Magnetic order from neutron diffraction : application of representation decomposition & Shubnikov symmetry

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This lecture, and some others:

http://sinq.web.psi.ch/sinq/instr/hrpt/praktikum.html

can be accessed from web page of neutron diffractometer HRPT

http://sinq.web.psi.ch/hrpt

Plan

- Intro to propagation vector description in zeroth block of the cell & neutron structure factors. (5)
- $Rb_xFe_{2-y}Se_2$: **k**=0 “simple” case. (6)
- $Ca_3Cu_1Ni_2(PO_4)_4$: multi-arm case. Shubnikov C_a2/c. (12)
- $TmMnO_3$:
    - Constraints on basis functions vs. superspace for the incommensurate two arm **k**=[±1/2±δ,0,0]. Both centrosymm and non-centrosymm.
    - One-arm multi dimensional irrep **k**=[1/2,0,0], Shubnikov P_bmn2_1.(24)

Propagation vector k formalism. Spin amplitudes S_0 are specified in zeroth block of the cell==parent cell w/o centering translations. All C, I, F, R -> Primitive

Magnetic moment below a phase transition

$$\mathbf{S}(\mathbf{t}_n) = \frac{1}{2}\left(\mathbf{S}_0 e^{2\pi i \mathbf{t}_n(+\mathbf{k})} + \mathbf{S}_0^* e^{2\pi i \mathbf{t}_n(-\mathbf{k})}\right)$$

Bragg peaks at

$$\mathbf{q} = \mathbf{H} \mp \mathbf{k}$$

In general
-k is nonequivalent to **+k**
i.e. **-k**≠**k**+'recip. latt. period'

multi-**k** or multi-*arm** structure
(non-equivalent $\mathbf{k}_1$, $\mathbf{k}_2$, … $\mathbf{k}_m$).

$$\mathbf{S}(\mathbf{t}_n) = \sum_{l=1}^{m} \frac{1}{2}\left(\mathbf{S}_{0l} e^{2\pi i \mathbf{t}_n(+\mathbf{k})} + \mathbf{S}_{0l}^* e^{2\pi i \mathbf{t}_n(-\mathbf{k})}\right)$$

---

* One must distinguish between the *arms* and the *twin* domains

Propagation vector formalism k≠0

Magnetic moment $$\mathbf{S}(\mathbf{t}_n) = \frac{1}{2}(\mathbf{S}_0 e^{+2\pi i \mathbf{t}_n \mathbf{k}} + \mathbf{S}_0^* e^{-2\pi i \mathbf{t}_n \mathbf{k}})$$

Bloch waves

Fourier amplitude is complex (In general, one can not avoid this in 3D for **k**≠ 0 or 1/2)

$$\mathbf{S}_0 = \mathbf{S}_x e^{i\phi_x} + \mathbf{S}_y e^{i\phi_y} + \mathbf{S}_z e^{i\phi_z}$$

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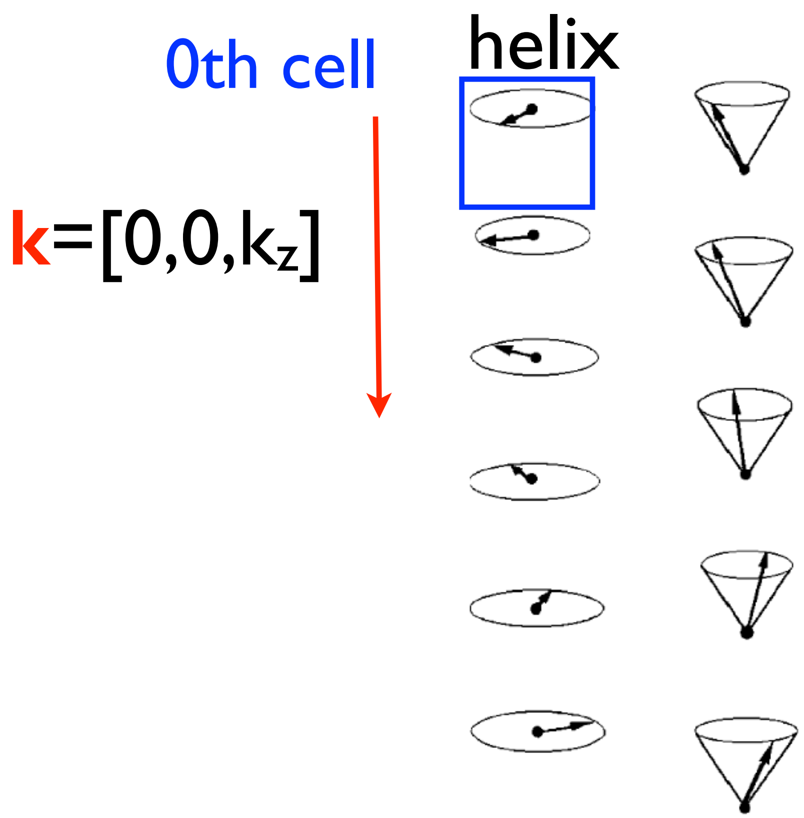
modulated (in)commensurate



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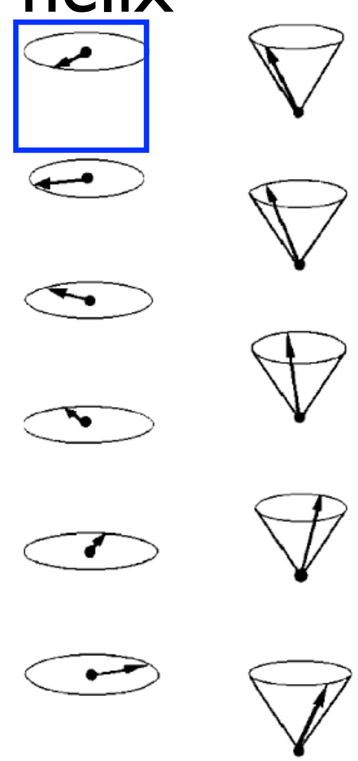
0th cell

helix

k=[0,0,k_z]



helix

$$\mathbf{S}_{01} = \mathbf{S}_x + \mathbf{S}_y e^{\frac{i\pi}{2}} = \mathbf{S}_x + i\mathbf{S}_y$$

$$\varphi_n = 2\pi i \mathbf{t}_n \mathbf{k}$$

$$\mathbf{S}(\mathbf{t}_n) = \mathbf{S}_x \cos(\varphi_n) + \mathbf{S}_y \sin(\varphi_n)$$

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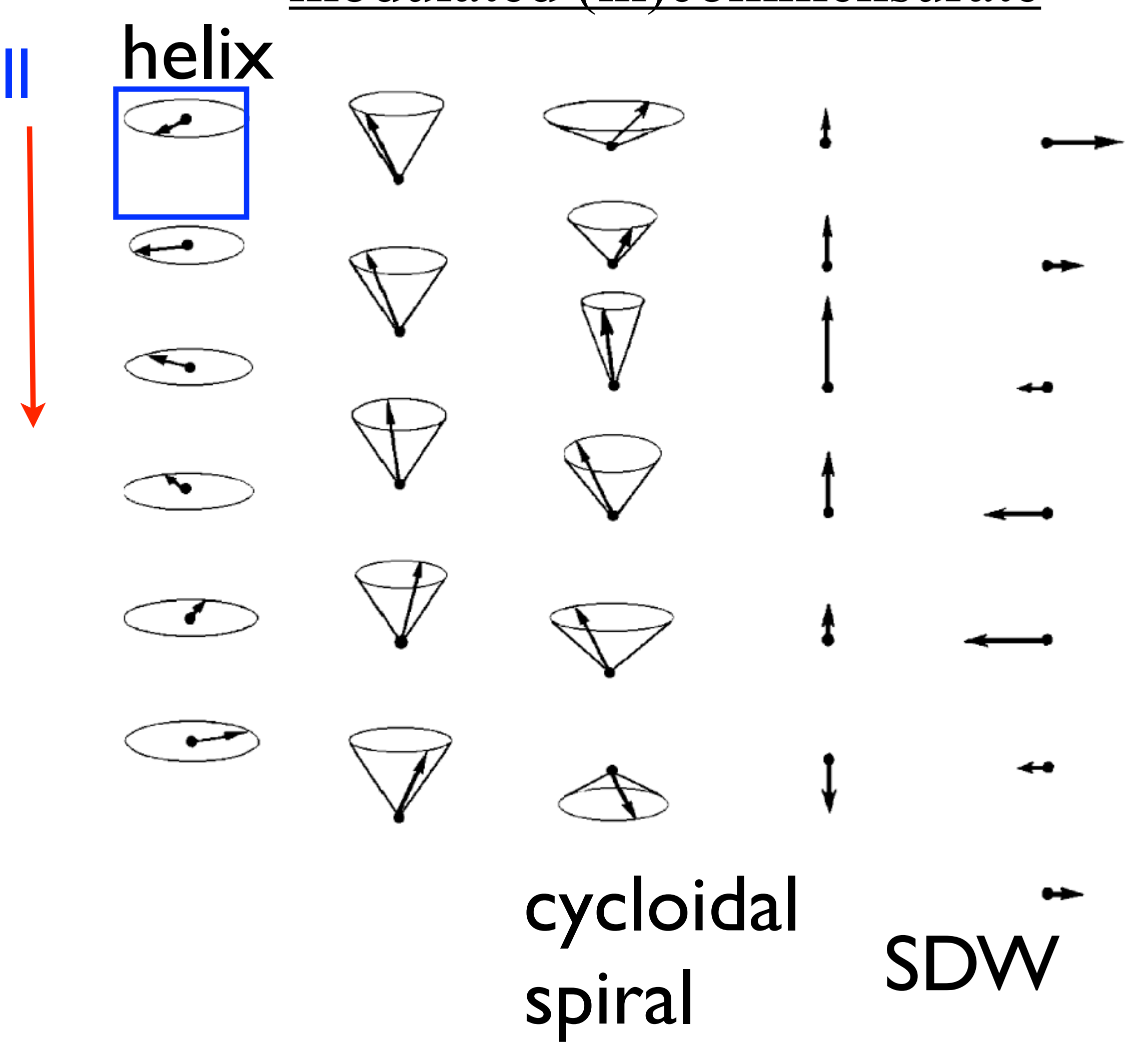

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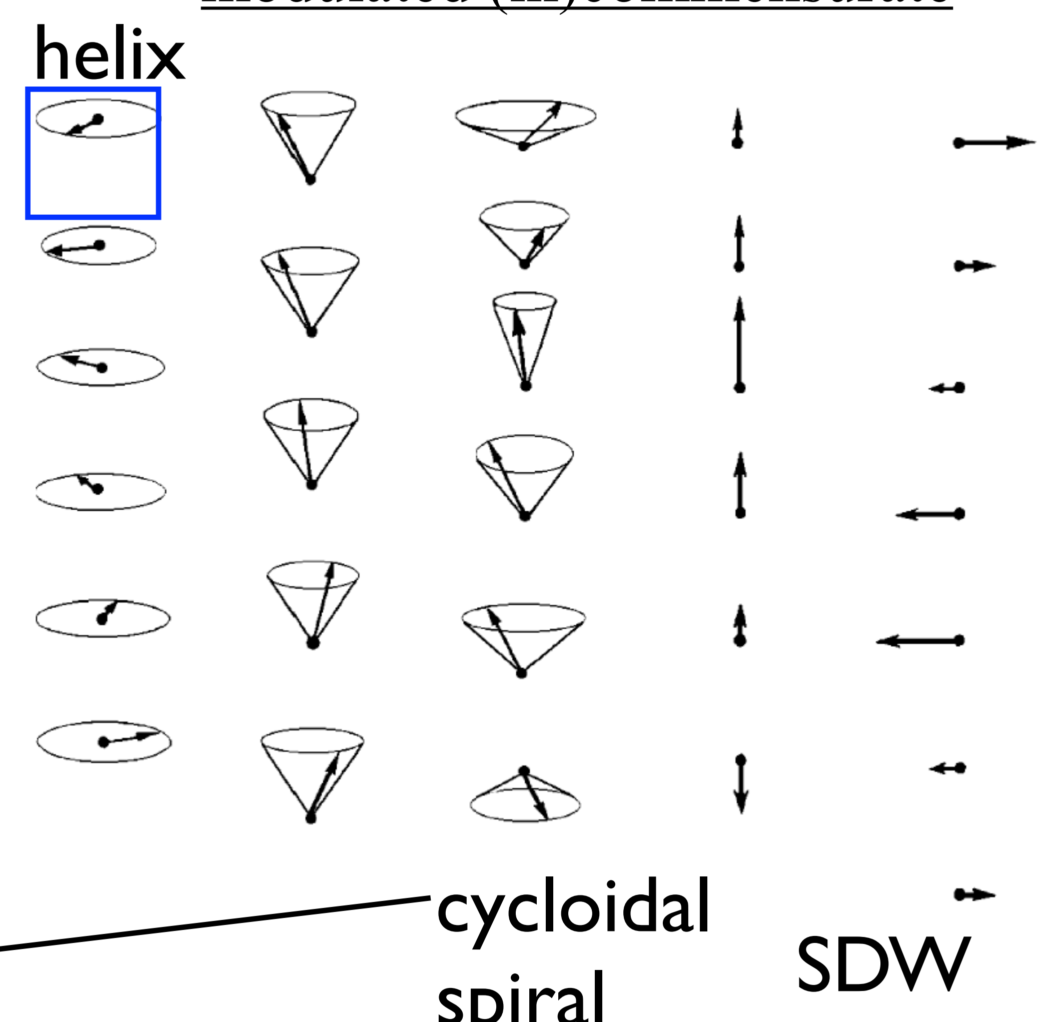

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cycloidal spiral

$$\mathbf{S}_{01} = \mathbf{S}_x + i\mathbf{S}_y + \mathbf{S}_z e^{i\phi_z}$$

Calculations of the scattering intensity:

structure factors in zeroth block of the cell are calculated using complex scattering amplitudes

Scattering from the lattice of spins. Structure factor F(q)

In ND experiment we measure correlators of Fourier transform of magnetic lattice

$$\frac{d\sigma}{d\Omega} \propto (\mathbf{F}(\mathbf{q}) \cdot \mathbf{F}^*(\mathbf{q}) + i\mathbf{P} \cdot [\mathbf{F}(\mathbf{q}) \times \mathbf{F}^*(\mathbf{q})]) \cdot \delta(\mathbf{H} \pm \mathbf{k} - \mathbf{q})$$

structure factor

polarized neutron (chiral) term.

Bragg peak at $\mathbf{q} = \mathbf{H} \mp \mathbf{k}$

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Sum runs over all atoms in zeroth cell

$$\mathbf{F}(\mathbf{q})_{-\boldsymbol{k}} = \sum_j \frac{1}{2}\mathbf{S}_{\perp 0j} \exp(i\mathbf{r}_j\mathbf{q}) \qquad \mathbf{F}(\mathbf{q})_{+\boldsymbol{k}} = \sum_j \frac{1}{2}\mathbf{S}^*_{\perp 0j} \exp(i\mathbf{r}_j\mathbf{q})$$

Complex amplitude of spin modulation perpendicular to $\mathbf{q}$

position of spin in the zeroth cell

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Example: one atom in a cell for helical structure

$$\mathbf{F}(\mathbf{q})_{+\boldsymbol{k}} = \frac{1}{2}\mathbf{S}^*_{01\perp} = \frac{s}{2}(1\mathbf{e}_x \pm i\mathbf{e}_y)$$

Complex amplitude of spin modulation perpendicular to **q**

spin in *xy*-plane

$$\mathbf{S}(\mathbf{t}_n) = s(\mathbf{e}_x \cos(2\pi i\mathbf{k}\mathbf{t}_n) \pm \mathbf{e}_y \sin(2\pi i\mathbf{k}\mathbf{t}_n))$$

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Complex amplitude of spin modulation perpendicular to $\mathbf{q}$

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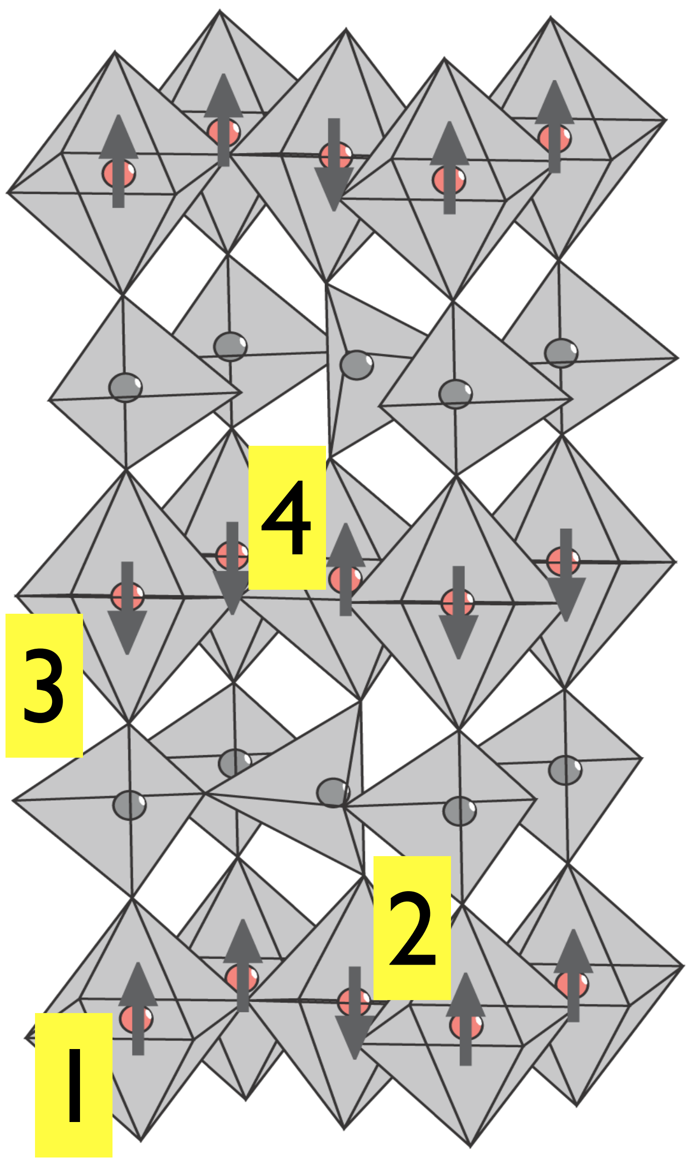
Chirality

$$\mathbf{S}(\mathbf{t}_n) = s(\mathbf{e}_x \cos(2\pi i\mathbf{k}\mathbf{t}_n) \pm \mathbf{e}_y \sin(2\pi i\mathbf{k}\mathbf{t}_n))$$

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. $\mathbf{S}(\mathbf{r}) = \mathbf{s}(\mathbf{r}_1) \oplus \mathbf{s}(\mathbf{r}_2) \oplus \mathbf{s}(\mathbf{r}_3) \oplus \mathbf{s}(\mathbf{r}_4)$



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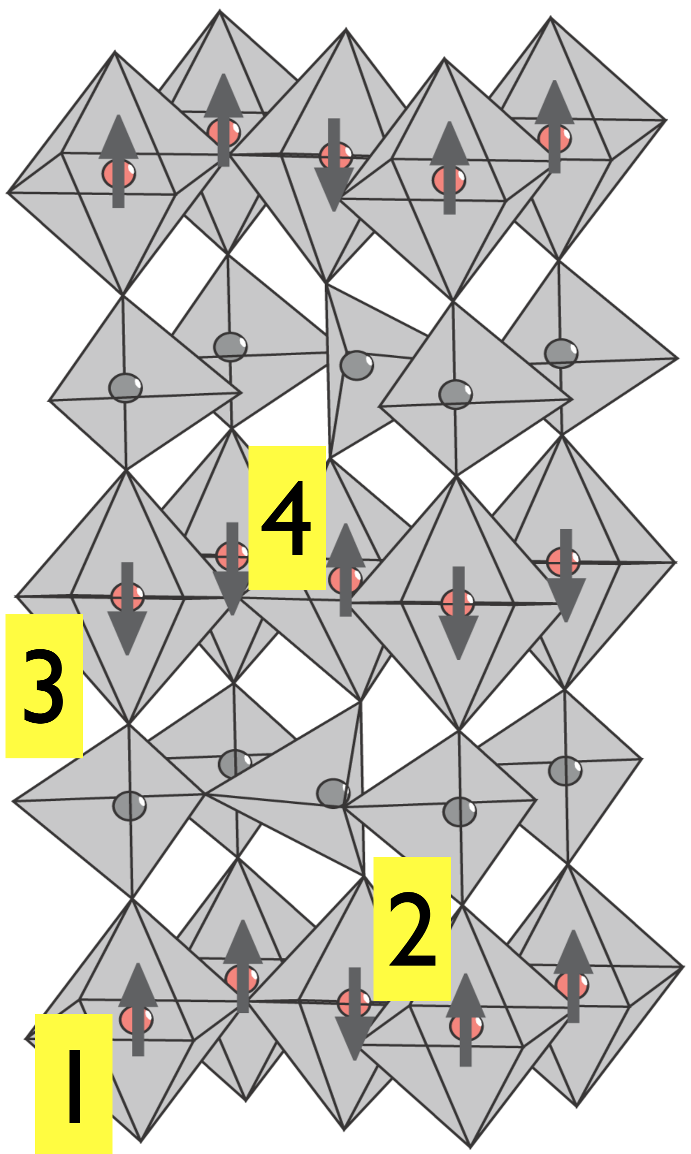

1. g**S**(**r**) = **S**(**r**) to itself, where g ∈ subgroup of SG⊗1’, 1’=spin/time reversal, SG (space group)

   or

2. g**S**(**r**) —> **S**’(**r**) to different function defined on the same system of points, g ∈ SG

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1. **Magnetic or Shubnikov groups MSG.** Historically the first way of description. A group that leaves **S(r)** invariant under a subgroup of G⊗1'. Identifying those symmetry elements that leave S(r) invariant.
   Similar to the space groups (SG 230). The MSG symbol looks similar to SG one, e.g. *I4/m'*

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<u>**S**(**r**) is transformed to $\mathbf{S}^i(\mathbf{r})$ under *g* ∈ G 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 space group G

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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

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τ_7	1	$-i$	-1	i	1	$-i$	-1	i

Relation of magnetic Shubnikov symmetry and irreducible representation of space group

Paramagnetic crystallographic space group (*PSG*)

Propagation vector of magnetic structure **k**

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magnetic symmetry

is irrep real and 1D?

Yes

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

representation

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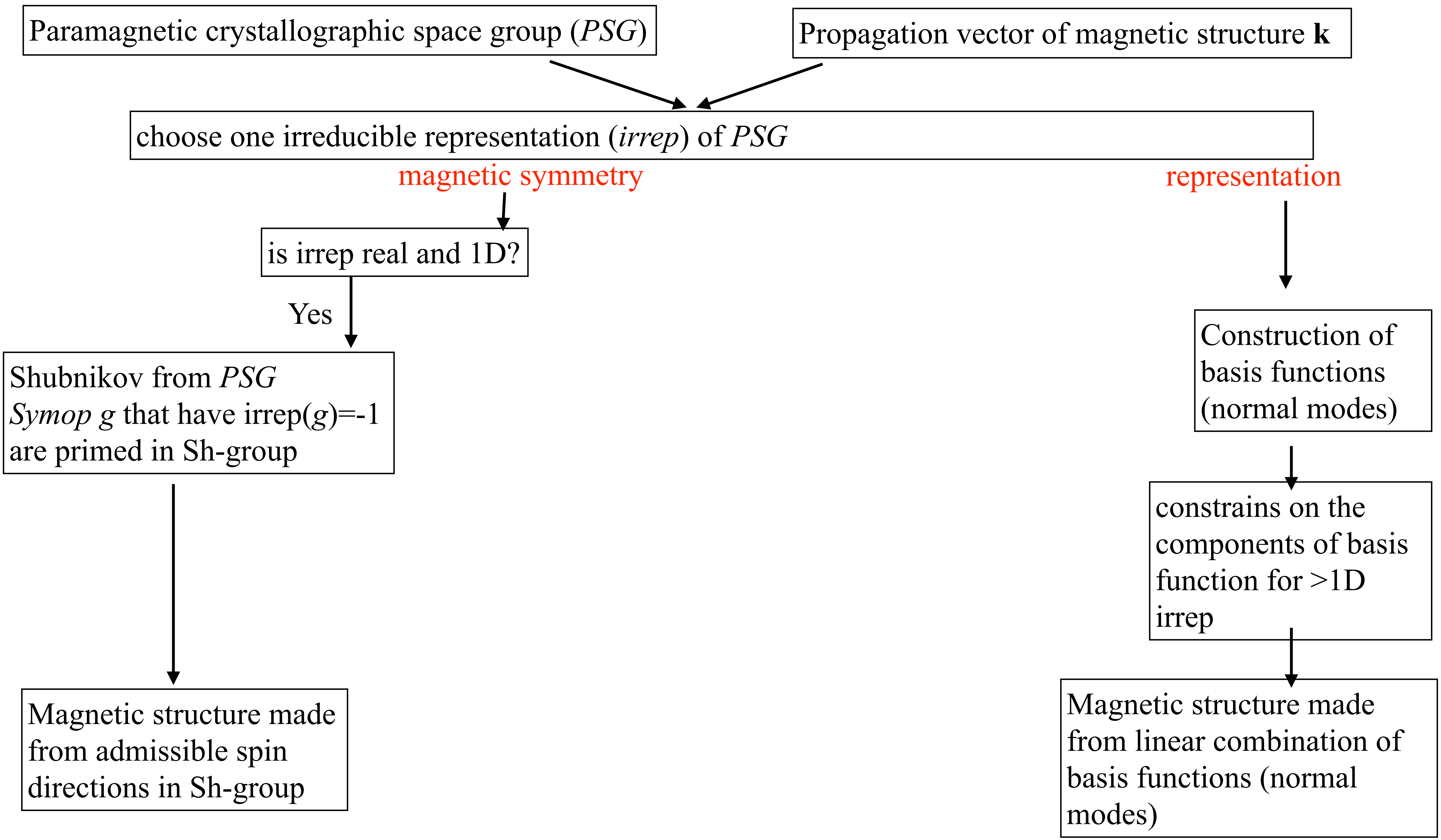

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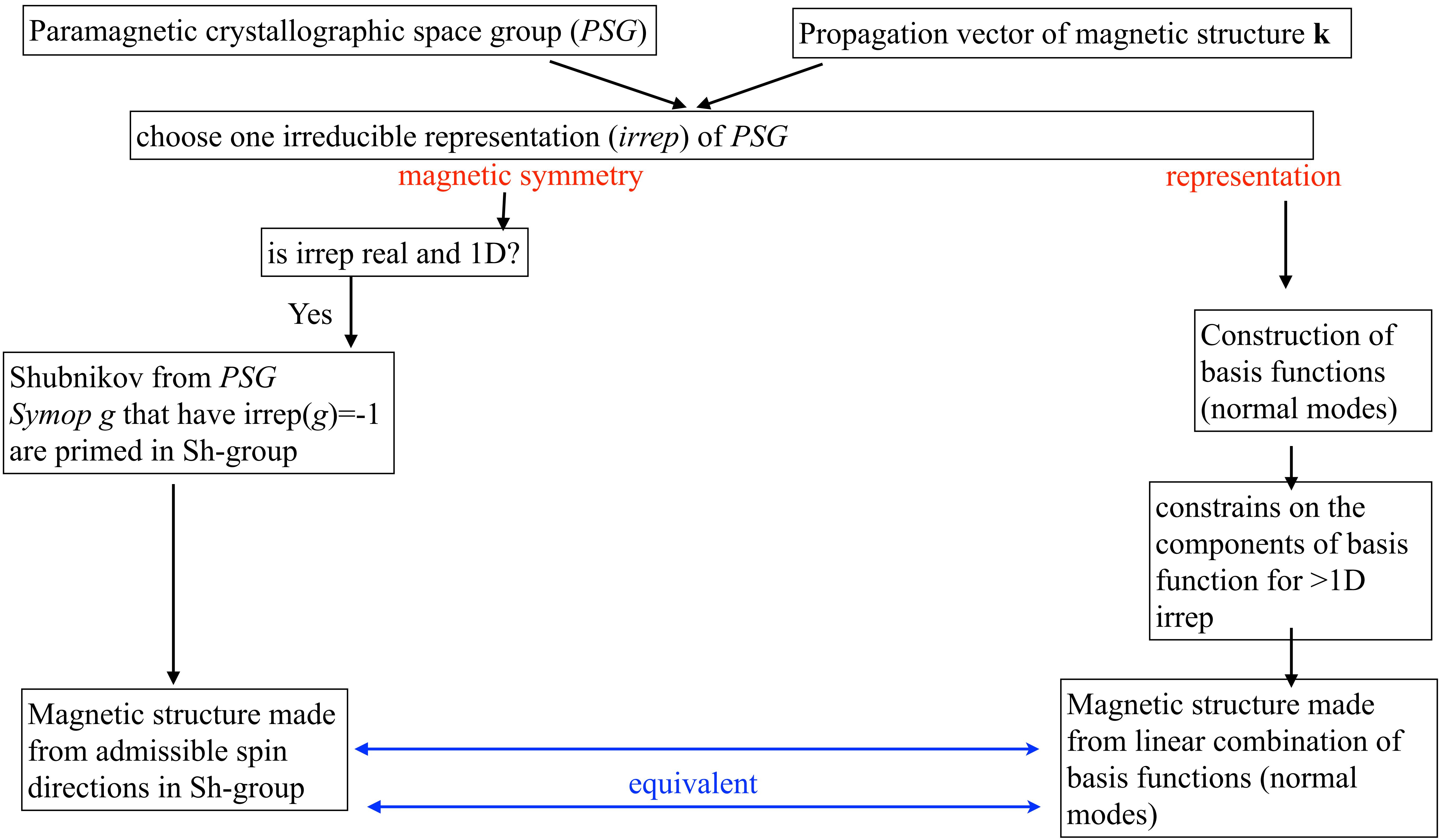

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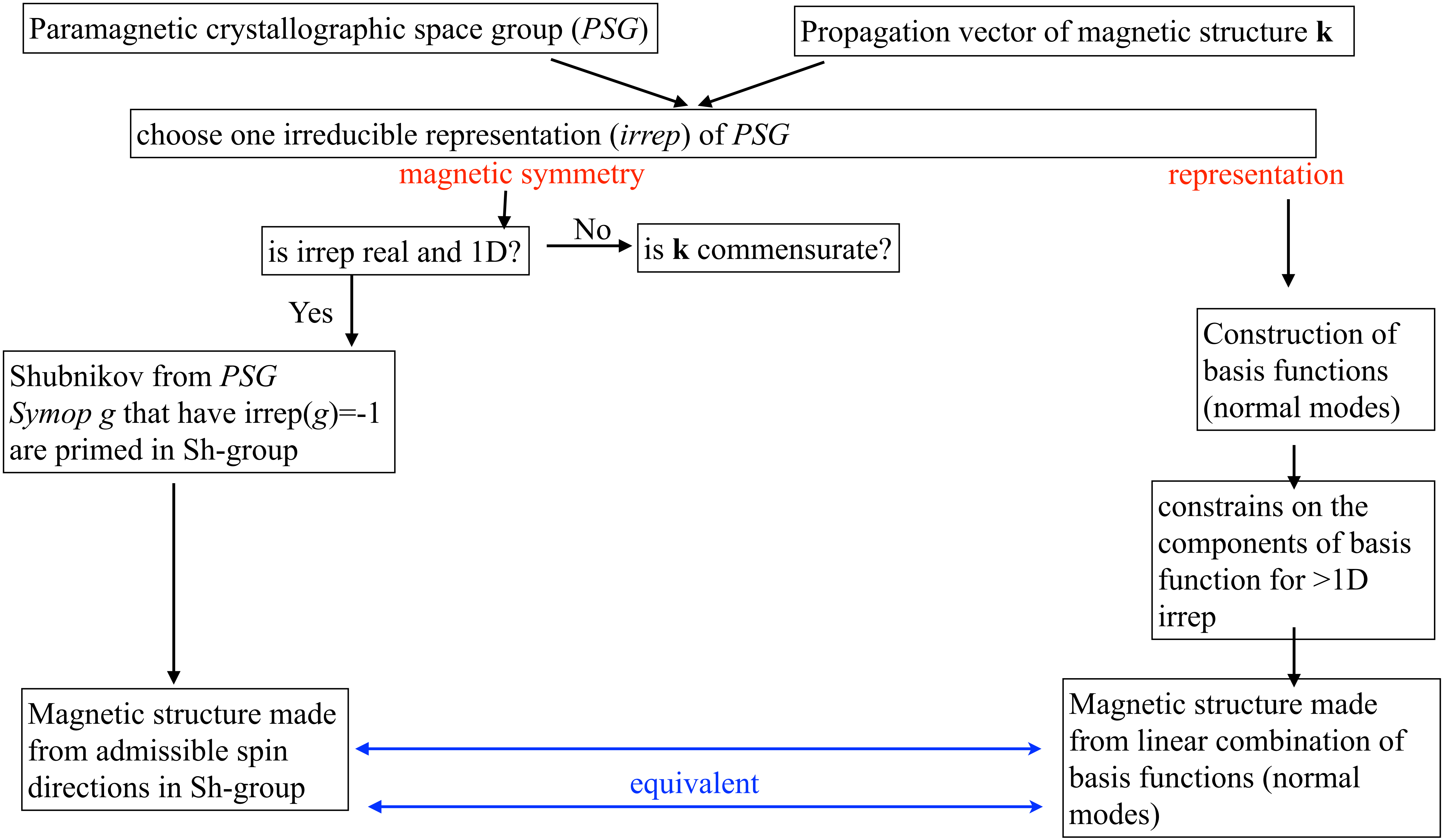

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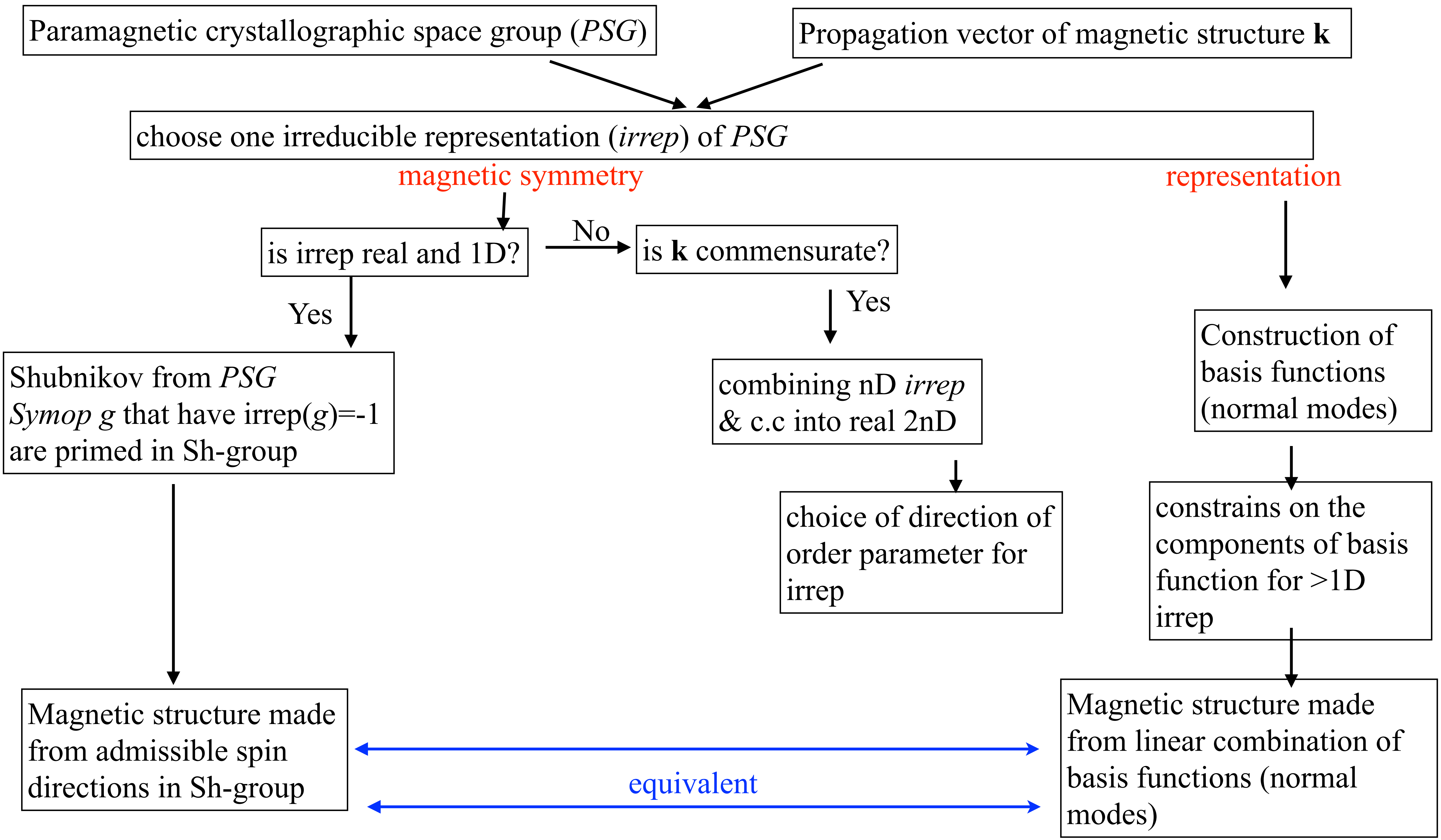

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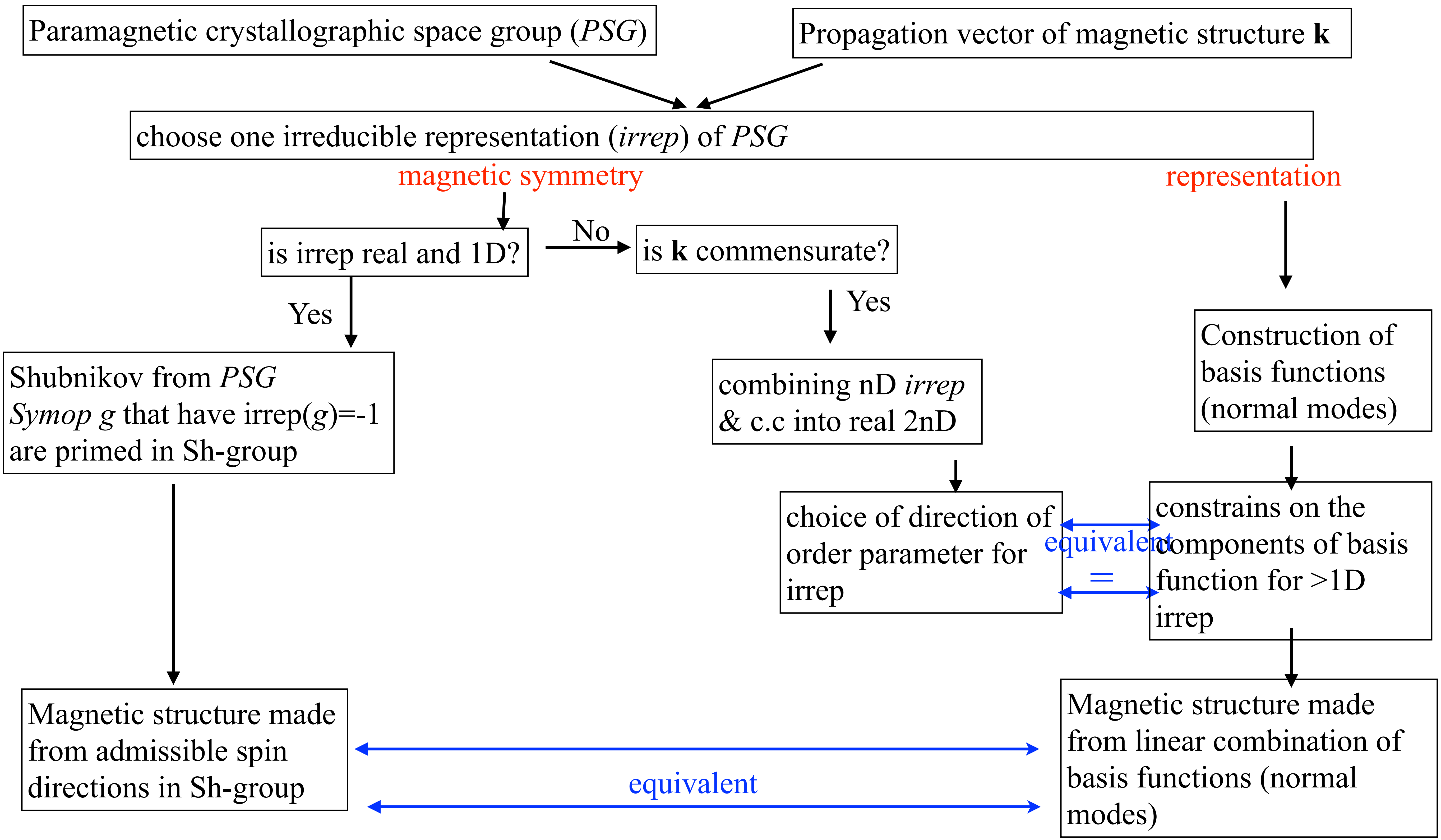

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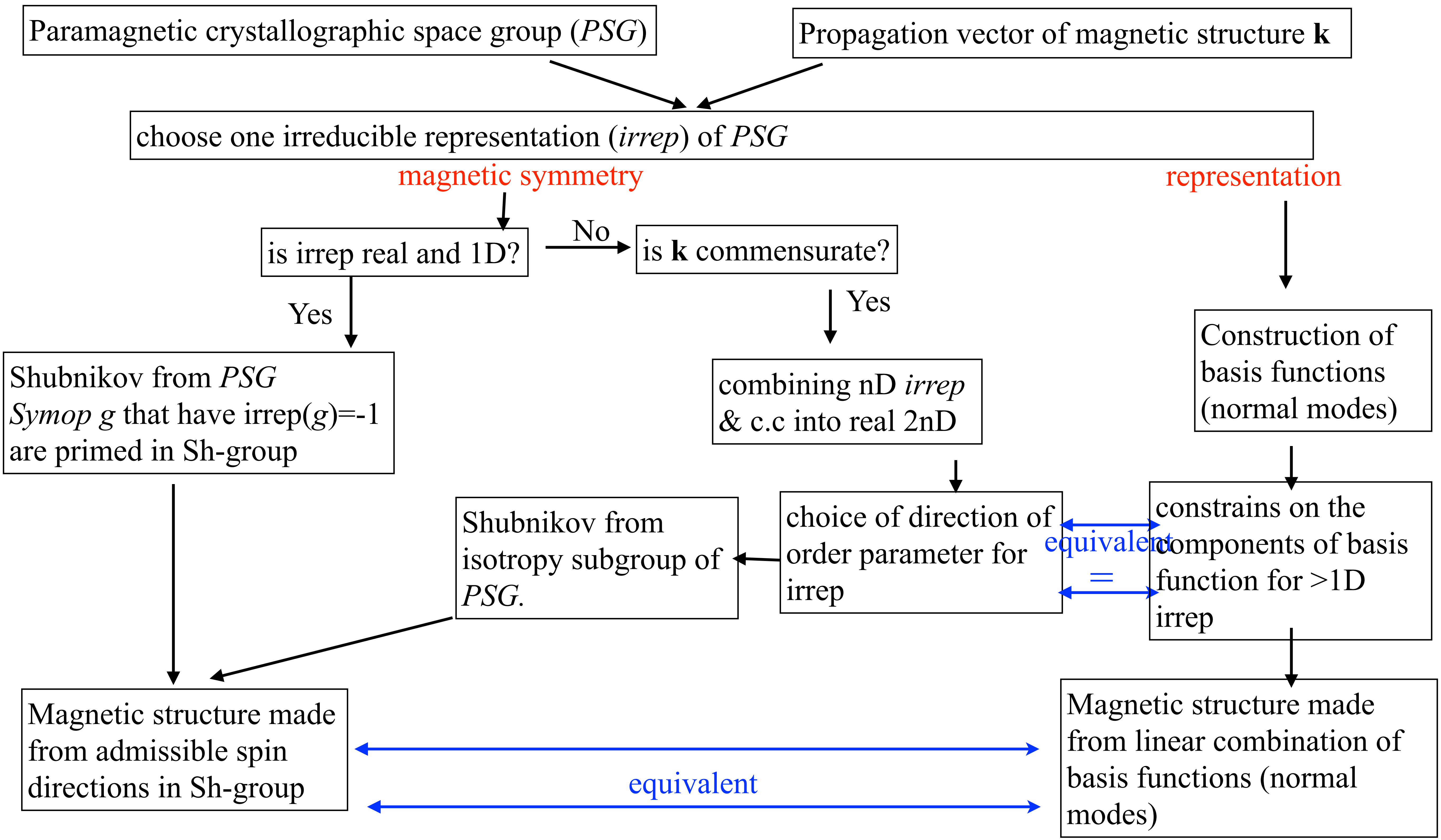

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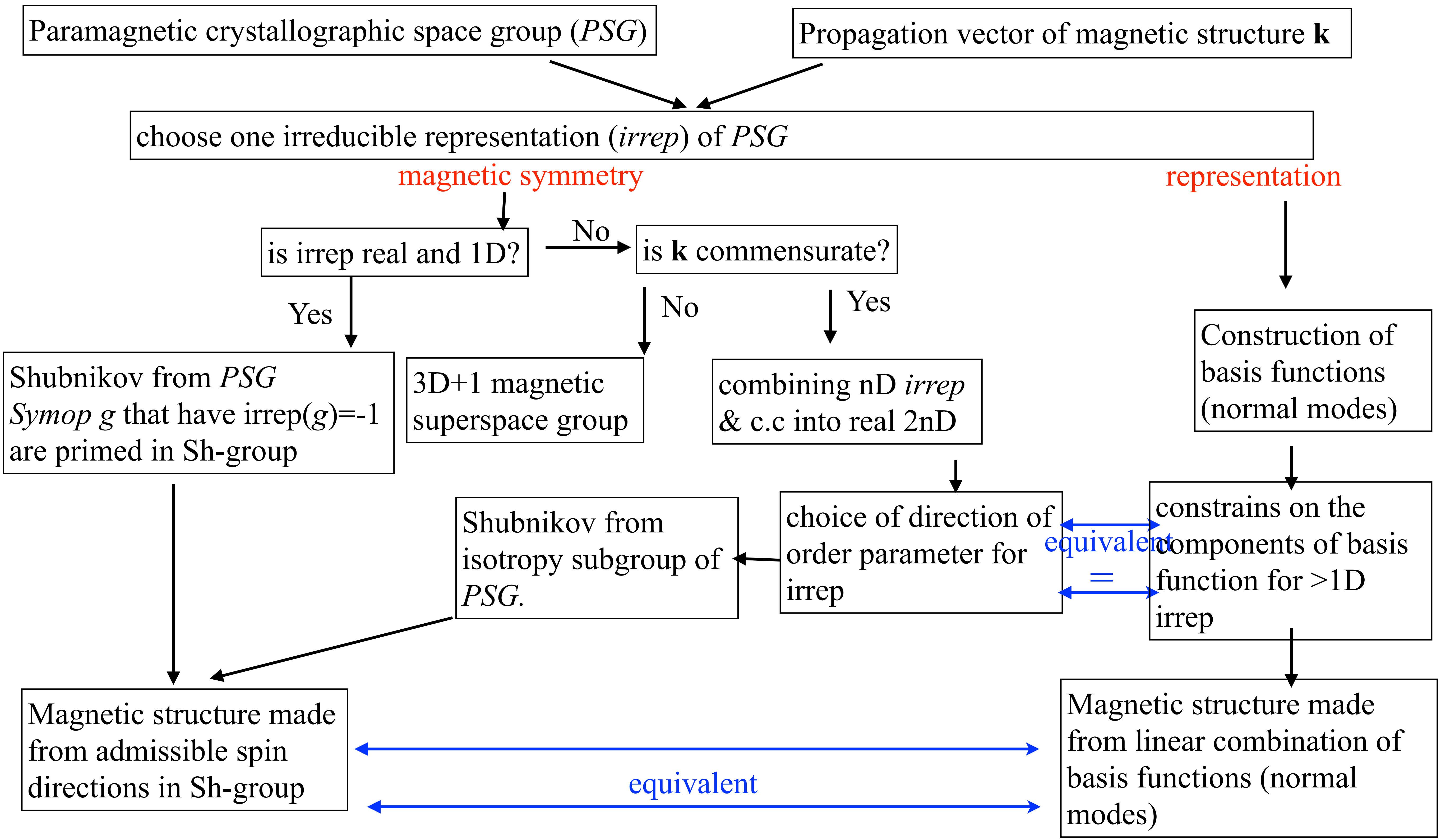
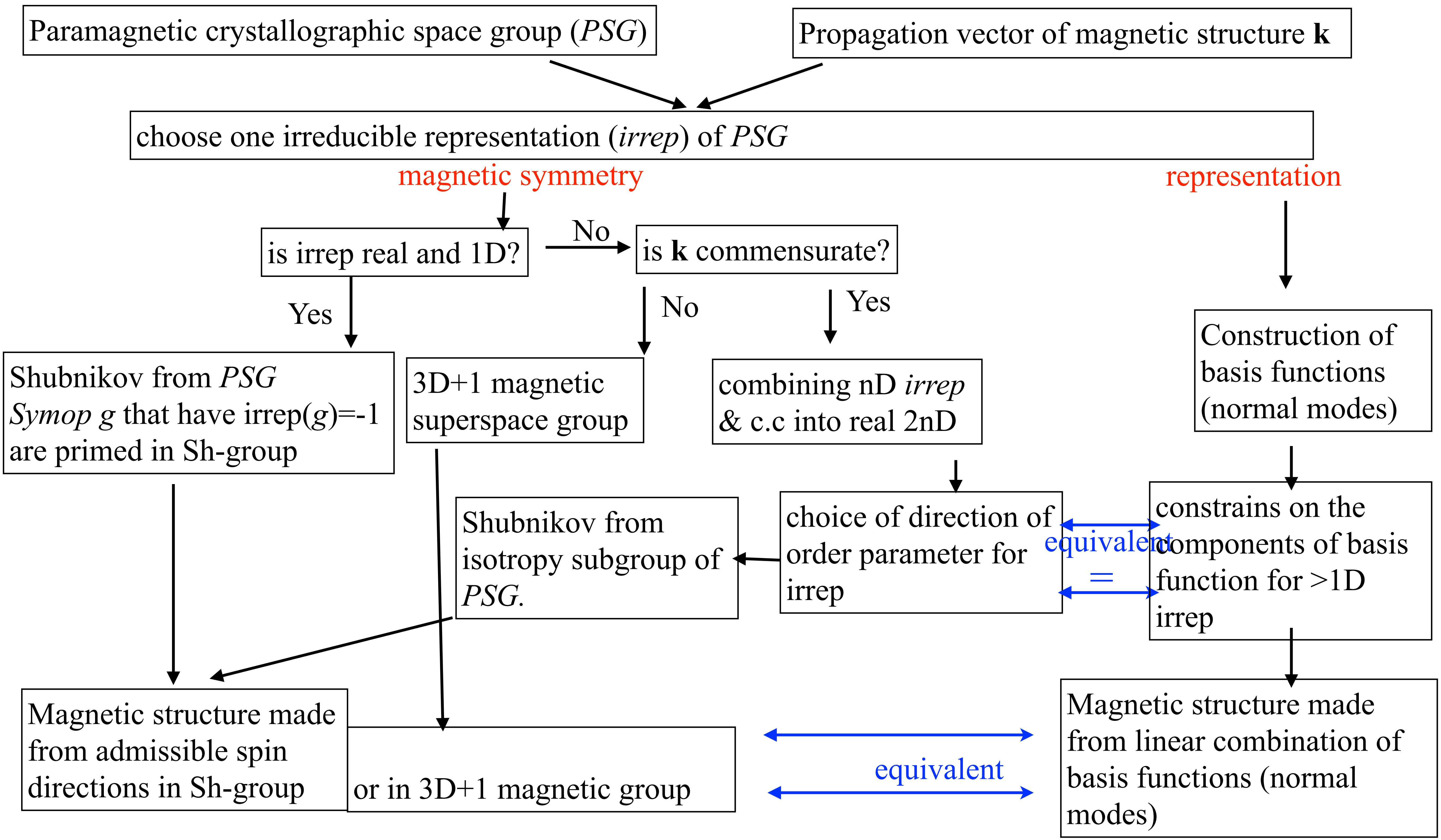
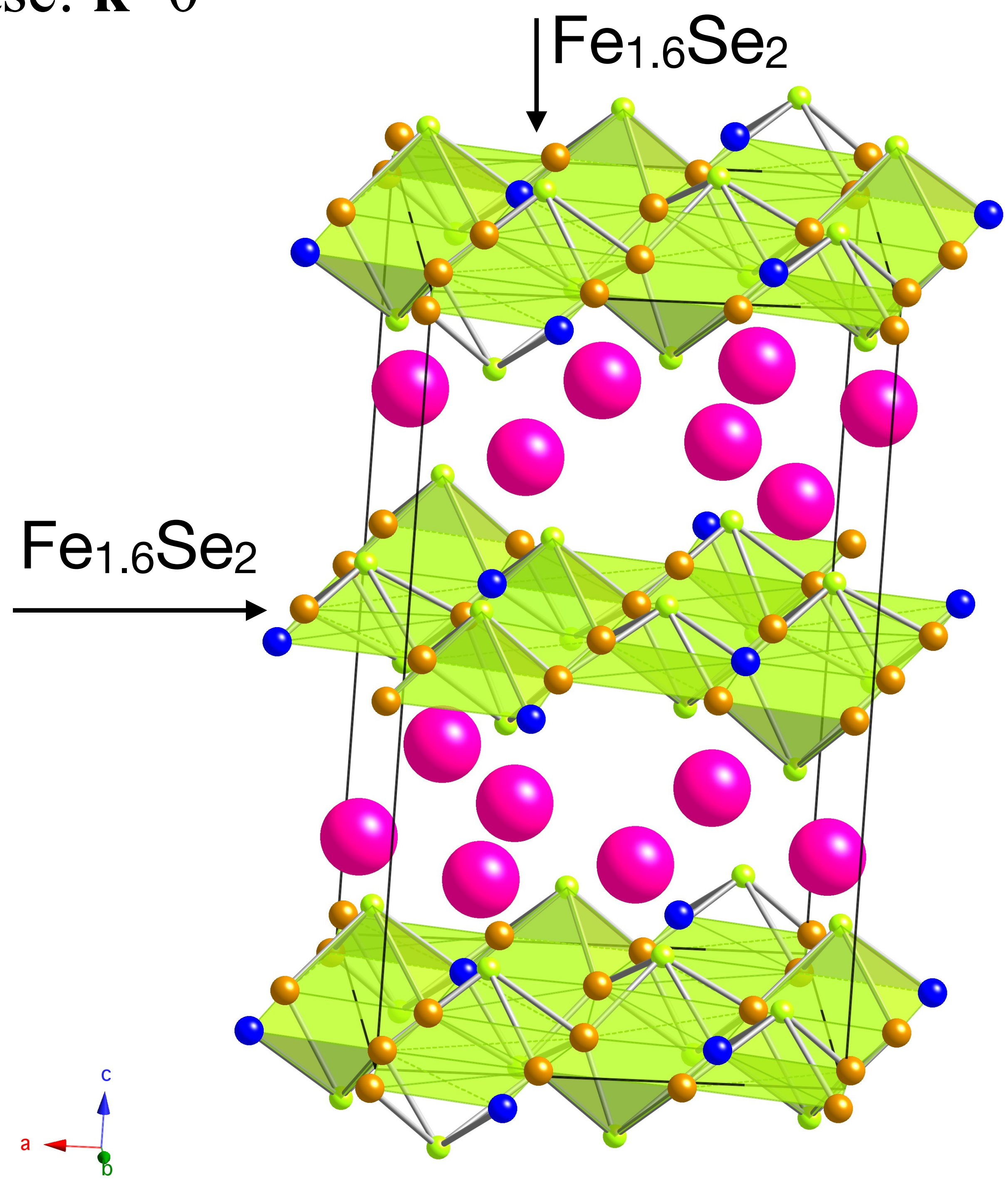


Relation of magnetic Shubnikov symmetry and irreducible representation of space group



Magnetic structure of $X_{0.8}Fe_{1.6}Se_2$, X=K, Rb, Cs

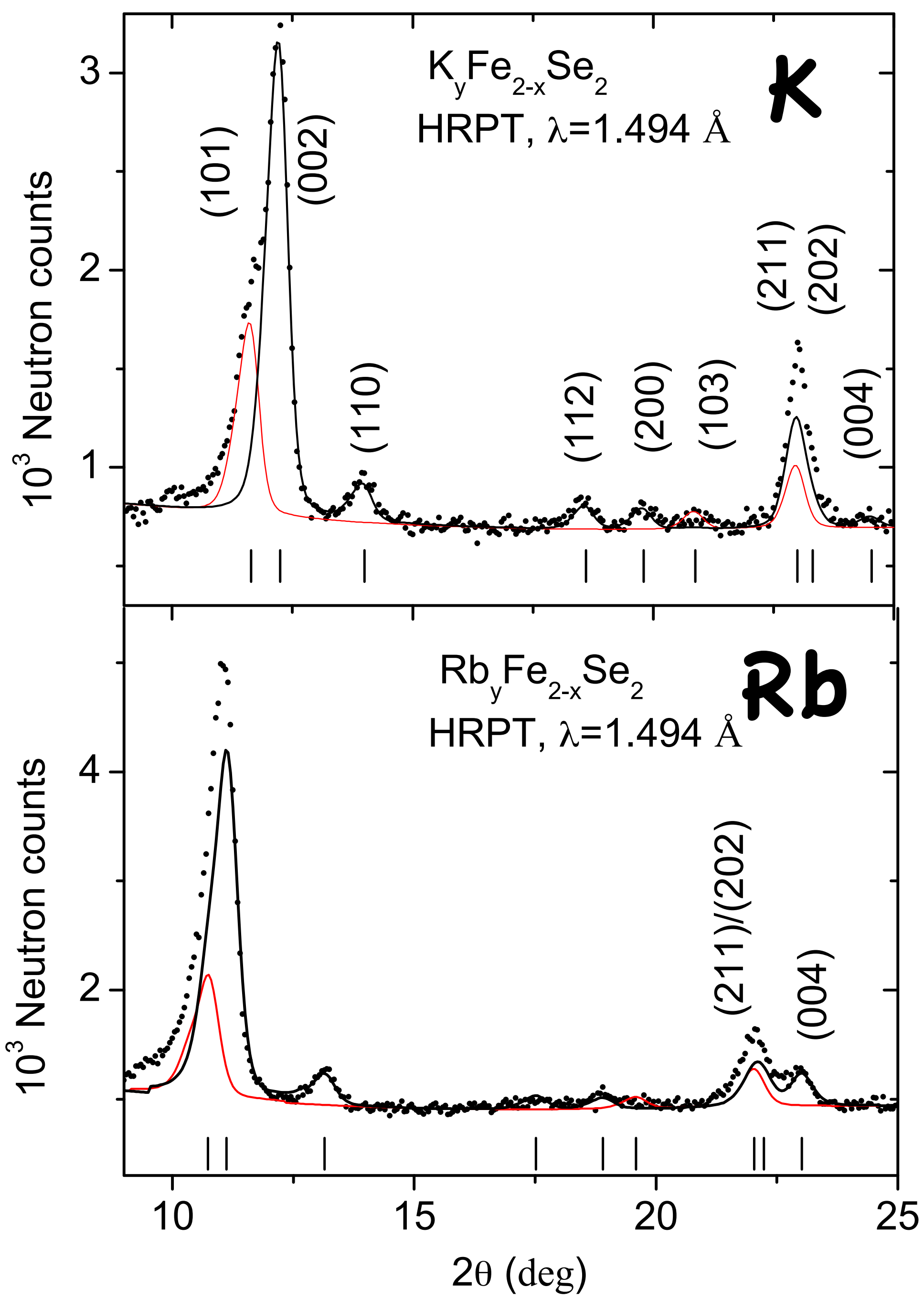
"Simple" case: **k**=0



J. Phys.: Condens. Matter **23** 156003 (2011);
Phys. Rev. **B 83**, 144410 (2011)

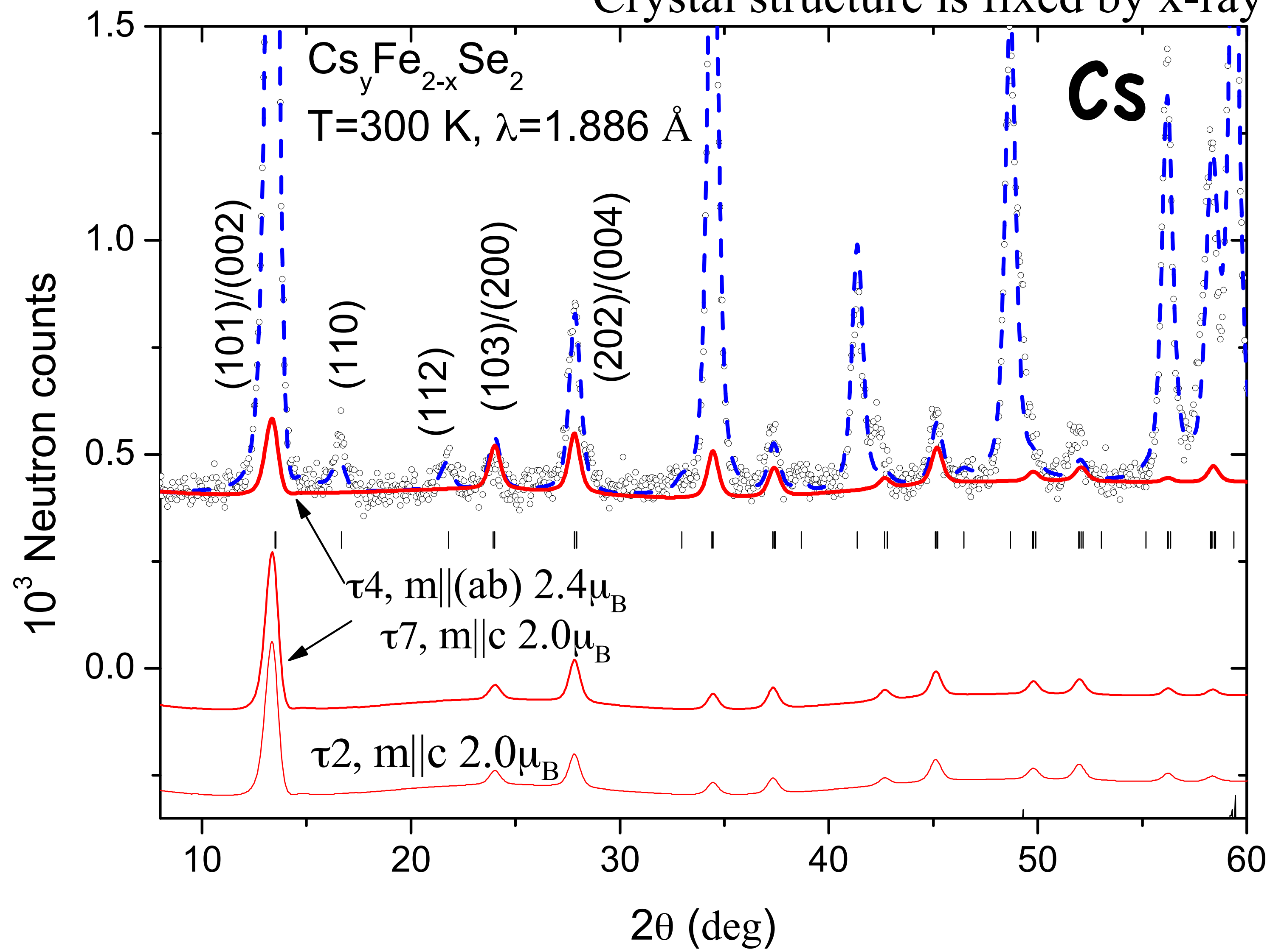
Neutron diffraction patterns Rb, K, Cs

Magnetic contribution is in red



τ2 or t7 with spins along c

Comparison of different models.
Crystal structure is fixed by x-ray



	K	Rb	Cs	
a=	8.7302	8.7996	8.8582 Å	is "difficult" for powder due to peak overlap
c=	14.1149	14.5762	15.2873 Å	
$(c/a)^2$ =	2.6140	2.7438	2.9783≈3	

$X_{0.8}Fe_{1.6}Se_2$, X=K, Rb, Cs. Magnetic representation. Symmetry adapted solutions.

I4/m, k=0 has 8 1D irreps τ_1,... τ_8.
4 real irreps <—> Shubnikov groups of *I4/m*
4 complex irreps <—> Lower symmetry Shubnikov

	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 *I4/m'*	1	1	1	1	-1	-1	-1	-1
τ_3	1	i	-1	$-i$	1	i	-1	$-i$
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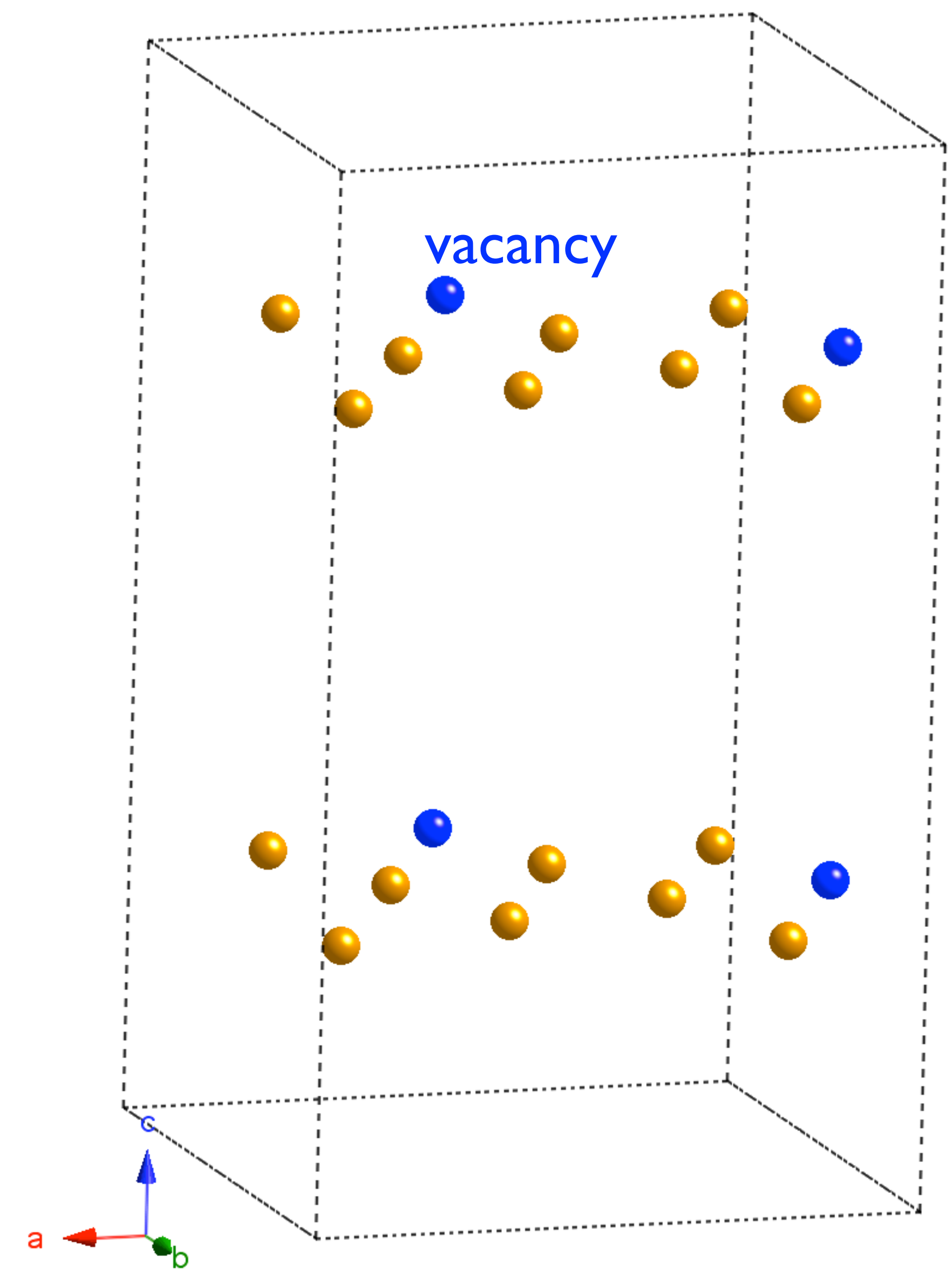
One unit cell with 16 Fe



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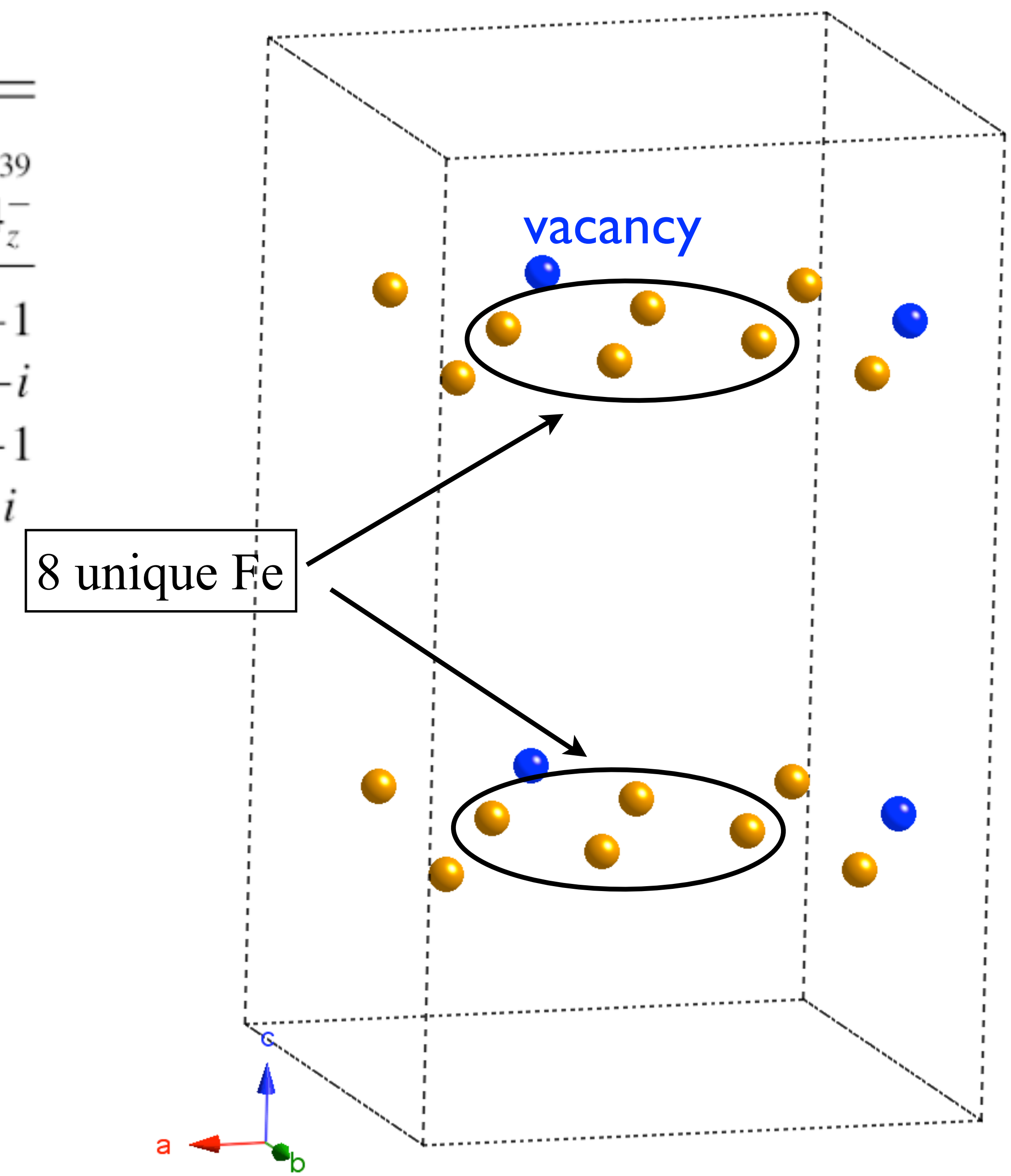

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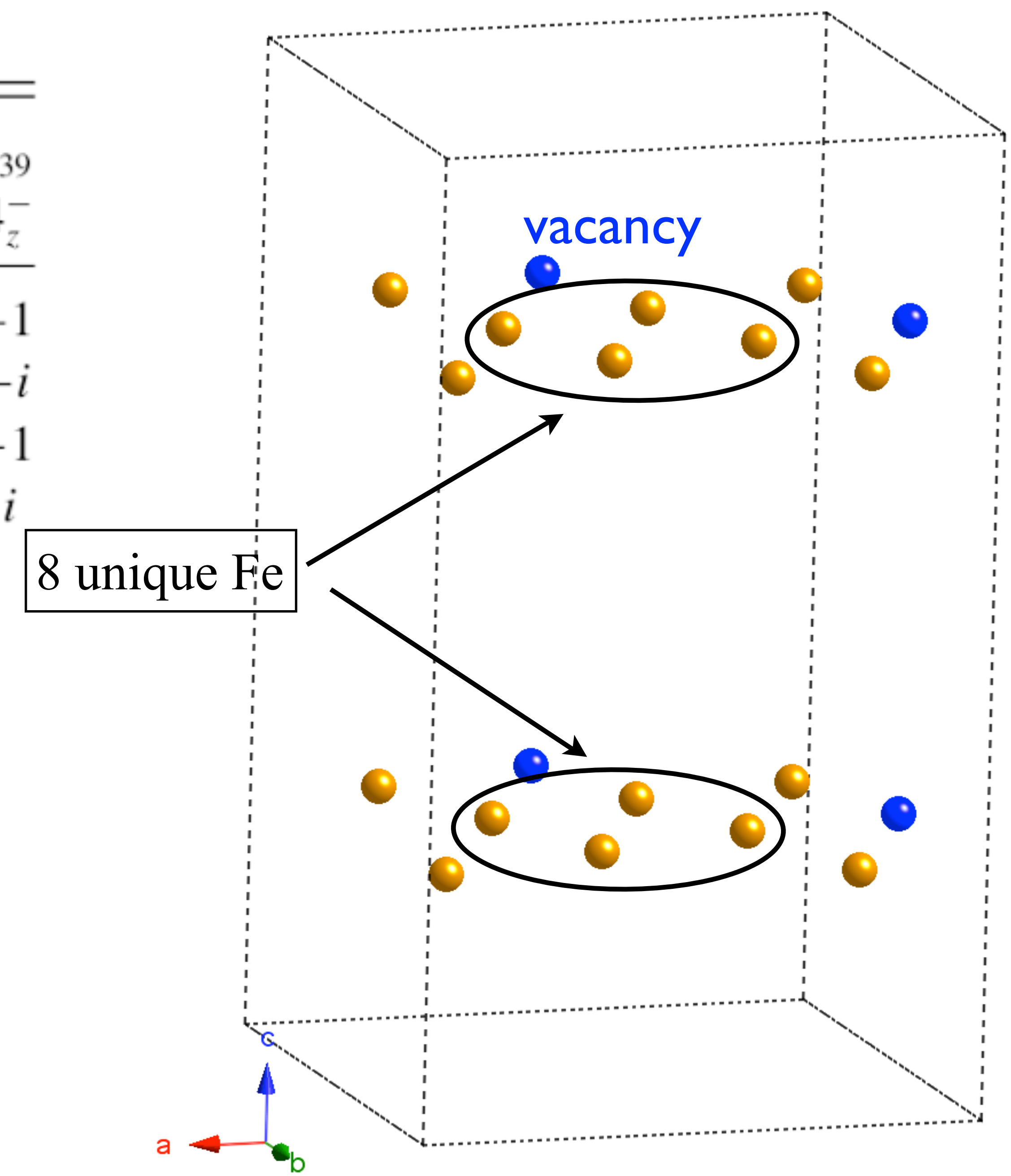

Fe

Magnetic representation (3x8=24D) of Fe spins **S** in(16i) (x,y,z): all eight irreps

$$\Gamma = 3\tau_1 \oplus 3\tau_2 \oplus 3... \oplus 3\tau_8$$

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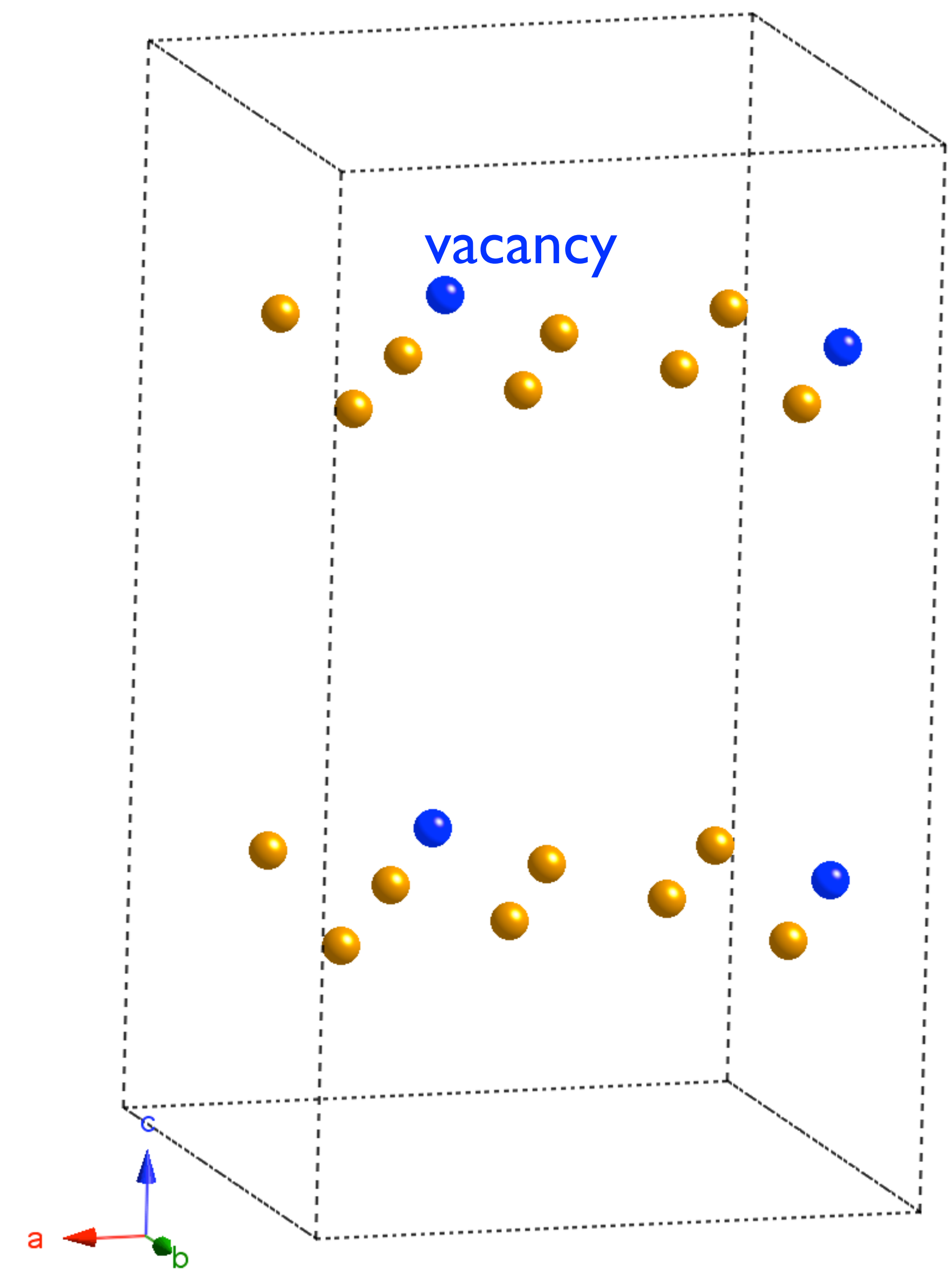
Example special case **S** || **c**:
irrep = "Fourier amplitude"

One unit cell with Fe



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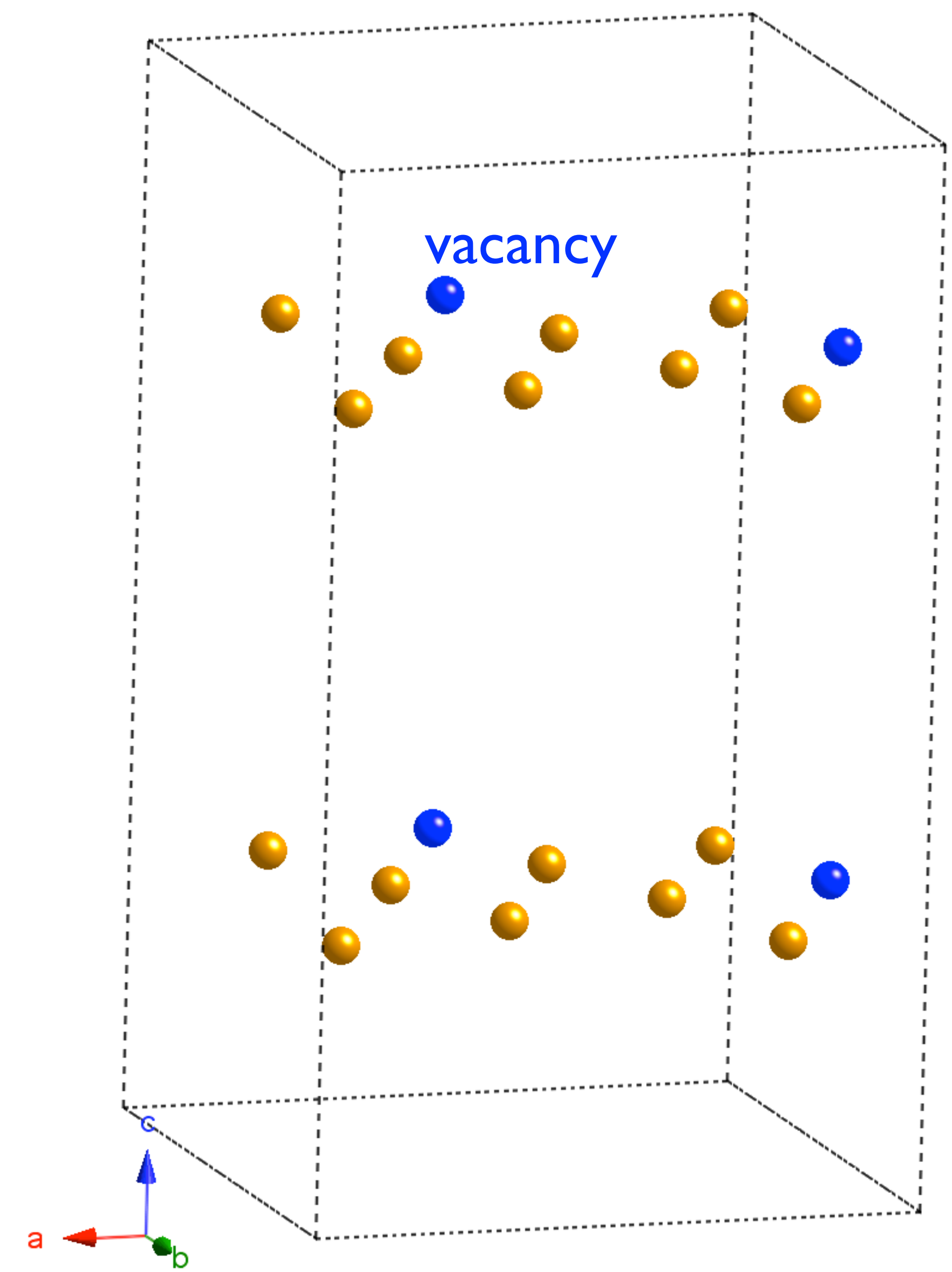
$$\mathbf{S}_0 = Ce^{i\phi_z}\mathbf{e}_z, \phi_z = 0, \frac{\pi}{2}, \pi$$

One unit cell with Fe



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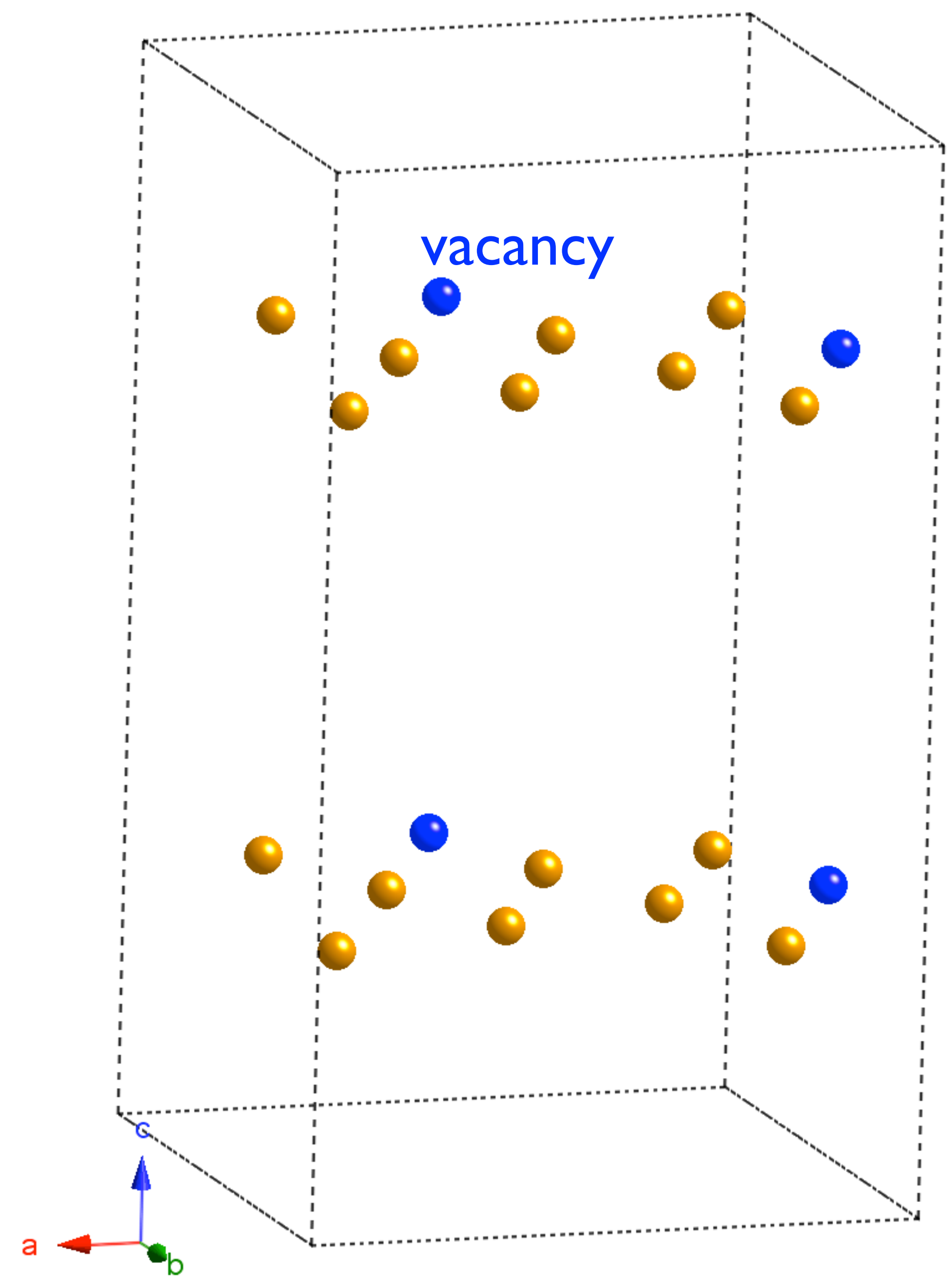
One unit cell with Fe



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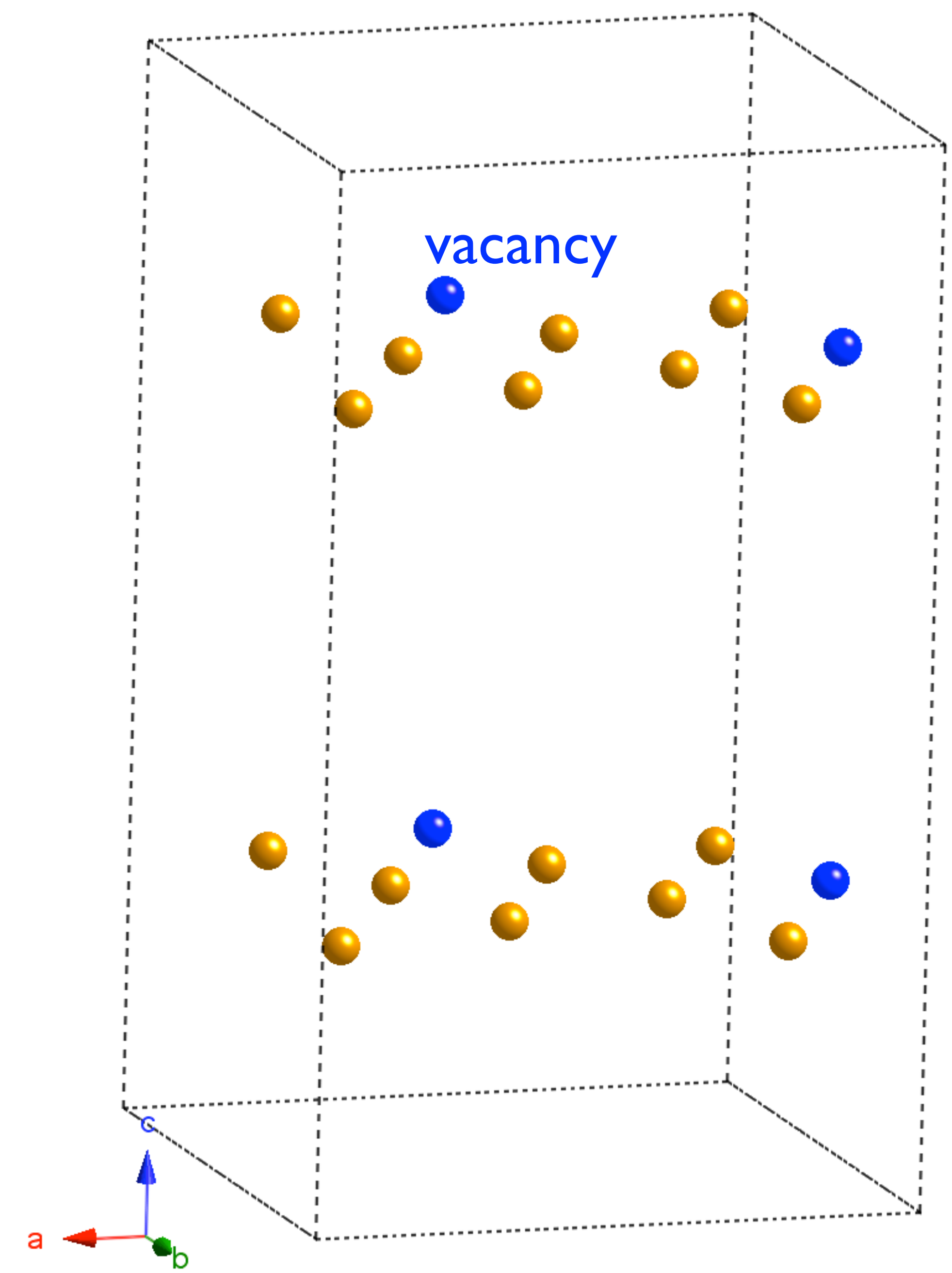
Spin $$\mathbf{S} = Re(\mathbf{S}_0) = |S_0|\cos(\phi_z + \varphi)\mathbf{e}_z$$

One unit cell with Fe



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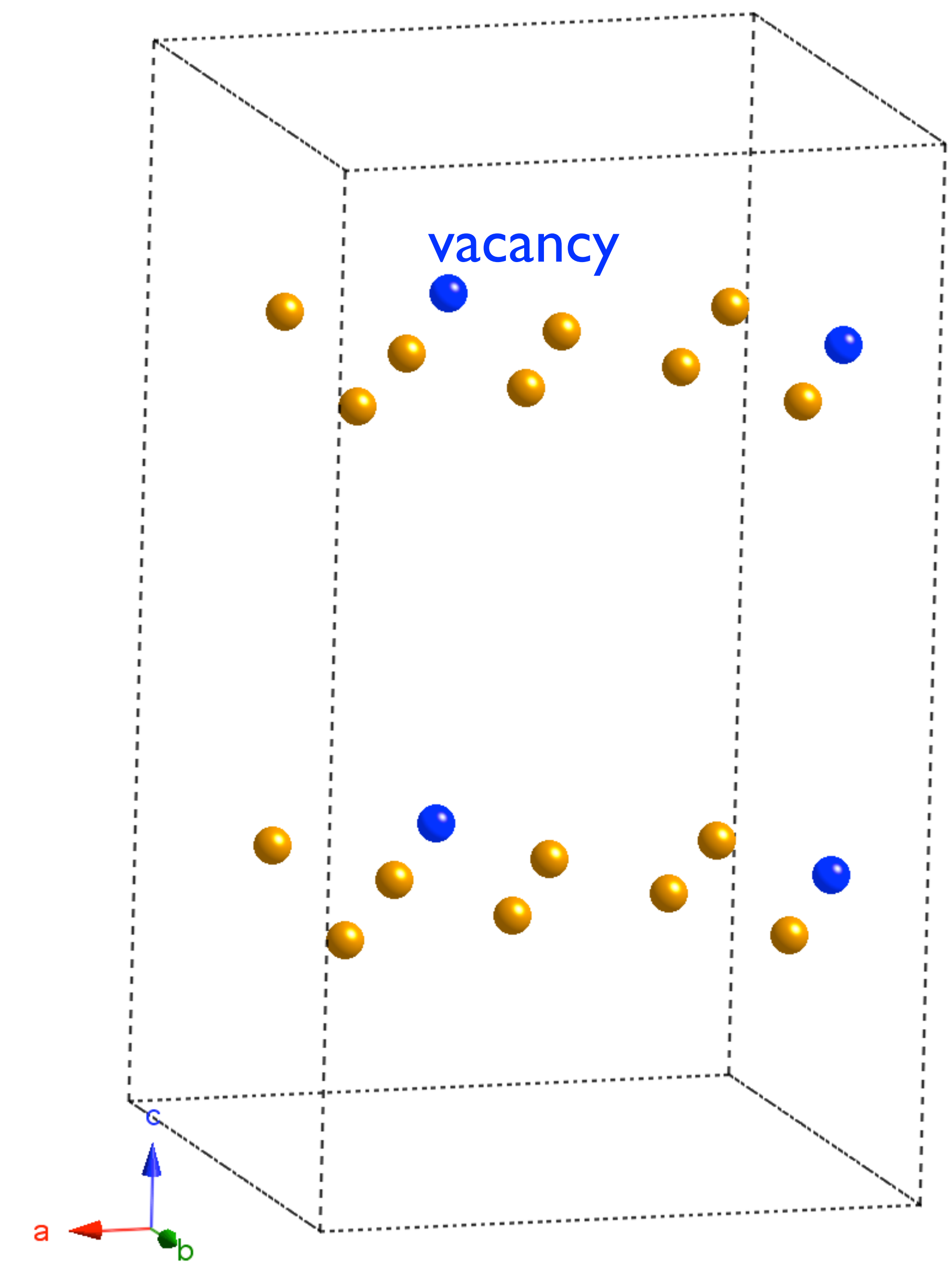
Spin $$\mathbf{S} = Re(\mathbf{S}_0) = |S_0|\cos(\phi_z + \varphi)\mathbf{e}_z$$

1. Real *irrep t2, t5*: angle φ=0 (a must). Tetragonal symmetry preserved.

One unit cell with Fe



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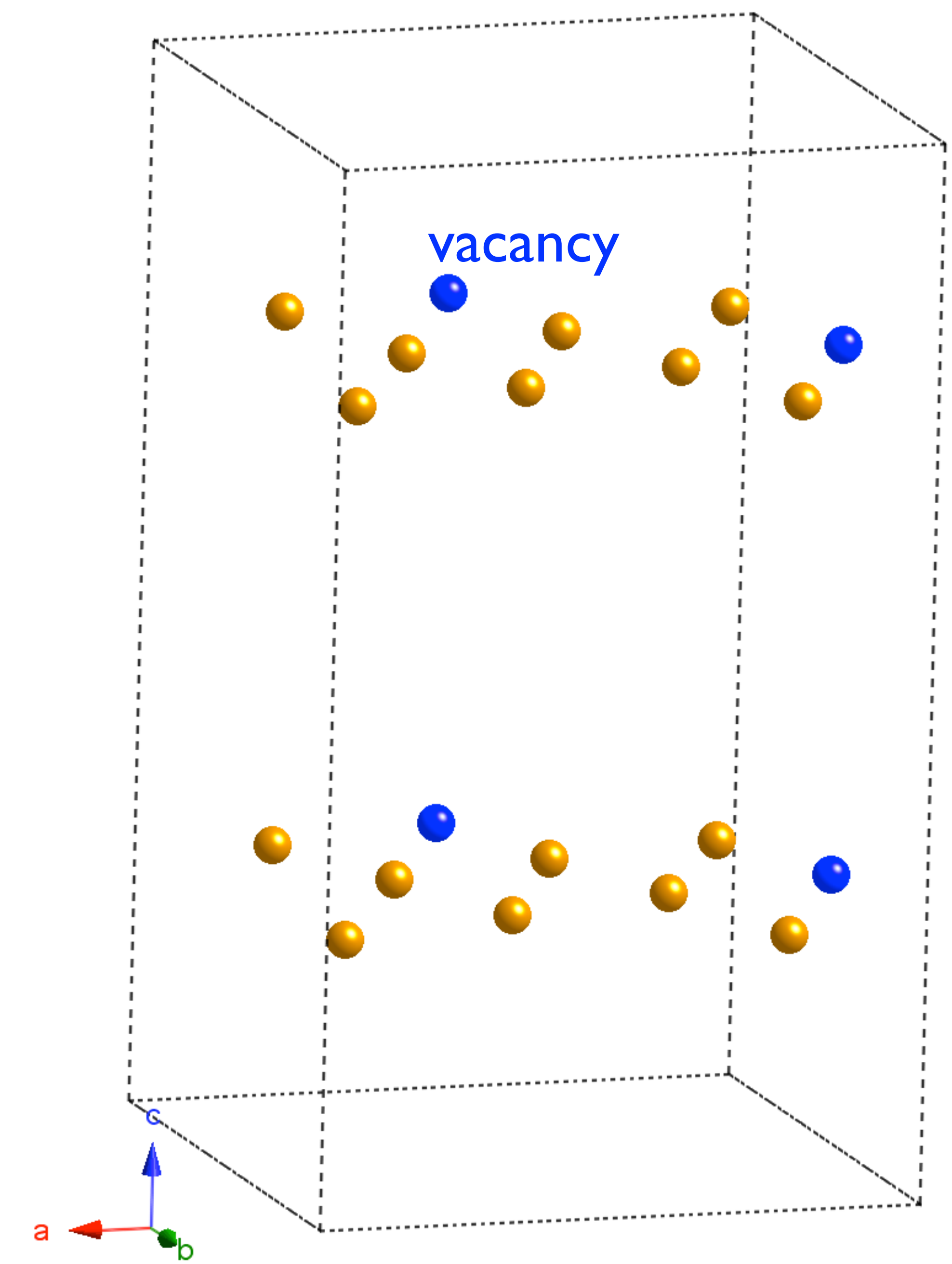

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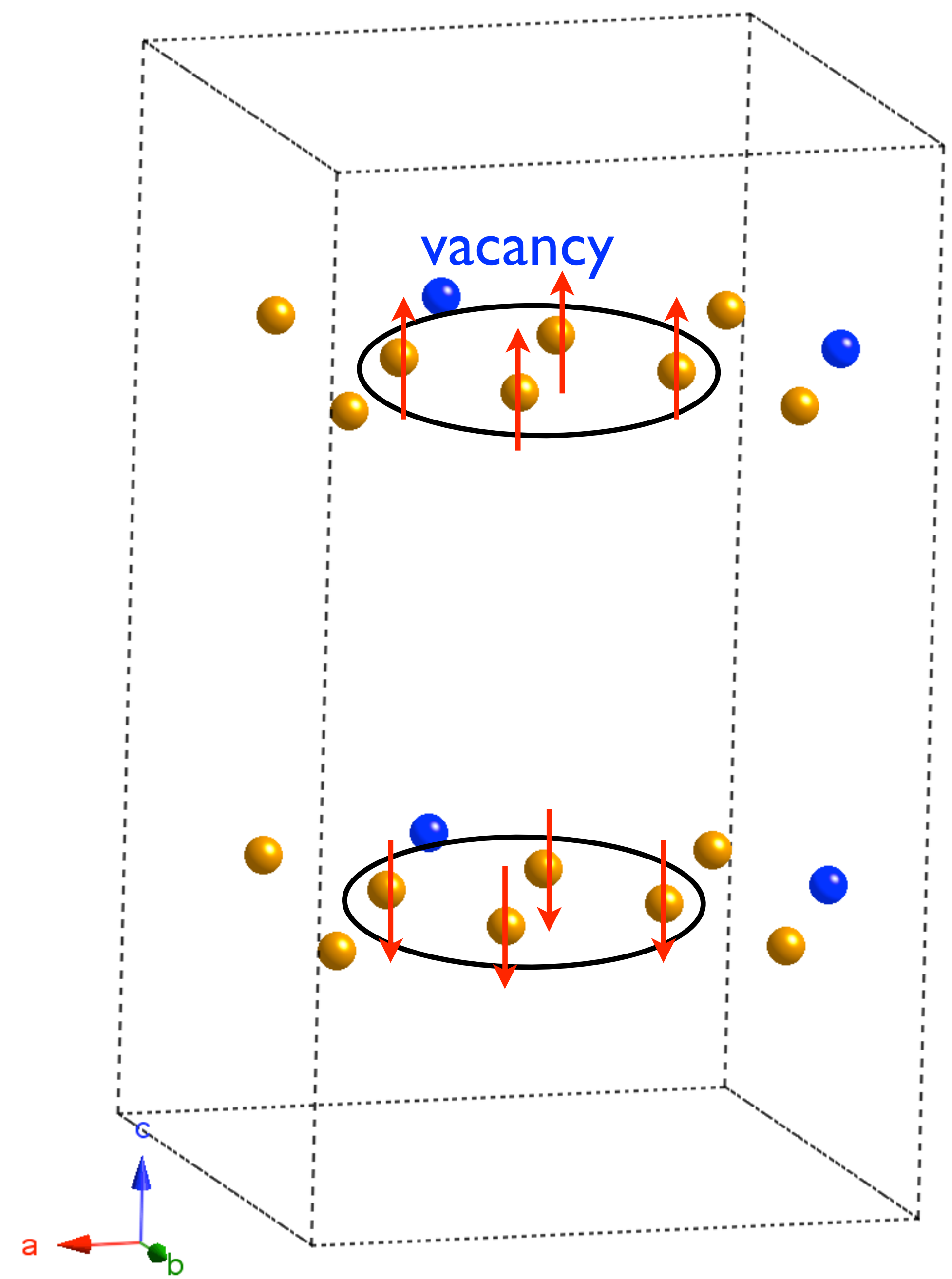

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4 complex irreps <—> Lower symmetry Shubnikov

τ,ψ	h_1 1	h_{14} 4_z^+	h_4 2_z	h_{15} 4_z^-	h_{25} -1	h_{38} -4_z^+	h_{28} m_z	h_{39} -4_z^-
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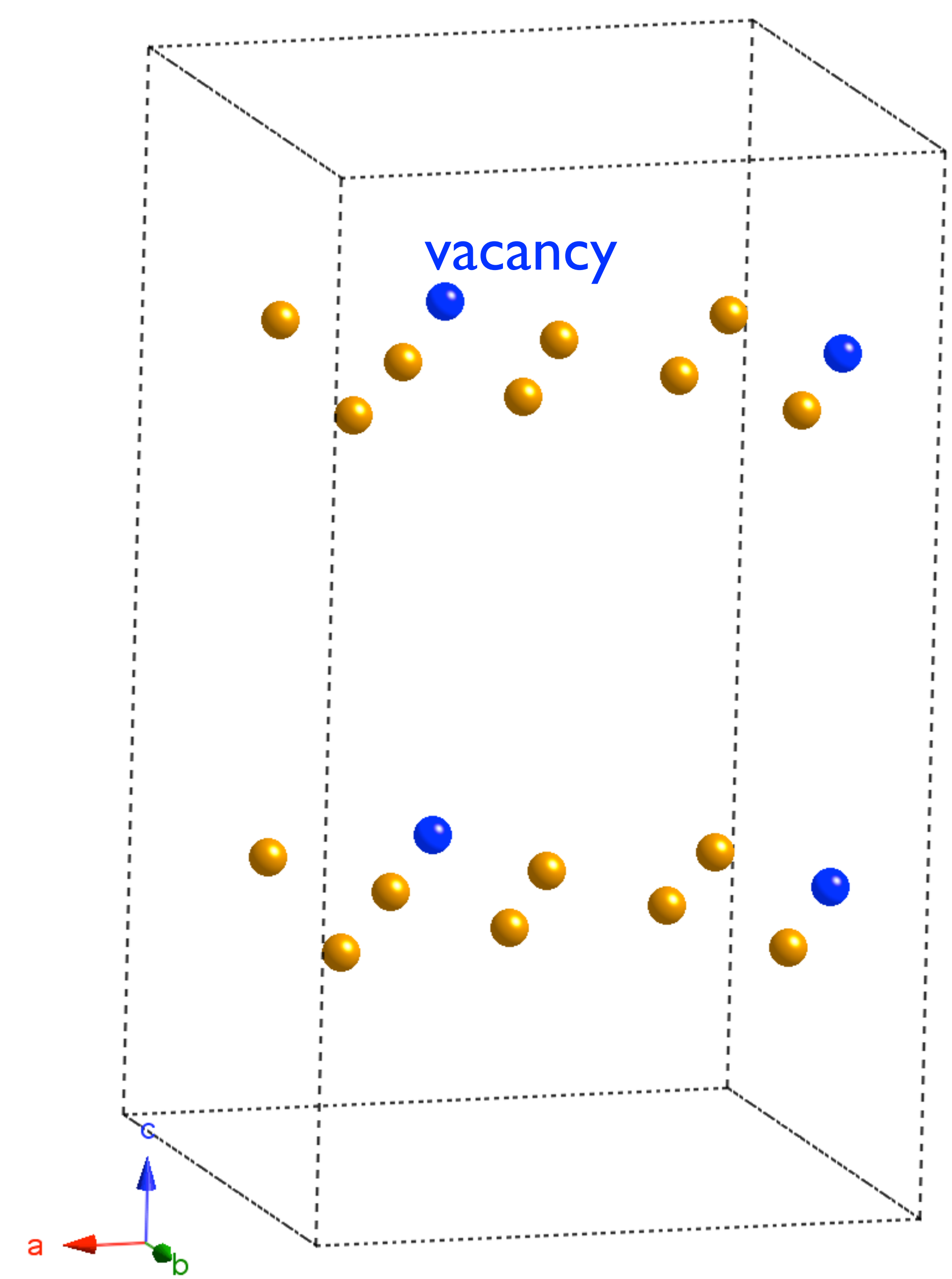
---

2. Complex *irrep t3, t7*:

One unit cell with Fe



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   Tetragonal symmetry preserved.

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$$\mathbf{S} = \pm|S_0|\cos(\varphi)\mathbf{e}_z$$
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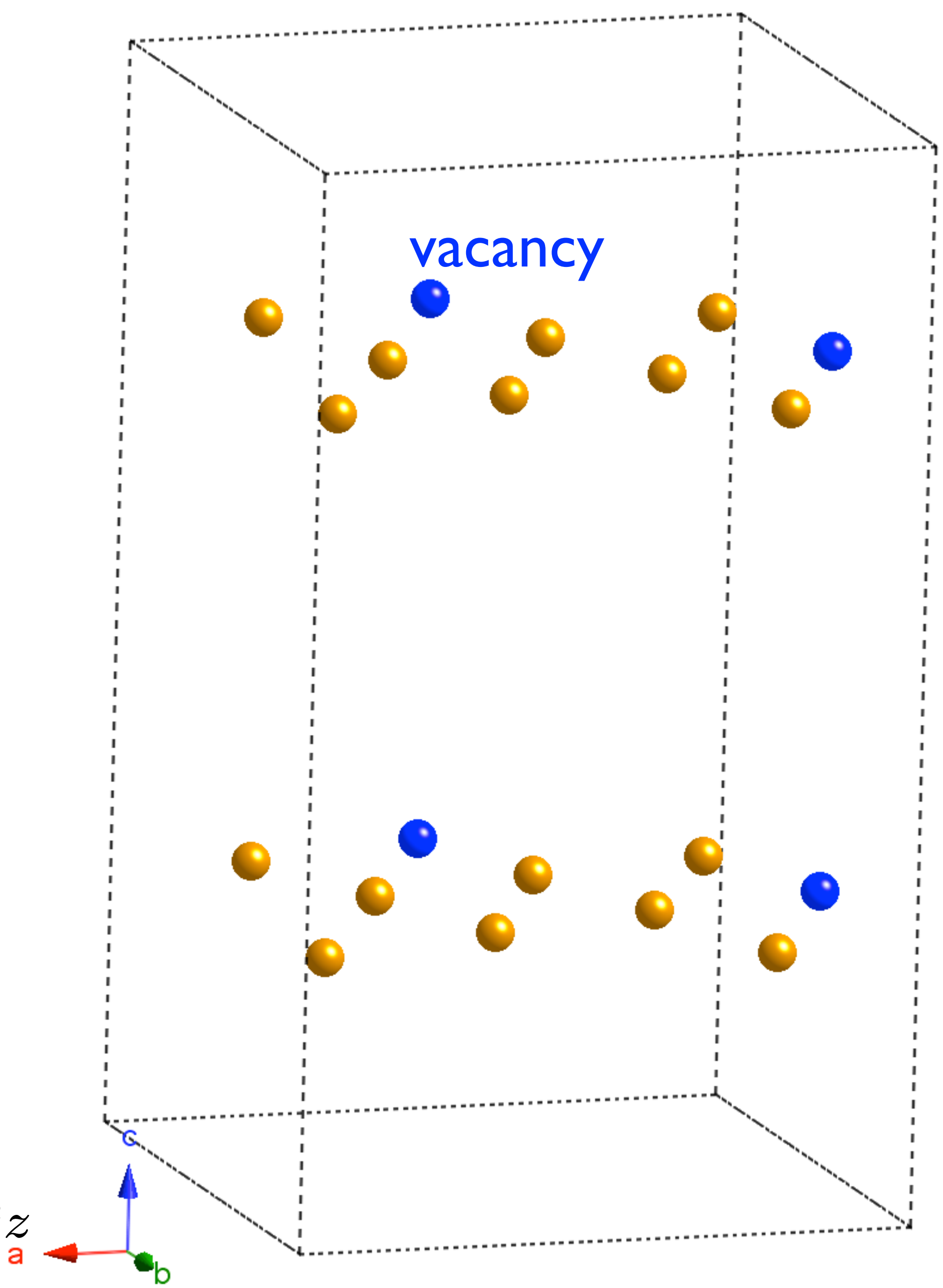
Amplitudes == spin for str. factor calculations for k=0, i.e. real

One unit cell with Fe



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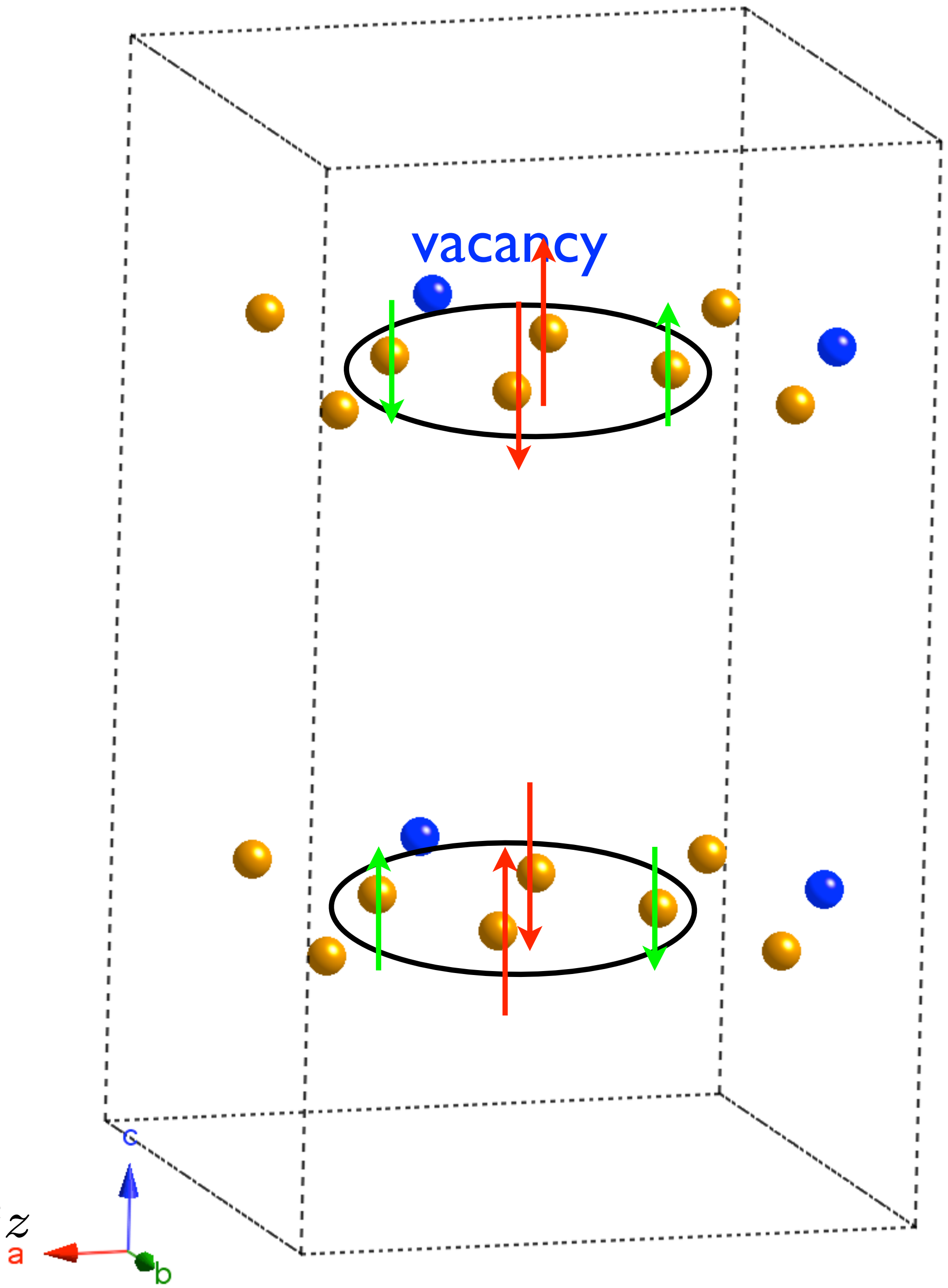
One unit cell with Fe



Example special case **S** ‖ **c**:
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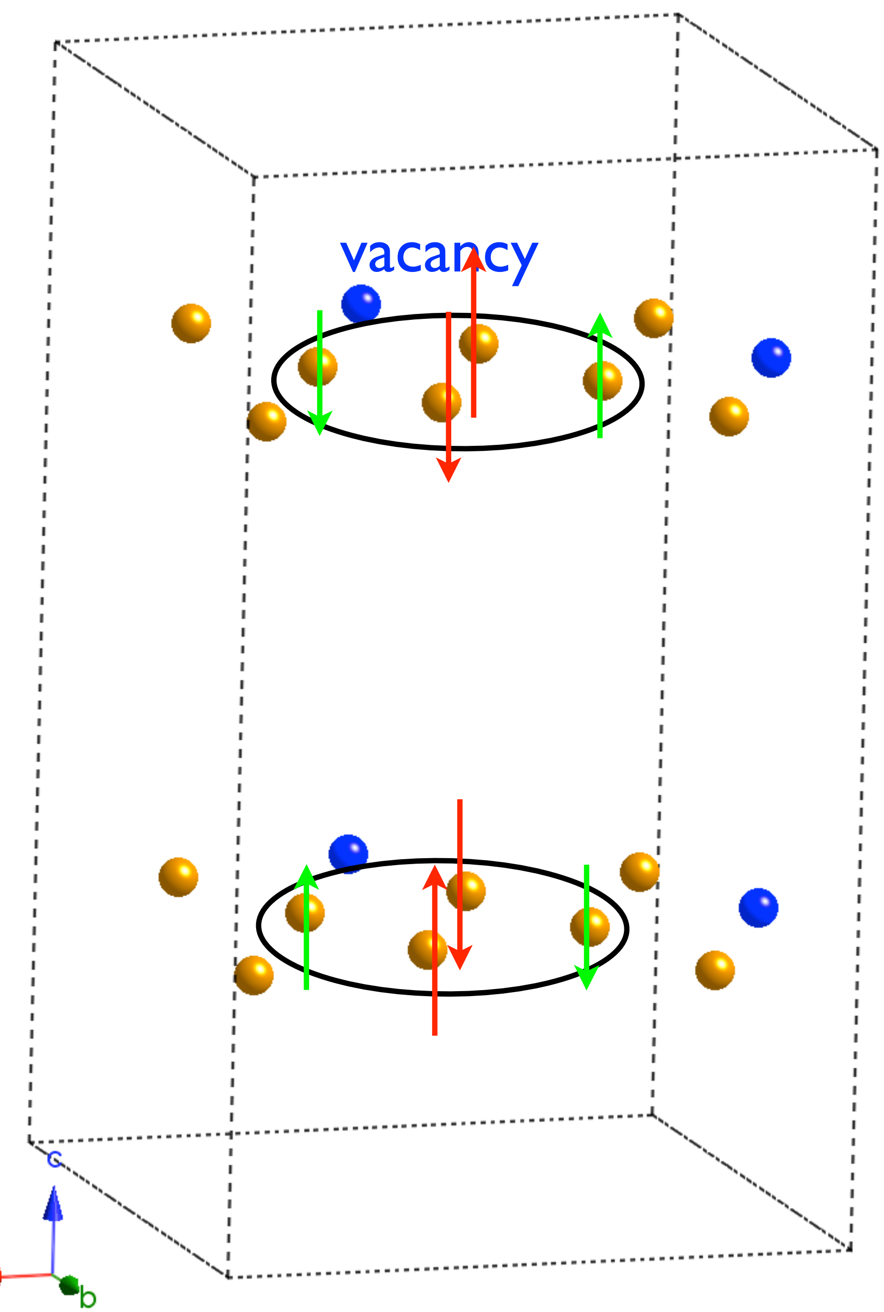
τ_7	1	$-i$	-1	i	1	$-i$	-1	i

One unit cell with Fe



Example special case **S** || **c**:
irrep = "Fourier amplitude"

$$\mathbf{S}_0 = Ce^{i\phi_z}\mathbf{e}_z, \phi_z = 0, \frac{\pi}{2}, \pi$$
$$\mathbf{S}_0 = |S_0|e^{i\varphi}e^{i\phi_z}\mathbf{e}_z$$

Spin $$\mathbf{S} = Re(\mathbf{S}_0) = |S_0|\cos(\phi_z + \varphi)\mathbf{e}_z$$

1. Real *irrep t2, t5*: angle φ=0 (a must). Tetragonal symmetry preserved. $$\mathbf{S} = \pm|S_0|\mathbf{e}_z$$

---

2. Complex *irrep t3, t7*:

$$\mathbf{S} = \pm|S_0|\cos(\varphi)\mathbf{e}_z$$
$$\mathbf{S} = \pm|S_0|\sin(\varphi)\mathbf{e}_z$$

Amplitudes == spin for str. factor calculations, i.e. real

Shubnikov subgroups of I4/m⊗1'

k=0, Gamma (GM) point of BZ

irrep		Shubnikov group	
mGM1+t1	P1 (a)	87.75 I4/m,	basis={(0,1,0),(-1,0,0),(0,0,1)}, origin=(0,0,0), s=1, i=2, k-active= (0,0,0)
mGM2+t5	P1 (a)	87.77 I4'/m,	basis={(-1,0,0),(0,-1,0),(0,0,1)}, origin=(0,0,0), s=1, i=2, k-active= (0,0,0)
mGM3+GM4+t3t7	C1 (a,b)	12.62 C2'/m',	basis={(-1,1,0),(0,0,-1),(0,-1,0)}, origin=(0,0,0), s=1, i=4, k-active= (0,0,0)
mGM1-t2	P1 (a)	87.78 I4/m',	basis={(0,1,0),(-1,0,0),(0,0,1)}, origin=(0,0,0), s=1, i=2, k-active= (0,0,0)
mGM2-t6	P1 (a)	87.79 I4'/m',	basis={(0,1,0),(-1,0,0),(0,0,1)}, origin=(0,0,0), s=1, i=2, k-active= (0,0,0)
mGM3-GM4-t4t8	C1 (a,b)	12.60 C2'/m,	basis={(-1,-1,0),(0,0,-1),(1,0,0)}, origin=(0,0,0), s=1, i=4, k-active= (0,0,0)

↑

Oder parameter direction
for multidimensional irreps

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,

Shubnikov subgroups of $I4/m\otimes1'$

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mGM2+t5	P1 (a)	87.77 I4'/m,	basis={(-1,0,0),(0,-1,0),(0,0,1)}, origin=(0,0,0), s=1, i=2, k-active= (0,0,0)
mGM3+GM4+t3t7	C1 (a,b)	12.62 C2'/m',	basis={(-1,1,0),(0,0,-1),(0,-1,0)}, origin=(0,0,0), s=1, i=4, k-active= (0,0,0)
mGM1-t2	P1 (a)	87.78 I4/m',	basis={(0,1,0),(-1,0,0),(0,0,1)}, origin=(0,0,0), s=1, i=2, k-active= (0,0,0)
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mGM3-GM4-t4t8	C1 (a,b)	12.60 C2'/m,	basis={(-1,-1,0),(0,0,-1),(1,0,0)}, origin=(0,0,0), s=1, i=4, k-active= (0,0,0)

↑ Oder parameter direction for multidimensional irreps

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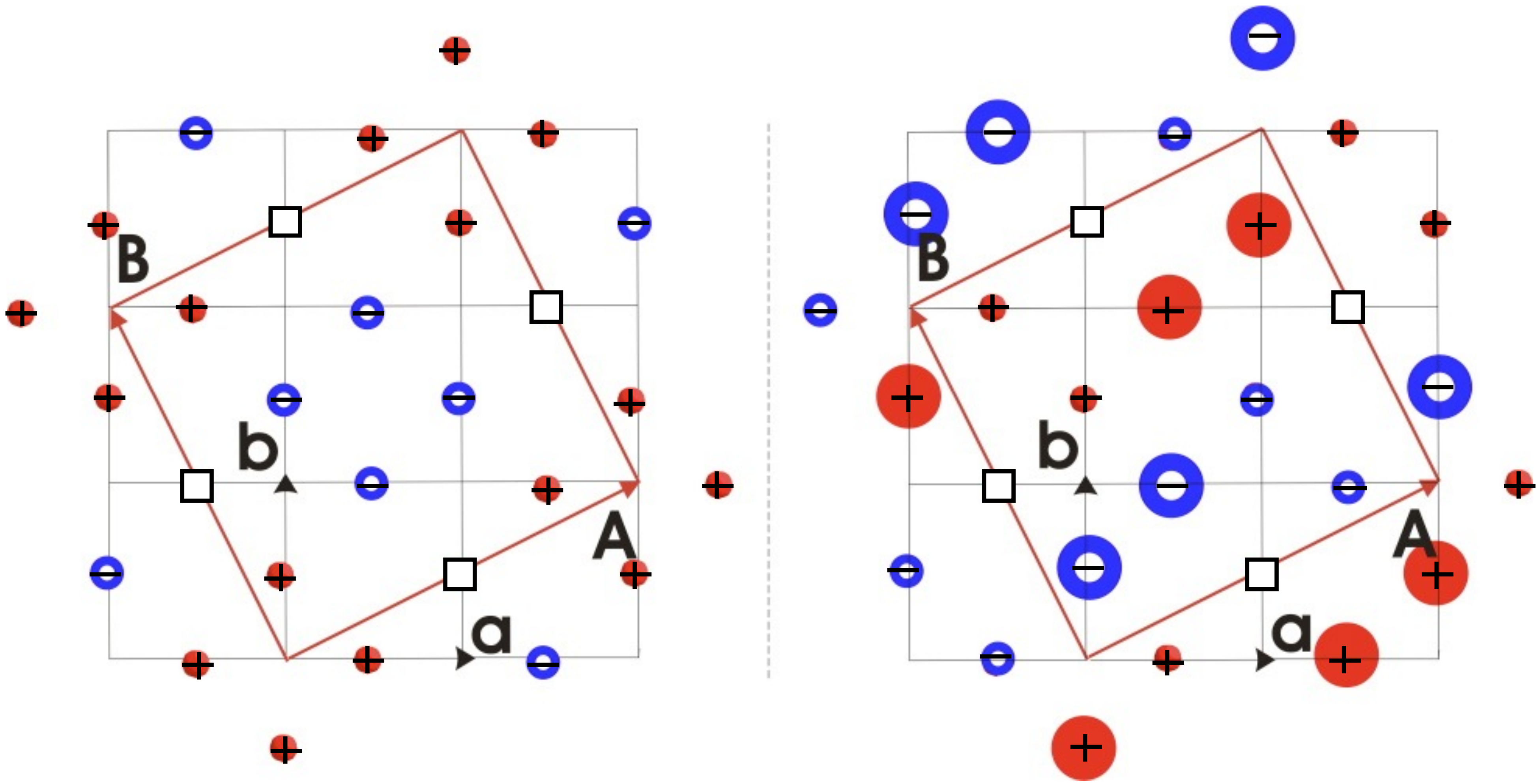
Harold T. Stokes, Dorian M. Hatch, and Branton J. Campbell, Department of Physics and Astronomy, Brigham Young University, Provo, Utah 84606, USA,

Magnetic structure of $X_{0.8}Fe_{1.6}Se_2$, X=K, Rb, Cs

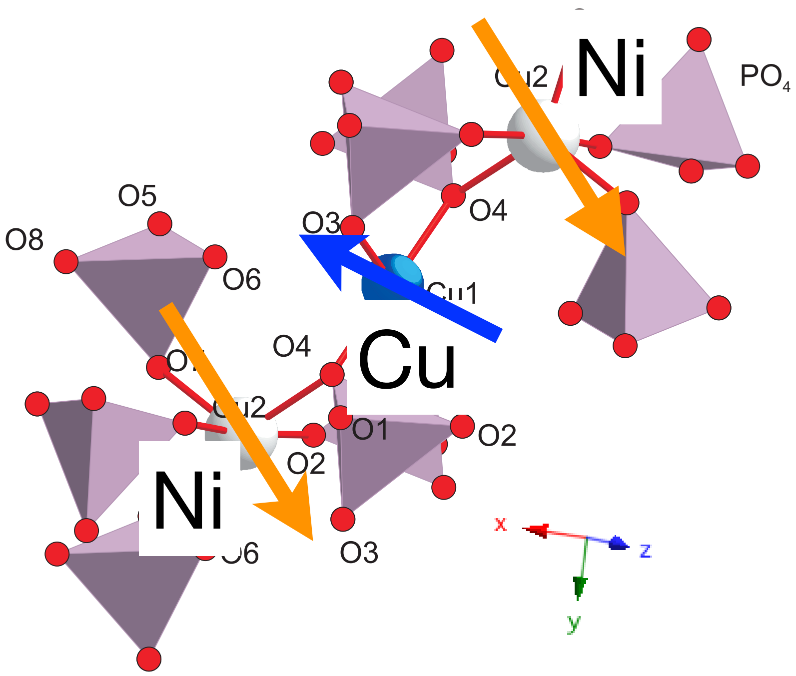
I4/m cell shown by red square. One *(ab)* layer of Fe-atoms is shown. Fe spins are parallel (+) or antiparallel (-) to c-axis

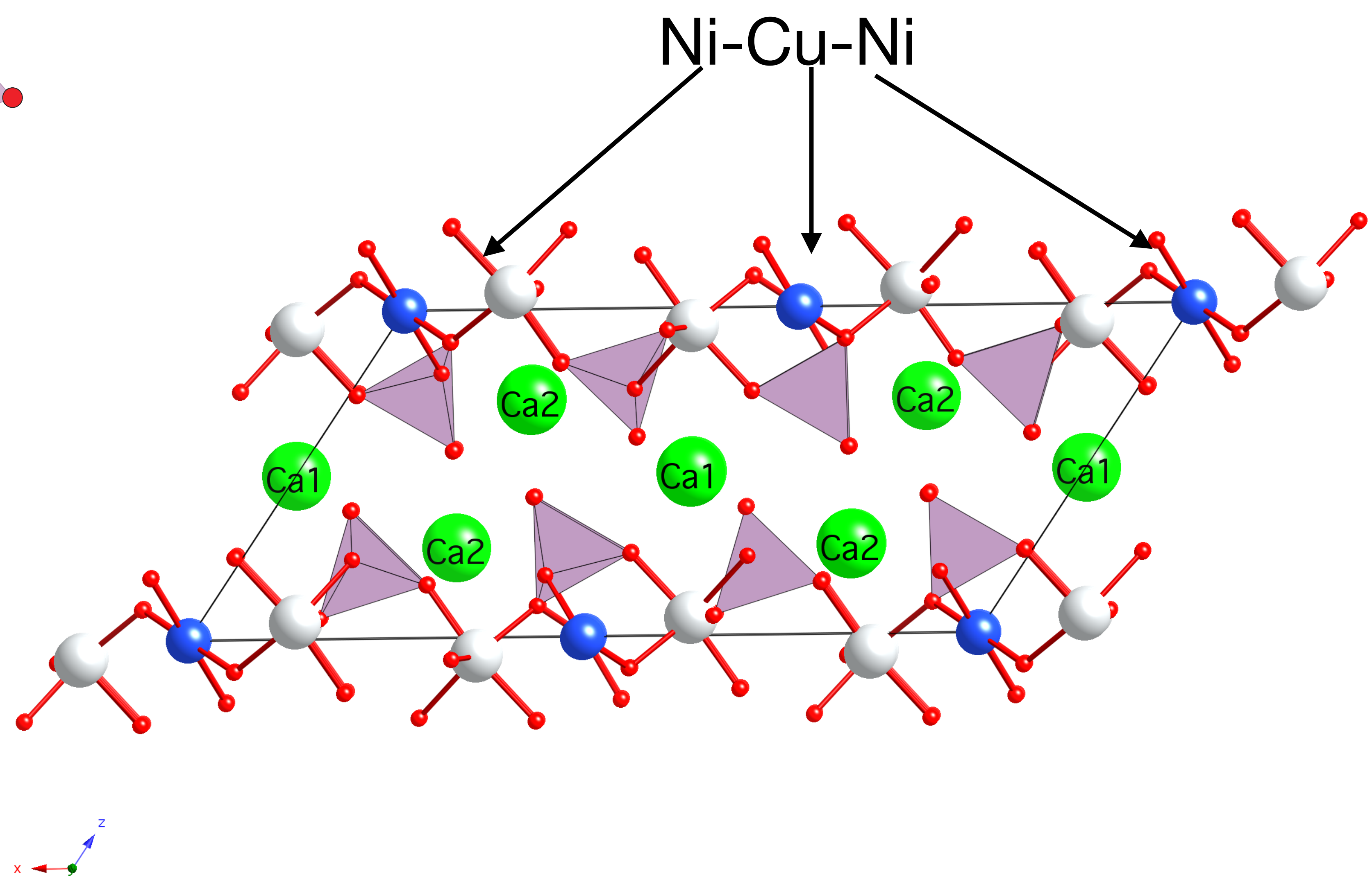


block checkerboard AFM
irrep τ_2, (Γ1-) *I4/m'*

zig-zag AFM
irrep τ_7/τ_3,(Γ4+/Γ3+), *C2'/m'*

Multi-arm magnetic order in quantum spin-trimer $Ca_3Cu_1Ni_2(PO_4)_4$





V. Pomjakushin, arXiv:1404.1683 (2014).

Symmetry group G_k of propagation vector k. k-star

space group of $Ca_3Cu_1Ni_2(PO_4)_4$

$C2/c$	C_{2h}^6	$2/m$	Monoclinic
No. 15	$C12/c1$		Patterson symmetry $C12/m1$

Symmetry operators *zeroth* block of SG

$h_1 = x, y, z$ $h_2 = \bar{x}, y, \bar{z} + \frac{1}{2}$ $h_3 = \bar{x}, \bar{y}, \bar{z}$ $h_4 = x, \bar{y}, z + \frac{1}{2}$

$+T(n_1\mathbf{t}_1 + n_2\mathbf{t}_2 + n_3\mathbf{t}_3)$

$(\frac{1}{2}, \frac{1}{2}, 0)+$

k-vector takes care about translations

$$\mathbf{S}_1(\mathbf{t}_n) = \sum_{l=1}^{m} \mathbf{S}_{01l} \cos(2\pi \mathbf{k}_l \mathbf{t}_n)$$

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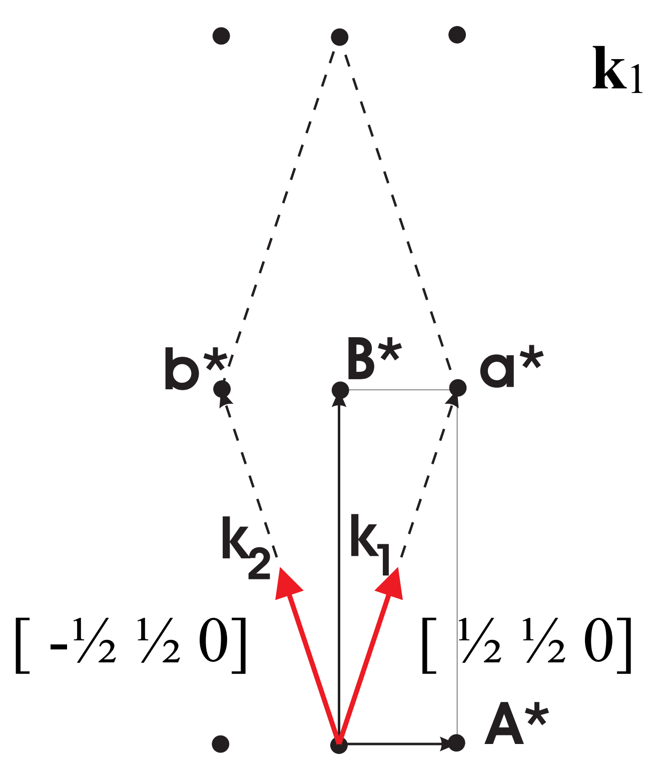
Reciprocal lattice. **a***,**b***:primitive, **A***, **B***: C-centered

$\mathbf{k}_1$=[½ ½ 0] *V*-point of BZ



{k}-star has two arms

Symmetry group G_k of propagation vector k. k-star

space group of $Ca_3Cu_1Ni_2(PO_4)_4$

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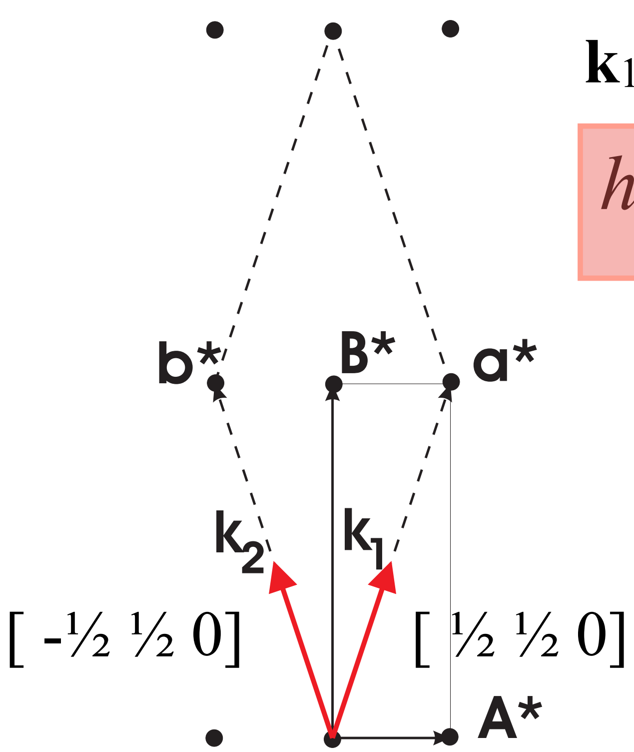

{k}-star has two arms

Symmetry group G_k of propagation vector k. k-star

space group of $Ca_3Cu_1Ni_2(PO_4)_4$

$C2/c$ C^6_{2h} $2/m$ Monoclinic

No. 15 $C\,1\,2/c\,1$ Patterson symmetry $C\,1\,2/m\,1$

Symmetry operators *zeroth* block of SG

$h_1 = x, y, z$ $h_2 = \bar{x}, y, \bar{z} + \frac{1}{2}$ $h_3 = \bar{x}, \bar{y}, \bar{z}$ $h_4 = x, \bar{y}, z + \frac{1}{2}$

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$(\frac{1}{2}, \frac{1}{2}, 0)+$

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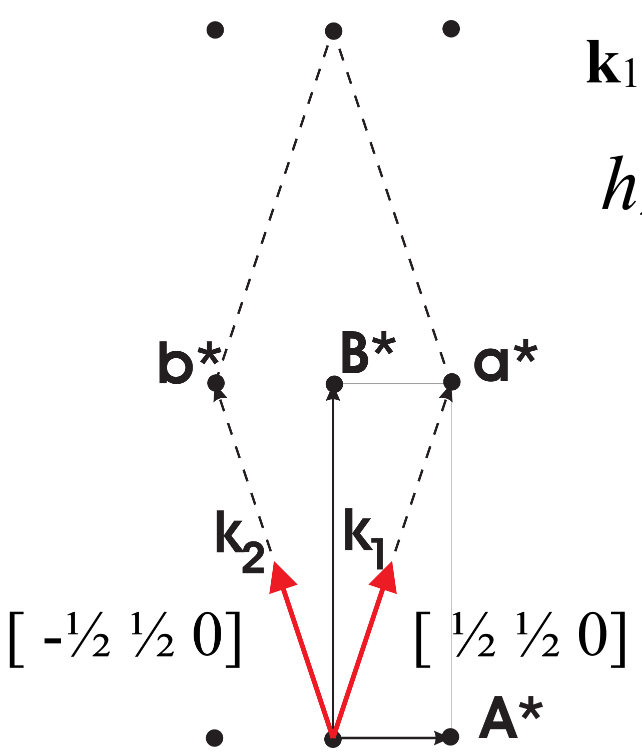
Reciprocal lattice. **a***,**b***:primitive, **A***, **B***: C-centered



$\mathbf{k}_1$=[½ ½ 0] *V*-point of BZ

$h_2\mathbf{k}_1 = \mathbf{k}_2$ $h_4\mathbf{k}_1 = -\mathbf{k}_2$

Manyfold of all non-equivalent $h_i\mathbf{k}$ == propagation vector star $\{\mathbf{k}\}$

{k}-star has two arms

Symmetry group G_k of propagation vector k. k-star

space group of $Ca_3Cu_1Ni_2(PO_4)_4$

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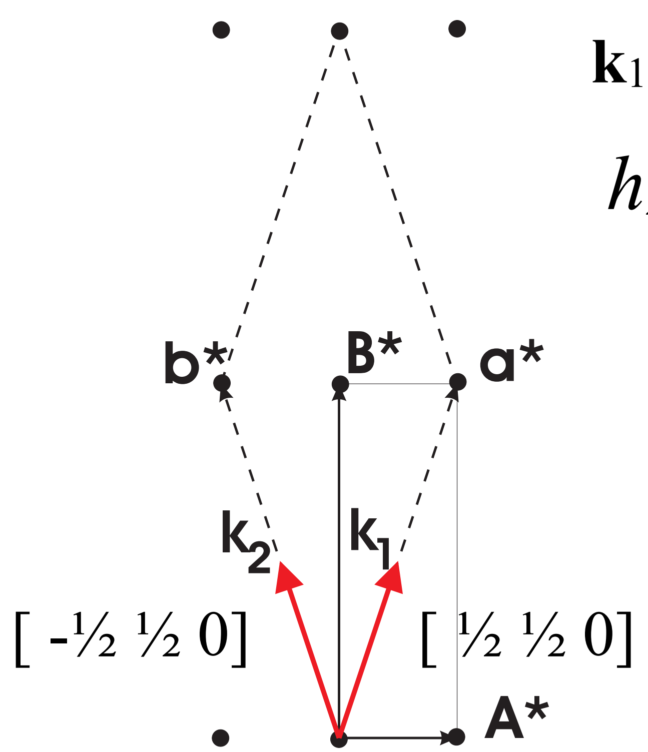

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Manyfold of all non-equivalent $h_i\mathbf{k}$ == propagation vector star $\{\mathbf{k}\}$

{k}-star has two arms

$G_k \in G$ that leaves ***k*** *invariant* == little group or propagation vector group

$h_1\ 1$ $\quad h_3\ \bar{1}$ $\quad G_k = C\bar{1}$

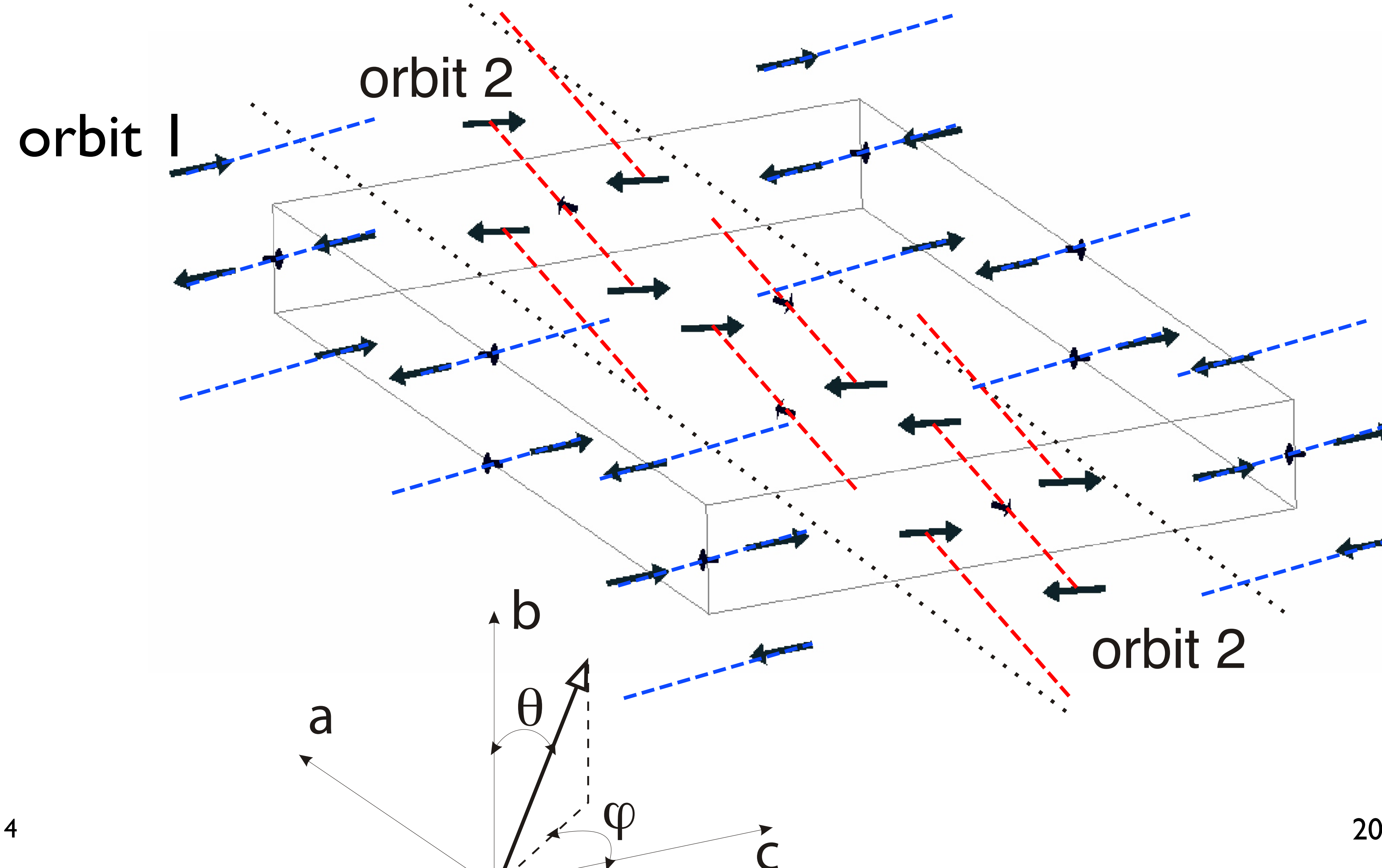
zeroth unit cell of $Ca_3Cu_1Ni_2(PO_4)_4$: orbits in k-vector formalism

Symmetry operators

$h_1 = x,y,z$ $\quad h_2 = \bar{x},y,\bar{z}+\frac{1}{2}$ $\quad h_3 = \bar{x},\bar{y},\bar{z}$ $\quad h_4 = x,\bar{y},z+\frac{1}{2}$ $\quad +T(n_1\mathbf{t}_1+n_2\mathbf{t}_2+n_3\mathbf{t}_3)$ $(\frac{1}{2},\frac{1}{2},0)+$

Unit cell

$a = 17.724$ Å, $b = 4.815$ Å, $c = 17.836$ Å, $\beta = 123.756°$



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orbit 1
$G_k = C\text{-}1$

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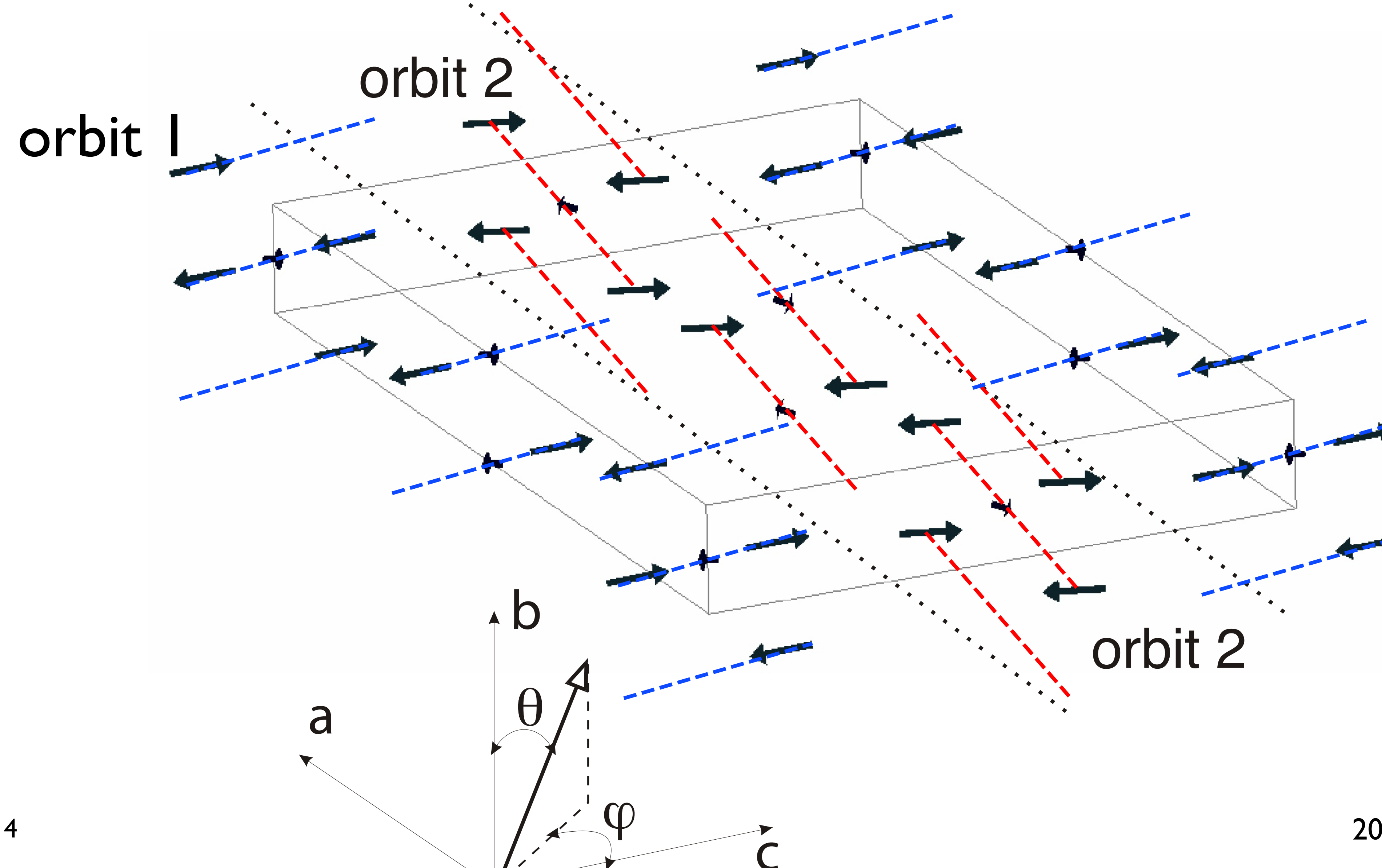

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orbit 1
$G_k = C\text{-}1$

orbit 2
$G_k = C\text{-}1$

Unit cell

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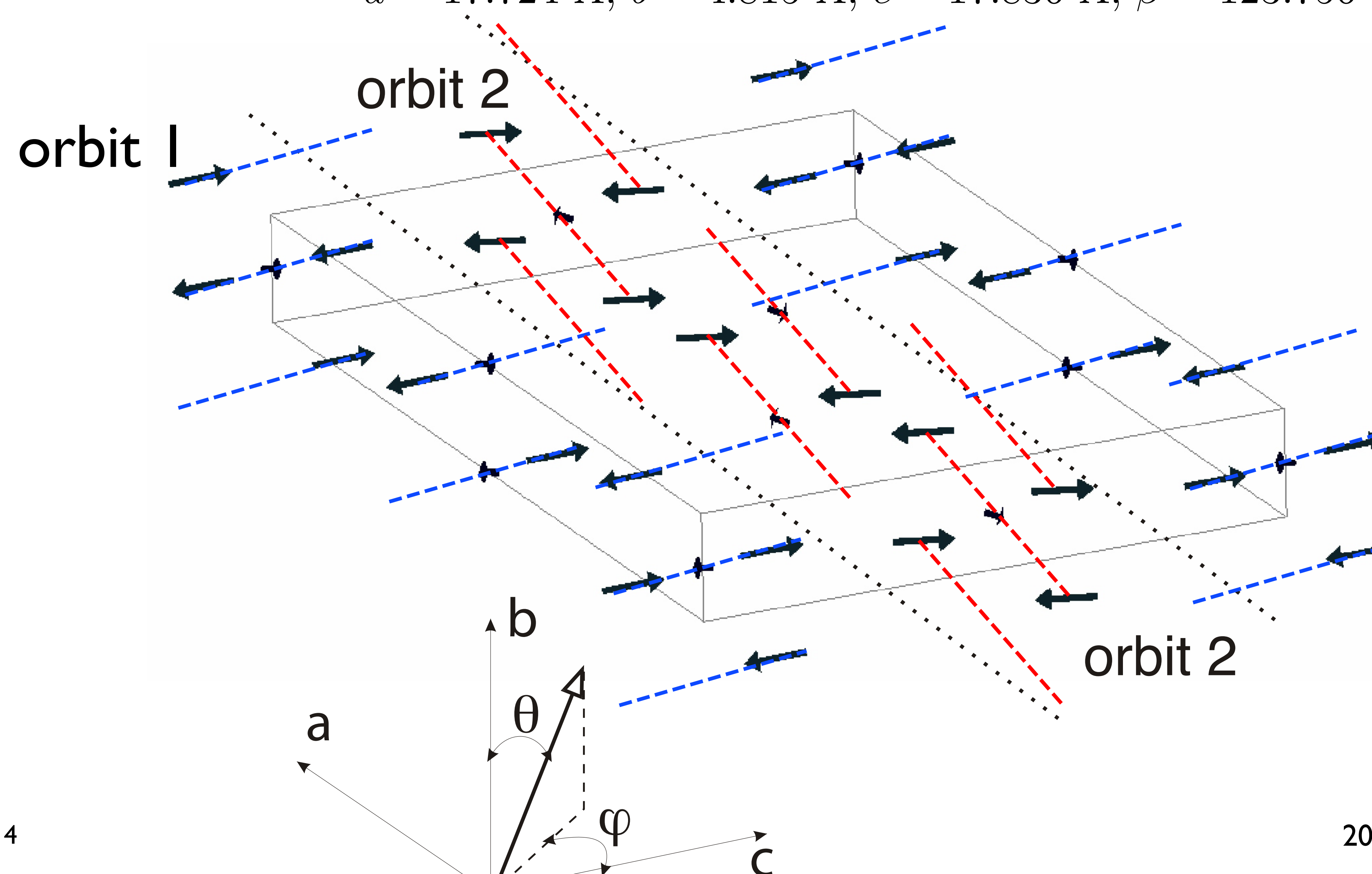
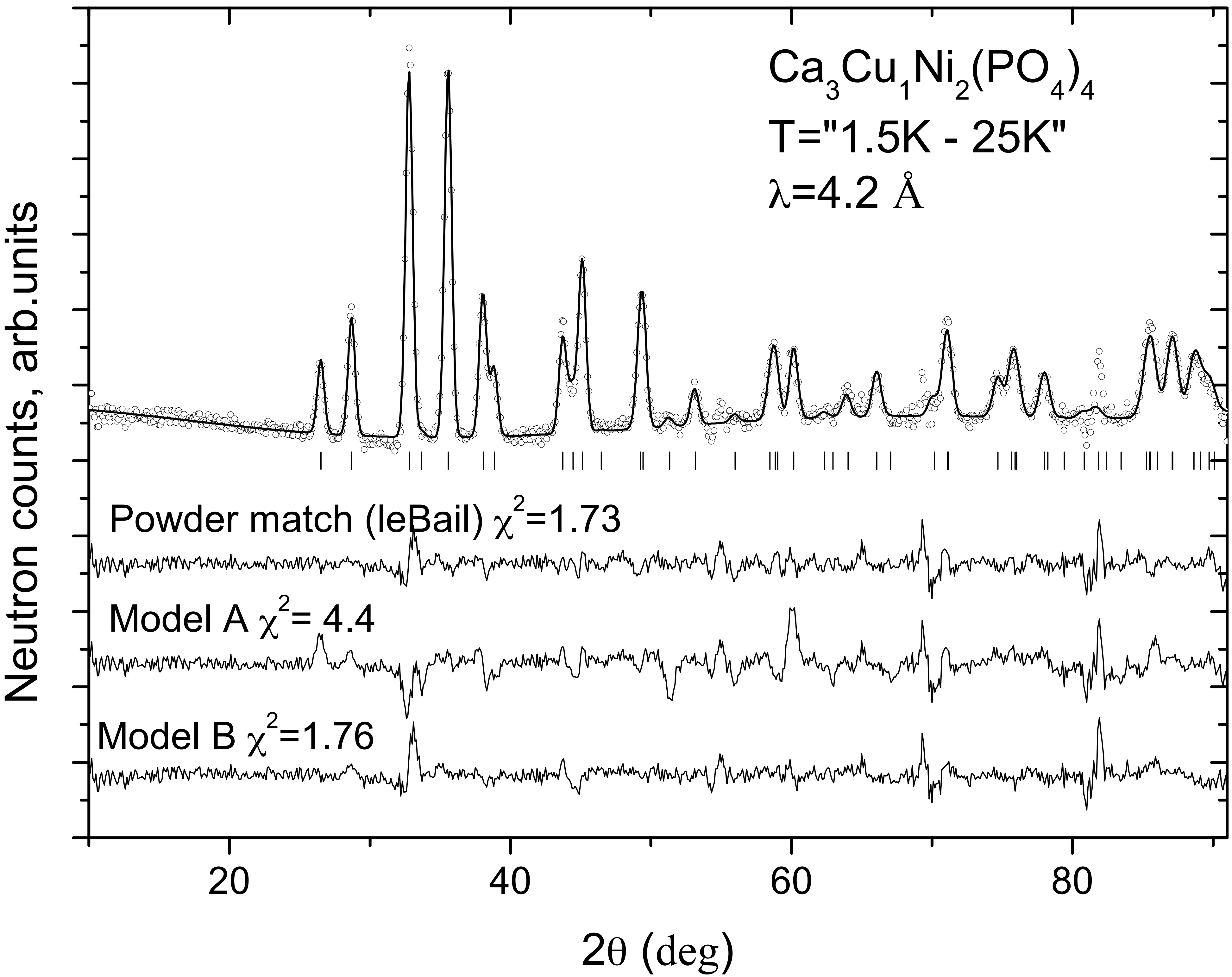


Magnetic order in $Ca_3Cu_1Ni_2(PO_4)_4$:
1) propagation vector arms

Magnetic neutron diffraction pattern



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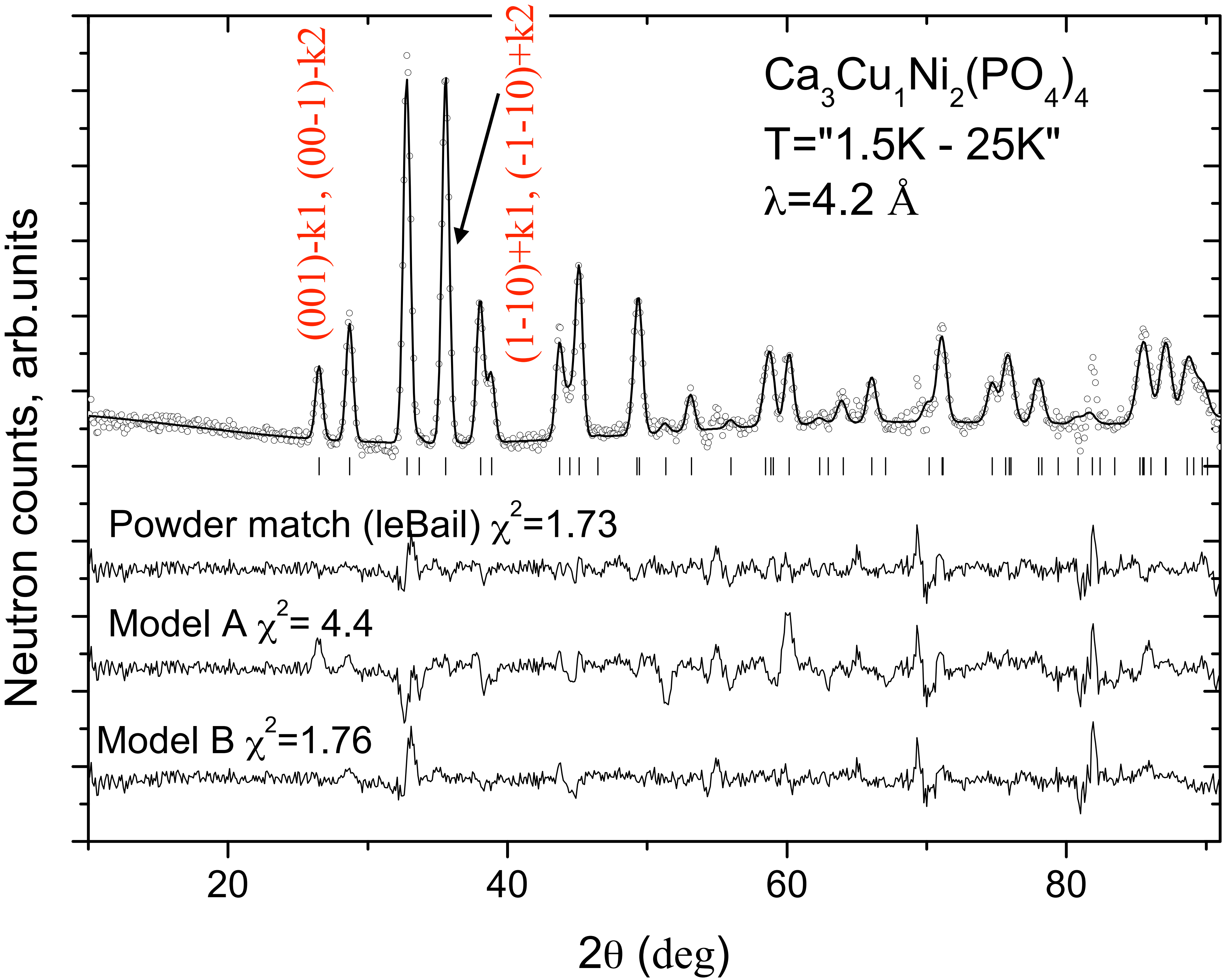
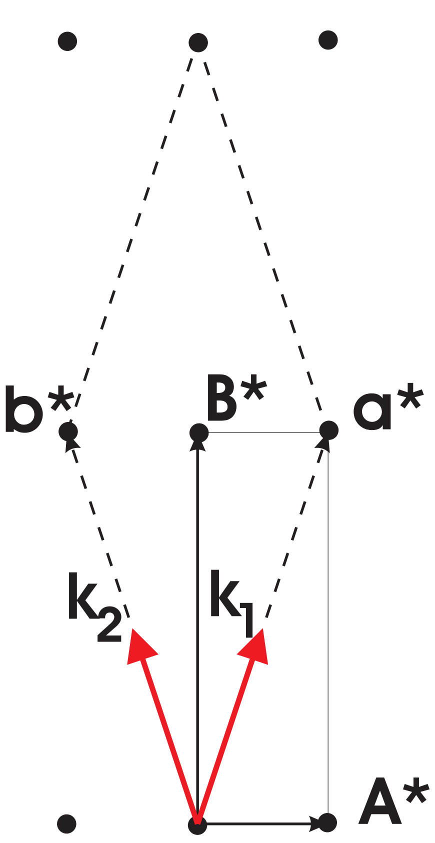


Space group *C2/c*

Reciprocal lattice.
a*,**b***:primitive,
A*, **B***: C-centered



Propagation vector star
{[½ ½ 0], [-½ ½ 0]}

zeroth unit cell of $Ca_3Cu_1Ni_2(PO_4)_4$:
2) orbits, irreps of G_k

Symmetry operators

$h_1 = x, y, z$ | $h_2 = \bar{x}, y, \bar{z} + \frac{1}{2}$ | $h_3 = \bar{x}, \bar{y}, \bar{z}$ | $h_4 = x, \bar{y}, z + \frac{1}{2}$ | $+T(n_1\mathbf{t}_1 + n_2\mathbf{t}_2 + n_3\mathbf{t}_3)$ $(\frac{1}{2}, \frac{1}{2}, 0)+$

orbit 1
$G_k = C\text{-}1$

orbit 2
$G_k = C\text{-}1$

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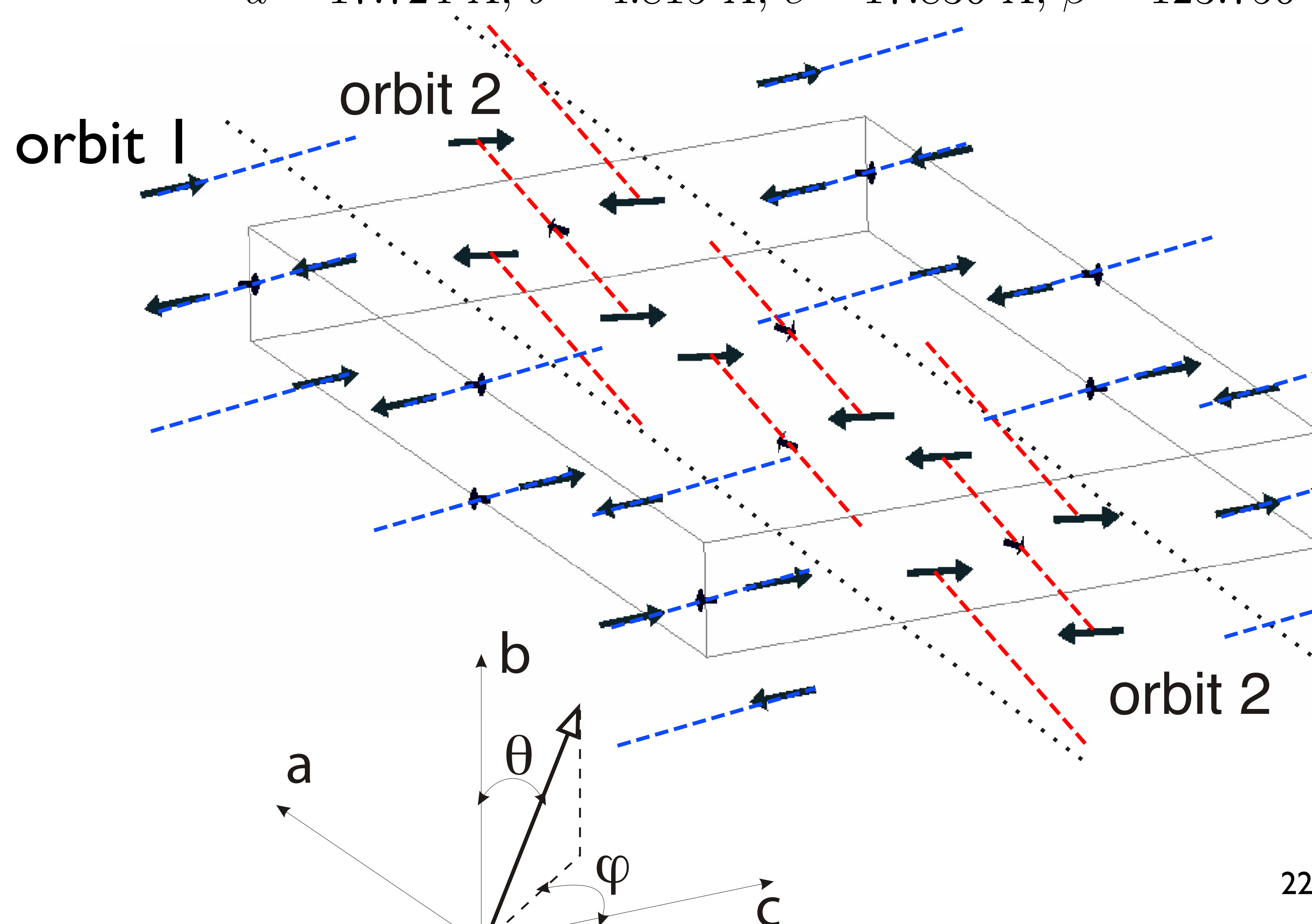


zeroth unit cell of $Ca_3Cu_1Ni_2(PO_4)_4$:
2) orbits, irreps of G_k

Symmetry operators

$h_1 = x, y, z$ — $h_2 = \bar{x}, y, \bar{z} + \frac{1}{2}$ — $h_3 = \bar{x}, \bar{y}, \bar{z}$ — $h_4 = x, \bar{y}, z + \frac{1}{2}$ — $+T(n_1\mathbf{t}_1 + n_2\mathbf{t}_2 + n_3\mathbf{t}_3)$ $(\frac{1}{2}, \frac{1}{2}, 0)+$

orbit 1
$G_k = C\text{-}\bar{1}$

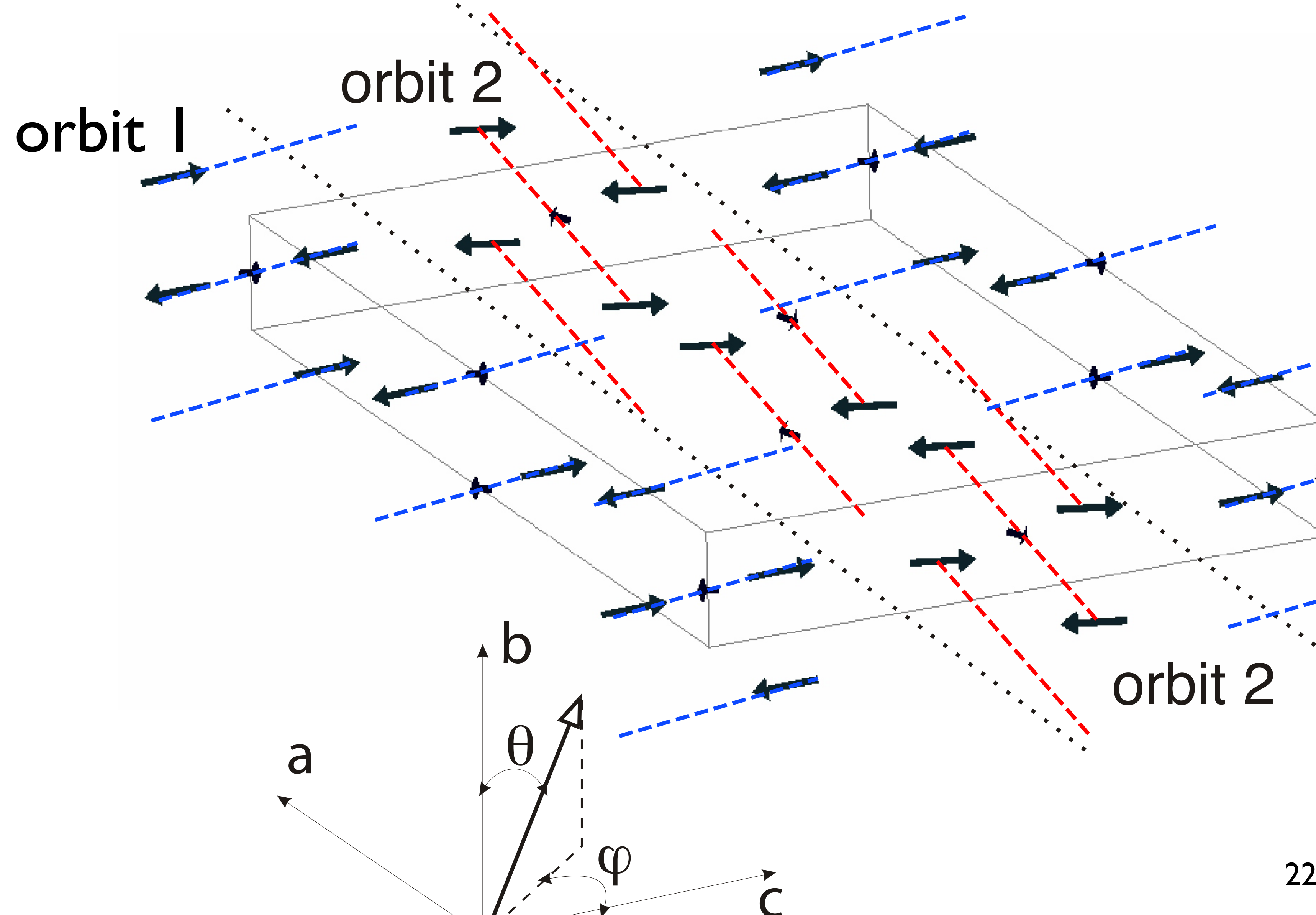
orbit 2
$G_k = C\text{-}\bar{1}$

Unit cell

$a = 17.724$ Å, $b = 4.815$ Å, $c = 17.836$ Å, $\beta = 123.756°$

Group $G_k = C\bar{1}$ that relates spins in the orbit has **two 1D irreducible representations (irreps) τ_1 and τ_2**

	h_1 1	h_3 $\bar{1}$
τ_1	1	1
τ_2	1	-1



$Ca_3Cu_1Ni_2(PO_4)_4$: magnetic representation decomposition

G_k= C-*1* has two 1D *irreps* τ_1 and τ_2

$Ca_3Cu_1Ni_2(PO_4)_4$: magnetic representation decomposition

G_k= C-*1* has two 1D *irreps* τ_1 and τ_2

Axial vector representations for Cu and Ni sites read:

Ni (8f)-position : **6D=2·3** magn. representation
+2 orbits, +C-centering $= 3\tau_1 \oplus 3\tau_2$

$Ca_3Cu_1Ni_2(PO_4)_4$: magnetic representation decomposition

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Cu (4b)-position: **3D=1·3** magn. representation
+2 orbits, +C-centering = $3\tau_2$

$Ca_3Cu_1Ni_2(PO_4)_4$: magnetic representation decomposition

G_k= C-*1* has two 1D *irreps* τ_1 and τ_2

Axial vector representations for Cu and Ni sites read:

Ni (8f)-position : **6D=2·3** magn. representation
+2 orbits, +C-centering = $3\tau_1 \oplus 3\tau_2$

Cu (4b)-position: **3D=1·3** magn. representation
+2 orbits, +C-centering = $3\tau_2$

To get non-zero Cu-spins

Magnetic order in $Ca_3Cu_1Ni_2(PO_4)_4$: 2k structure

irrep τ_2

Independently for both Cu-spins and Ni-spins we have:

Orbit 1

basis functions

$$\mathbf{S}_0 = \sum_{\lambda=1}^{3} (C_{\lambda,\mathbf{k}_1} \boldsymbol{\psi}_\lambda(\mathbf{k}_1) + C_{\lambda,\mathbf{k}_2} \boldsymbol{\psi}_\lambda(\mathbf{k}_2))$$

$\lambda = x, y, z$

Orbit 2

$$\mathbf{S}'_0 = \sum_{\lambda=1}^{3} \left(C'_{\lambda,\mathbf{k}_1} \boldsymbol{\psi}_\lambda(\mathbf{k}_1) + C'_{\lambda,\mathbf{k}_2} \boldsymbol{\psi}_\lambda(\mathbf{k}_2)\right)$$

Magnetic order in $Ca_3Cu_1Ni_2(PO_4)_4$: 2k structure

irrep τ_2

Independently for both Cu-spins and Ni-spins we have:

Orbit 1 — basis functions

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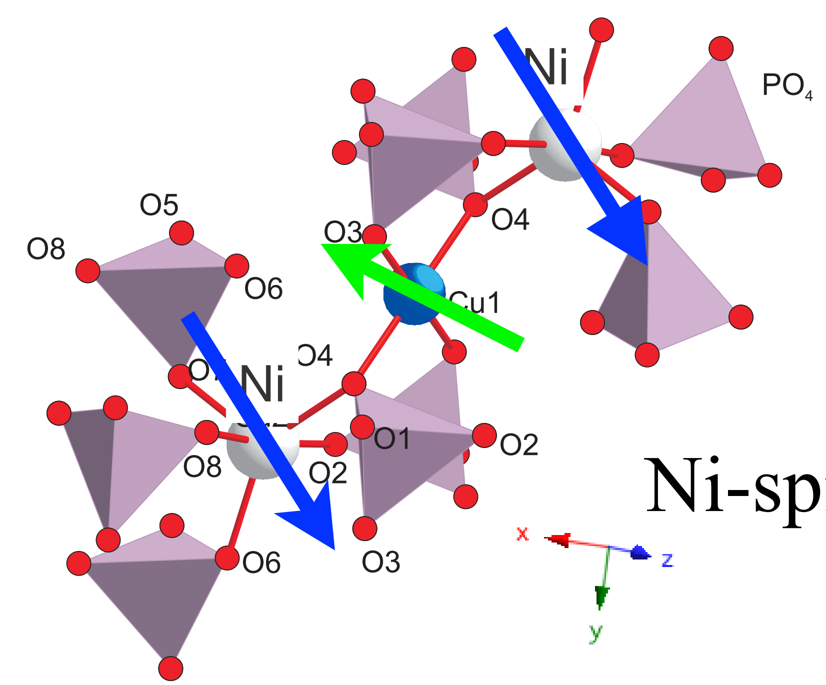
Orbit 2

$$\mathbf{S}'_0 = \sum_{\lambda=1}^{3} \left(C'_{\lambda,\mathbf{k}_1} \psi_\lambda(\mathbf{k}_1) + C'_{\lambda,\mathbf{k}_2} \psi_\lambda(\mathbf{k}_2) \right)$$

Solution that fits experiment:
Both Cu and Ni propagate with the same **k**-arm
and



τ_2

Ni-spins ⇈ in trimer

Magnetic order in $Ca_3Cu_1Ni_2(PO_4)_4$: 2k structure

irrep τ_2

Independently for both Cu-spins and Ni-spins we have:

Orbit 1 (basis functions)

$$\mathbf{S}_0 = \sum_{\lambda=1}^{3} (C_{\lambda,\mathbf{k}_1}\psi_\lambda(\mathbf{k}_1) + C_{\lambda,\mathbf{k}_2}\psi_\lambda(\mathbf{k}_2))$$

$\lambda = x, y, z$

$$C_{\lambda,\mathbf{k}_1} = C'_{\lambda,\mathbf{k}_2}$$

Orbit 2

$$\mathbf{S}'_0 = \sum_{\lambda=1}^{3} (C_{\lambda,\mathbf{k}_1}\psi_\lambda(\mathbf{k}_1) + C'_{\lambda,\mathbf{k}_2}\psi_\lambda(\mathbf{k}_2))$$

$$C_{\lambda,\mathbf{k}_2} = C'_{\lambda,\mathbf{k}_1} = 0$$

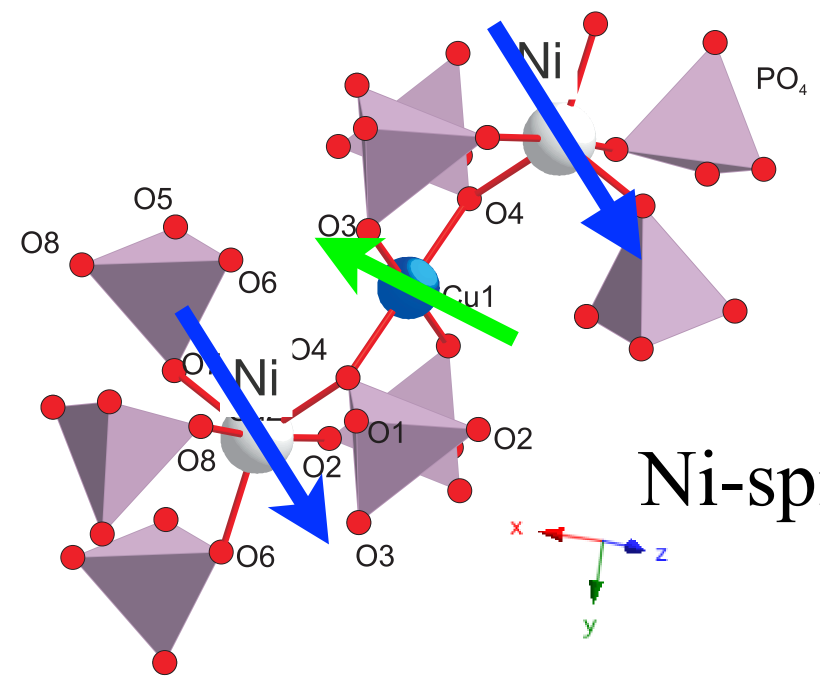
Solution that fits experiment:

Both Cu and Ni propagate with the same **k**-arm

and

$\mathbf{k}_1$ for orbit 1 and $\mathbf{k}_2$ for orbit 2

$$C_{\lambda,\mathbf{k}_1} = C'_{\lambda,\mathbf{k}_2}$$



τ_2

Ni-spins ⇑⇑ in trimer

Magnetic order in $Ca_3Cu_1Ni_2(PO_4)_4$: 2k structure

irrep τ_2

Independently for both Cu-spins and Ni-spins we have:

Orbit 1

basis functions

$$\mathbf{S}_0 = \sum_{\lambda=1}^{3} (C_{\lambda,\mathbf{k}_1}\psi_\lambda(\mathbf{k}_1) + \cancel{C_{\lambda,\mathbf{k}_2}}\psi_\lambda(\mathbf{k}_2))$$

$\lambda = x, y, z$

$C_{\lambda,\mathbf{k}_1} = C'_{\lambda,\mathbf{k}_2}$

$$C_{\lambda,\mathbf{k}_2} = C'_{\lambda,\mathbf{k}_1} = 0$$

Orbit 2

$$\mathbf{S}'_0 = \sum_{\lambda=1}^{3} (\cancel{C'_{\lambda,\mathbf{k}_1}}\psi_\lambda(\mathbf{k}_1) + C'_{\lambda,\mathbf{k}_2}\psi_\lambda(\mathbf{k}_2))$$

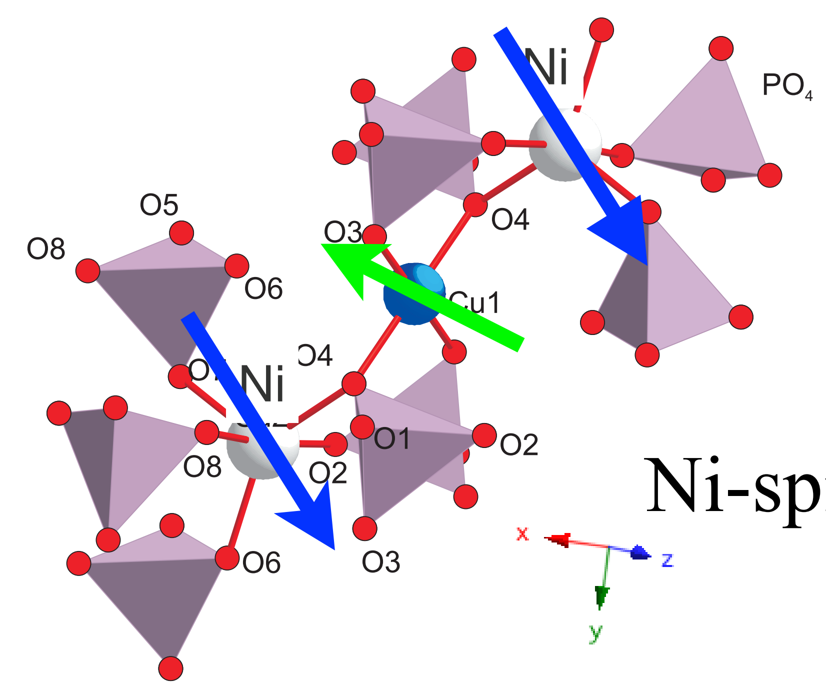
Solution that fits experiment:

Both Cu and Ni propagate with the same **k**-arm

and

$\mathbf{k}_1$ for orbit 1 and $\mathbf{k}_2$ for orbit 2

$$C_{\lambda,\mathbf{k}_1} = C'_{\lambda,\mathbf{k}_2}$$



τ_2

Ni-spins ⇑⇑ in trimer

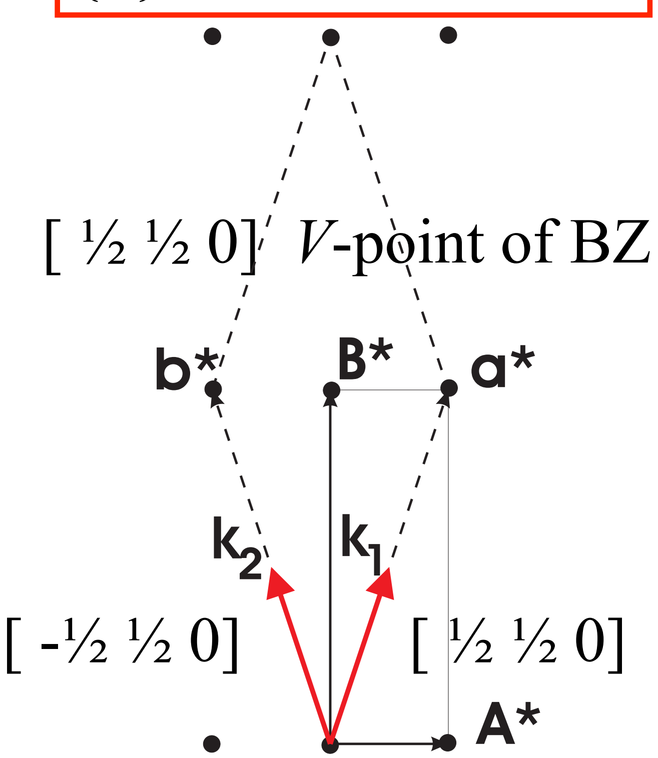
Symmetry analysis using full star {k} & Shubnikov

$C2/c$	C_{2h}^6	$2/m$	Monoclinic
No. 15	$C12/c1$		Patterson symmetry $C12/m1$

Symmetry operators

$h_1 = x,y,z$ $h_2 = \bar{x},y,\bar{z}+\frac{1}{2}$ $h_3 = \bar{x},\bar{y},\bar{z}$ $h_4 = x,\bar{y},z+\frac{1}{2}$ $+T(n_1\mathbf{t}_1 + n_2\mathbf{t}_2 + n_3\mathbf{t}_3)$ $(\frac{1}{2},\frac{1}{2},0)+$

{k}-star has two arms



h_1 1
h_3 -1

$G_k = C\text{-}1$

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ISOTROPY Software Suite

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$C2/c$ C_{2h}^{6} $2/m$ Monoclinic

No. 15 $C\,1\,2/c\,1$ Patterson symmetry $C\,1\,2/m\,1$

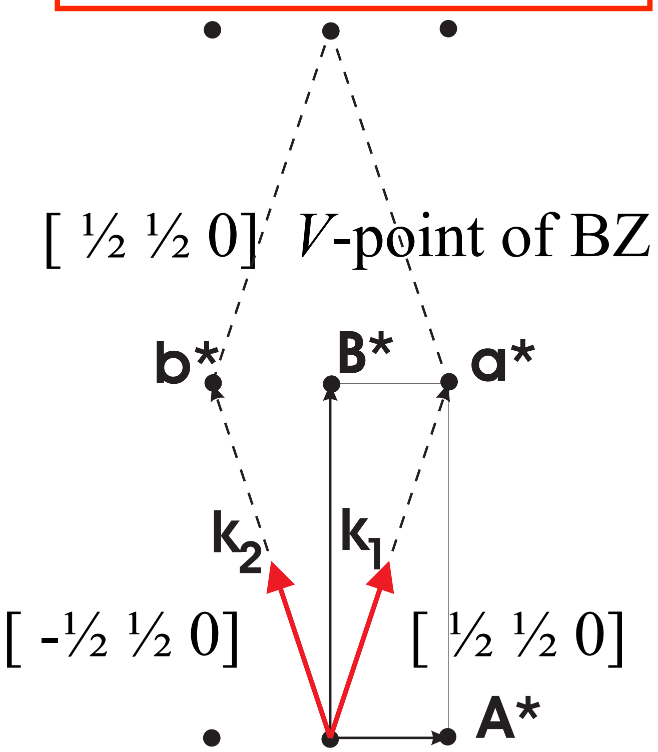
Symmetry operators

$h_1 = x, y, z$ $h_2 = \bar{x}, y, \bar{z} + \frac{1}{2}$ $h_3 = \bar{x}, \bar{y}, \bar{z}$ $h_4 = x, \bar{y}, z + \frac{1}{2}$ $+T(n_1\mathbf{t}_1 + n_2\mathbf{t}_2 + n_3\mathbf{t}_3)$ $(\frac{1}{2}, \frac{1}{2}, 0)+$

$\{[\frac{1}{2}, \frac{1}{2}, 0], [-\frac{1}{2}, \frac{1}{2}, 0]\}$ in $C2/c$ has 2D *irrep* (mV-), based on 1D *irrep* τ_2 of $G_k = C$-1

$$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \quad \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \quad \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix} \quad \begin{bmatrix} 0 & -1 \\ -1 & 0 \end{bmatrix}$$

{k}-star has two arms



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No. 15 $\quad C\,1\,2/c\,1$ $\quad$ Patterson symmetry $C\,1\,2/m\,1$

Symmetry operators

$h_1 = x, y, z \qquad h_2 = \bar{x}, y, \bar{z} + \frac{1}{2} \qquad h_3 = \bar{x}, \bar{y}, \bar{z} \qquad h_4 = x, \bar{y}, z + \frac{1}{2}$

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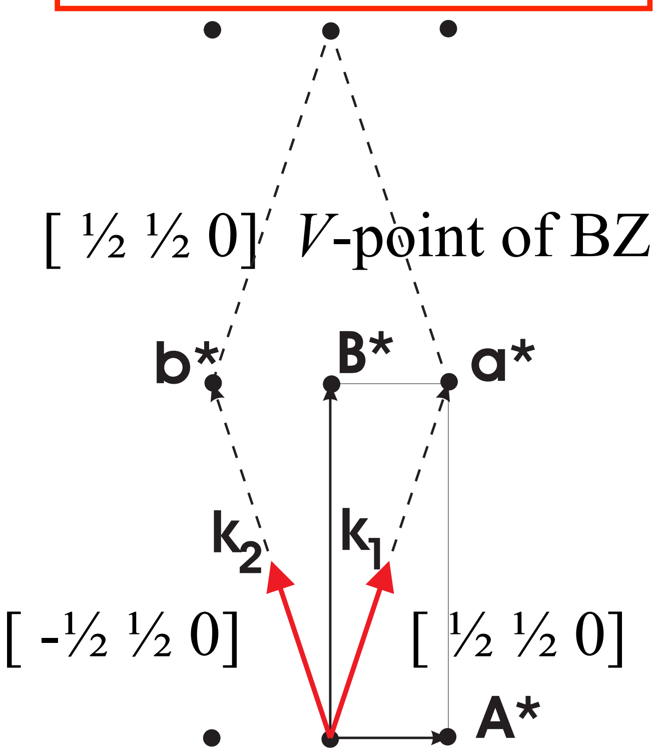

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Space Group: 15 C2/c C2h-6, Lattice parameters: a=17.71770, b=4.82100, c=17.84720, alpha=90.00000, beta=123.63700, gamma=90.00000

Cu 4b (0,1/2,0), Ni 8f (x,y,z), x=-0.12000 , y=0.03750 , z=-0.46700

k point: V, k4 (1/2,1/2,0)
IR: mV1-, mk4t2

P1 (a,a) 15.91 C_a2/c, basis={(2,0,2),(0,-2,0),(0,0,-1)}, origin=(0,1/2,0), s=4, i=4, k-active= (1/2,1/2,0),(-1/2,1/2,0)

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C1 (a,b) 2.7 P_S-1, basis={(0,0,-1),(1,1,1),(0,-2,0)}, origin=(0,1/2,0), s=4, i=8, k-active= (1/2,1/2,0),(-1/2,1/2,0)

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Order parameter direction | Shubnikov Space group | Active arms of propagation vector star

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Order parameter direction

Shubnikov Space group

Active arms of propagation vector star

solution

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"Conventional" one-**k** case does not give physically reasonable solution

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Shubnikov group

C_a2/c 15.91 BNS
P_c2/c 13.8.84 OG

Shubnikov subgroup generated by *2*D-*irrep mV-* and P1 (a,a)

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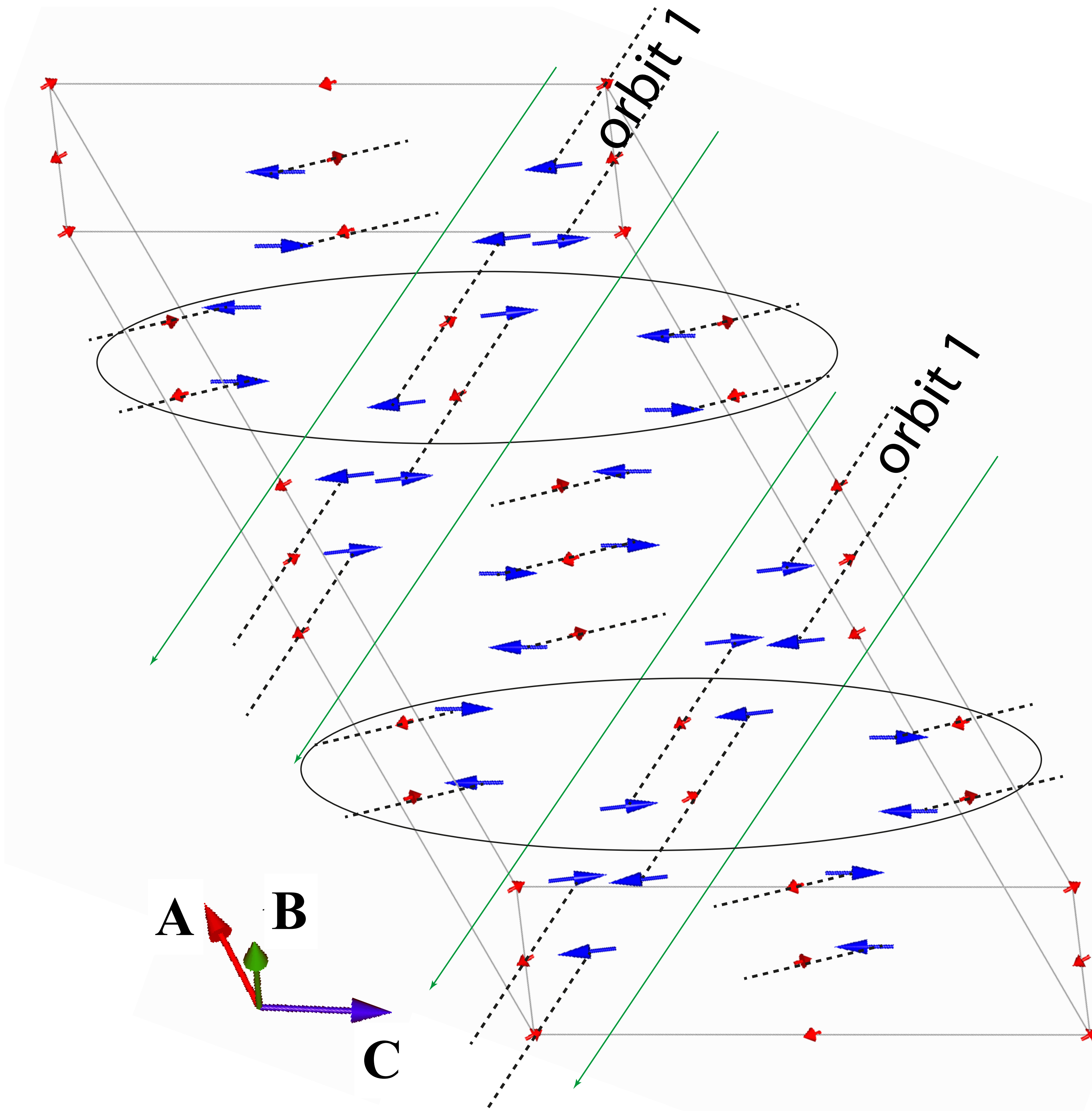
Shubnikov subgroup generated by *2*D-*irrep mV-* and P1 (a,a)

C2/c —> Sh. group C_a2/c

Basis transformation

$\mathbf{A} = 2\mathbf{a} + 2\mathbf{c}, \mathbf{B} = -2\mathbf{b}, \mathbf{C} = -\mathbf{c}$



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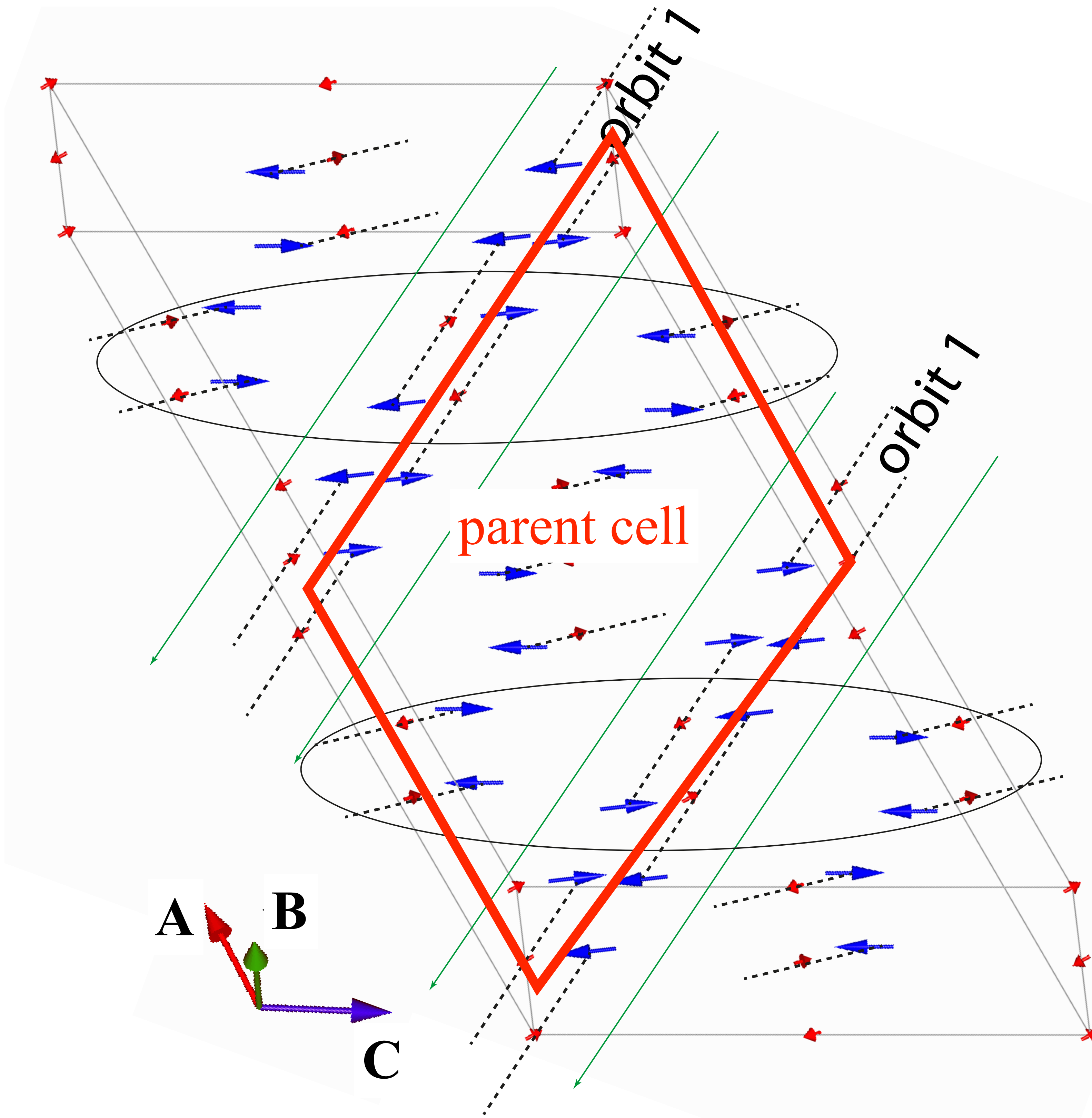

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Spin configuration

two Ni in (16g), two Cu in (8a)

Independently for both Cu-spins and Ni-spins we have two normal modes, constructed from parent *C2/c*::

$$\mathbf{S} = \sum_{\lambda=1}^{3} (C_{\lambda,o_1\mathbf{k}_1}\boldsymbol{\psi}_\lambda(o_1\mathbf{k}_1) + C_{\lambda,o_1\mathbf{k}_2}\boldsymbol{\psi}_\lambda(o_1\mathbf{k}_2))$$

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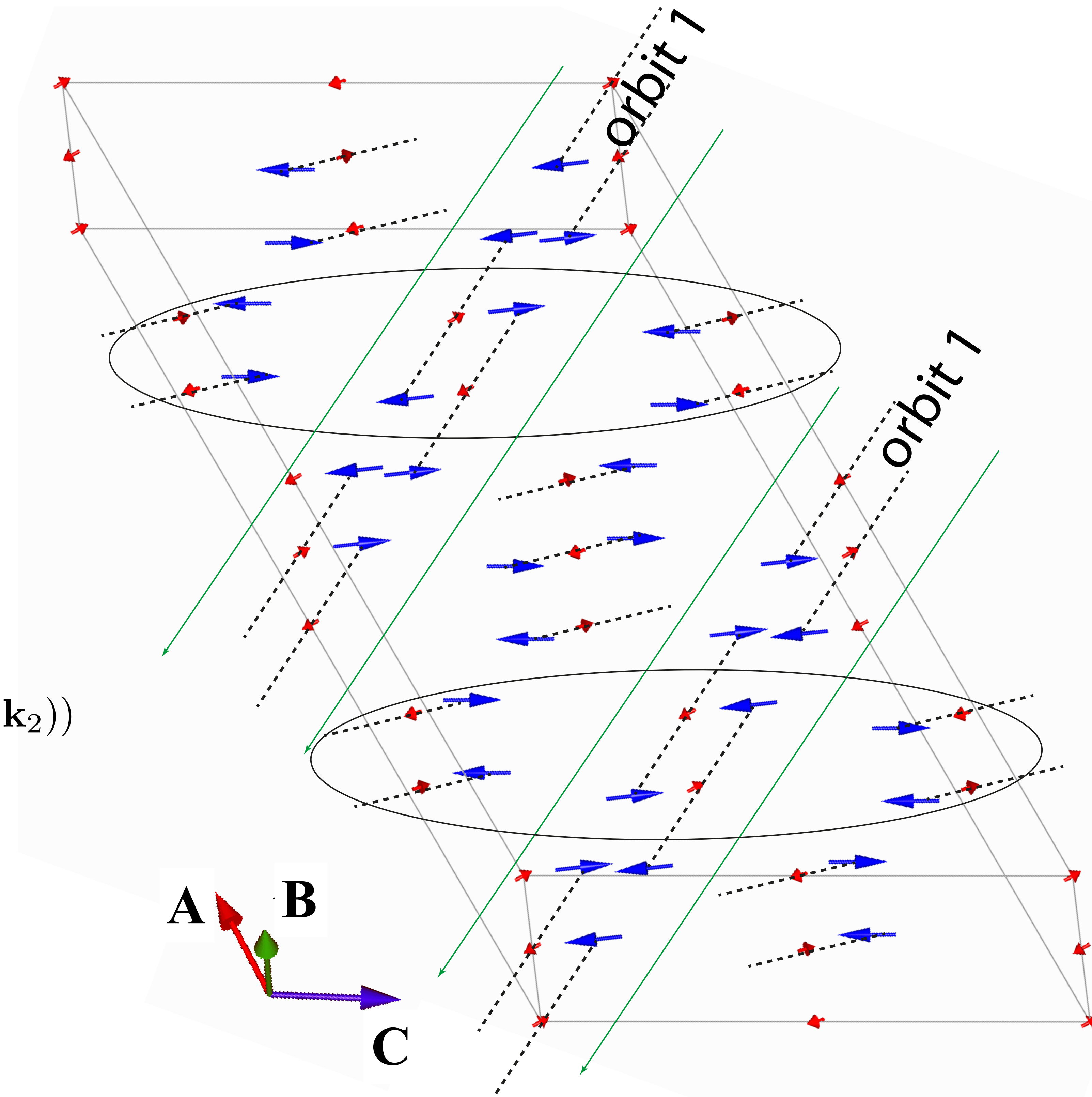

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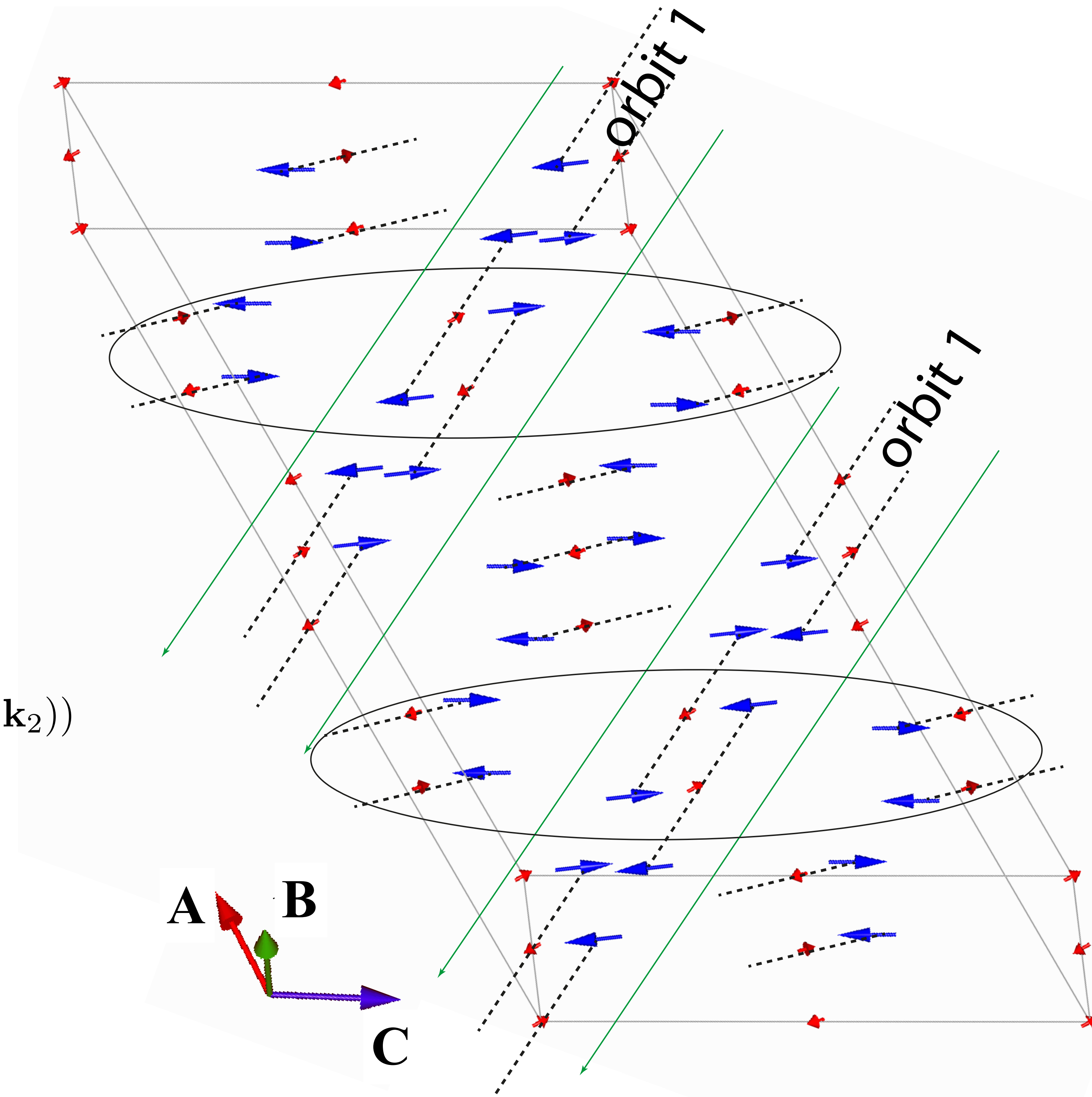
$\lambda = x, y, z$

In parent *C-1* group

orbit1 with $\mathbf{k}_1$
+
orbit2 with $\mathbf{k}_2$



Shubnikov group

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Shubnikov subgroup generated by *2*D-*irrep mV*- and P1 (a,a)

C2/c —> Sh. group C_a2/c

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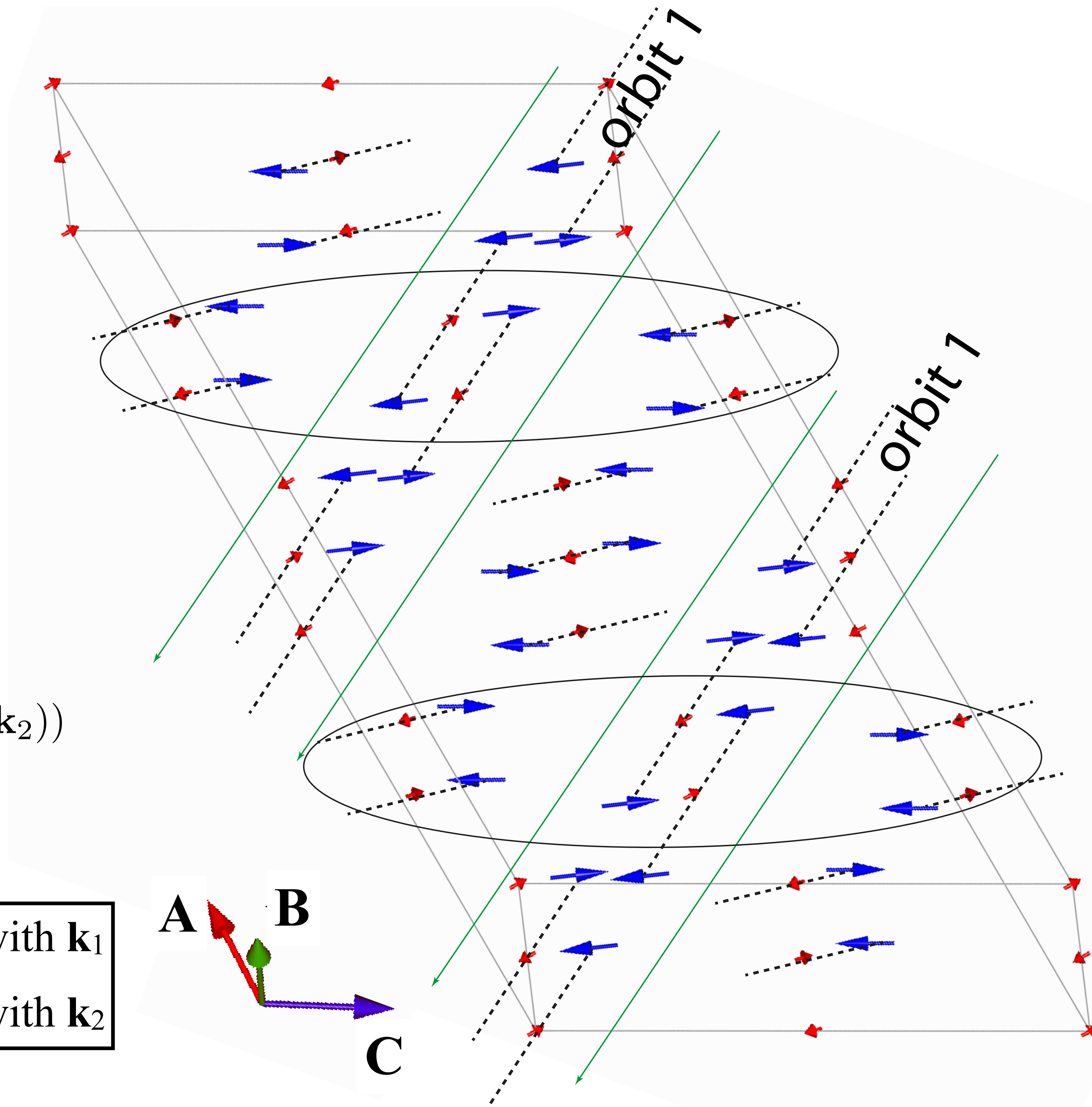
$\lambda = x, y, z$

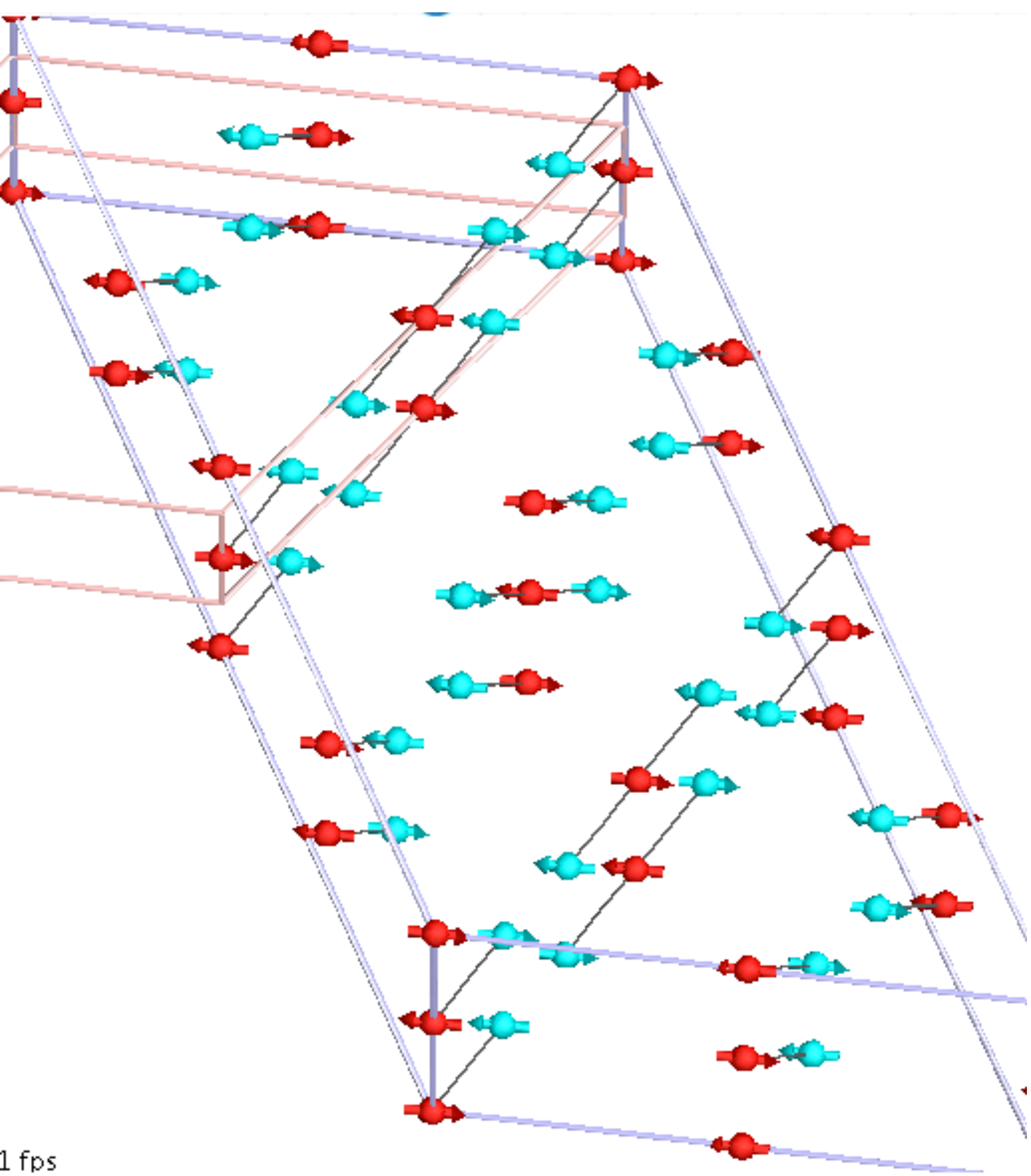
In parent *C-1* group →

orbit1 with $\mathbf{k}_1$ + orbit2 with $\mathbf{k}_2$	orbit2 with $\mathbf{k}_1$ + orbit1 with $\mathbf{k}_2$

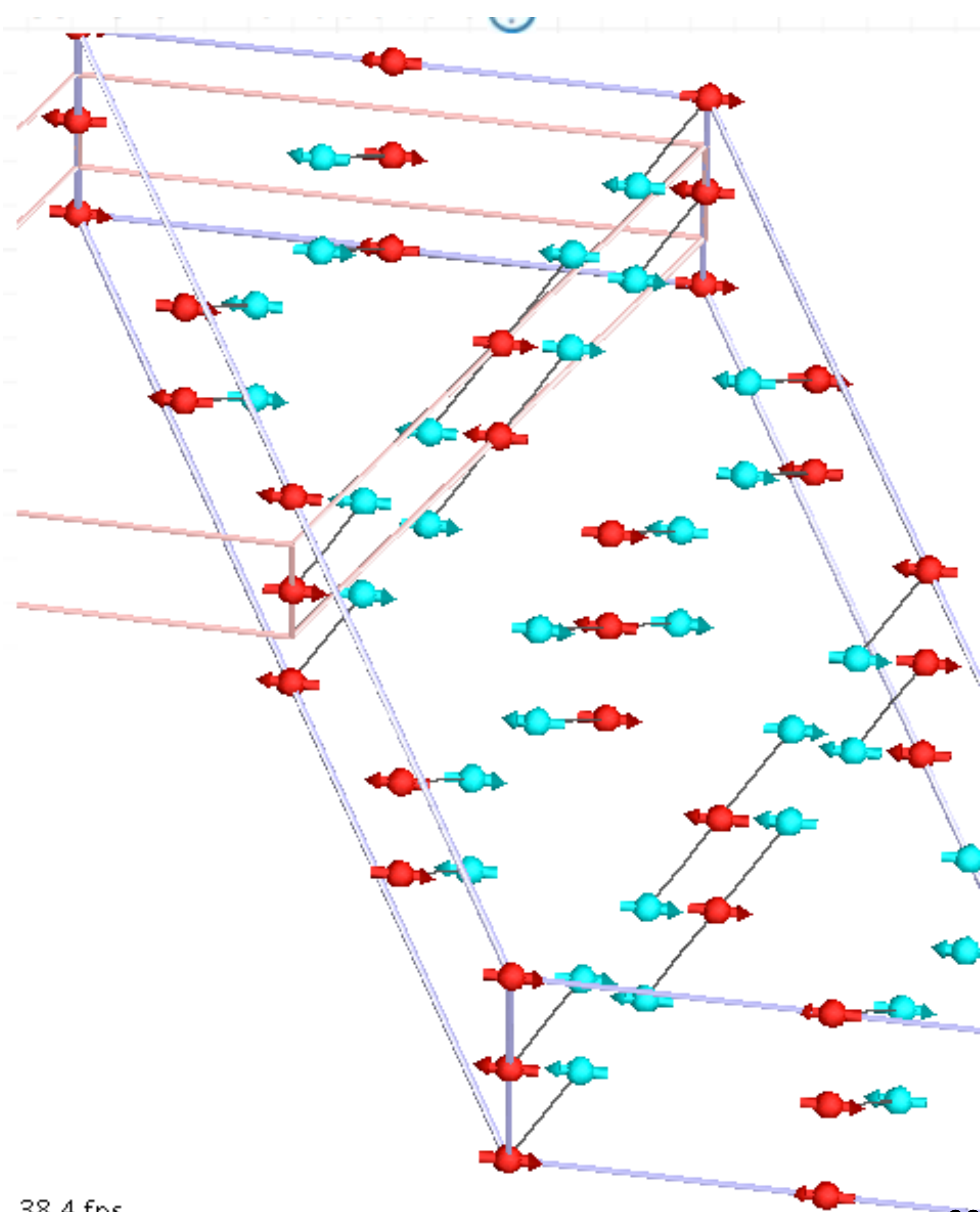


Comparison of two modes

$\psi_{\lambda}(o_1\mathbf{k}_1)$ [½ ½ 0]



$\psi_{\lambda}(o_1\mathbf{k}_2)$ [-½ ½ 0]



Comparison of two modes

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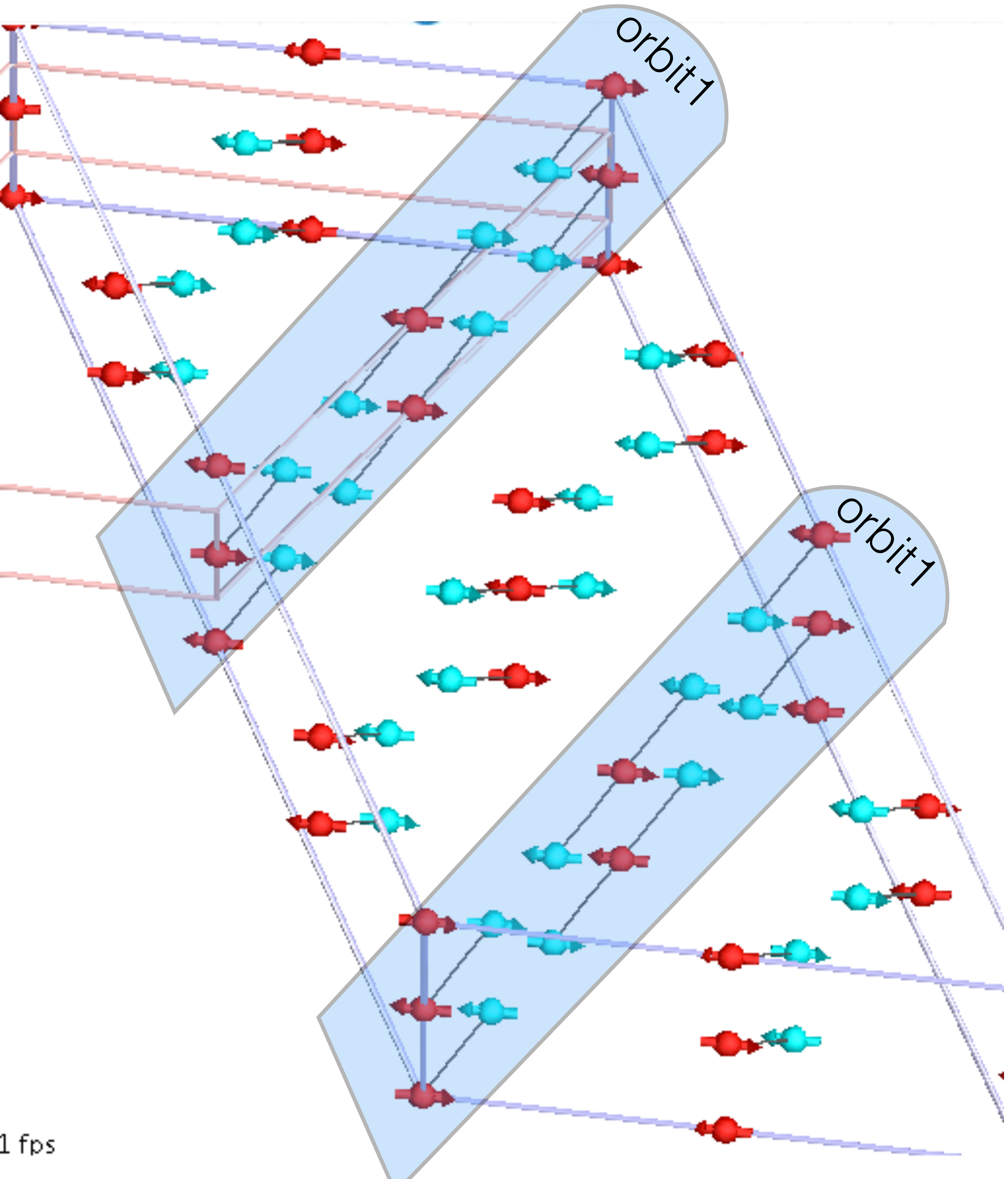
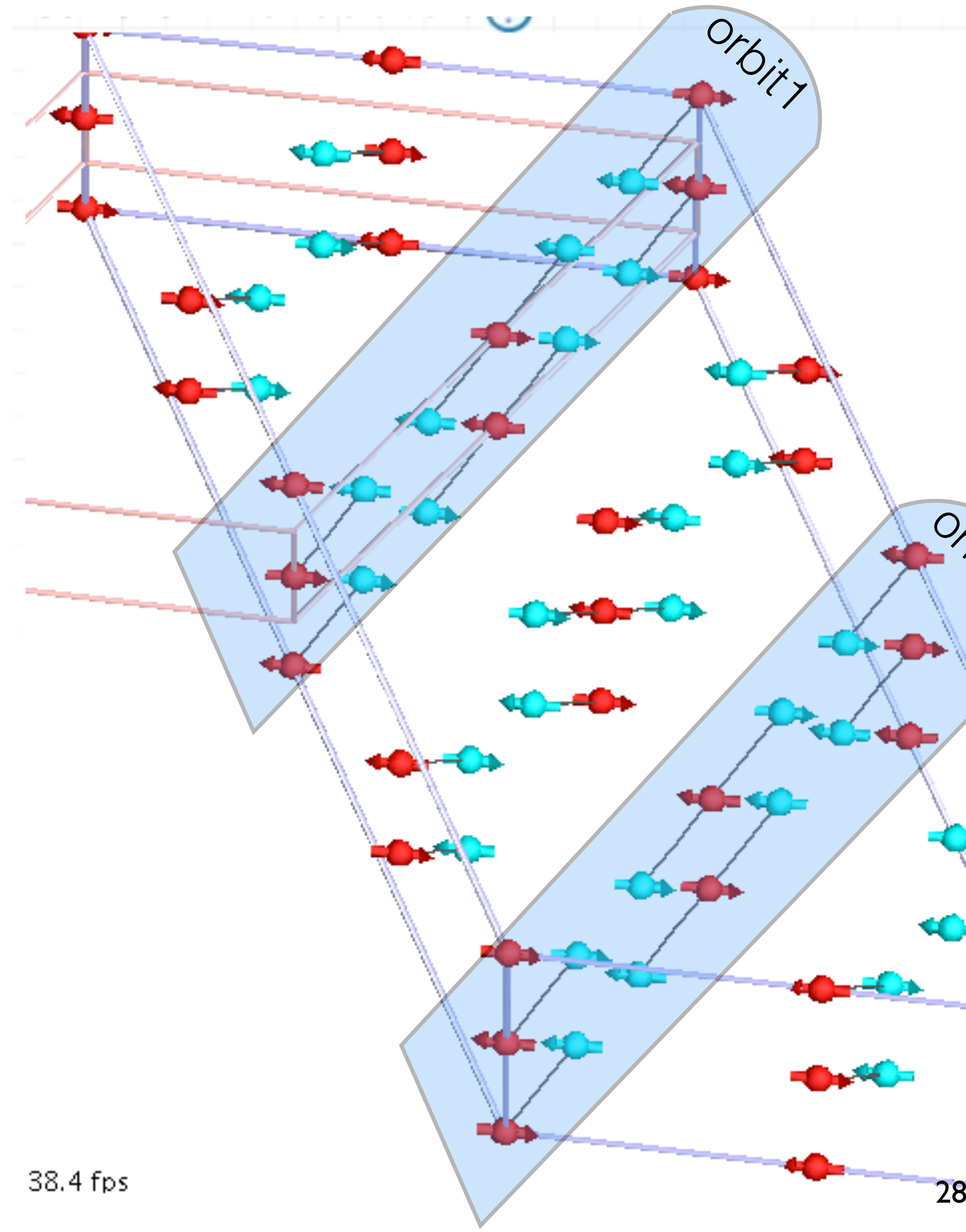
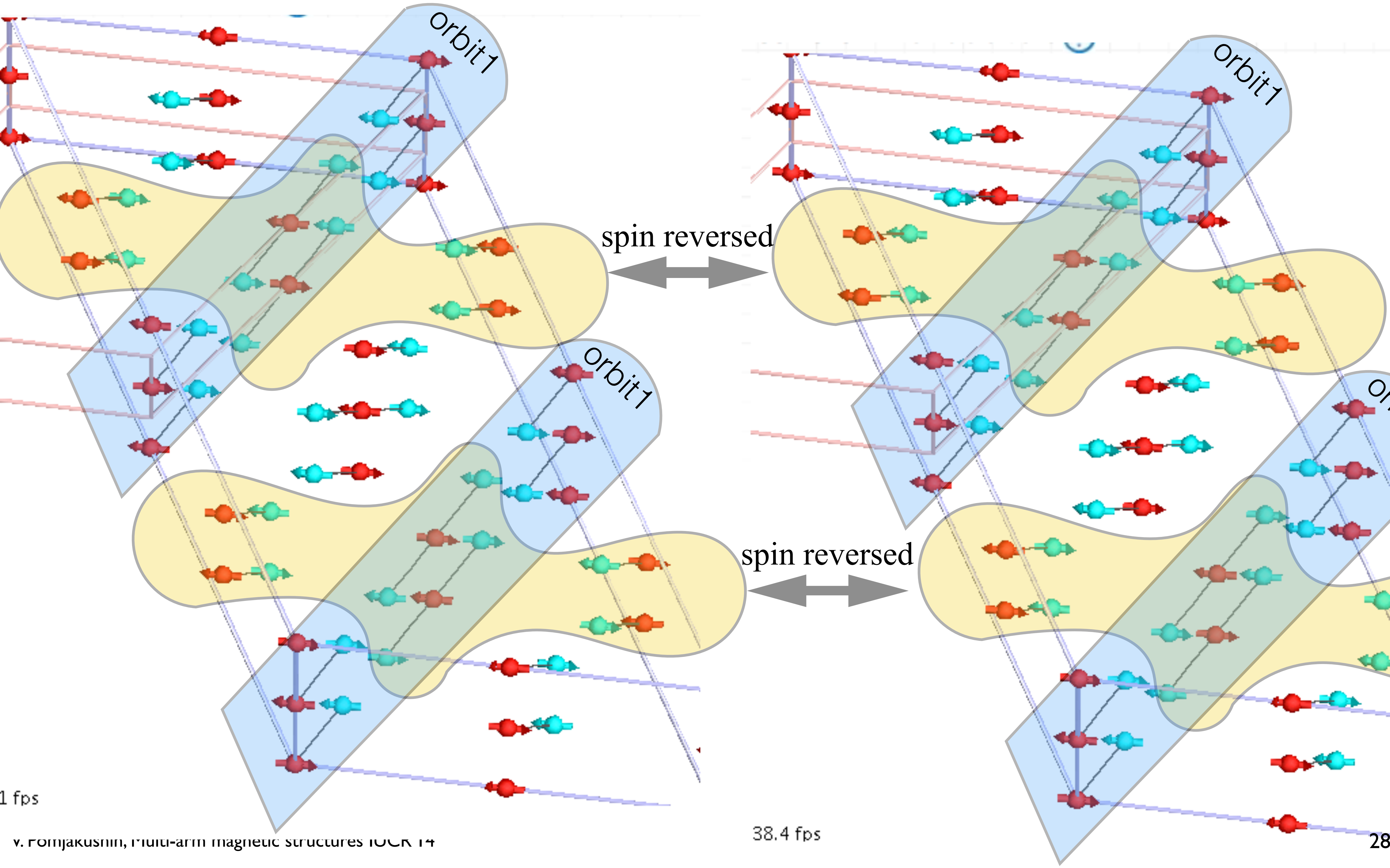


$\psi_\lambda(o_1\mathbf{k}_2)$ [-½ ½ 0]



Comparison of two modes

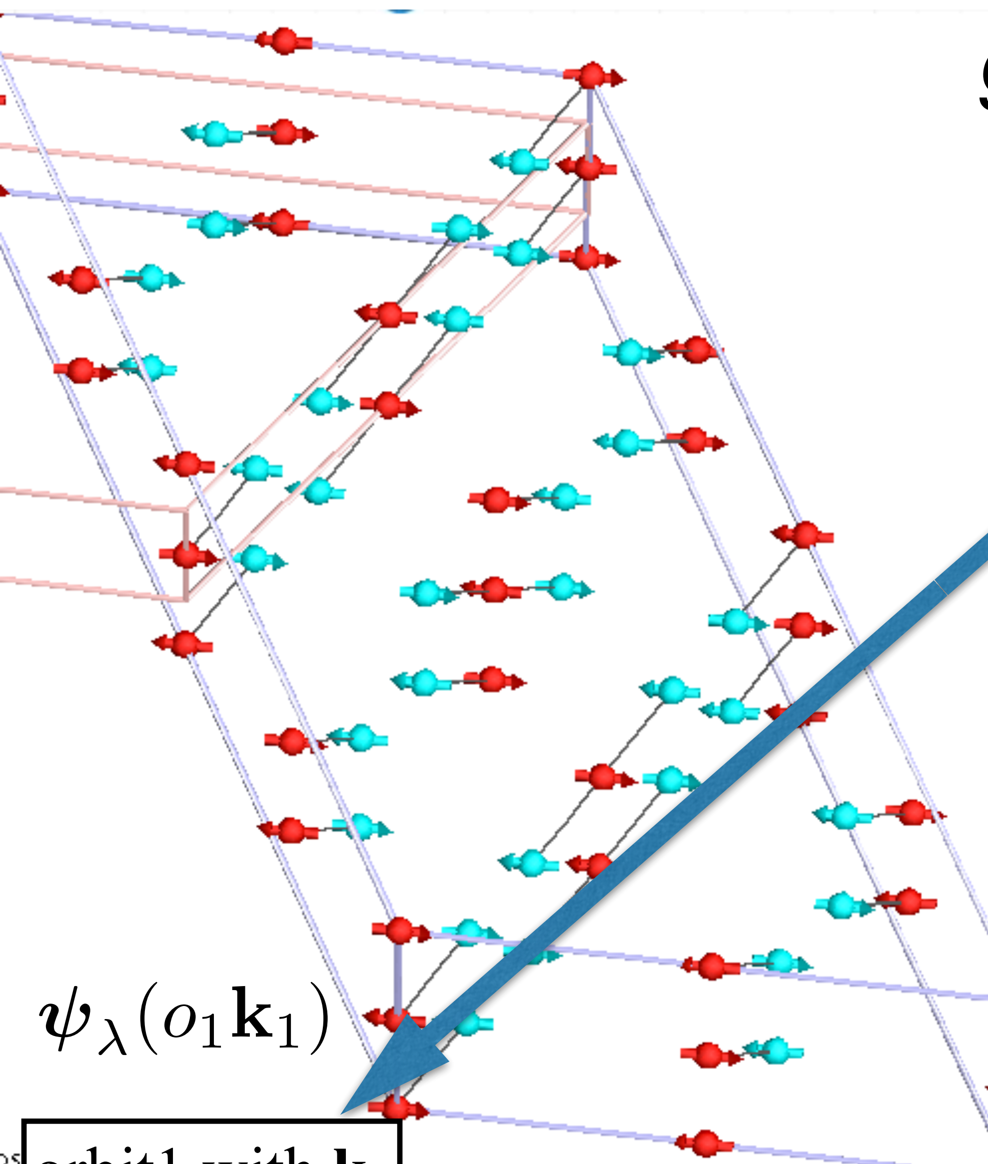
$\psi_\lambda(o_1\mathbf{k}_1)$ [½ ½ 0] $\psi_\lambda(o_1\mathbf{k}_2)$ [-½ ½ 0]



Only one mode fits experimental data

Shubnikov group C_a2/c

*g*enerated by full propagation vector star



$\psi_\lambda(o_1\mathbf{k}_1)$

orbit1 with $\mathbf{k}_1$
$+$
orbit2 with $\mathbf{k}_2$

experimental values

$\langle S_{Ni} \rangle = 0.945(5)$, $\langle S_{Cu} \rangle = 0.31(1)$

angle between $\langle \mathbf{S}_{Ni} \rangle$ and $\langle \mathbf{S}_{Cu} \rangle$

$\cong$ 160 degrees

k-vector and Shubnikov description

$C2/c$ —> Sh. group C_a2/c

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$\mathbf{A} = 2\mathbf{a} + 2\mathbf{c}, \mathbf{B} = -2\mathbf{b}, \mathbf{C} = -\mathbf{c}$

(8f)-Ni and (4b)-Cu in $C2/c$
splits into two orbits

		$C\text{-}1$ with $\mathbf{k}_1$& $\mathbf{k}_2$
	a, Å	17.68079
	b, Å	4.80421
	c, Å	17.79799
	β, deg	123.755
orbit 1 (4i)	Ni11 xyz	0.62065 0.5353 0.96795
	$m_x m_y m_z$	0.1539 -0.1984 -1.7917
(2c)	Cu1 xyz	0 $\frac{1}{2}$ 0
	$m_x m_y m_z$	0.3238 -0.1426 -0.3601
orbit 2 (4i)	Ni21 xyz	0.37935 0.5353 0.53205
	$m_x m_y m_z$	0.1539 0.1984 -1.7917
(2c)	Cu2 xyz	0 $\frac{1}{2}$ $\frac{1}{2}$
	$m_x m_y m_z$	-0.3238 -0.1426 0.3601
$\mathbf{t} = -(\frac{1}{2}, \frac{1}{2}, 0)$	Ni11c xyz	0.12065 0.0353 0.96795
	$m_x m_y m_z$	-0.1539 0.1984 1.7917
	Cu1c xyz	$-\frac{1}{2}$ 0 0
	$m_x m_y m_z$	-0.3238 0.1426 0.3601

k-vector and Shubnikov description

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		$m_x m_y m_z$	0.3238 -0.1426 -0.3601
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		$m_x m_y m_z$	-0.3238 -0.1426 0.3601
$\mathbf{t} = -(\frac{1}{2}, \frac{1}{2}, 0)$		Ni11c xyz	0.12065 0.0353 0.96795
		$m_x m_y m_z$	-0.1539 0.1984 1.7917
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		$m_x m_y m_z$	0.1539 -0.1984 -1.7917
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$\mathbf{t} = -(\frac{1}{2}, \frac{1}{2}, 0)$		Ni11c xyz	0.12065 0.0353 0.96795
		$m_x m_y m_z$	-0.1539 0.1[illegible] [illegible].7917
		Cu1c xyz	$-\frac{1}{2}$ 0 [illegible]
		$m_x m_y m_z$	-[illegible] [illegible].1426 0.3601

generated by k

$$\mathbf{m}(\mathbf{t}) = \mathbf{m}_0 \cos(2\pi \mathbf{k}_1 \mathbf{t})$$

k-vector and Shubnikov description

C2/c —> Sh. group C_a2/c

$\mathbf{A}=2\mathbf{a}+2\mathbf{c}, \mathbf{B}=-2\mathbf{b}, \mathbf{C}=-\mathbf{c}$

$$\mathbf{S}=\sum_{\lambda=1}^{3}(C_{\lambda,o_1\mathbf{k}_1}\psi_\lambda(o_1\mathbf{k}_1)+C_{\lambda,o_1\mathbf{k}_2}\psi_\lambda(o_1\mathbf{k}_2))$$

Mix generates two Ni and two Cu positions

(8f)-Ni and (4b)-Cu in *C2/c* splits into two orbits

		C-1 with $\mathbf{k}_1$& $\mathbf{k}_2$	C_a2/c 15.91 BNS P_c2/c 13.8.84 OG
	a, Å	17.68079	33.44705
	b, Å	4.80421	9.608429
	c, Å	17.79799	17.79799
	β, deg	123.755	118.477
(4i)	Ni11 xyz	0.62065 0.5353 0.96795	
orbit 1	$m_xm_ym_z$	0.1539 -0.1984 -1.7917	
(2c)	Cu1 xyz	0 $\frac{1}{2}$ 0	
	$m_xm_ym_z$	0.3238 -0.1426 -0.3601	
(4i)	Ni21 xyz	0.37935 0.5353 0.53205	
orbit 2	$m_xm_ym_z$	0.1539 0.1984 -1.7917	
(2c)	Cu2 xyz	0 $\frac{1}{2}$ $\frac{1}{2}$	
	$m_xm_ym_z$	-0.3238 -0.1426 0.3601	
	Ni11c xyz	0.12065 0.035[illegible].96795	
$\mathbf{t}=-(\frac{1}{2},\frac{1}{2},0)$	$m_xm_ym_z$	-0.1539 0.[illegible]917	
	Cu1c xyz	$-\frac{1}{2}$ 0 [illegible]	
	$m_xm_ym_z$	-[illegible].1426 0.3601	

generated by **k**

$\mathbf{m}(\mathbf{t})=\mathbf{m}_0\cos(2\pi\mathbf{k}_1\mathbf{t})$

k-vector and Shubnikov description

C2/c —> Sh. group C_a2/c

$\mathbf{A} = 2\mathbf{a} + 2\mathbf{c}, \mathbf{B} = -2\mathbf{b}, \mathbf{C} = -\mathbf{c}$

$$\mathbf{S} = \sum_{\lambda=1}^{3} (C_{\lambda,o_1\mathbf{k}_1}\psi_\lambda(o_1\mathbf{k}_1) + C_{\lambda,o_1\mathbf{k}_2}\psi_\lambda(o_1\mathbf{k}_2))$$

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	c, Å	17.79799	17.79799	
	β, deg	123.755	118.477	
orbit 1 (4i)	Ni11 xyz	0.62065 0.5353 0.96795	0.31033 -0.01765 -0.3473	Ni11 (16g)
	$m_xm_ym_z$	0.1539 -0.1984 -1.7917	0.1456 0.1984 1.9466	
(2c)	Cu1 xyz	0 $\frac{1}{2}$ 0	0 0 0	Cu1 (8a)
	$m_xm_ym_z$	0.3238 -0.1426 -0.3601	0.3063 0.1426 0.6860	
orbit 2 (4i)	Ni21 xyz	0.37935 0.5353 0.53205		
	$m_xm_ym_z$	0.1539 0.1984 -1.7917		
(2c)	Cu2 xyz	0 $\frac{1}{2}$ $\frac{1}{2}$		
	$m_xm_ym_z$	-0.3238 -0.1426 0.3601		
	Ni11c xyz	0.12065 0.035[illegible].96795	0.06033 0.23235 -0.8473	Ni11c (16g)
$\mathbf{t} = -(\frac{1}{2}, \frac{1}{2}, 0)$	$m_xm_ym_z$	-0.1539 0.1[illegible].7917	-0.1456 -0.19843 -1.9466	
	Cu1c xyz	$-\frac{1}{2}$ 0 [illegible]	$-\frac{1}{4}$ $\frac{1}{4}$ -$\frac{1}{2}$	Cu1c (8b)
	$m_xm_ym_z$	-[illegible].1426 0.3601	-0.3063 -0.1426 -0.6860	

generated by k

$$\mathbf{m}(\mathbf{t}) = \mathbf{m}_0 \cos(2\pi\mathbf{k}_1\mathbf{t})$$

k-vector and Shubnikov description

C2/c —> Sh. group C_a2/c

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C_a2/c 15.91 BNS

P_c2/c 13.8.84 OG

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	$m_xm_ym_z$	0.1539 -0.1984 -1.7917	0.1456 0.1984 1.9466	
(2c)	Cu1 xyz	0 $\frac{1}{2}$ 0	0 0 0	Cu1 (8a)
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(2c)	Cu2 xyz	0 $\frac{1}{2}$ $\frac{1}{2}$		
	$m_xm_ym_z$	-0.3238 -0.1426 0.3601		
	Ni11c xyz	0.12065 0.0353 0.96795	0.06033 0.23235 -0.8473	Ni11c (16g)
$\mathbf{t} = -(\frac{1}{2}, \frac{1}{2}, 0)$	$m_xm_ym_z$	-0.1539 0.1[illegible] [illegible]917	-0.1456 -0.19843 -1.9466	
	Cu1c xyz	$-\frac{1}{2}$ 0 [illegible]	$-\frac{1}{4}$ $\frac{1}{4}$ $-\frac{1}{2}$	Cu1c (8b)
	$m_xm_ym_z$	-[illegible] [illegible].1426 0.3601	-0.3063 -0.1426 -0.6860	

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$$\mathbf{m}(\mathbf{t}) = \mathbf{m}_0 \cos(2\pi\mathbf{k}_1\mathbf{t})$$

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	$m_xm_ym_z$	-0.1539 0.1[illegible] [illegible]917	-0.1456 -0.19843 -1.9466	
	Cu1c xyz	$-\frac{1}{2}$ 0 [illegible]	$-\frac{1}{4}$ $\frac{1}{4}$ -$\frac{1}{2}$	Cu1c (8b)
	$m_xm_ym_z$	-[illegible].1426 0.3601	-0.3063 -0.1426 -0.6860	

generated by Sh. group

generated by k

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orbit 2 (4i)	Ni21 xyz	0.37935 0.5353 0.53205		
	$m_xm_ym_z$	0.1539 0.1984 -1.7917		
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	$m_xm_ym_z$	-0.3238 0.1426 0.3601	-0.3063 -0.1426 -0.6860	

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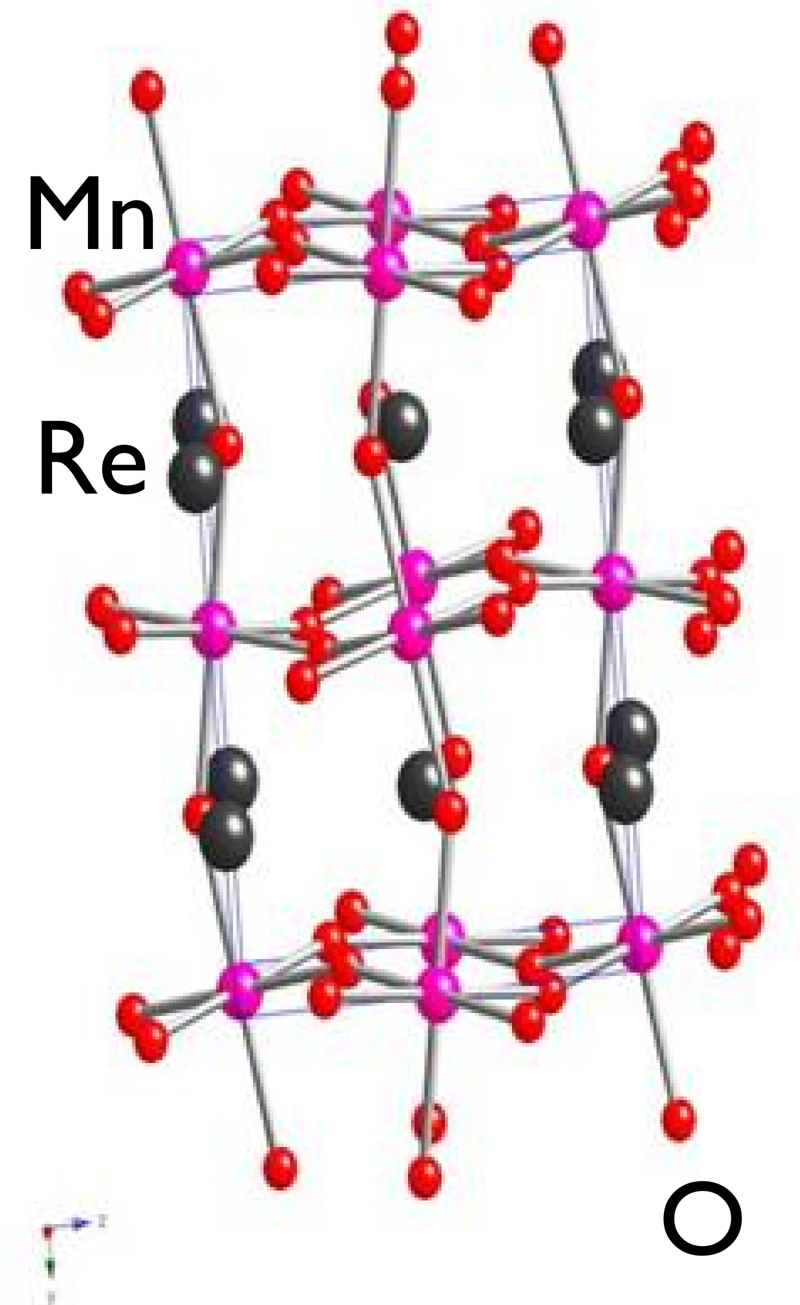
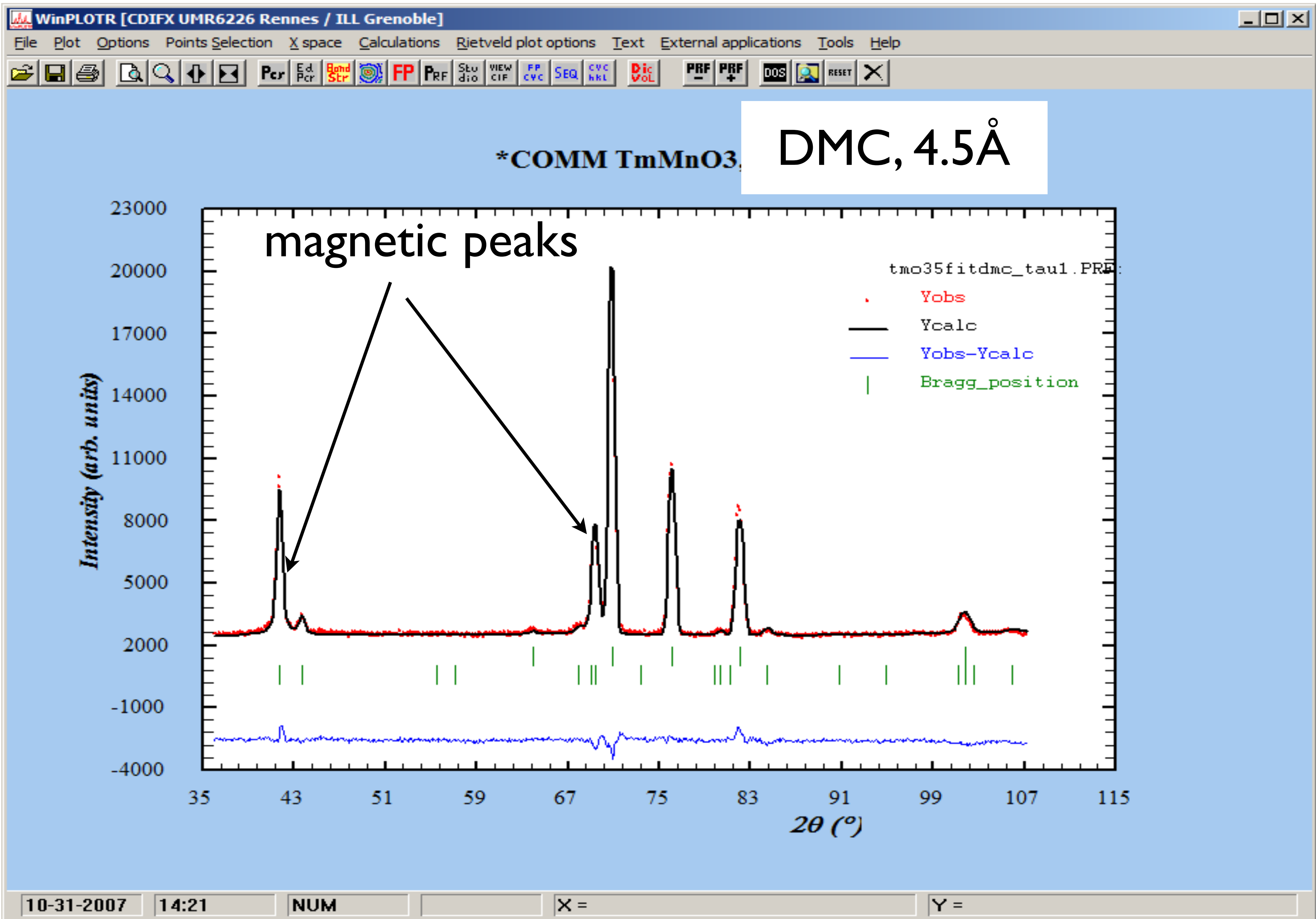
Antiferromagnetic order in orthorhombic multiferroic $TmMnO_3$

1. Constraints on basis functions vs. superspace for the incommensurate two arm **k**=[1/2±δ,0,0]. {**k**}={-**k**,+**k**}
2. one-arm multi dimensional irrep **k**=[1/2,0,0]

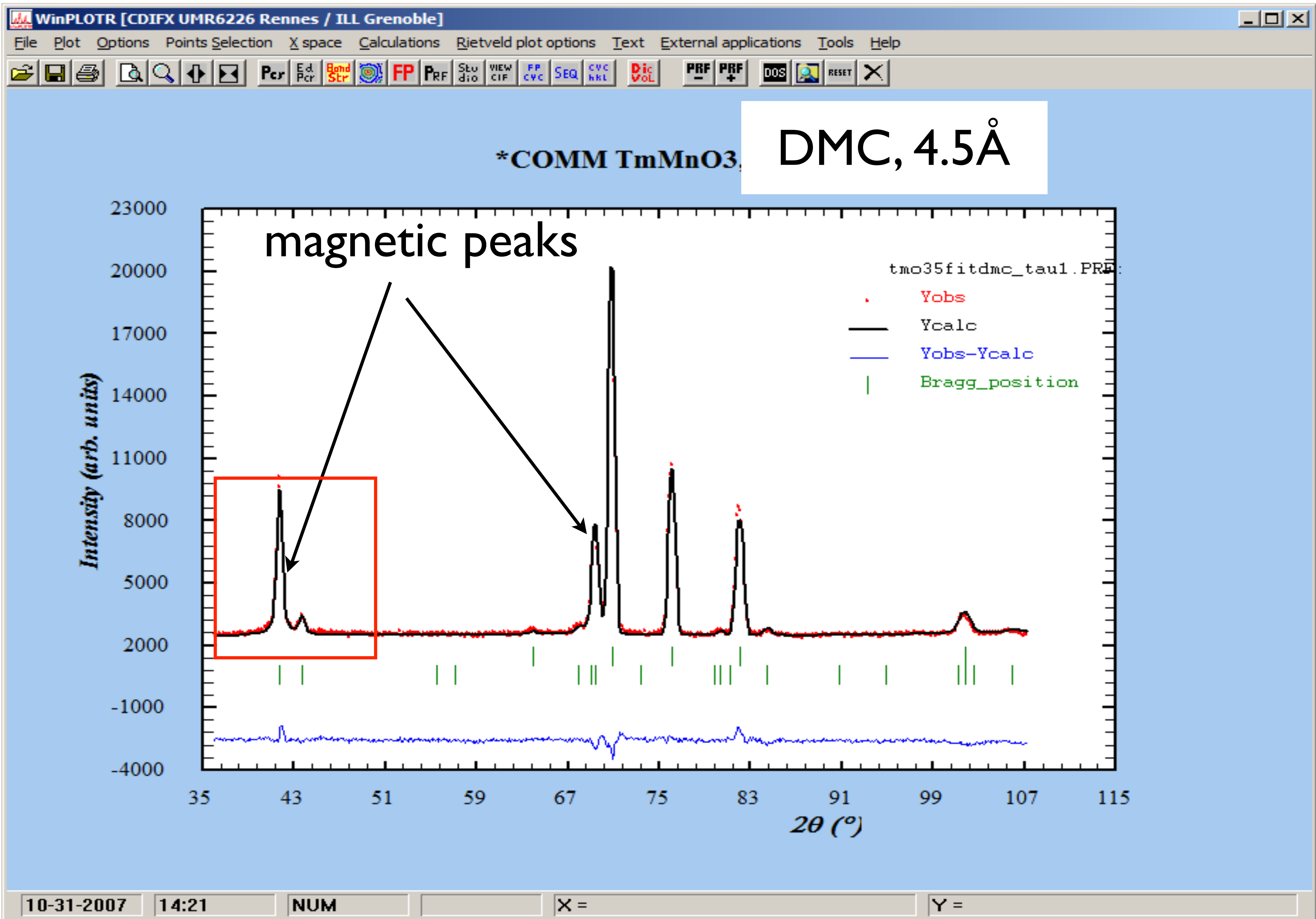


New Journal of Physics 11, 043019 (2009)

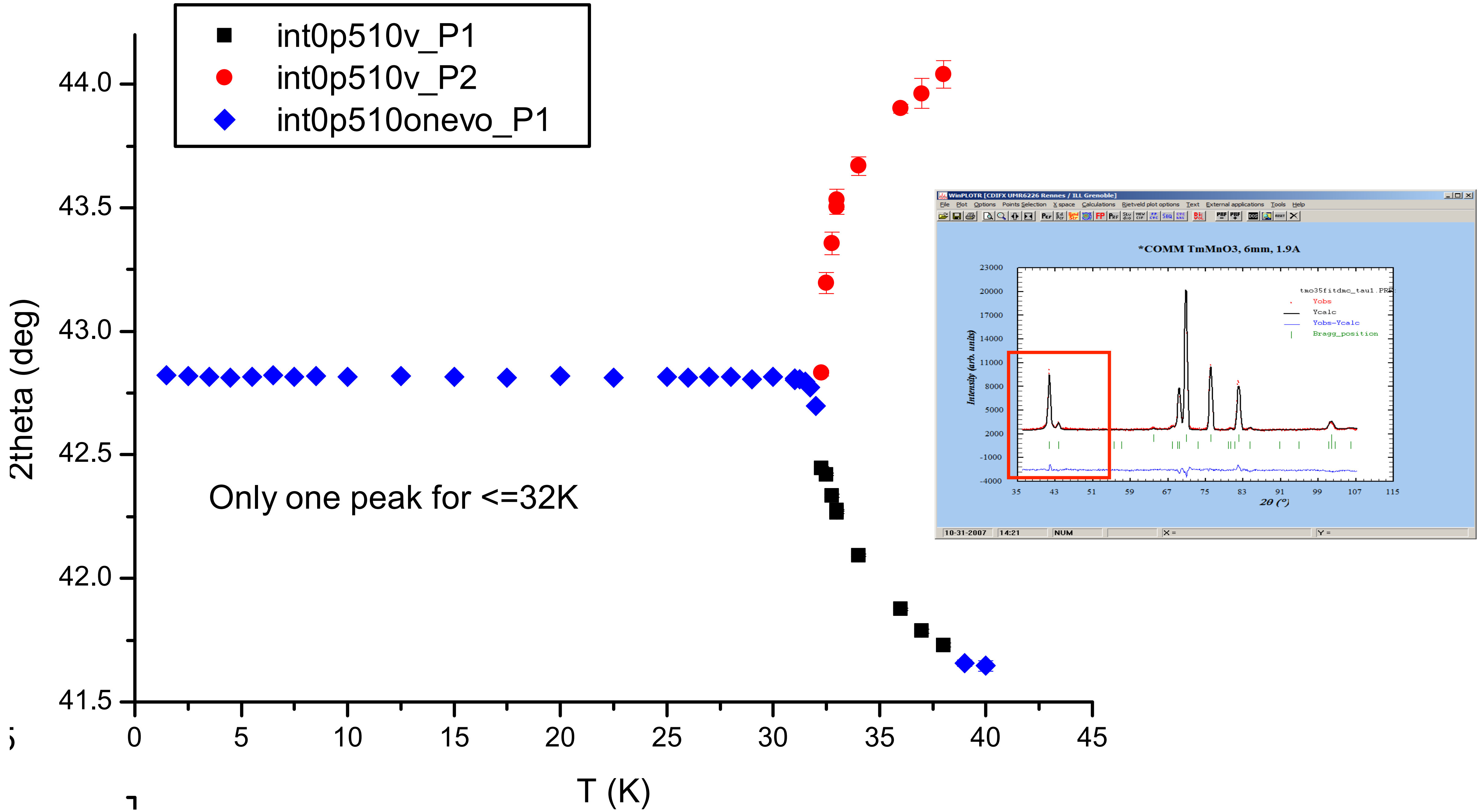
Diffraction pattern $TmMnO_3$



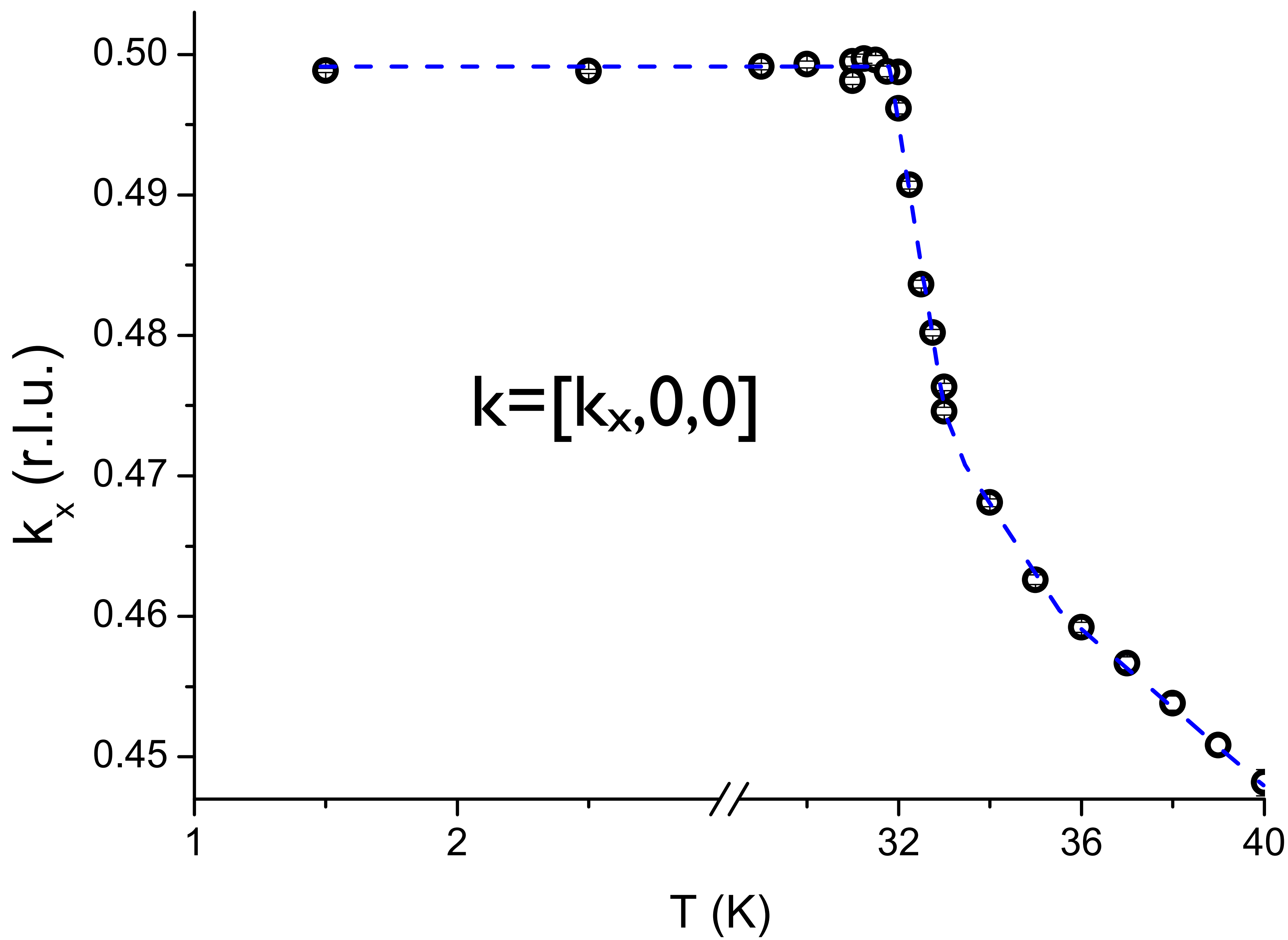
Diffraction pattern $TmMnO_3$



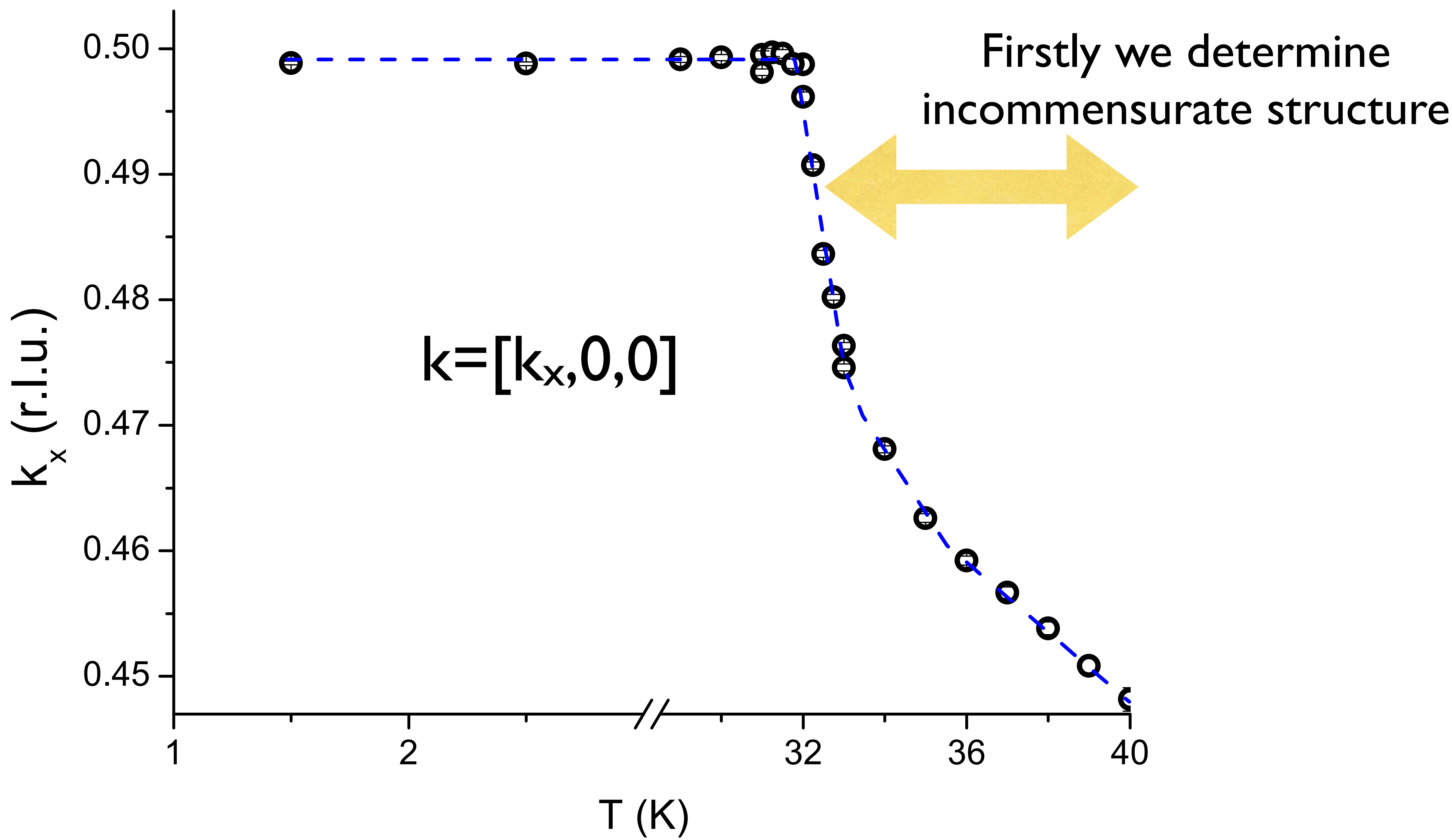
T-dependence of Bragg peak positions



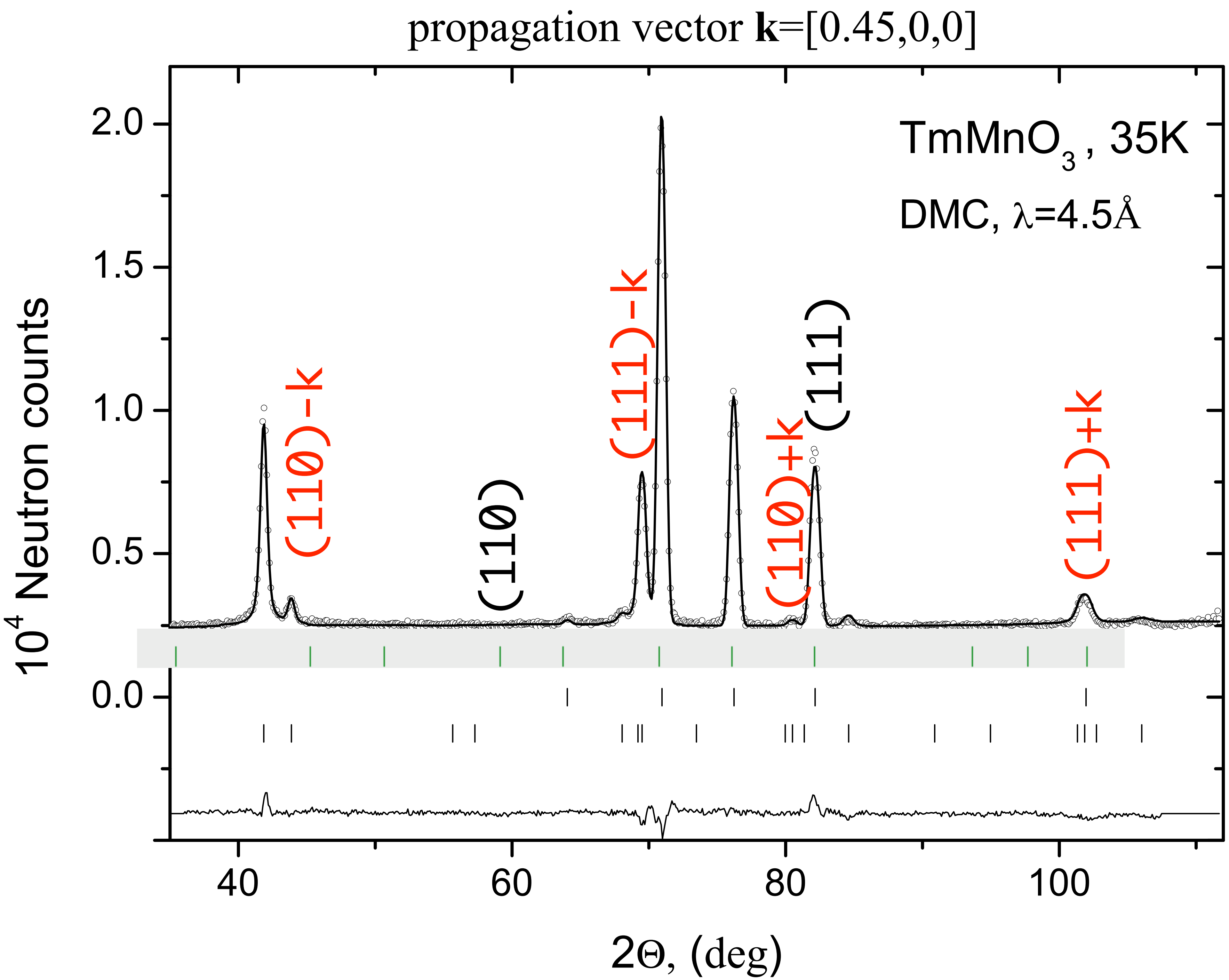
Refining the propagation k-vector from profile matching fit



Refining the propagation k-vector from profile matching fit



Indexed diffraction pattern



Classifying possible magnetic structures k-vector group

Group *G: Pnma,* no.62: 8 symmetry operators

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

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Little group G_k, k=[0.45,0,0]=[μ,0,0] SM point of BZ

Little group of propagation vector G_k contains only the elements of *G* that do not change **k**

Classifying possible magnetic structures k-vector group

Group *G: Pnma*, no.62: 8 symmetry operators

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

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$P2_1ma\ (Pmc2_1, 26)$

(1) x,y,z (4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$ (7) $x,\bar{y}+\frac{1}{2},z$ (6) $x+\frac{1}{2},y,\bar{z}+\frac{1}{2}$

rotation+ translation

$$E\begin{pmatrix}100\\010\\001\end{pmatrix}\begin{pmatrix}0\\0\\0\end{pmatrix}\quad 2_x\begin{pmatrix}100\\0\bar{1}0\\00\bar{1}\end{pmatrix}\begin{pmatrix}\frac{1}{2}\\\frac{1}{2}\\\frac{1}{2}\end{pmatrix}\quad m_y\begin{pmatrix}100\\0\bar{1}0\\001\end{pmatrix}\begin{pmatrix}0\\\frac{1}{2}\\0\end{pmatrix}\quad m_z\begin{pmatrix}100\\010\\00\bar{1}\end{pmatrix}\begin{pmatrix}\frac{1}{2}\\0\\\frac{1}{2}\end{pmatrix}$$

Classifying possible magnetic structures
k-vector group

Group *G*: *Pnma*, no.62: 8 symmetry operators

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

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

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$$E\begin{pmatrix}100\\010\\001\end{pmatrix}\begin{pmatrix}0\\0\\0\end{pmatrix}\quad 2_x\begin{pmatrix}100\\0\bar{1}0\\00\bar{1}\end{pmatrix}\begin{pmatrix}\frac{1}{2}\\\frac{1}{2}\\\frac{1}{2}\end{pmatrix}\quad m_y\begin{pmatrix}100\\0\bar{1}0\\001\end{pmatrix}\begin{pmatrix}0\\\frac{1}{2}\\0\end{pmatrix}\quad m_z\begin{pmatrix}100\\010\\00\bar{1}\end{pmatrix}\begin{pmatrix}\frac{1}{2}\\0\\\frac{1}{2}\end{pmatrix}$$

star {**k**}
has two arms

-k ← → **k**

-k is nonequivalent to +**k**
i.e. -**k**≠**k**+'recip. latt. period'

Constructing normal modes of magnetic structure from irreps

$TmMnO_3$

Space Group *G: Pnma,* no.62
propagation vector k=[μ,0,0] SM point of BZ

has 4 1D irreducible representations

symmetry
irreps

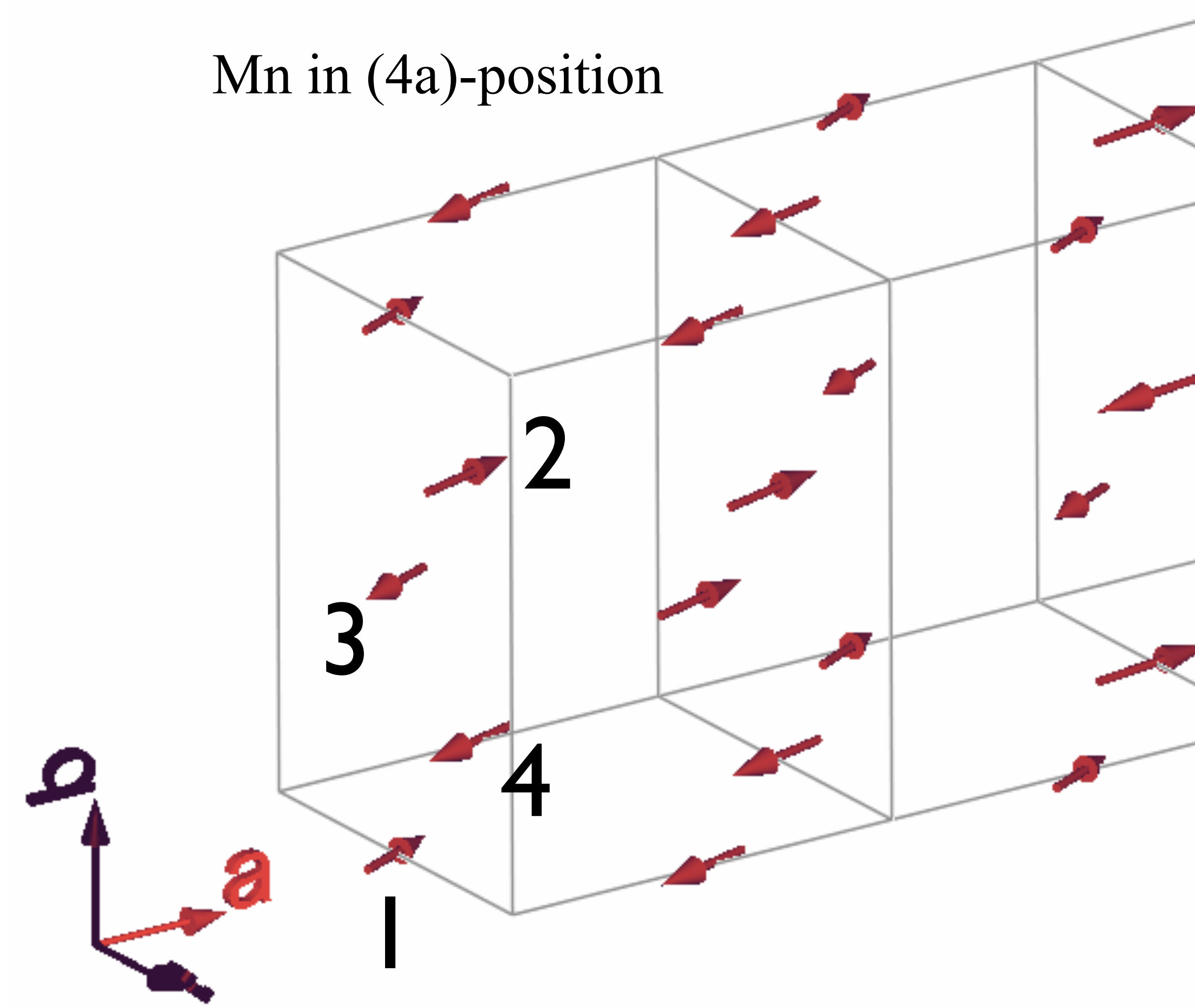
Constructing normal modes of magnetic structure from irreps

$TmMnO_3$

Space Group *G: Pnma,* no.62
propagation vector k=[μ,0,0] SM point of BZ

↓

has 4 1D irreducible representations



symmetry irreps | linear space spanned by Mn spins

$TmMnO_3$. Classifying possible magnetic structures basis functions $S_{\tau 1}$, $S_{\tau 2}$, $S_{\tau 3}$, ...

Pnma, k=[-0.45,0,0]
Mn in (4a)-position in -1 → 12D magnetic representation

	$0,0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,0$
Mn-position	1	2	3	4

Magnetic representation is reduced to four one-dimensional irreps

$$3\tau_1 \oplus 3\tau_2 \oplus 3\tau_3 \oplus 3\tau 4$$

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	E	2_x	m_y	m_z
	g_1	g_2	g_3	g_4
τ_1	1	a	1	a
τ_2	1	a	-1	$-a$
τ_3	1	$-a$	1	$-a$
τ_4	1	$-a$	-1	a

$$a = e^{\pi i k_x}$$

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$$S'_{\tau 3} = +1\mathbf{e}_{1x} - a^*\mathbf{e}_{2x} - 1\mathbf{e}_{3x} + a^*\mathbf{e}_{4x}$$
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	g_1	g_2	g_3	g_4
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τ_3	1	$-a$	1	$-a$
τ_4	1	$-a$	-1	a

$$a = e^{\pi i k_x}$$

For irreducible representation τ3 the spins of all four atoms are specified by 3 *complex* variables.

$$C_1 S'_{\tau 3} + C_2 S''_{\tau 3} + C_3 S'''_{\tau 3}$$

Refinement of the data for τ3

$$\mathbf{S}(\mathbf{r}) = \frac{1}{2}(C_1 S'_{\tau 3} + C_2 S''_{\tau 3} + C_3 S'''_{\tau 3}) e^{2\pi i \mathbf{k}\boldsymbol{r}} + c.c.$$

k=[-0.45,0,0]

$$S'_{\tau 3} = +1\mathbf{e}_{1x} - a^*\mathbf{e}_{2x} - 1\mathbf{e}_{3x} + a^*\mathbf{e}_{4x}$$

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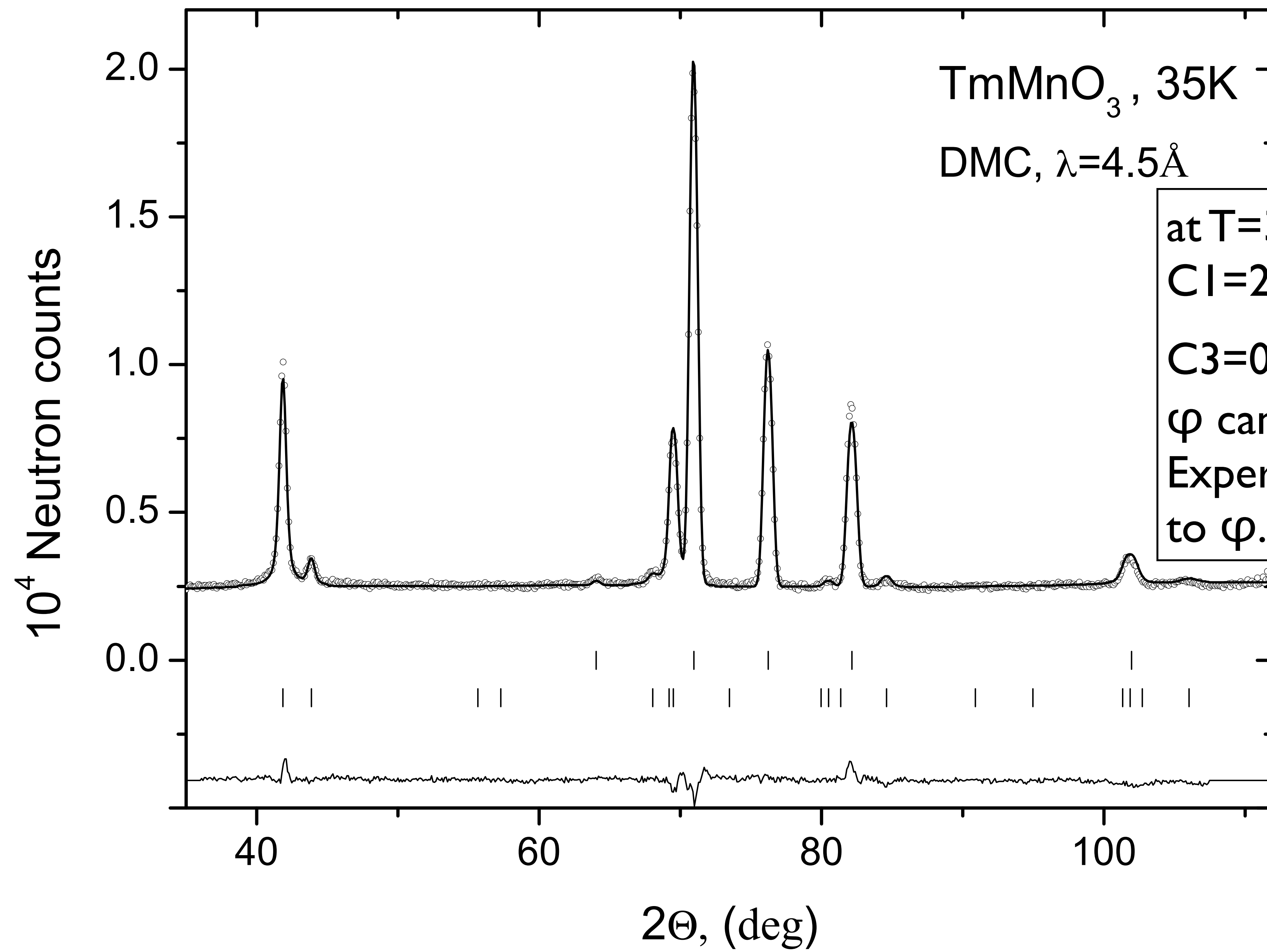
Refinement of the data for τ_3

$$\mathbf{S}(\mathbf{r}) = \frac{1}{2}(C_1 S'_{\tau 3} + C_2 S''_{\tau 3} + C_3 S'''_{\tau 3}) e^{2\pi i \mathbf{k}\boldsymbol{r}} + c.c.$$



at T=35K
C1=2.11(1)μ_B, C2=0,
C3=0.67(2) $e^{i\varphi}$ μ_B
φ can be fixed to any value.
Experiment data are insensitive to φ.

Visualization of the magnetic structure

a cycloid structure propagating along x-direction

$$\mathbf{S}(\mathbf{r}) = Re\left[(C_1 S'_{\tau 3} + |C_3| \exp(i\varphi) S'''_{\tau 3}) \exp(2\pi i \mathbf{k}\boldsymbol{r})\right]$$

$$S'_{\tau 3} = +1\mathbf{e}_{1x} - a^*\mathbf{e}_{2x} - 1\mathbf{e}_{3x} + a^*\mathbf{e}_{4x}$$

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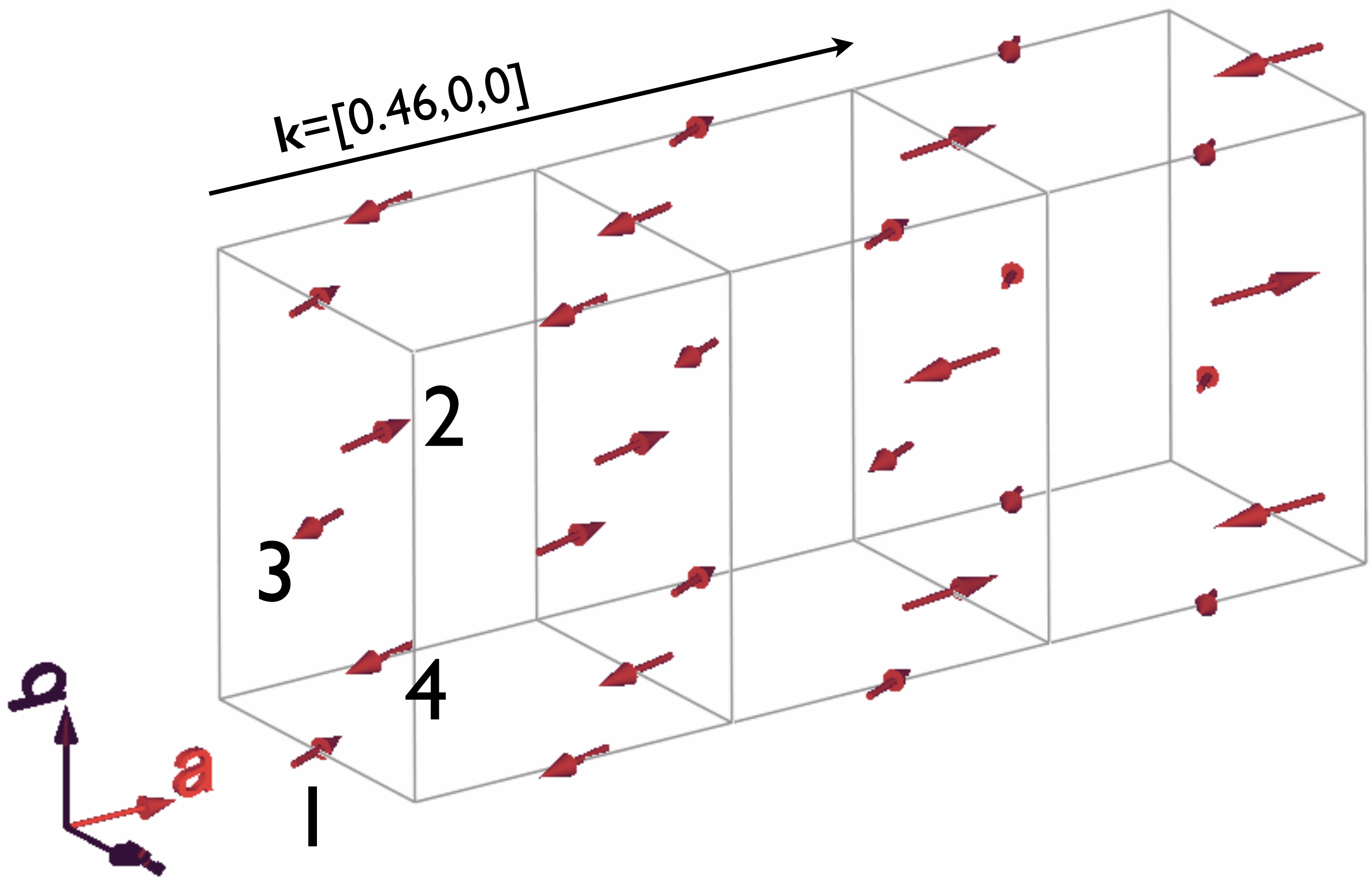

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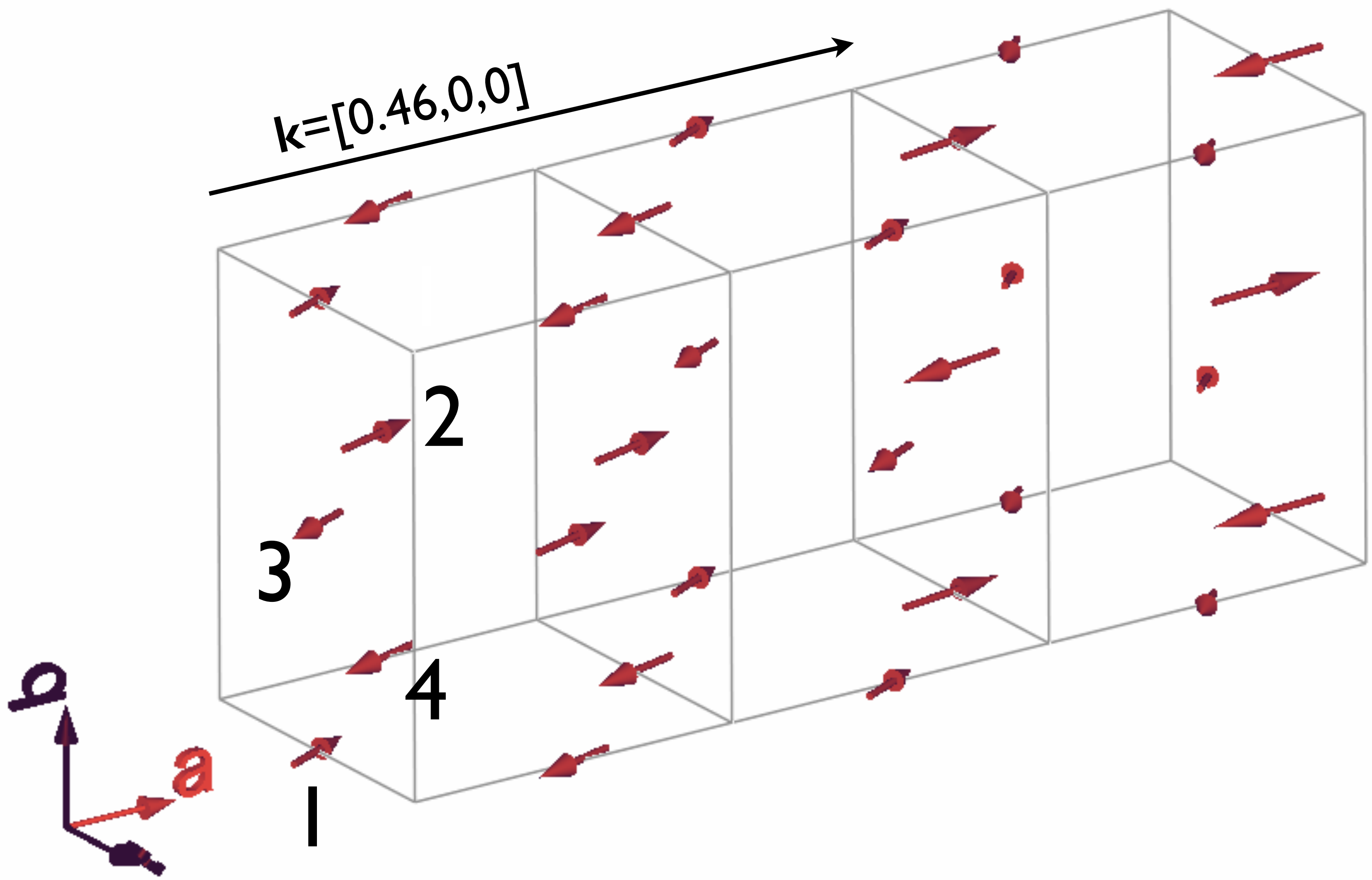
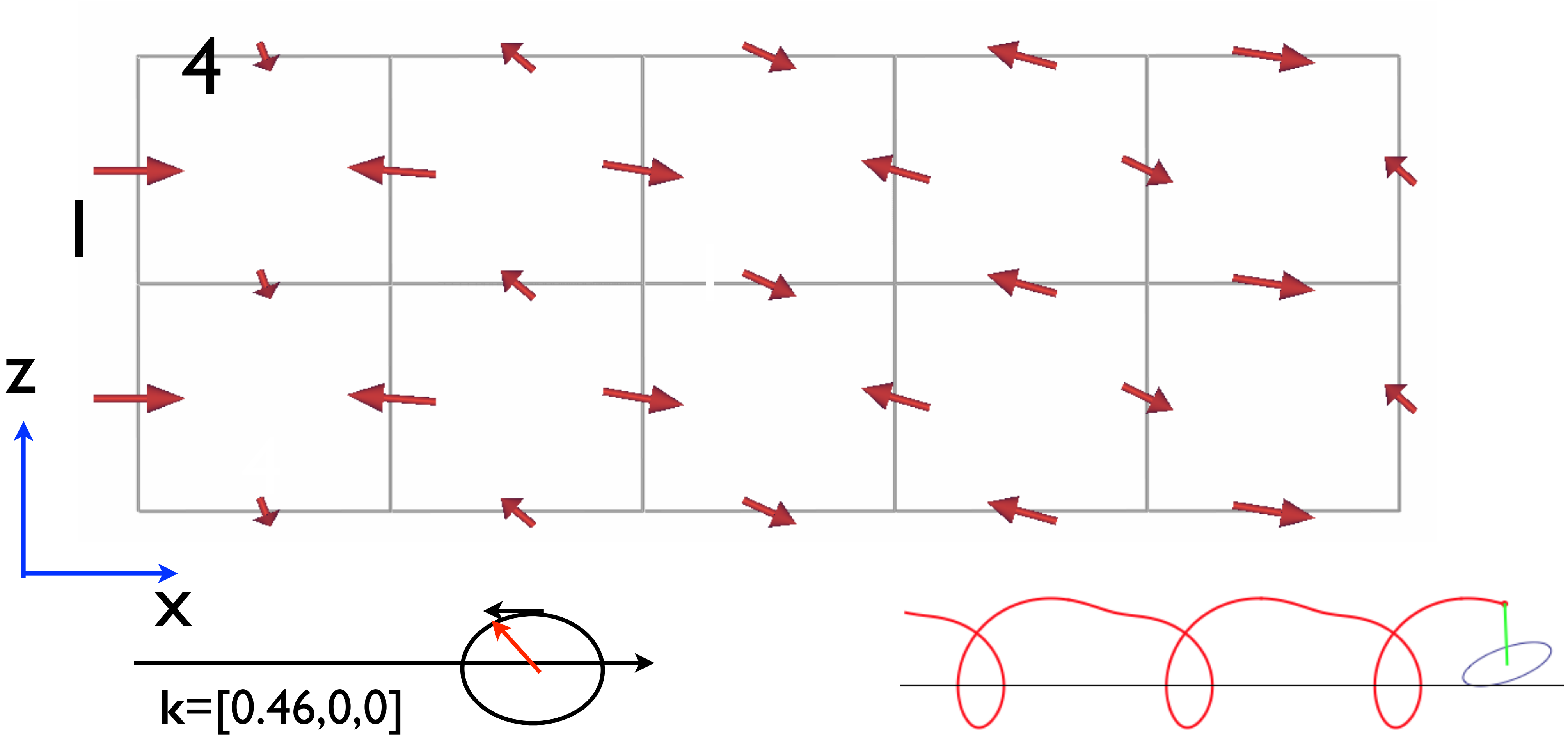
Propagation of the spin, e.g. for atom no. 1

$$\mathbf{S}_1(x) = C_1 \cos(kx)\mathbf{e}_x + |C_3| \cos(kx + \varphi)\mathbf{e}_z$$



Visualization of the magnetic structure: xz-projection

for arbitrary φ cycloid:
both direction and size of S_1 are changed



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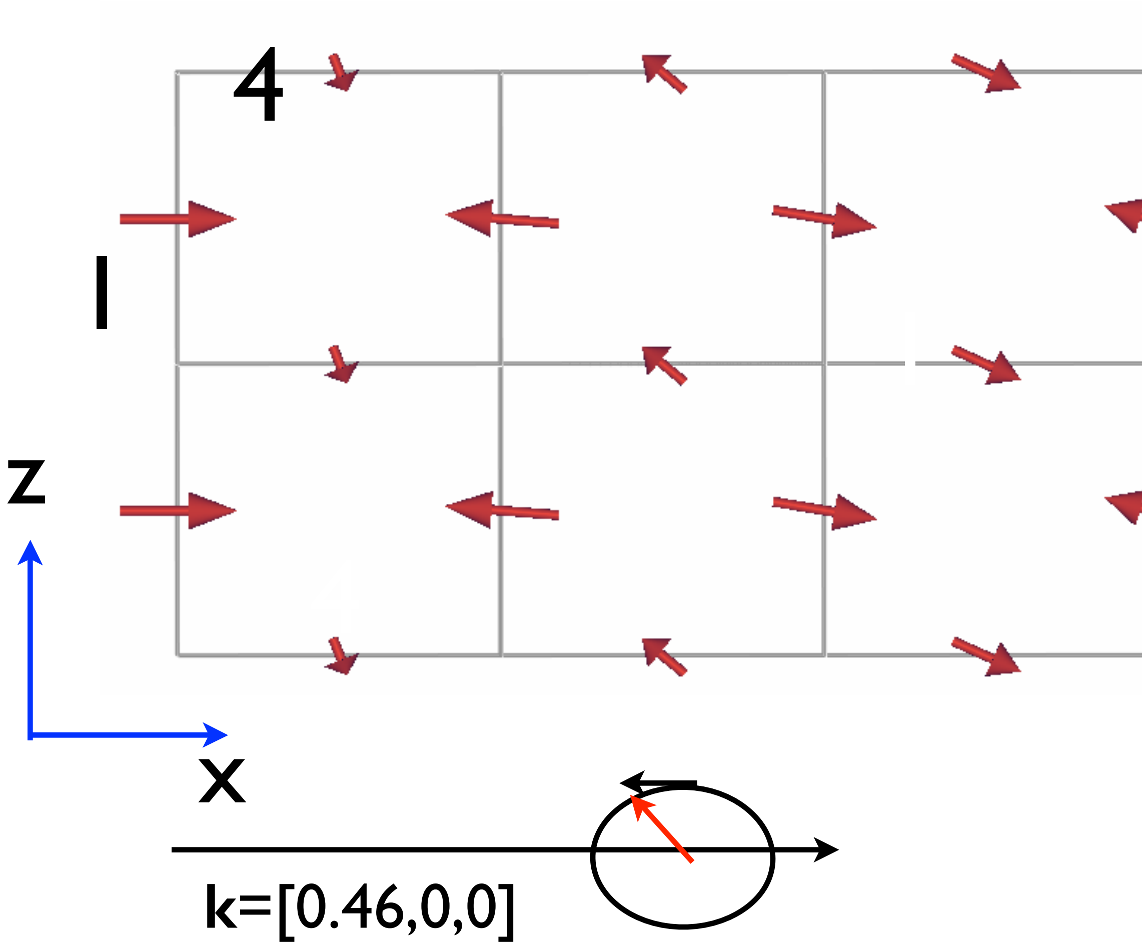
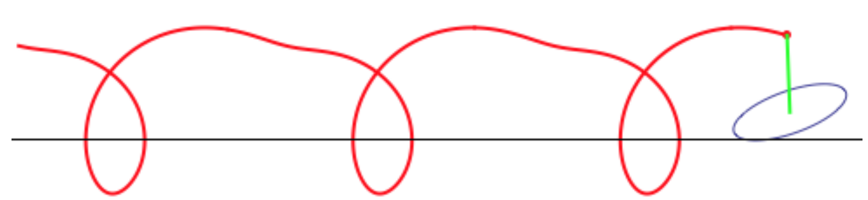
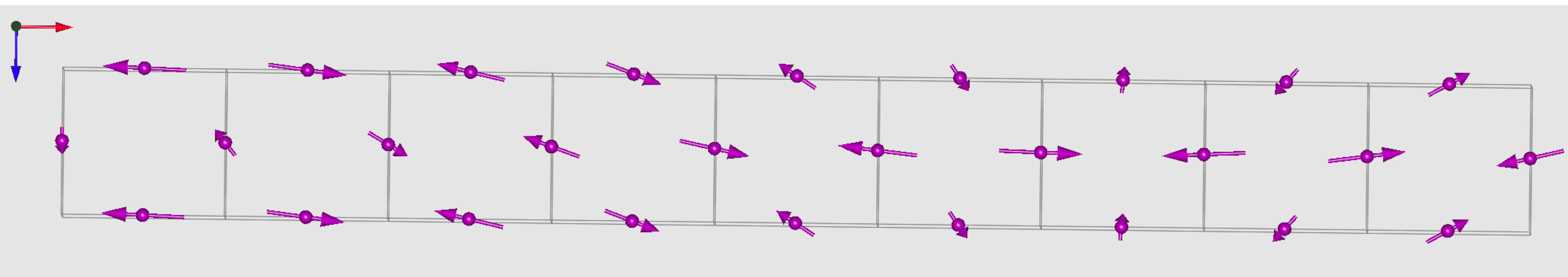
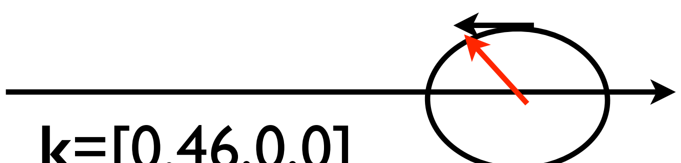




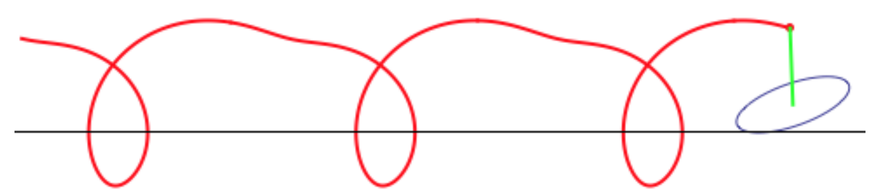
Visualization of the magnetic structure: xz-projection

for arbitrary φ:
both direction and size of S_l are changed





k=[0.46,0,0]

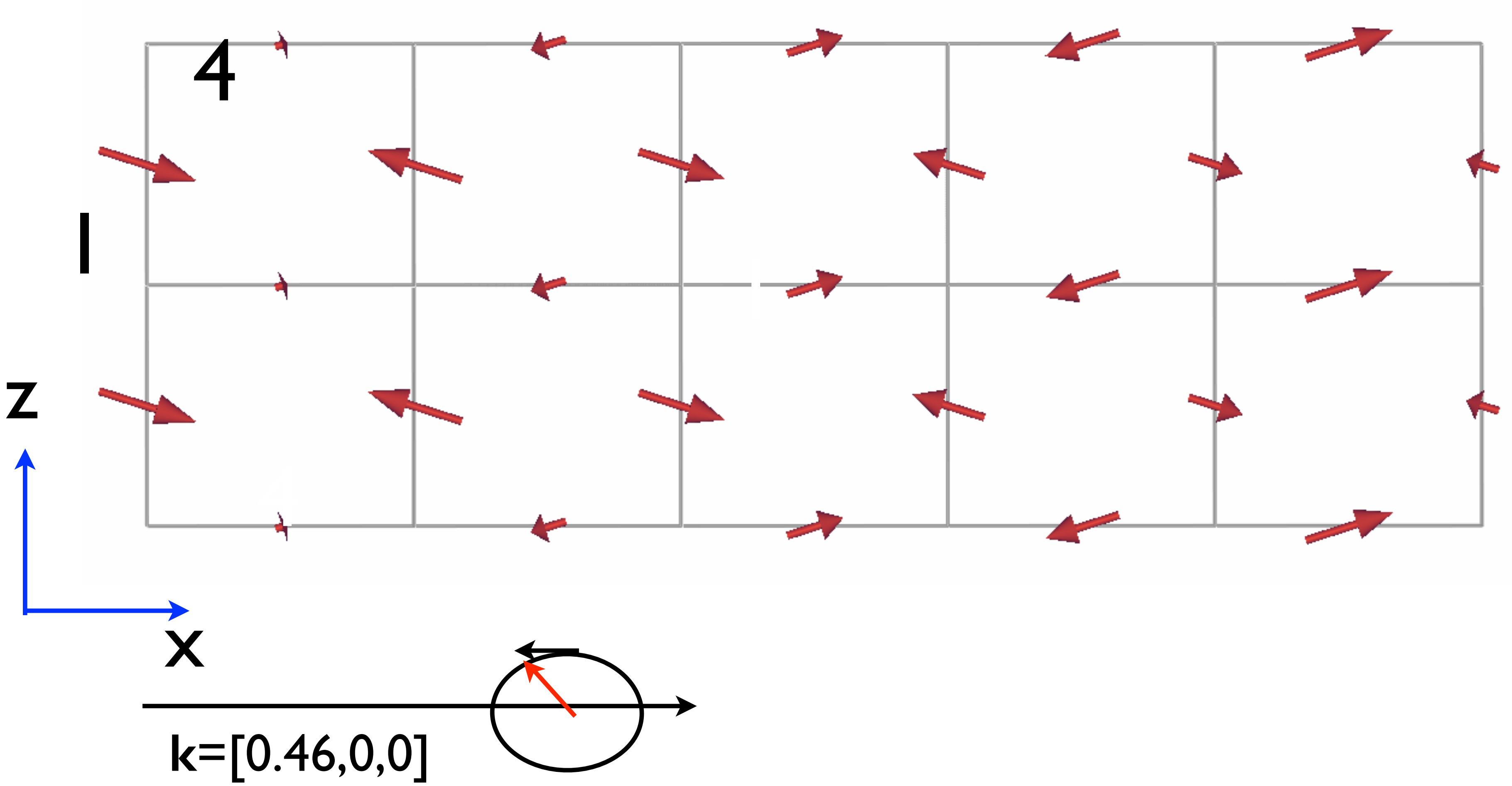


Visualization of the magnetic structure: xz-projection. Inversion.

for φ=0:
only the size of S_1 are changed:
Incommensurate amplitude-modulated order

Propagation of the spin, e.g. for atom no. 1

$$\mathbf{S}_1(x) = (C_1\mathbf{e}_x + |C_3|\mathbf{e}_z)\cos(kx)$$



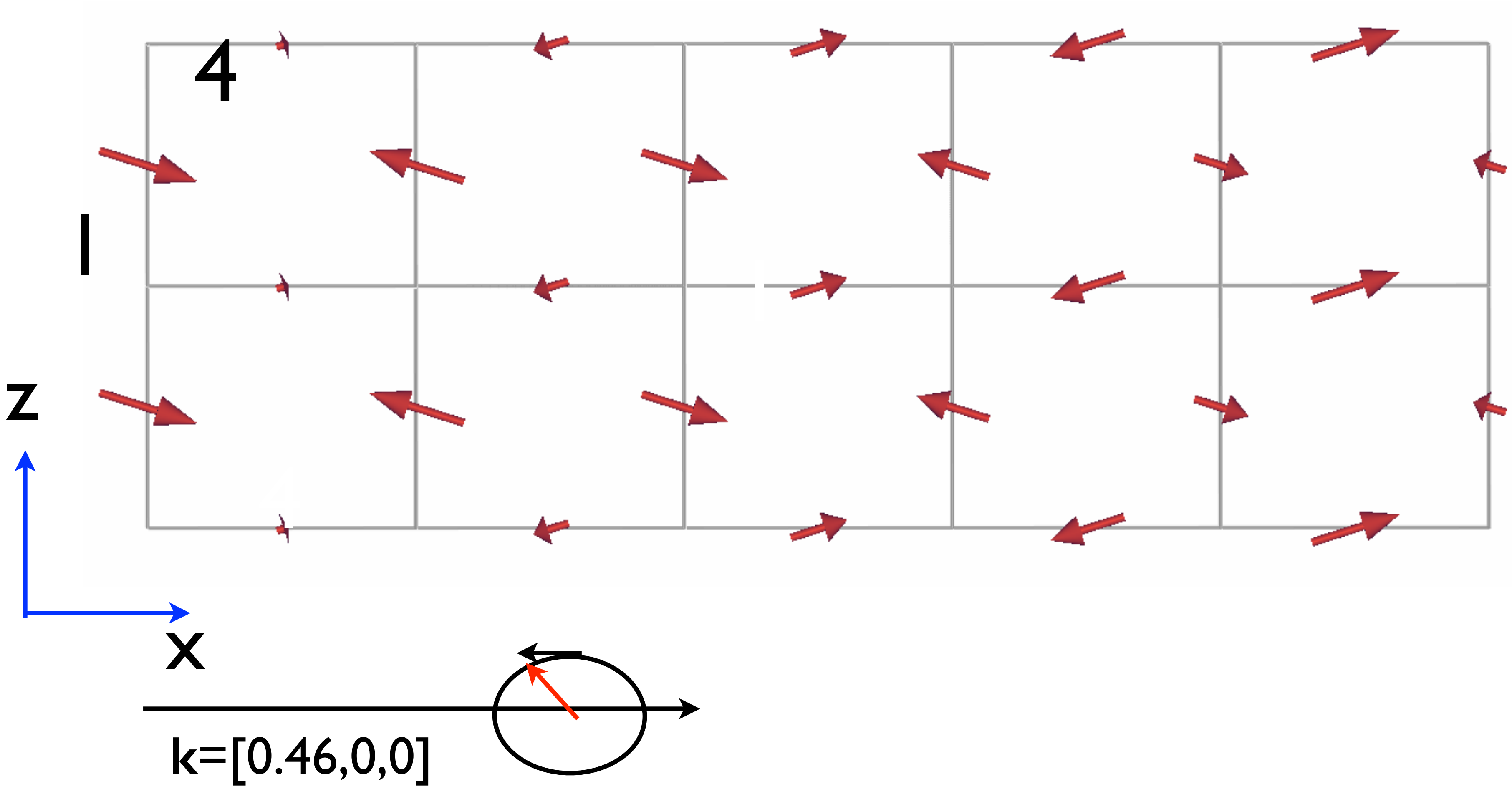
Visualization of the magnetic structure: xz-projection. Inversion.

for φ=0:
only the size of S_1 are changed:
Incommensurate amplitude-modulated order

requirement to preserve inversion symmetry $I(C_3)=C_3^*$

Propagation of the spin, e.g. for atom no. 1

$$\mathbf{S}_1(x) = (C_1\mathbf{e}_x + |C_3|\mathbf{e}_z)\cos(kx)$$



Constraints on basis functions with irreps in k-vector group

vs.

Magnetic superspace group

Magnetic group vs constraints on basis functions. Case 1: φ≠0

$$\mathbf{S}_1(x) = C_1\cos(kx)\mathbf{e}_x + |C_3|\cos(kx+\varphi)\mathbf{e}_z$$

φ≠0: Inversion symmetry is lost

Magnetic group vs constraints on basis functions. Case 1: φ≠0

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Firstly we go to the isotropy space subgroup

Pnma —> propagation vector group $P2_1ma\ (Pmc2_1, 26)$

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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,

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Firstly we go to the isotropy space subgroup

Pnma —> propagation vector group $P2_1ma$ ($Pmc2_1$, 26)

ISODISTORT: distortion.

Space Group: 62 **Pnma** D2h-16, Lattice parameters: a=5.80520, b=7.31070, c=5.23350, alpha=90.00000, beta=90.00000, gamma=90.00000

MN 4b (0,0,1/2), O1 4c (x,1/4,z), x=0.45960 , z=0.11820, O2 8d (x,y,z), x=0.33010 , y=0.05490 , z=-0.30160, Tm 4c (x,1/4,z), x=0.08460 , z=-0.01860

Irrep matrices: 2011 version for all k points

Include displacive distortions

k point: GM, k19 (0,0,0)

IR: GM3-, k19t6

P1 (a) 26 Pmc2_1, basis={(0,1,0),(0,0,1),(1,0,0)}, origin=(0,1/4,1/4), s=1, i=2, k-active= (0,0,0)

Lattice parameters of undistorted supercell: a=7.31070, b=5.23350, c=5.80520, alpha=90.00000, beta=90.00000, gamma=90.00000

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Magnetic group vs. k-vector irrep description

Magnetic group vs. k-vector irrep description

Secondly, we go to the 3D+1 magnetic group

ISODISTORT: distortion

Space Group: 26 **Pmc2_1** C2v-2, Lattice parameters: a=7.31070, b=5.23350, c=5.80520, alpha=90.00000, beta=90.00000, gamma=90.00000
MN_1 4c (x,y,z), x=-0.25000 , y=0.25000 , z=0.00000, Tm_2 2b (1/2,y,z), y=-0.23140 , z=-0.08460
IInclude strain, magnetic MN_1 Tm_1 Tm_2 distortions
k point: LD (0,0,g), g=0.46000 (1 incommensurate modulation)
IR: mLD3LE3
P1P1 (a,b) 26.1 Pmc2_11'(00g)000s, basis={(1,0,0,0),(0,1,0,0),(0,0,1,1),(0,0,0,1)}, origin=(0,0,0,0)

Magnetic group vs. k-vector irrep description

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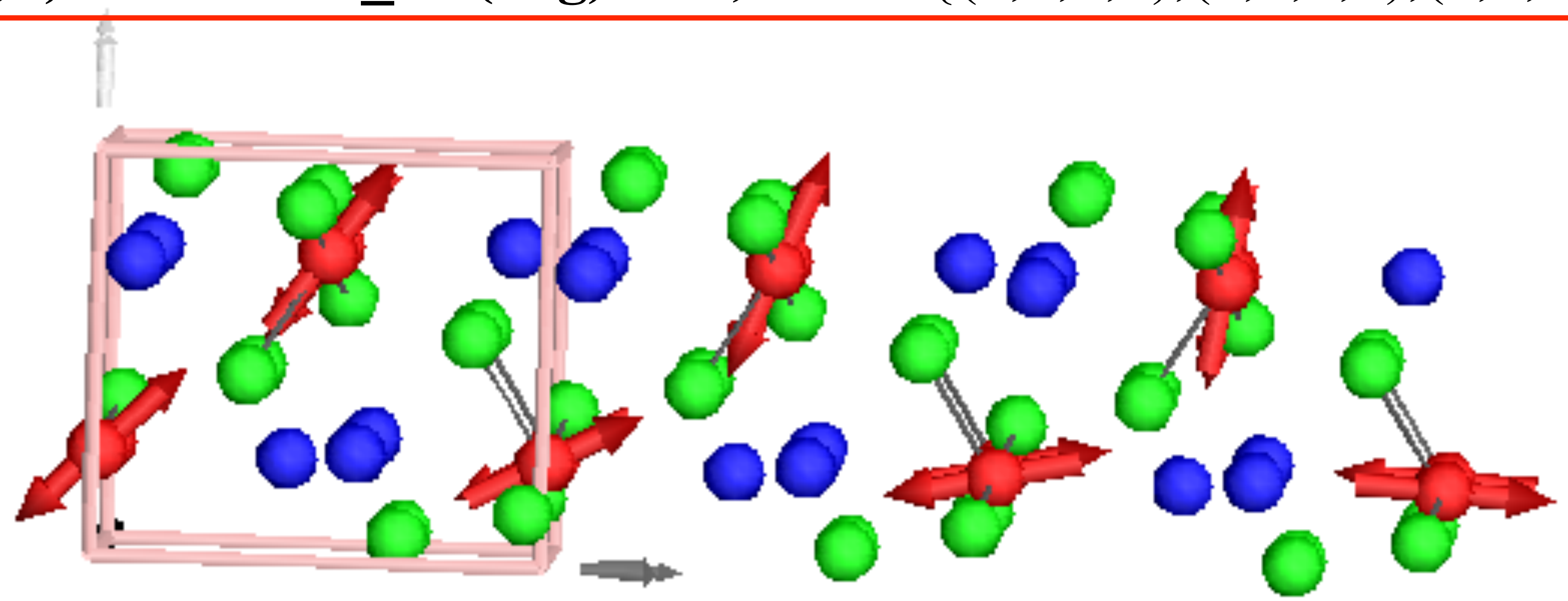

Magnetic group vs. k-vector irrep description

Secondly, we go to the 3D+1 magnetic group

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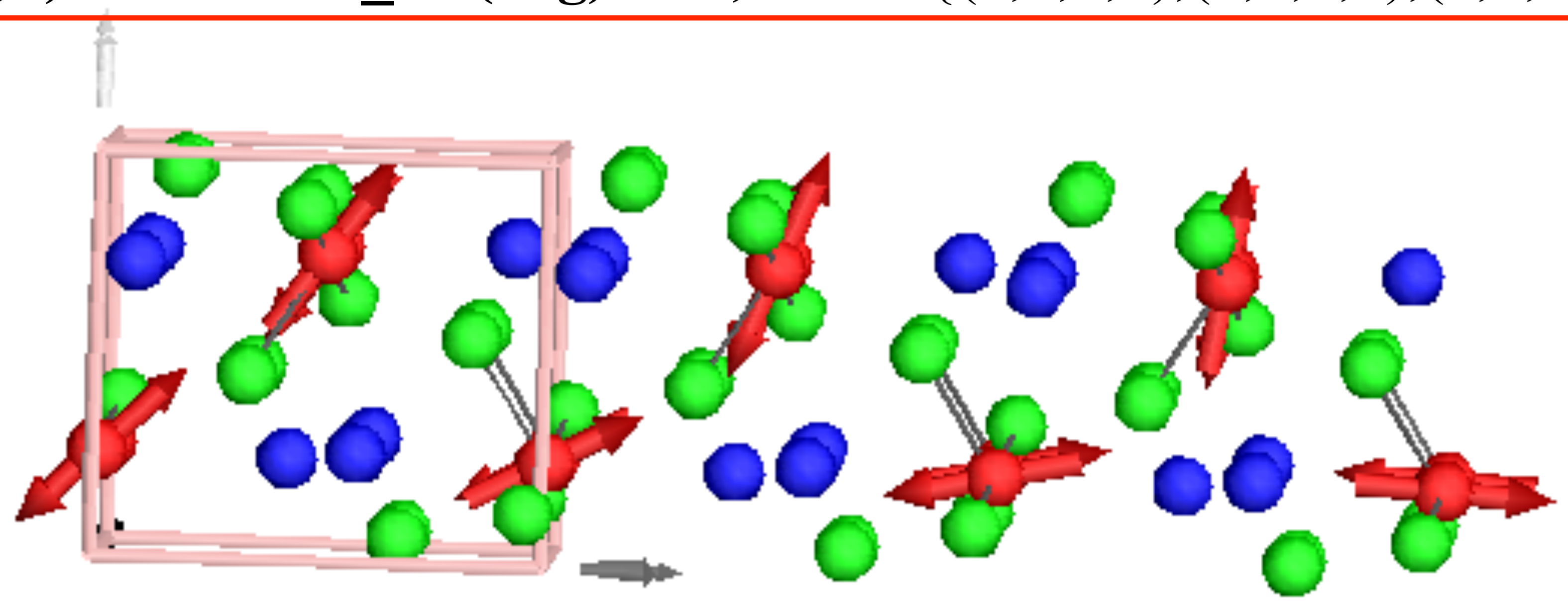
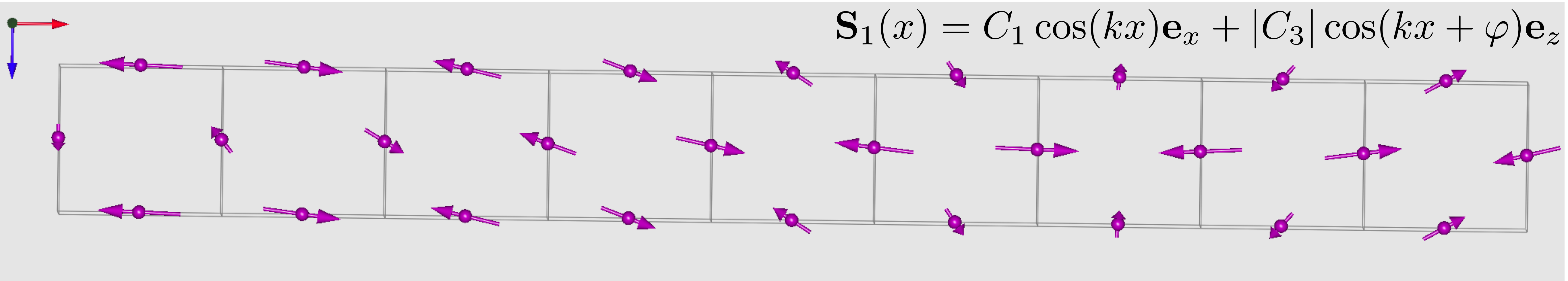
P1P1 (a,b) 26.1 Pmc2_11'(00g)000s, basis={(1,0,0,0),(0,1,0,0),(0,0,1,1),(0,0,0,1)}, origin=(0,0,0,0)



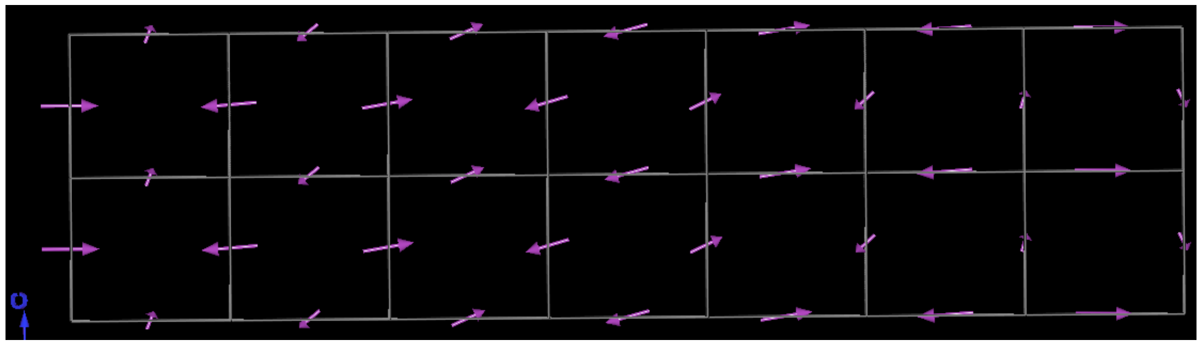


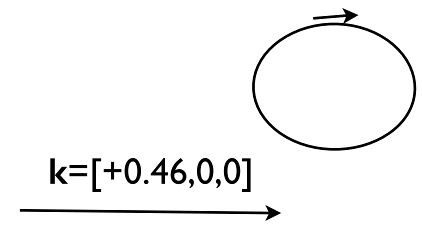
$$\mathbf{S}_1(x) = C_1 \cos(kx)\mathbf{e}_x + |C_3| \cos(kx+\varphi)\mathbf{e}_z$$

"Chirality"

$$\mathbf{S}(\mathbf{r}) = Re\left[(C_1 S'_{\tau 3} + |C_3| \exp(i\varphi) S'''_{\tau 3}) \exp(2\pi i \mathbf{k}\boldsymbol{r})\right]$$

a cycloid structure propagating along x-direction





$$\frac{d\sigma}{d\Omega} \propto (\mathbf{F}(\mathbf{q}) \cdot \mathbf{F}^*(\mathbf{q}) + i\mathbf{P} \cdot [\mathbf{F}(\mathbf{q}) \times \mathbf{F}^*(\mathbf{q})]) \cdot \delta(\mathbf{H} \pm \mathbf{k} - \mathbf{q})$$

polarised neutron (chiral) term.

$$S'_{\tau 3} = (+1\mathbf{e}_{1x} - a^*\mathbf{e}_{2x} - 1\mathbf{e}_{3x} + a^*\mathbf{e}_{4x})$$

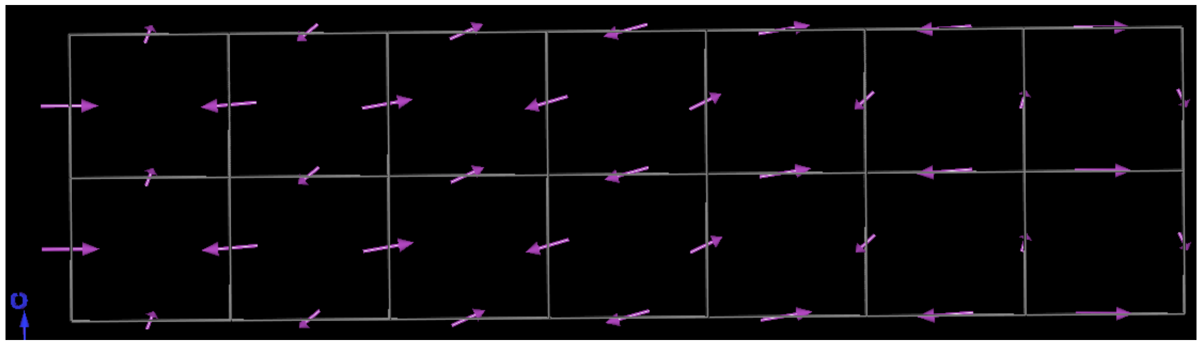
$$S''_{\tau 3} = (+1\mathbf{e}_{1z} + a^*\mathbf{e}_{2z} - 1\mathbf{e}_{3z} - a^*\mathbf{e}_{4z})$$

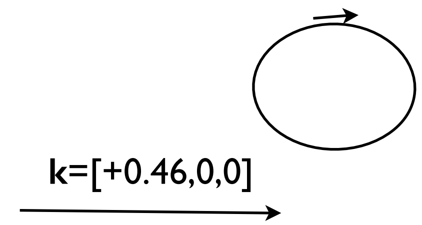
$$a = e^{\pi i k_x}$$

“Chirality”

$$\mathbf{S}(\mathbf{r}) = Re\left[(C_1 S'_{\tau 3} + |C_3| \exp(i\varphi) S'''_{\tau 3}) \exp(2\pi i \mathbf{k}\boldsymbol{r})\right]$$

a cycloid structure propagating along x-direction





$$\frac{d\sigma}{d\Omega} \propto (\mathbf{F}(\mathbf{q}) \cdot \mathbf{F}^*(\mathbf{q}) + i\mathbf{P} \cdot [\mathbf{F}(\mathbf{q}) \times \mathbf{F}^*(\mathbf{q})]) \cdot \delta(\mathbf{H} \pm \mathbf{k} - \mathbf{q})$$

polarised neutron (chiral) term. “+” —> “-“ @

“Chirality”

$$S'_{\tau 3} = (+1\mathbf{e}_{1x} - a^*\mathbf{e}_{2x} - 1\mathbf{e}_{3x} + a^*\mathbf{e}_{4x})$$

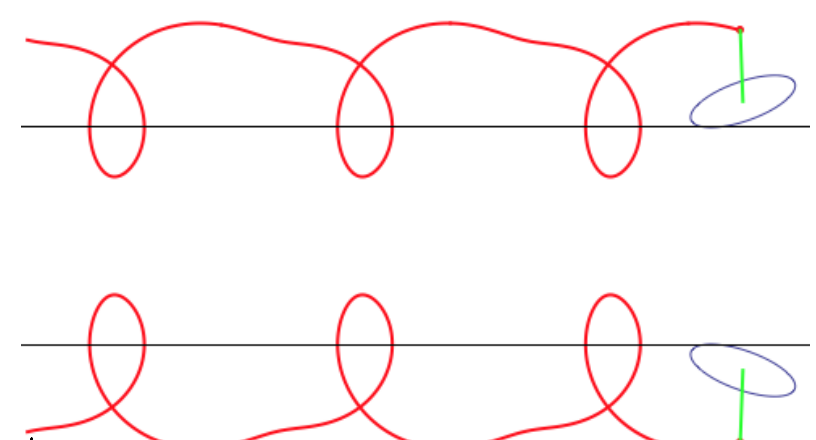
$$S''_{\tau 3} = (+1\mathbf{e}_{1z} + a^*\mathbf{e}_{2z} - 1\mathbf{e}_{3z} - a^*\mathbf{e}_{4z})$$

$\times(+i), \varphi = \pi/2$

$$a = e^{\pi i k_x}$$

or

$\times(-i), \varphi = -\pi/2$



+1

-1

Magnetic group vs. constraints on basis functions. Case 2: φ=0

$$\mathbf{S}_1(x) = C_1\cos(kx)\mathbf{e}_x + |C_3|\cos(kx+\varphi)\mathbf{e}_z$$

φ = 0: all symmetry elements of *Pnma*

Pnma —> group of propagation vector star *Pnma*

2D irreps of the star {k}

ISODISTORT: IR matrices

Irrep matrices: 2011 version for all k points

Space Group 62 Pnma

For each representative symmetry element ofthe parent space group, we display (1) the space-group operator, (2) the character of the IR of the little group of k if the operator is contained in the little group of k, and (3) the IR matrix.

IR mSM3

Star of k: (a,0,0), (-a,0,0), a=0.480

IR matrix of phase shift d: T(d)=(c, s /-s, c) where c=cos(2*pi*d), s=sin(2*pi*d), k=(a, 0,0), a=0.480

(1)	(2)	(3)
1:(x1,x2,x3,x4;m1,m2,m3)	1	(1, 0 /0, 1)
2[100]:(x1+1/2,-x2+1/2,-x3+1/2,x4;m1,-m2,-m3)	-0.063-0.998i	(-1, 0 /0, -1)
2[010]:(-x1,x2+1/2,-x3,-x4;-m1,m2,-m3)		(1, 0 /0, -1)
2[001]:(-x1+1/2,-x2,x3+1/2,-x4;-m1,-m2,m3)		(-1, 0 /0, 1)
-1:(-x1,-x2,-x3,-x4;m1,m2,m3)		(1, 0 /0, -1)
-2[100]:(-x1+1/2,x2+1/2,x3+1/2,-x4;m1,-m2,-m3)		(-1, 0 /0, 1)
-2[010]:(x1,-x2+1/2,x3,x4;-m1,m2,-m3)	1	(1, 0 /0, 1)
-2[001]:(x1+1/2,x2,-x3+1/2,x4;-m1,-m2,m3)	-0.063-0.998i	(-1, 0 /0, -1)
1':(x1,x2,x3,x4;-m1,-m2,-m3)	-1	(-1, 0 /0, -1)
2'[100]:(x1+1/2,-x2+1/2,-x3+1/2,x4;-m1,m2,m3)	0.063+0.998i	(1, 0 /0, 1)
2'[010]:(-x1,x2+1/2,-x3,-x4;m1,-m2,m3)		(-1, 0 /0, 1)
2'[001]:(-x1+1/2,-x2,x3+1/2,-x4;m1,m2,-m3)		(1, 0 /0, -1)
-1':(-x1,-x2,-x3,-x4;-m1,-m2,-m3)		(-1, 0 /0, 1)
-2'[100]:(-x1+1/2,x2+1/2,x3+1/2,-x4;-m1,m2,m3)		(1, 0 /0, -1)
-2'[010]:(x1,-x2+1/2,x3,x4;m1,-m2,m3)	-1	(-1, 0 /0, -1)
-2'[001]:(x1+1/2,x2,-x3+1/2,x4;m1,m2,-m3)	0.063+0.998i	(1, 0 /0, 1)

2D irreps of the star {k}

ISODISTORT: IR matrices

Irrep matrices: 2011 version for all k points

Space Group 62 Pnma

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2[100]:(x1+1/2,-x2+1/2,-x3+1/2,x4;m1,-m2,-m3)	-0.063-0.998i	(-1, 0 /0, -1)
2[010]:(-x1,x2+1/2,-x3,-x4;-m1,m2,-m3)		(1, 0 /0, -1)
2[001]:(-x1+1/2,-x2,x3+1/2,-x4;-m1,-m2,m3)		(-1, 0 /0, 1)
-1:(-x1,-x2,-x3,-x4;m1,m2,m3)		(1, 0 /0, -1)
-2[100]:(-x1+1/2,x2+1/2,x3+1/2,-x4;m1,-m2,-m3)		(-1, 0 /0, 1)
-2[010]:(x1,-x2+1/2,x3,x4;-m1,m2,-m3)	1	(1, 0 /0, 1)
-2[001]:(x1+1/2,x2,-x3+1/2,x4;-m1,-m2,m3)	-0.063-0.998i	(-1, 0 /0, -1)
1':(x1,x2,x3,x4;-m1,-m2,-m3)	-1	(-1, 0 /0, -1)
2'[100]:(x1+1/2,-x2+1/2,-x3+1/2,x4;-m1,m2,m3)	0.063+0.998i	(1, 0 /0, 1)
2'[010]:(-x1,x2+1/2,-x3,-x4;m1,-m2,m3)		(-1, 0 /0, 1)
2'[001]:(-x1+1/2,-x2,x3+1/2,-x4;m1,m2,-m3)		(1, 0 /0, -1)
-1':(-x1,-x2,-x3,-x4;-m1,-m2,-m3)		(-1, 0 /0, 1)
-2'[100]:(-x1+1/2,x2+1/2,x3+1/2,-x4;-m1,m2,m3)		(1, 0 /0, -1)
-2'[010]:(x1,-x2+1/2,x3,x4;m1,-m2,m3)	-1	(-1, 0 /0, -1)
-2'[001]:(x1+1/2,x2,-x3+1/2,x4;m1,m2,-m3)	0.063+0.998i	(1, 0 /0, 1)

2D irreps of the star {k}

ISODISTORT: IR matrices

Irrep matrices: 2011 version for all k points

Space Group 62 Pnma

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IR matrices

(1)	(2)	(3)
1:(x1,x2,x3,x4;m1,m2,m3)	1	(1, 0 /0, 1)
2[100]:(x1+1/2,-x2+1/2,-x3+1/2,x4;m1,-m2,-m3)	-0.063-0.998i	(-1, 0 /0, -1)
2[010]:(-x1,x2+1/2,-x3,-x4;-m1,m2,-m3)		(1, 0 /0, -1)
2[001]:(-x1+1/2,-x2,x3+1/2,-x4;-m1,-m2,m3)		(-1, 0 /0, 1)
-1:(-x1,-x2,-x3,-x4;m1,m2,m3)		(1, 0 /0, -1)
-2[100]:(-x1+1/2,x2+1/2,x3+1/2,-x4;m1,-m2,-m3)		(-1, 0 /0, 1)
-2[010]:(x1,-x2+1/2,x3,x4;-m1,m2,-m3)	1	(1, 0 /0, 1)
-2[001]:(x1+1/2,x2,-x3+1/2,x4;-m1,-m2,m3)	-0.063-0.998i	(-1, 0 /0, -1)
1':(x1,x2,x3,x4;-m1,-m2,-m3)	-1	(-1, 0 /0, -1)
2'[100]:(x1+1/2,-x2+1/2,-x3+1/2,x4;-m1,m2,m3)	0.063+0.998i	(1, 0 /0, 1)
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-2'[100]:(-x1+1/2,x2+1/2,x3+1/2,-x4;-m1,m2,m3)		(1, 0 /0, -1)
-2'[010]:(x1,-x2+1/2,x3,x4;m1,-m2,m3)	-1	(-1, 0 /0, -1)
-2'[001]:(x1+1/2,x2,-x3+1/2,x4;m1,m2,-m3)	0.063+0.998i	(1, 0 /0, 1)

Case 2: φ=0. Superspace magnetic centrosymmetric group

ISODISTORT: distortion

Space Group: 62 **Pnma** D2h-16, Lattice parameters: a=5.80520, b=7.31070, c=5.23350, alpha=90.00000, beta=90.00000, gamma=90.00000
Default space-group preferences: monoclinic axes a(b)c, monoclinic cell choice 1, orthorhombic axes abc, origin choice 2, hexagonal axes, SSG standard setting
MN 4b (0,0,1/2), O1 4c (x,1/4,z), x=0.45960 , z=0.11820, O2 8d (x,y,z), x=0.33010 , y=0.05490 , z=-0.30160, Tm 4c (x,1/4,z), x=0.08460 , z=-0.01860
Irrep matrices: 2011 version for all k points
Include magnetic MN Tm distortions

k point: SM (a,0,0), a=0.48000 (1 incommensurate modulation)
IR: mSM3
P1Z (a,0) 62.5 **Pmcn1'(00g)000s, basis={(0,1,0,0),(0,0,1,0),(1,0,0,1),(0,0,0,1)}**, origin=(0,0,0,0), s=1, i=1

Case 2: φ=0. Superspace magnetic centrosymmetric group

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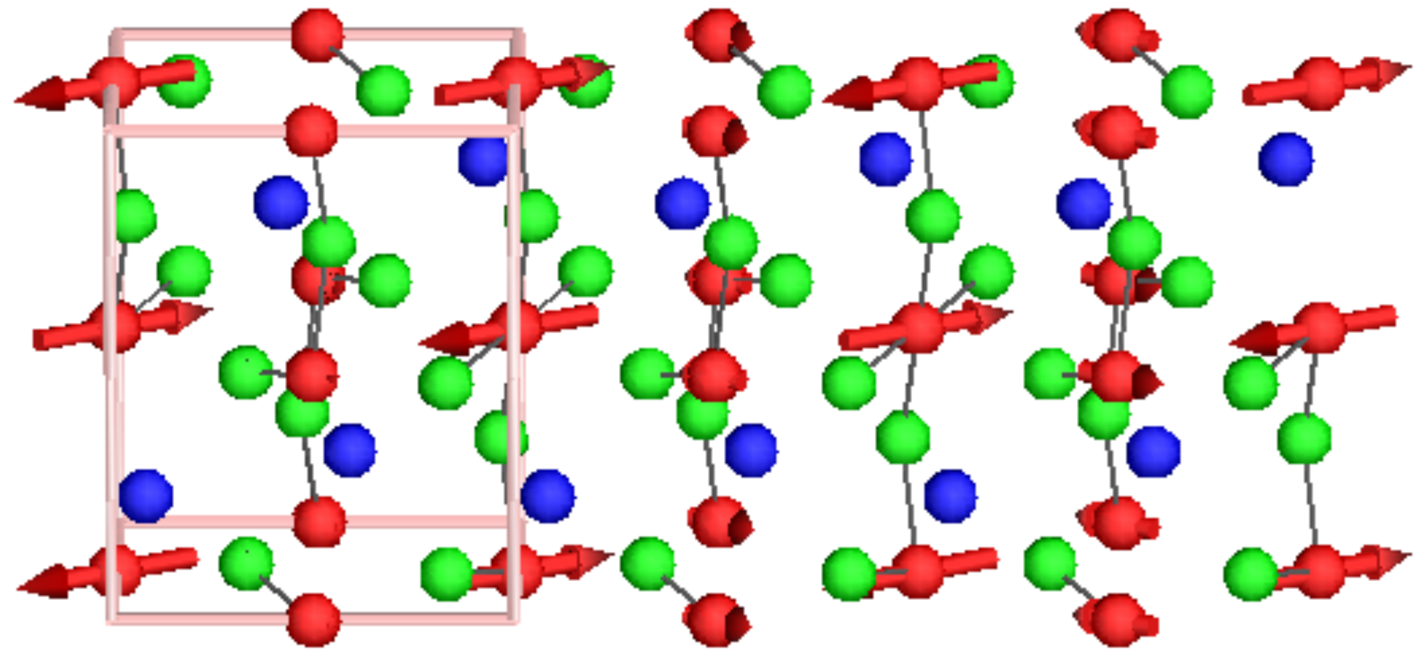
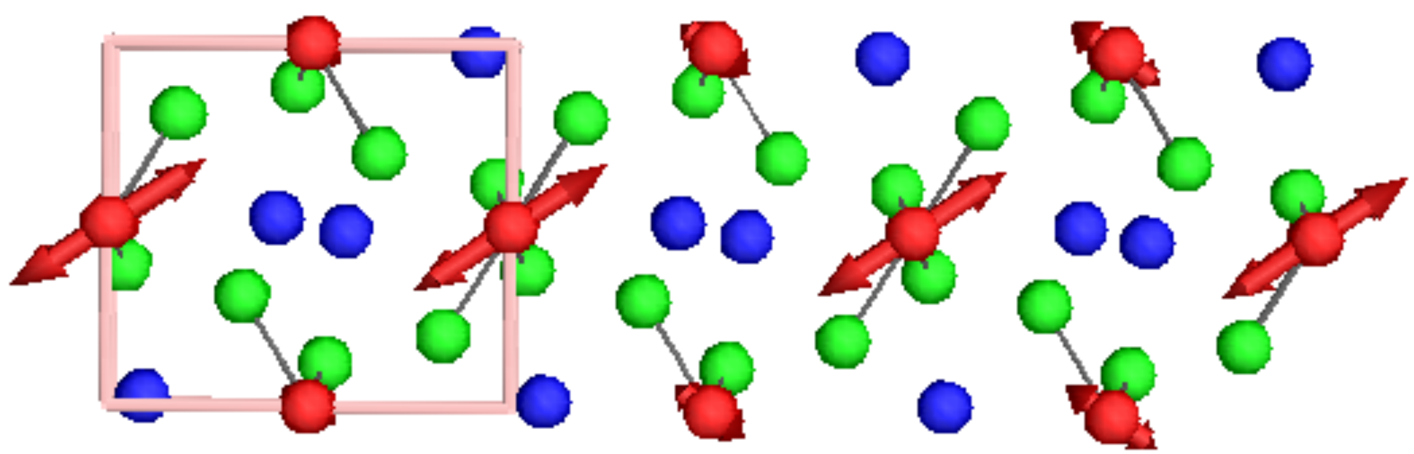
Pnma -> **bca** *Pmcn*

Vizualization of Pmcn1'(00g)000s by ISODISTORT

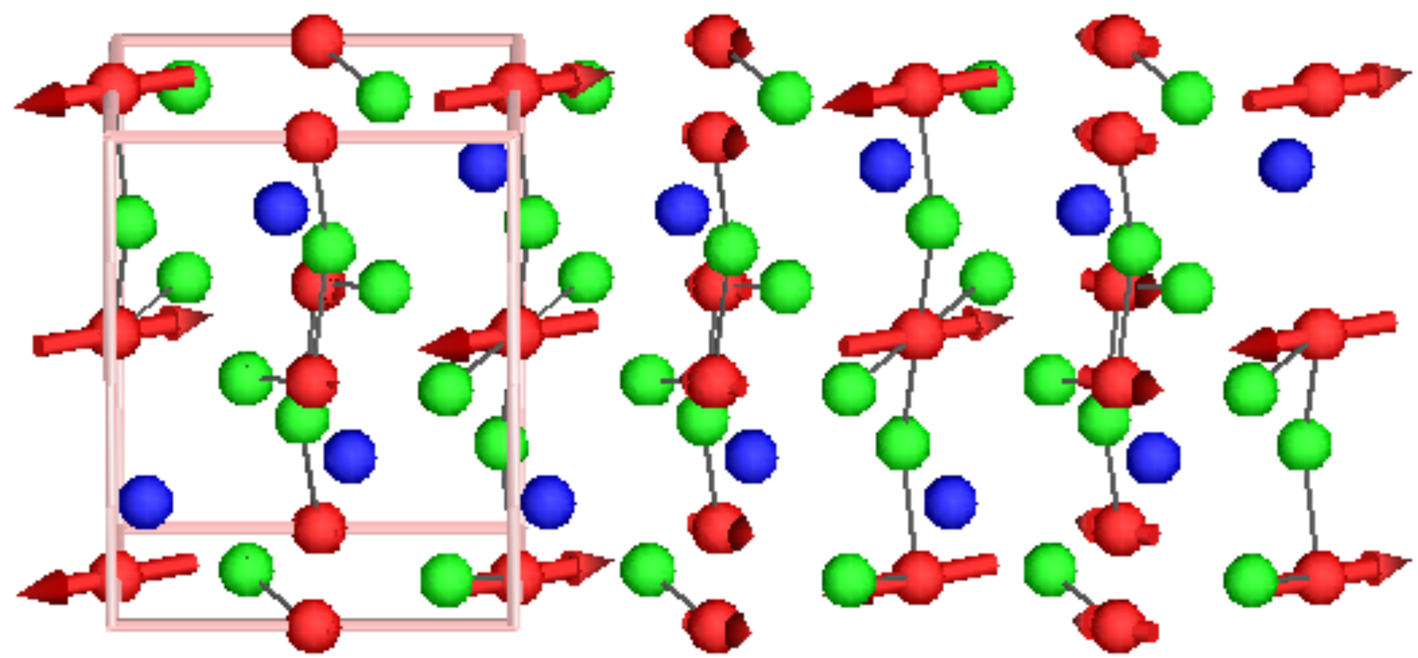


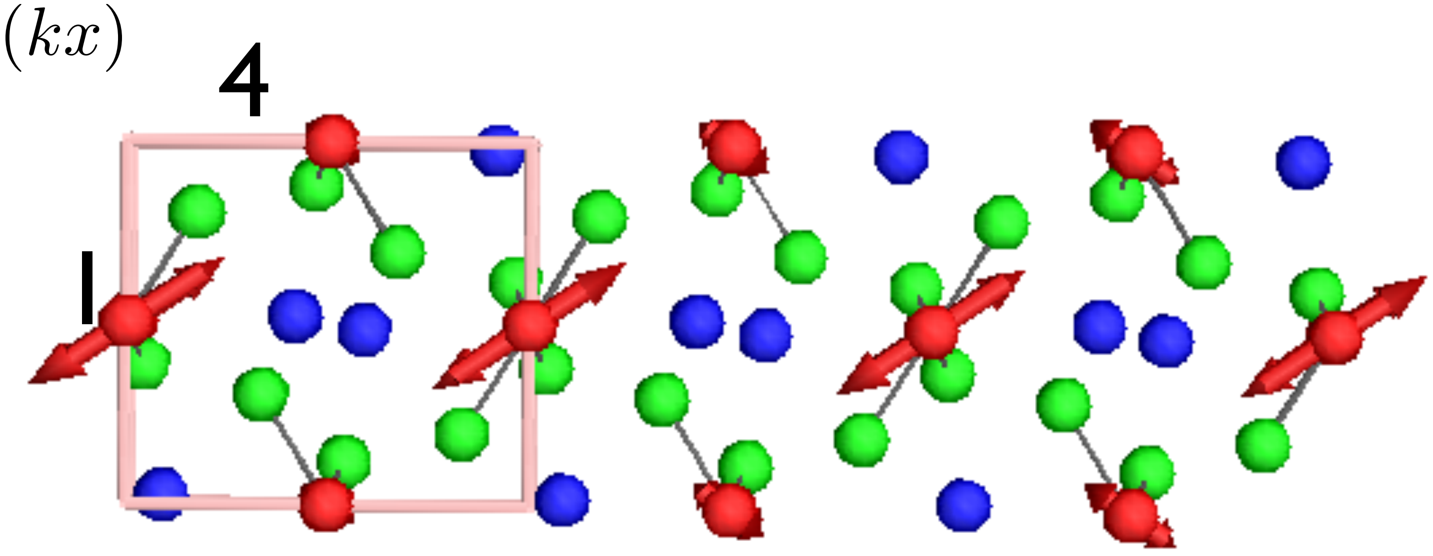


Vizualization of Pmcn1'(00g)000s by ISODISTORT

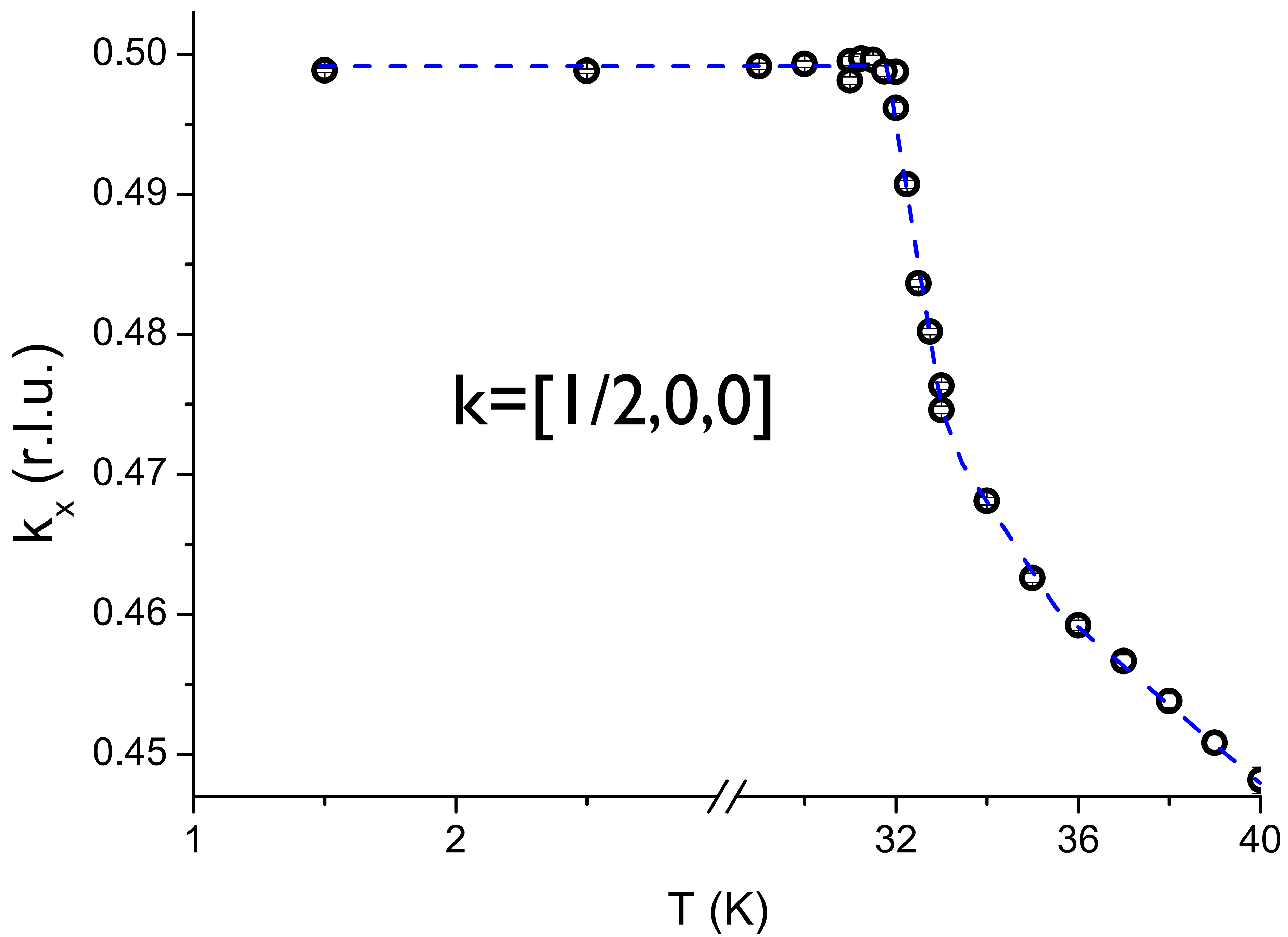
Recap: In the propagation vector approach:
requirement of φ=0.
only the sizes of spins are changed: Incommensurate amplitude-modulated order

$$\mathbf{S}_1(x) = (C_1\mathbf{e}_x + |C_3|\mathbf{e}_z)\cos(kx)$$





Magnetic structure of commensurate phase (ferroelectric)



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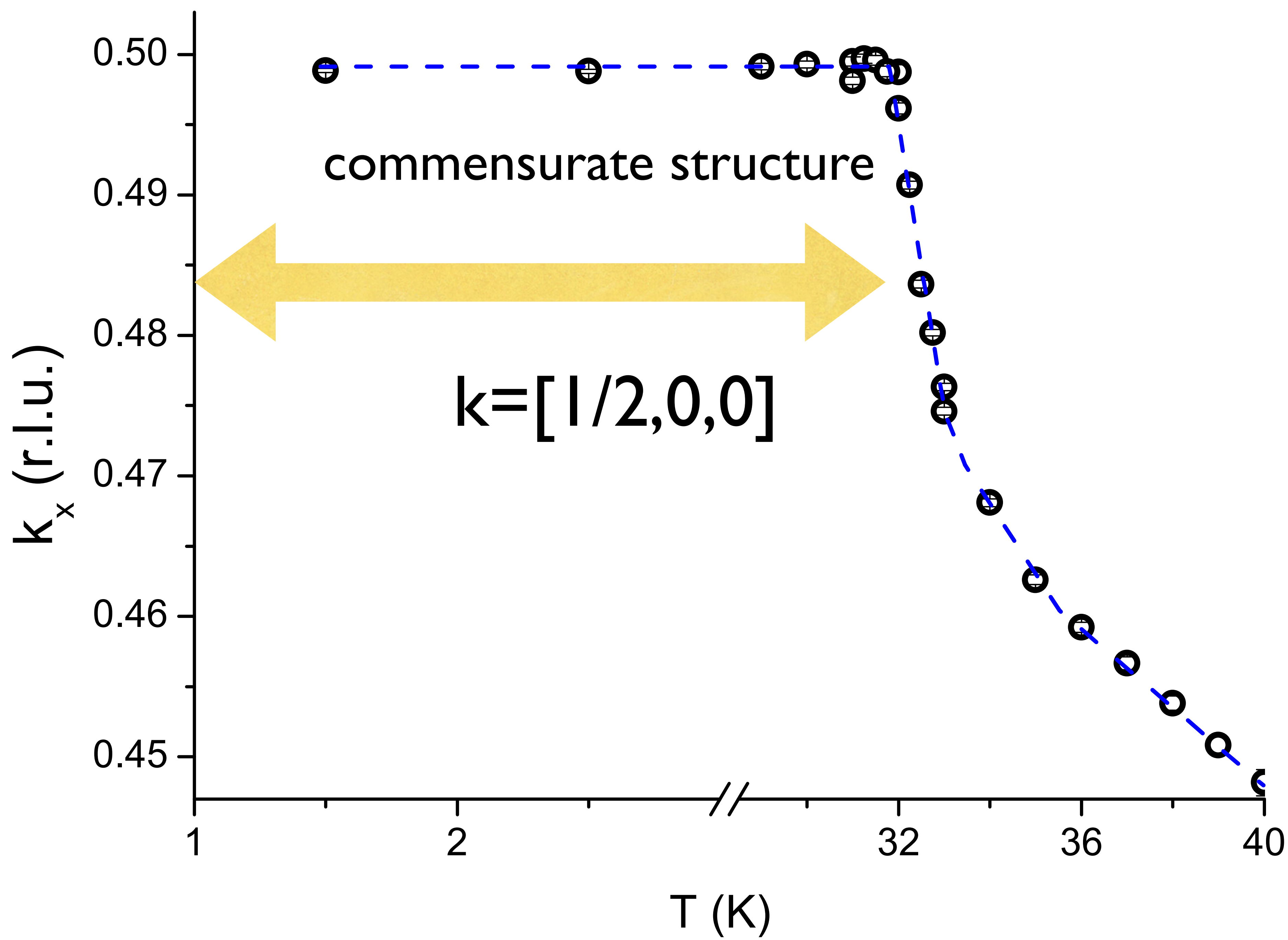
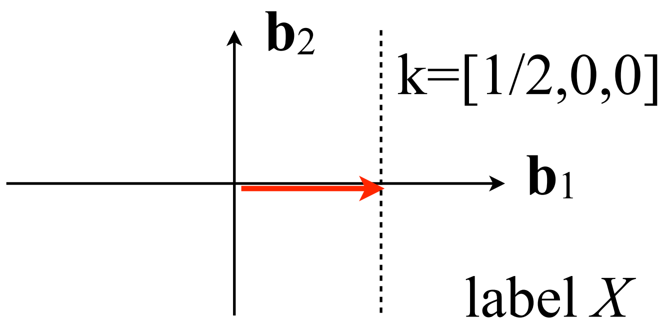


Commensurate phase (ferroelectric)

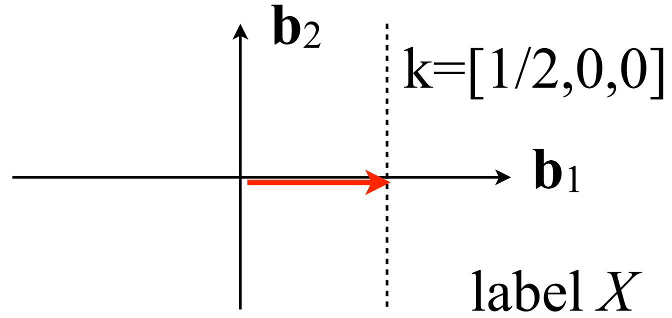
star {**k**}



$G_k = G$

Commensurate phase (ferroelectric)

star {**k**}



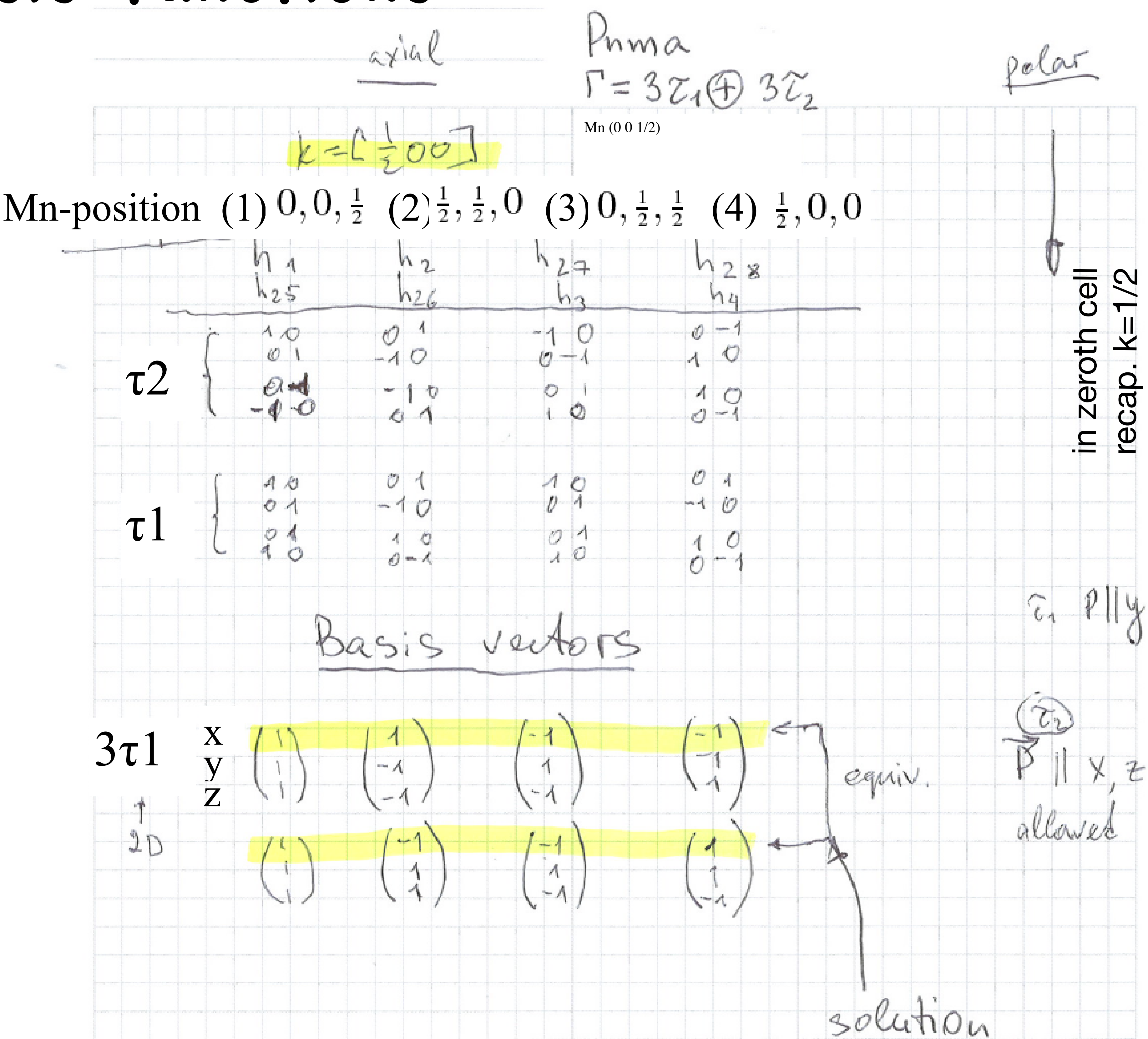
$G_k = G$

Pnma k=[1/2,0,0], k20, *X*
irreps: two 2D τ_1, τ_2

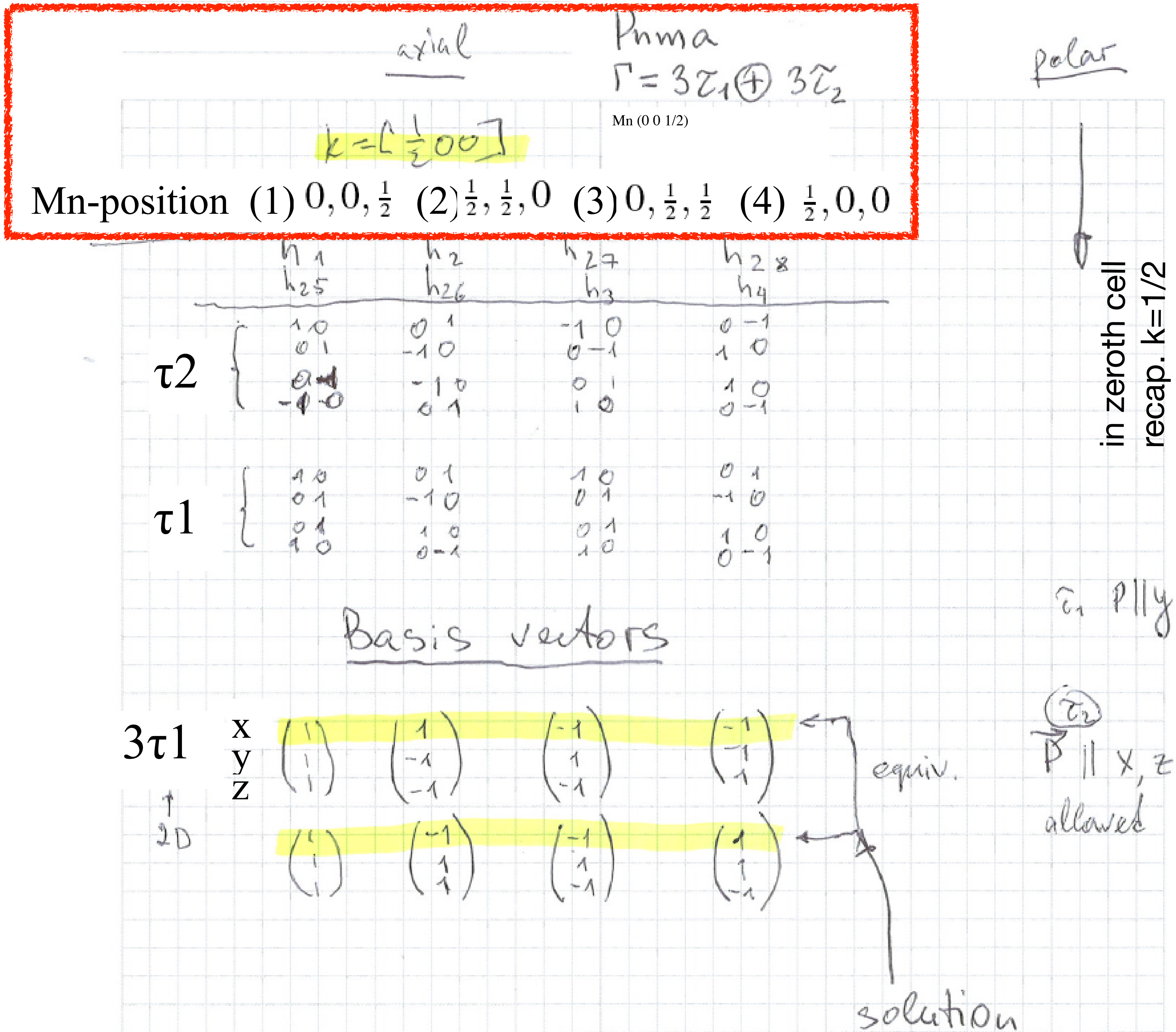
(LIR)

$d^{\mathbf{k}\nu}(g)$							
IT	2_x	2_y	2_z	$\bar{1}$	n_x	m_y	a_z
g Kovalev	/2	/3	/4	/25	/26	/27	/28
$\hat{\tau}1$	$\begin{pmatrix}1 & 0\\0 & -1\end{pmatrix}$	$\begin{pmatrix}0 & 1\\1 & 0\end{pmatrix}$	$\begin{pmatrix}0 & 1\\-1 & 0\end{pmatrix}$	$\begin{pmatrix}0 & 1\\1 & 0\end{pmatrix}$	$\begin{pmatrix}0 & 1\\-1 & 0\end{pmatrix}$	$\begin{pmatrix}1 & 0\\0 & 1\end{pmatrix}$	$\begin{pmatrix}1 & 0\\0 & -1\end{pmatrix}$
$\hat{\tau}2 = \hat{\tau}1 \times$	1	1	1	-1	-1	-1	-1

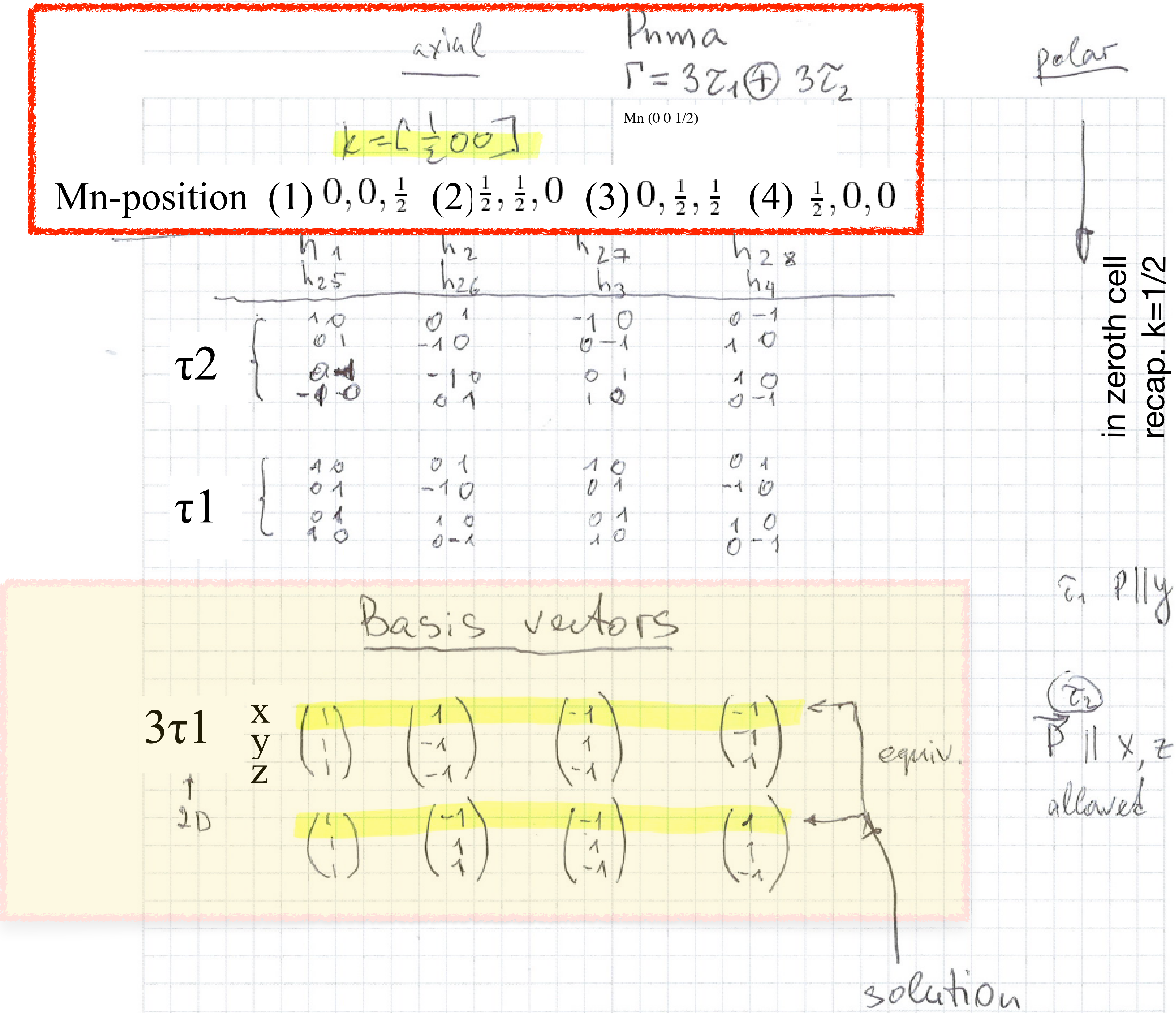
Classifying possible magnetic structures
basis functions



Classifying possible magnetic structures basis functions

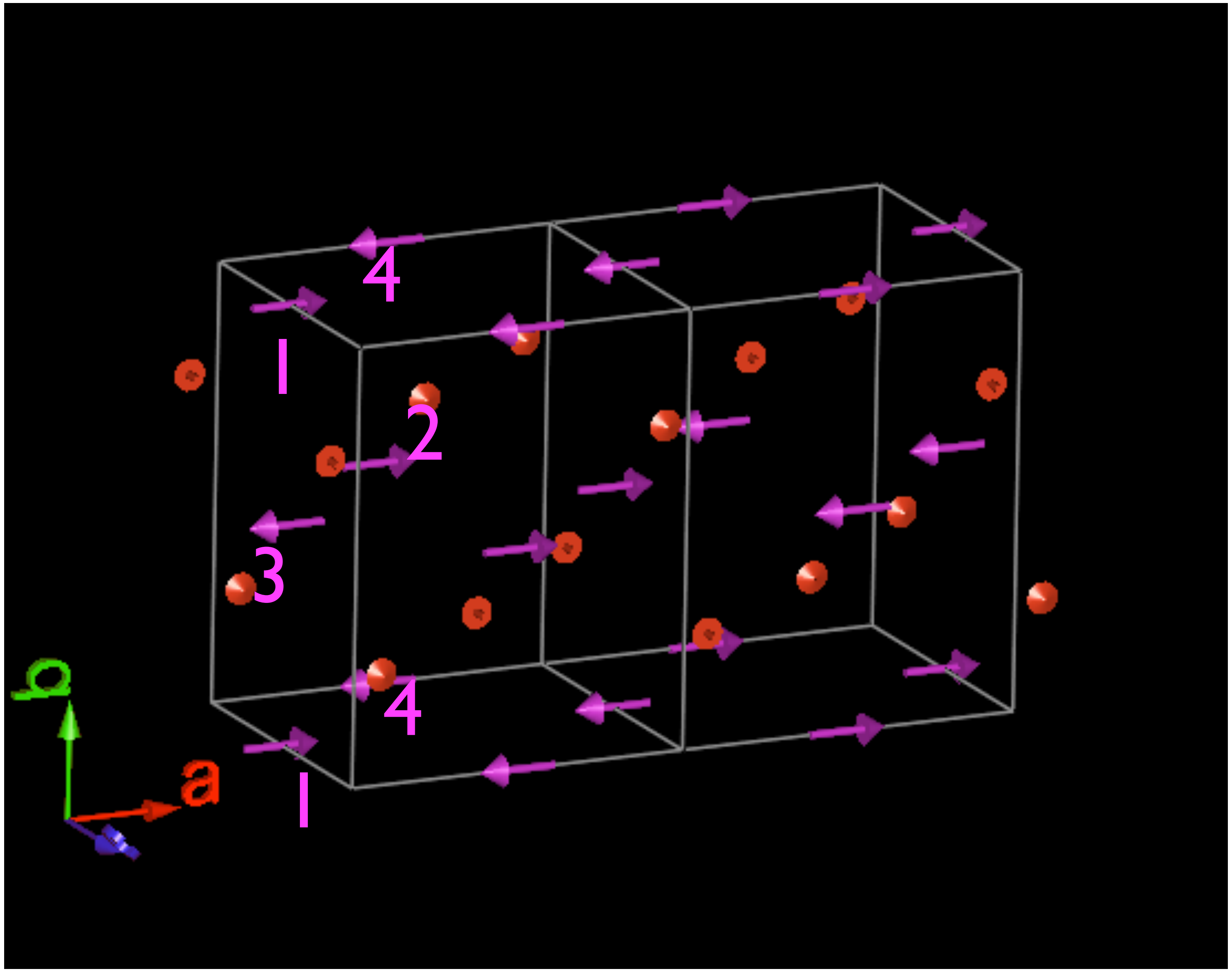


Classifying possible magnetic structures
basis functions



Two basis functions E1 and E2 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) $\frac{1}{2},0,0$
$E1=$	+1	+1	-1	-1
$E2=$	+1	-1	-1	+1



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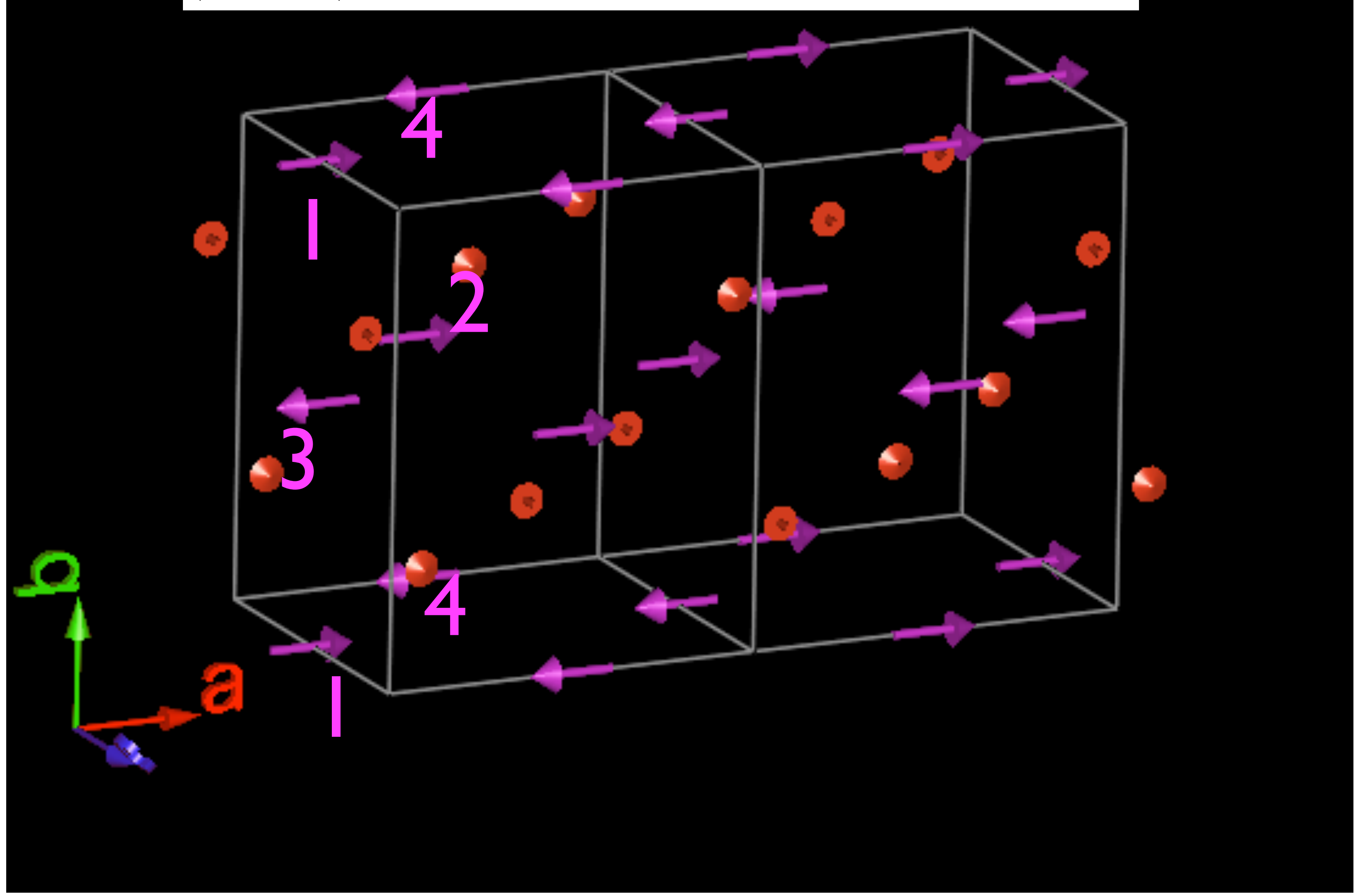
Mn-position	(1) $0,0,\frac{1}{2}$	(2) $\frac{1}{2},\frac{1}{2},0$	(3) $0,\frac{1}{2},\frac{1}{2}$	(4) $\frac{1}{2},0,0$
E1 =	+1	+1	-1	-1
E2 =	+1	-1	-1	+1

Any linear combination, in general

(E1+E2)/2 =	+1	0	-1	0
(E1-E2)/2 =	0	1	0	-1



function E1 -> Sh. group P_bmn2_1

ISODISTORT: order parameter direction

Space Group: 62 Pnma D2h-16, Lattice parameters: a=5.80520, b=7.31070, c=5.23350, alpha=90.00000, beta=90.00000, gamma=90.00000
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Irrep matrices: 2011 version for all k points
Include magnetic MN Tm distortions
k point: X, k21 (1/2,0,0)
IR: mX1, mk21t1

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)

function E1 -> Sh. group P_bmn2_1

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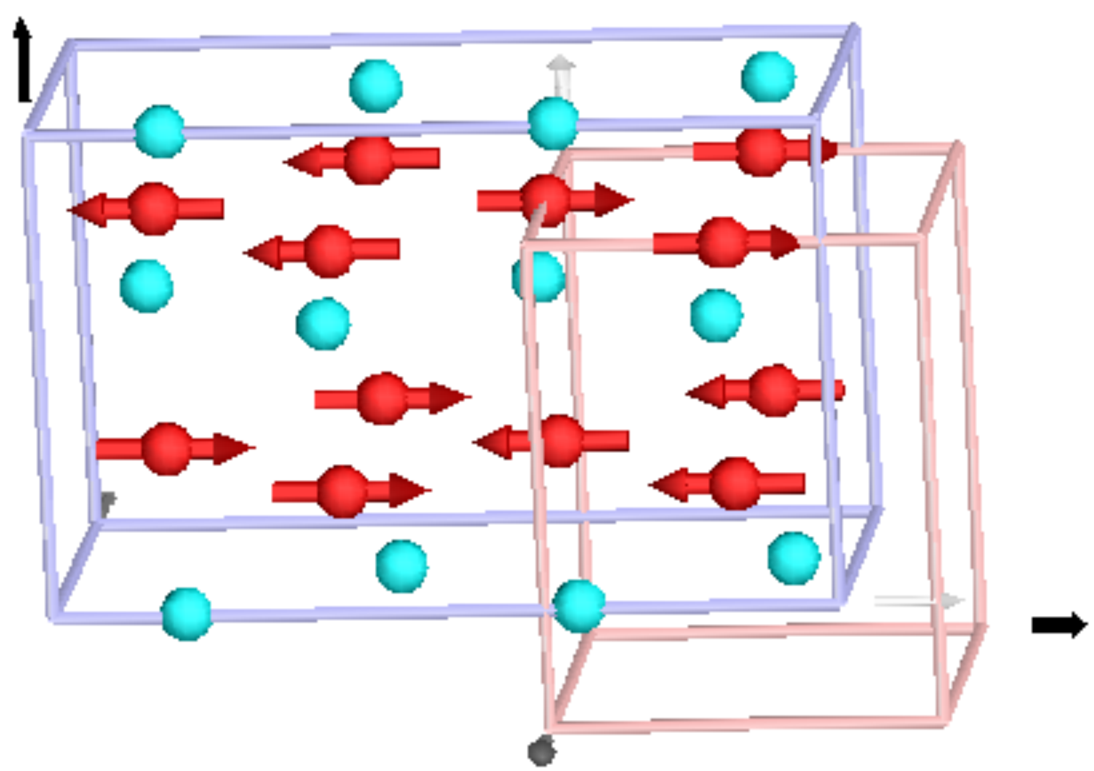
Default space-group preferences: monoclinic axes a(b)c, monoclinic cell choice 1, orthorhombic axes abc, origin choice 2, hexagonal axes, SSG standard setting
MN 4b (0,0,1/2), O1 4c (x,1/4,z), x=0.45960 , z=0.11820, O2 8d (x,y,z), x=0.33010 , y=0.05490 , z=-0.30160, Tm 4c (x,1/4,z), x=0.08460 , z=-0.01860
Irrep matrices: 2011 version for all k points
Include magnetic MN Tm distortions
k point: X, k21 (1/2,0,0)
IR: mX1, mk21t1

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)

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

$Pmn2_1$



function $C_1E1 + C_2E2$ -> Sh. group P_am

ISODISTORT: order parameter direction

Space Group: 62 Pnma D2h-16, Lattice parameters: a=5.80520, b=7.31070, c=5.23350, alpha=90.00000, beta=90.00000, gamma=90.00000
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Irrep matrices: 2011 version for all k points
Include magnetic MN Tm distortions
k point: X, k21 (1/2,0,0)
IR: mX1, mk21t1

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)

function $C_1E1 + C_2E2$ -> Sh. group P_am

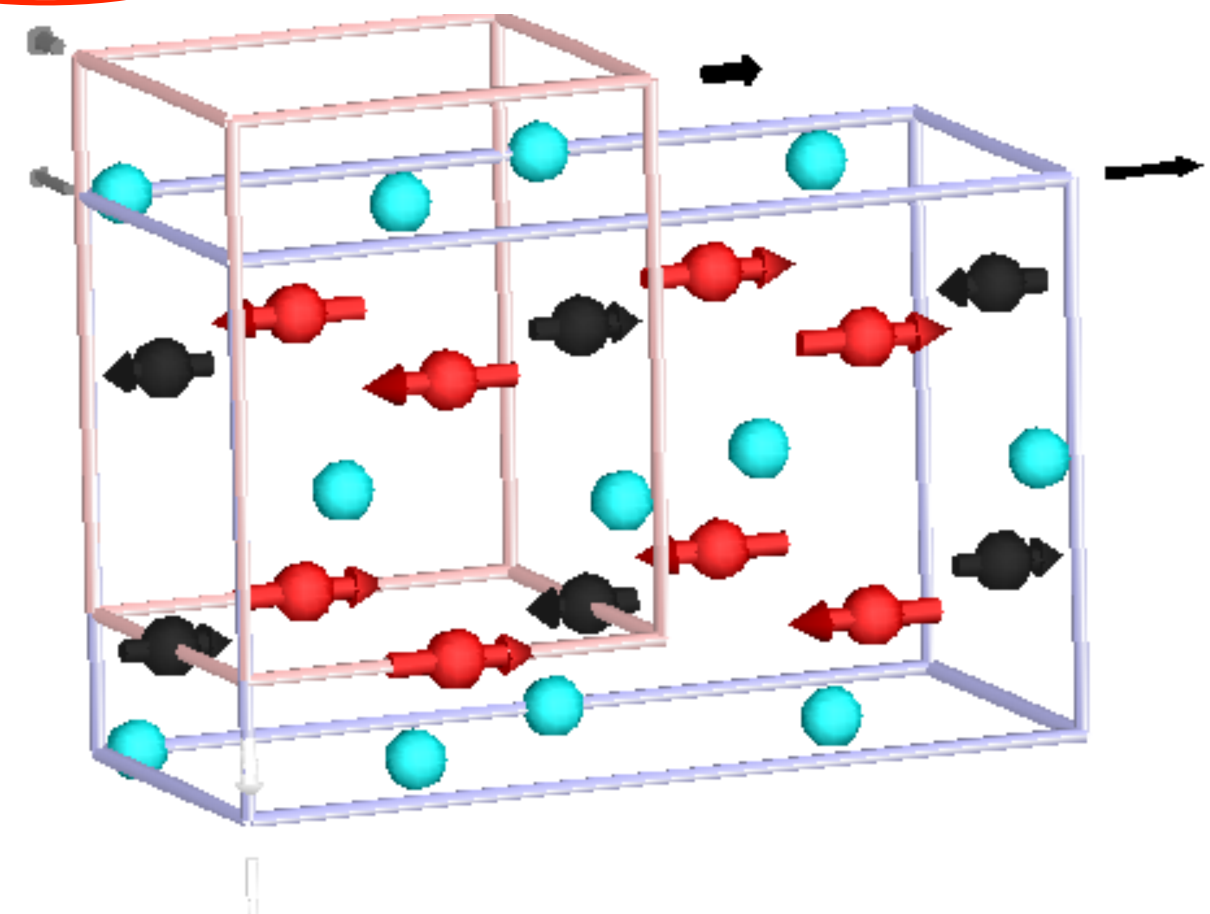
ISODISTORT: order parameter direction

Space Group: 62 Pnma D2h-16, Lattice parameters: a=5.80520, b=7.31070, c=5.23350, alpha=90.00000, beta=90.00000, gamma=90.00000
Default space-group preferences: monoclinic axes a(b)c, monoclinic cell choice 1, orthorhombic axes abc, origin choice 2, hexagonal axes, SSG standard setting
MN 4b (0,0,1/2), O1 4c (x,1/4,z), x=0.45960 , z=0.11820, O2 8d (x,y,z), x=0.33010 , y=0.05490 , z=-0.30160, Tm 4c (x,1/4,z), x=0.08460 , z=-0.01860
Irrep matrices: 2011 version for all k points
Include magnetic MN Tm distortions
k point: X, k21 (1/2,0,0)
IR: mX1, mk21t1

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)

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

Pm



The end