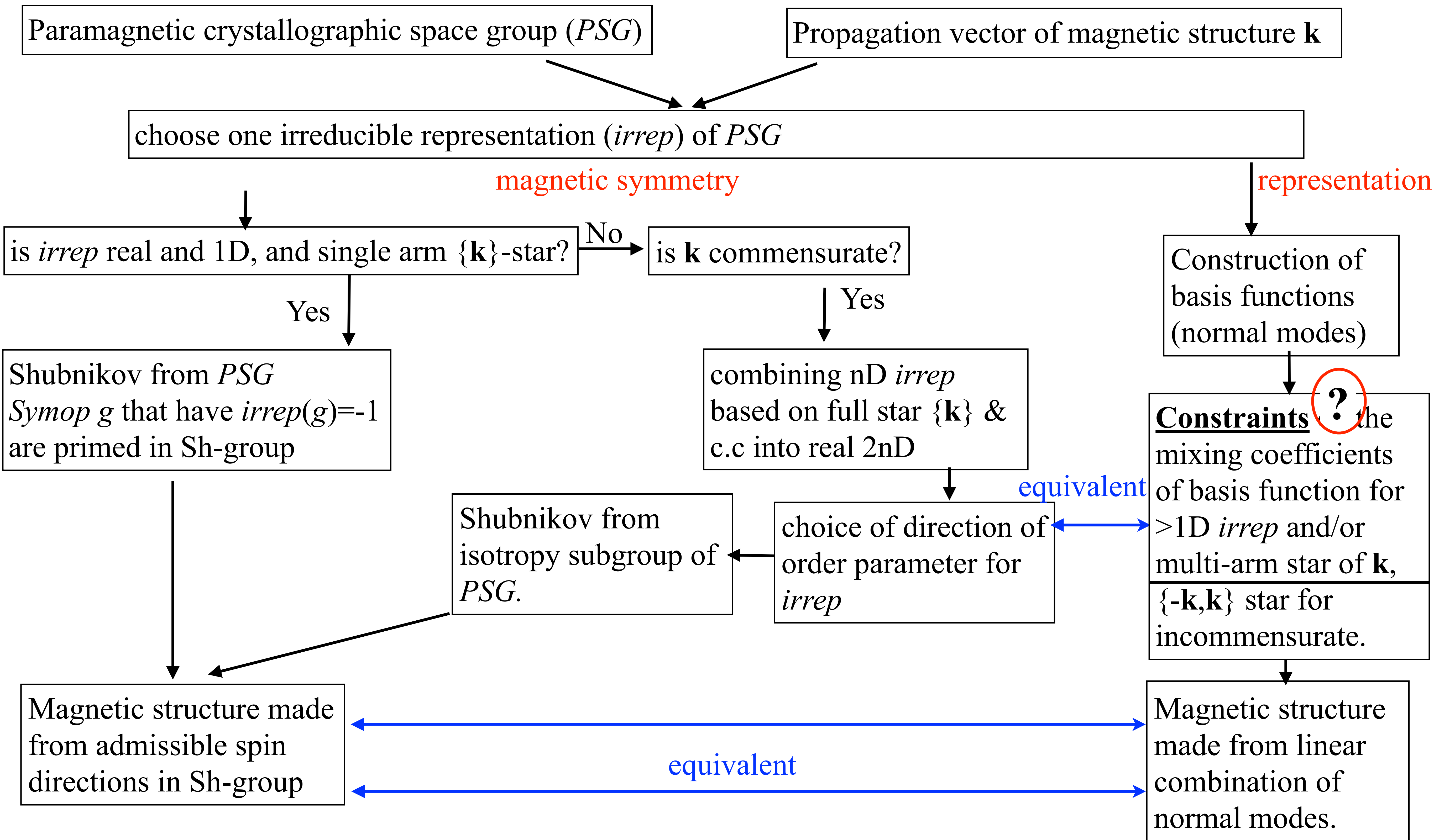
equivalent

Magnetic structure made from linear combination of normal modes.

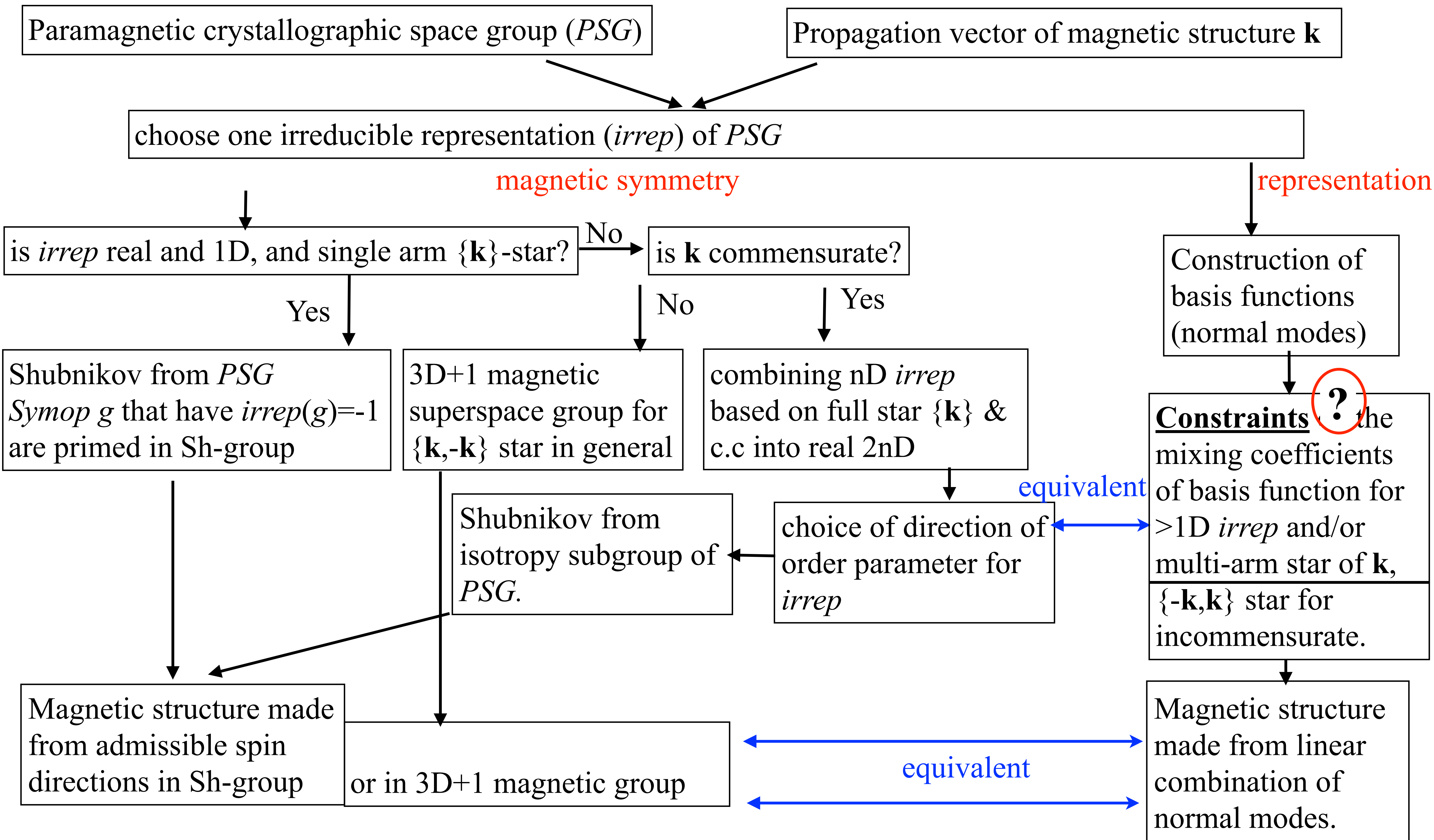
Relation of magnetic Shubnikov/superspace symmetry and representation analysis RA



Relation of magnetic Shubnikov/superspace symmetry and representation analysis RA



Relation of magnetic Shubnikov/superspace symmetry and representation analysis RA



Relation of magnetic Shubnikov/superspace symmetry and representation analysis RA

Paramagnetic crystallographic space group (*PSG*)

Propagation vector of magnetic structure **k**

The disadvantage of using only RA:

?

In general: there are no rules to make **constraints**, (except ones based on physical grounds)

but the **constraints** appear in a natural way from magnetic group symmetry arguments

Shubnikov from *PSG*
Symop g that have *irrep*(*g*)=-1 are primed in Sh-group

3D+1 magnetic superspace group for {**k**,-**k**} star in general

combining nD *irrep* based on full star {**k**} & c.c into real 2nD

Constraints ? the mixing coefficients of basis function for >1D *irrep* and/or multi-arm star of **k**, {-**k**,**k**} star for incommensurate.

equivalent

choice of direction of order parameter for *irrep*

Shubnikov from isotropy subgroup of *PSG*.

Magnetic structure made from admissible spin directions in Sh-group

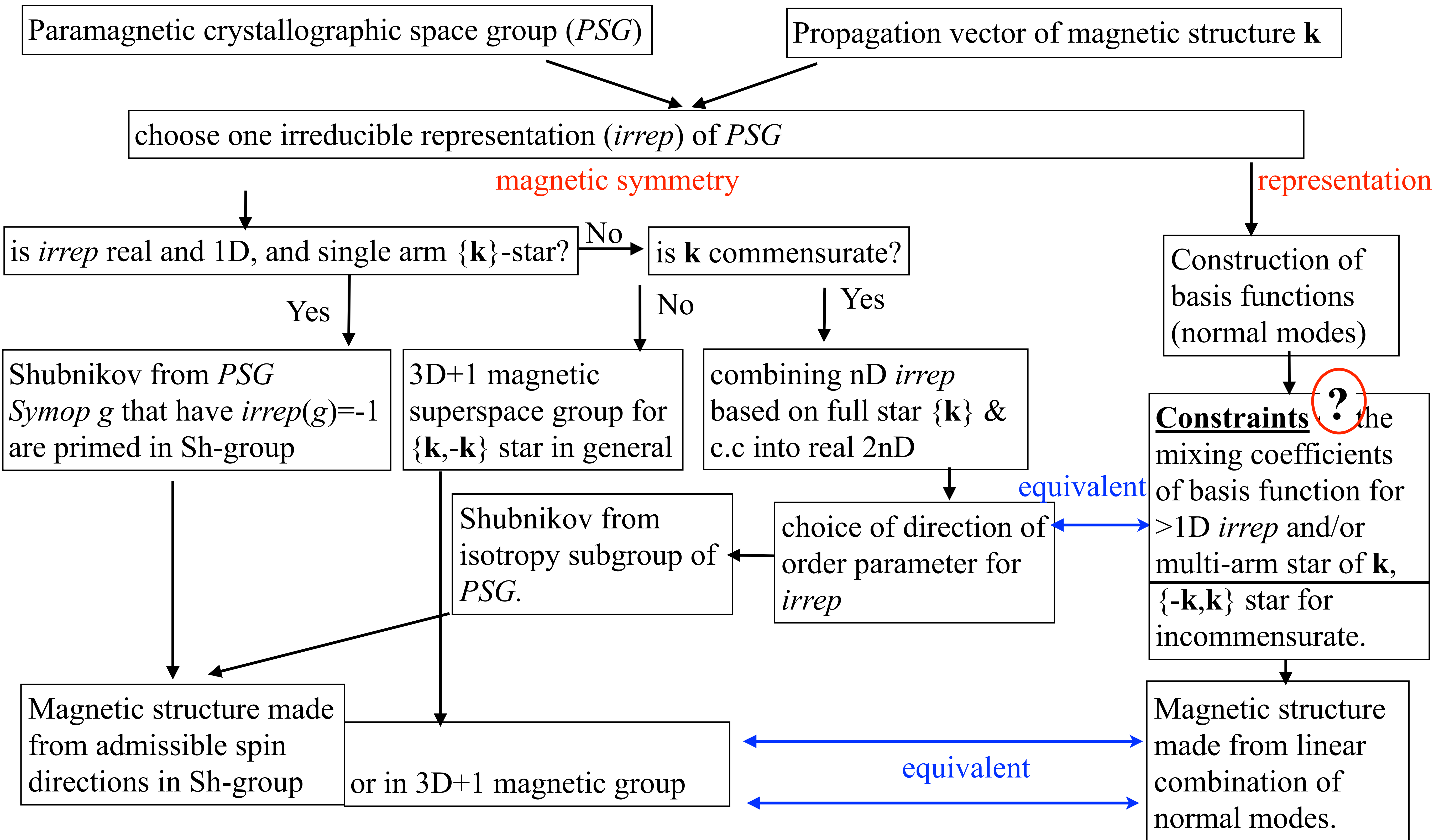
or in 3D+1 magnetic group

equivalent

Magnetic structure made from linear combination of normal modes.

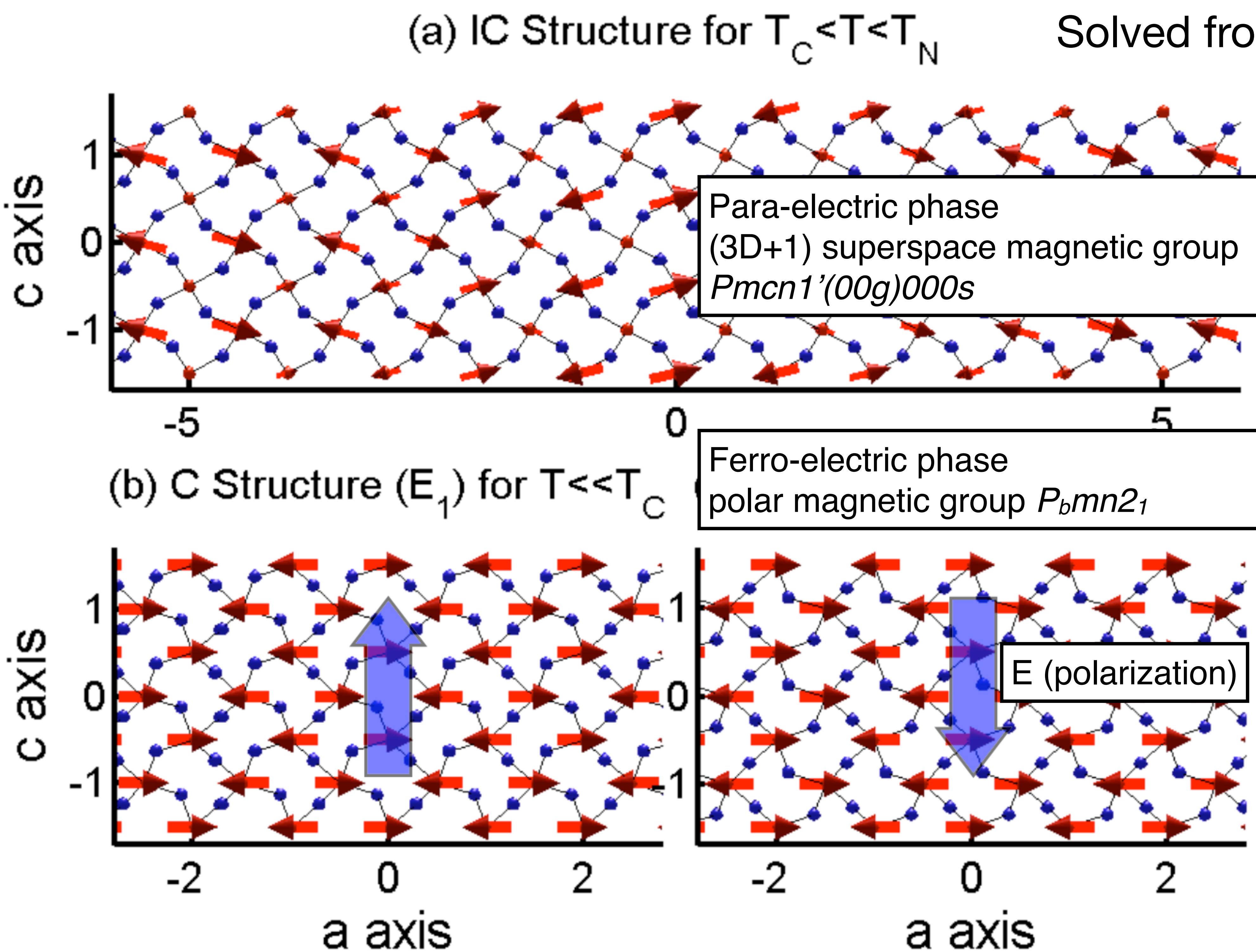
Thank you!

Relation of magnetic Shubnikov/superspace symmetry and representation analysis RA



Magnetic structure $TmMnO_3$

Solved from DMC



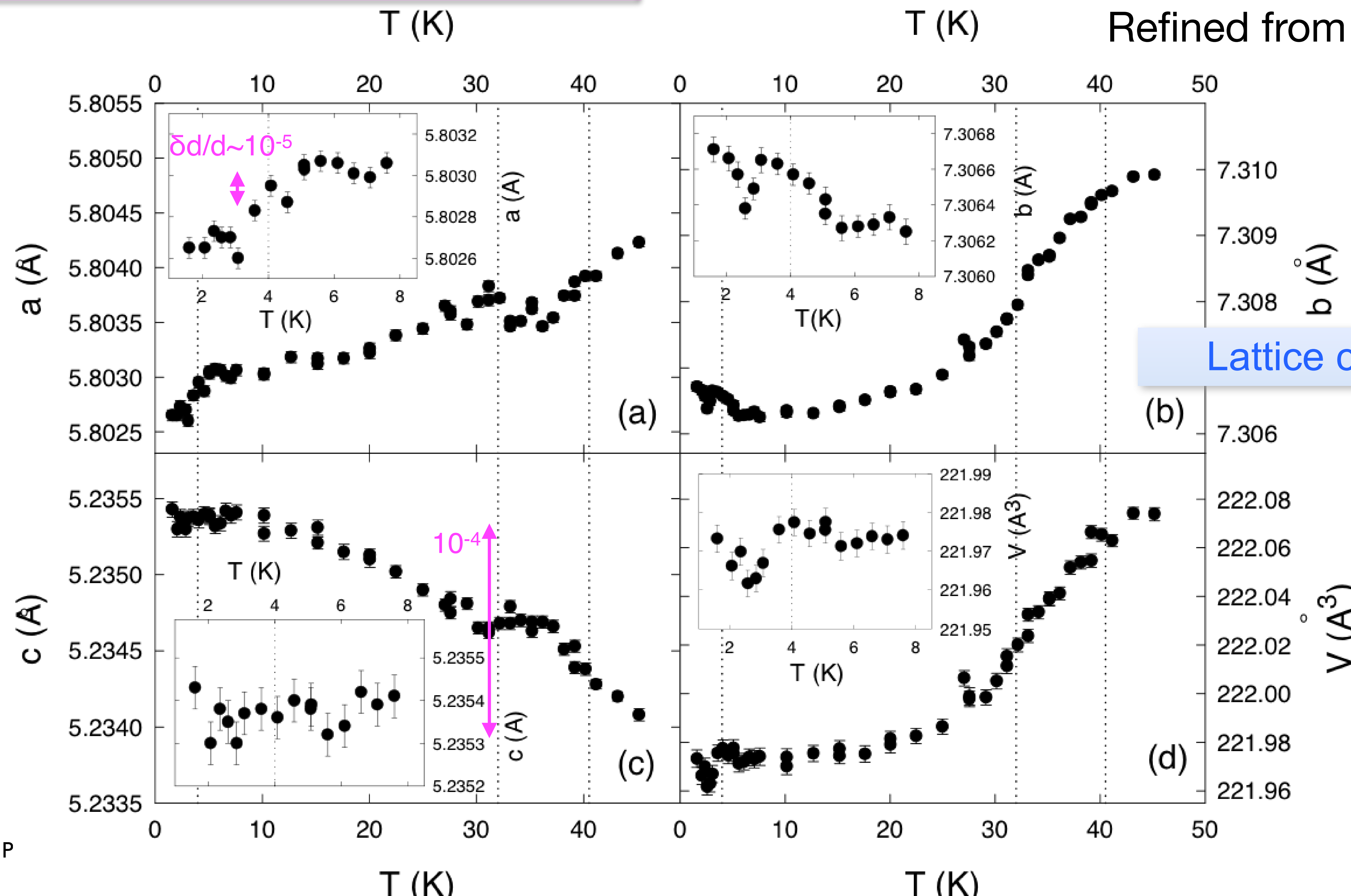
E = 0

Example of accuracy on metric: orthorhombic multiferroic $TmMnO_3$

material that have coupled electric, magnetic and structural order

accuracy ~0.0001Å=10 fm

Refined from HRPT



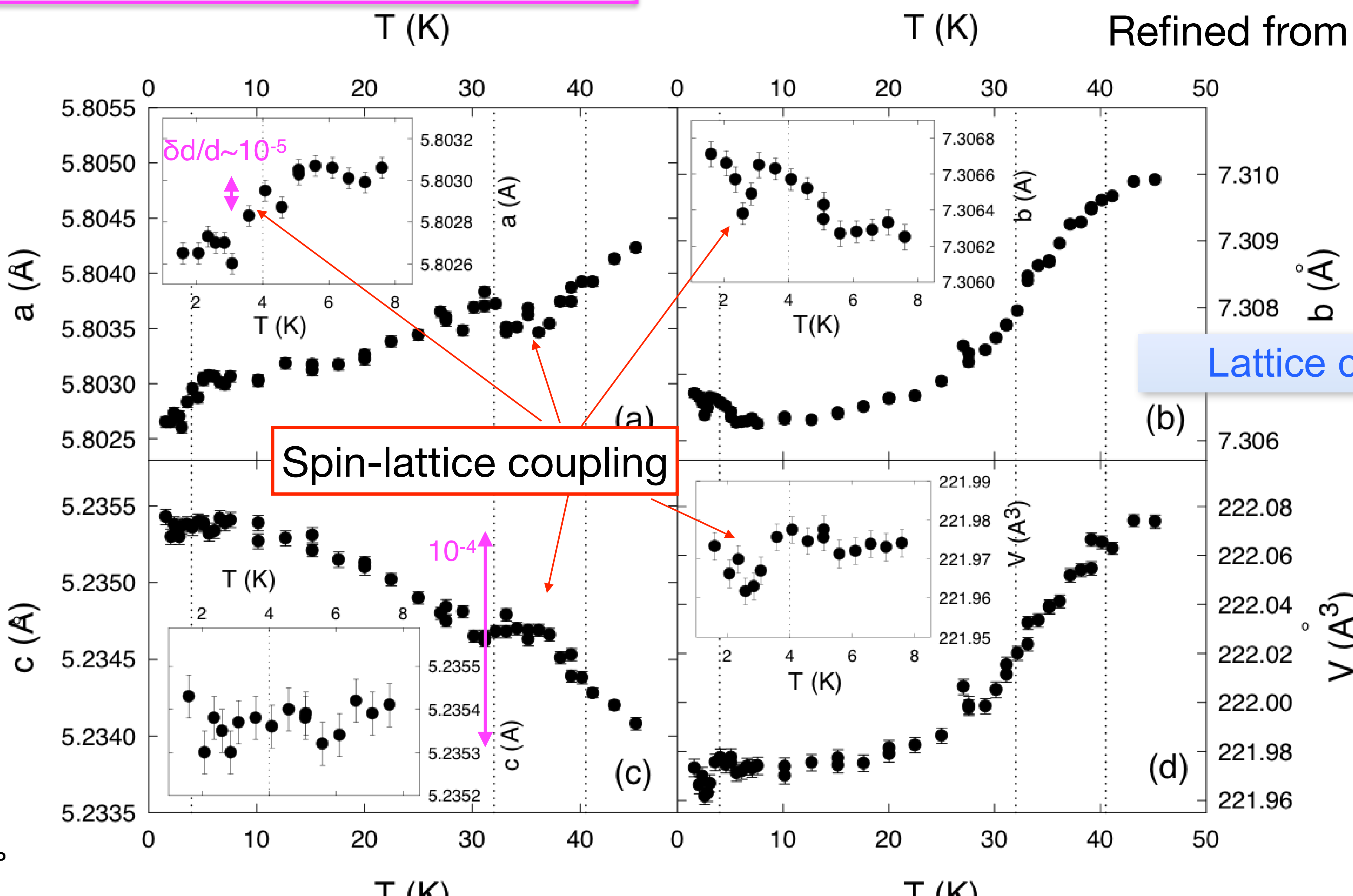
Lattice constants

Example of accuracy on metric: orthorhombic multiferroic $TmMnO_3$

accuracy ~0.0001Å=10 fm

material that have coupled electric, magnetic and structural order

Refined from HRPT



Lattice constants

P