Symmetry Analysis of the Magnetic Structure of Hexagonal Manganites and Ferrites

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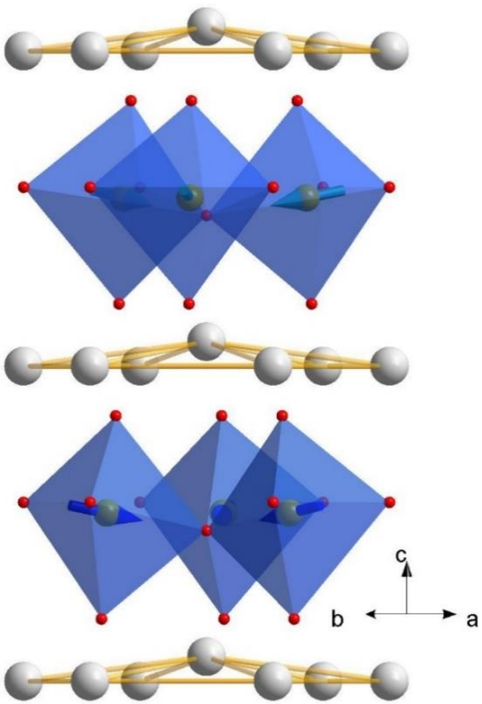
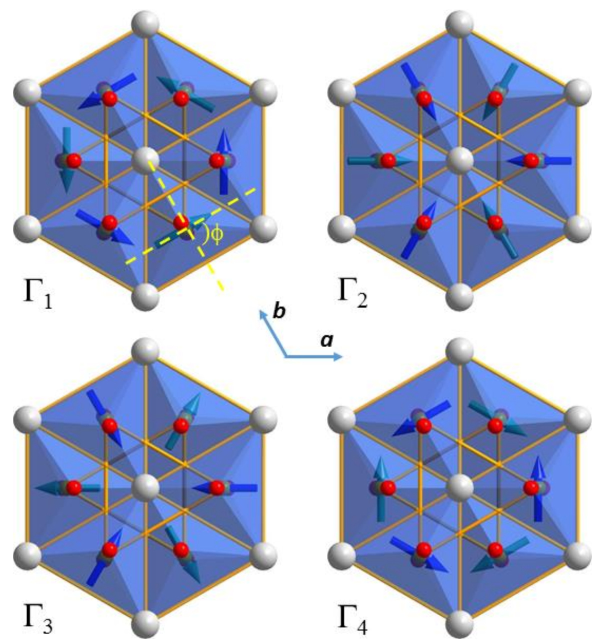
What is magnetic structure?

- Magnetic structure is also called spin structure, which is the arrangement of the magnetic moments in the crystal (solid).



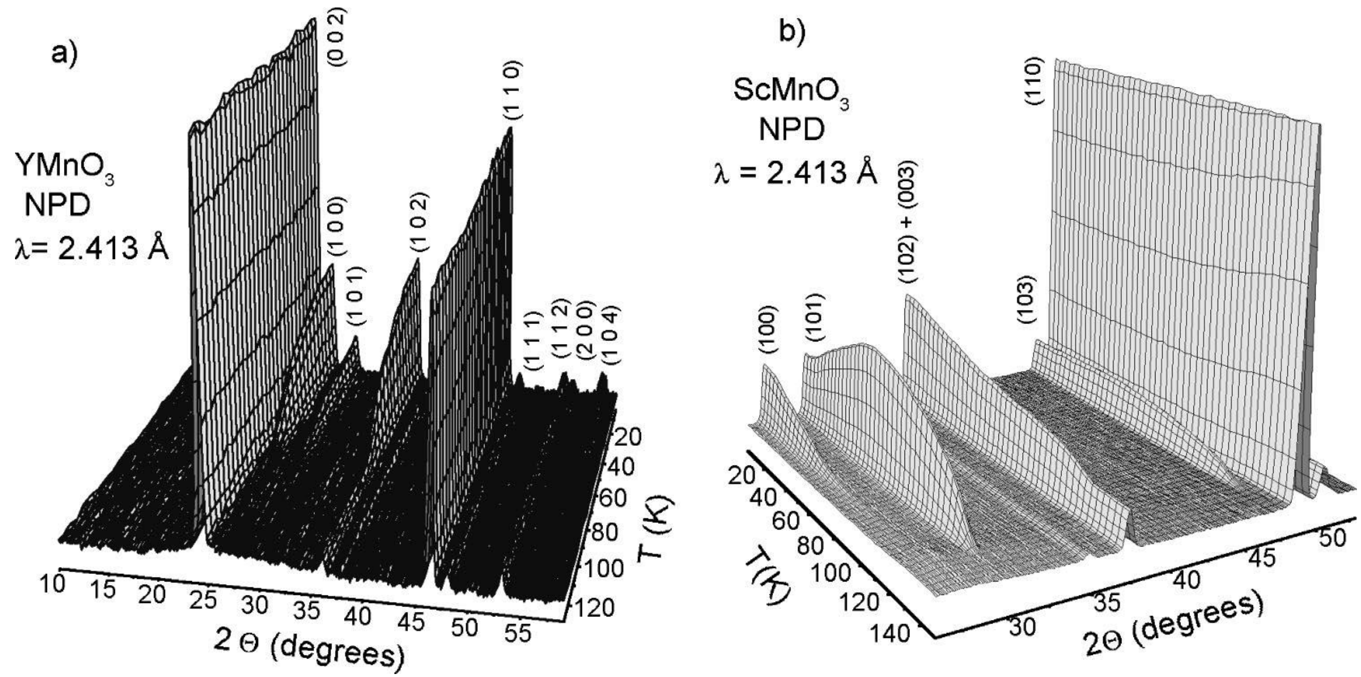


How to determine the magnetic structure?

- Symmetry (Group theory) analysis
  - 1. Determine the symmetry of the magnetic structure
    - Start from symmetry of the crystal structure
    - Find relation between the crystal structure and magnetic structure (propagation vector). Or the relation between the magnetic unit cell and magnetic unit cell.
      - This can be found from magnetic (neutron) diffractions
      - If there is no peak at **fractional index**, the magnetic propagation vector is (0,0,0). In other words, the magnetic and structural unit cells are the same.
  - 2. Analyze the possible magnetic structure
- Calculate the diffraction patterns from possible magnetic structures and compare with the experiments
  - 1. Quick determination according to the existence of certain peaks.
  - 2. Fit the diffraction spectra using magnetic structures

Symmetry analysis

1. Determine the symmetry of the magnetic structure



There is no peaks of fractional indices.

- The propagation vector is (0,0,0).
- The symmetry of the magnetic structure is the same as that of the crystal structure ($P6_3cm$).

PRB, v. 62, p. 9498, 2000.

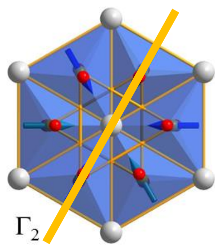
2. Analyze the possible magnetic structure

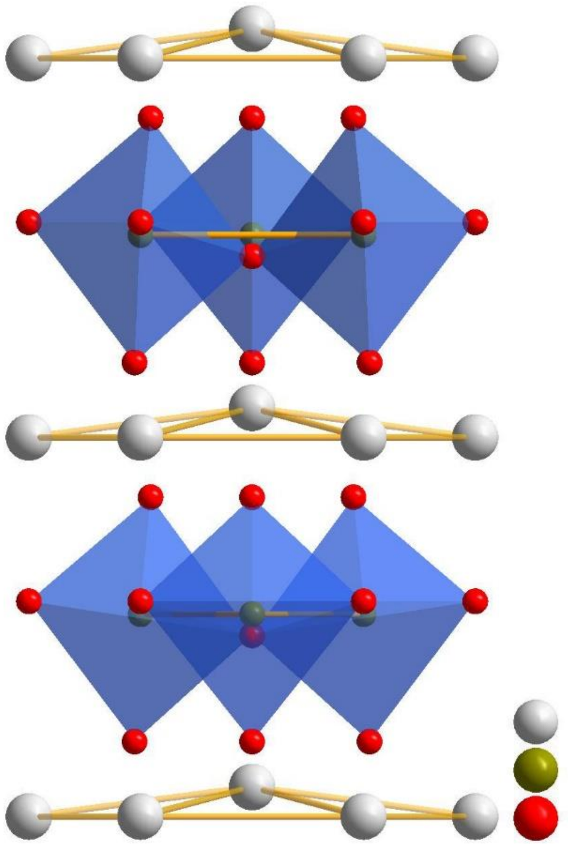
- Symmetry $P6_3cm$ (185), or $P6_3cm$ group.
- A set of symmetry operation that can bring the crystal structure back to itself. These operations are also called symmetry operations.
- 12 operations, here x and y refers to the first and second coordinates

X,Y,Z
-Y,X-Y,Z
Y-X,-X,Z
Y,X,Z
X-Y,-Y,Z
-X,Y-X,Z
-X,-Y,1/2+Z
Y,Y-X,1/2+Z
X-Y,X,1/2+Z
-Y,-X,1/2+Z
Y-X,Y,1/2+Z
X,X-Y,1/2+Z

Counter-clockwise rotation by 120 degree

Mirror plane





2.2 Group theory and representations

- What's important for a symmetry group is its effect on vectors.
- The effect of a group on different vectors are different.
- We call the effect of a **group** on a **vector** a **representation**.
- For any certain group, there are a finite number of fundamental representations, called **irreducible representations** (IR).
- Any representations can be decomposed into the linear combination of the irreducible representations (IR).
- Example:
  - group P2 [(X,Y,Z)(-X,Y,-Z)]
  - Effect on (001) is to transform it into (001) and (00-1)
  - Effect on (010) is to transform it into (010) and (010)

2.3 For $P6_3cm$ (185), there are six irreducible representations (IR)

TABLE IV. Irreducible representations of the space group $G_k = P6_3cm$ for $\mathbf{k}=0$. The symmetry operators are given in Kovalev's notation (KV) and in a notation based in Hermann-Mauguins symbols (IT). $\omega = e^{i\pi/3}$.

KV	h_1	$h_2/(\boldsymbol{\tau}^{a})$	h_3	$h_4/(\boldsymbol{\tau})$	h_5	$h_6/(\boldsymbol{\tau})$	$h_{19}/(\boldsymbol{\tau})$	h_{20}	$h_{21}/(\boldsymbol{\tau})$	h_{22}	$h_{23}/(\boldsymbol{\tau})$	h_{24}
IT	1	6^{+}_{3z}	3^{+}_{z}	2_{1z}	3^{-}_{z}	6^{-}_{3z}	$c(2x,x,z)$	$m(x,x,z)$	$c(x,2x,z)$	$m(0,y,z)$	$c(x,\bar{x},z)$	$m(x,0,z)$
Pos.	x	$x-y$	$\bar{y}$	$\bar{x}$	$\bar{x}+y$	y	x	y	$\bar{x}+y$	$\bar{x}$	$\bar{y}$	$x-y$
	y	x	$x-y$	$\bar{y}$	$\bar{x}$	$\bar{x}+y$	$x-y$	x	y	$\bar{x}+y$	$\bar{x}$	$\bar{y}$
	z	$z+\frac{1}{2}$	z	$z+\frac{1}{2}$	z	$z+\frac{1}{2}$	$z+\frac{1}{2}$	z	$z+\frac{1}{2}$	z	$z+\frac{1}{2}$	z
Γ_1	1	1	1	1	1	1	1	1	1	1	1	1
Γ_2	1	1	1	1	1	1	-1	-1	-1	-1	-1	-1
Γ_3	1	-1	1	-1	1	-1	1	-1	1	-1	1	-1
Γ_4	1	-1	1	-1	1	-1	-1	1	-1	1	-1	1
Γ_5	I	B_1	$-B_2$	$-I$	$-B_1$	B_2	A	C_1	$-C_2$	$-A$	$-C_1$	C_2
Γ_6	I	$-B_1$	$-B_2$	I	$-B_1$	$-B_2$	A	$-C_1$	$-C_2$	A	$-C_1$	$-C_2$

Where: $I=\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}$ $A=\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}$ $B_1=\begin{pmatrix}\omega & 0\\ 0 & \omega^{\star}\end{pmatrix}$ $B_2=\begin{pmatrix}\omega^{\star} & 0\\ 0 & \omega\end{pmatrix}$ $C_1=\begin{pmatrix}0 & \omega\\ \omega^{\star} & 0\end{pmatrix}$ $C_2=\begin{pmatrix}0 & \omega^{\star}\\ \omega & 0\end{pmatrix}$

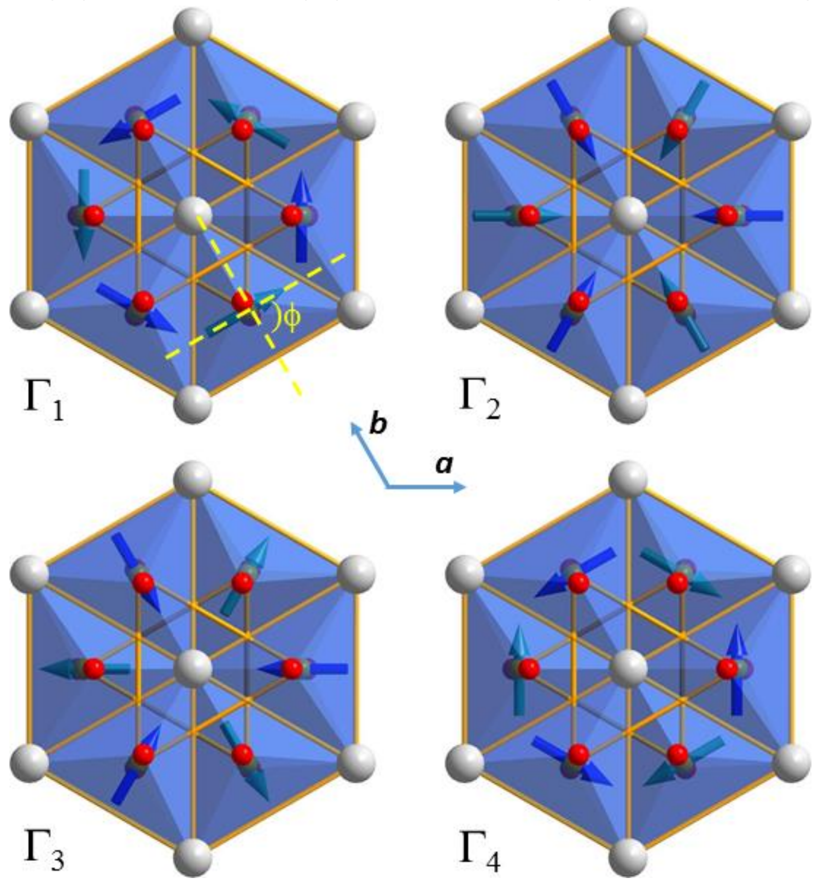
12 operations

6 IRs

PRB, v. 62, p. 9498, 2000.

2.4 About the vector for Γ_1 to Γ_4

Γ_1	Re	(1 2 0)	(-1 -2 0)	(-2 -1 0)	(2 1 0)	(1 -1 0)	(-1 1 0)
Γ_2	Re	(1 0 0)	(-1 0 0)	(0 1 0)	(0 -1 0)	(-1 -1 0)	(1 1 0)
	Re	(0 0 1)	(0 0 1)	(0 0 1)	(0 0 1)	(0 0 1)	(0 0 1)
Γ_3	Re	(1 0 0)	(1 0 0)	(0 1 0)	(0 1 0)	(-1 -1 0)	(-1 -1 0)
	Re	(0 0 1)	(0 0 -1)	(0 0 1)	(0 0 -1)	Re (0 0 1)	(0 0 -1)
Γ_4	Re	(1 2 0)	(1 2 0)	(-2 -1 0)	(-2 -1 0)	(1 -1 0)	(1 -1 0)



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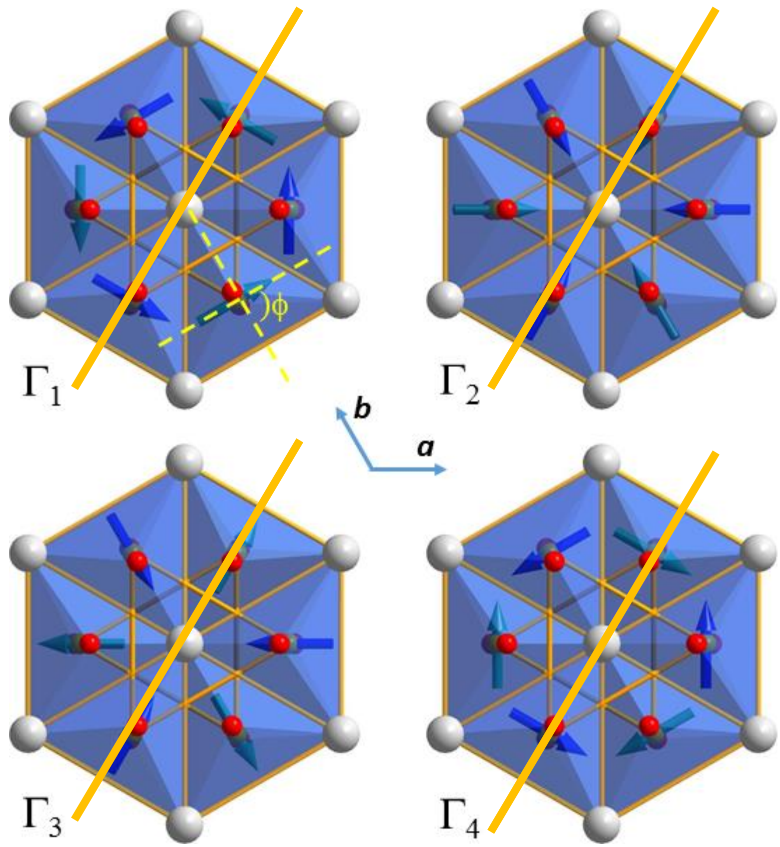
2.5 Example of Γ_1 to Γ_4

Pos.	x, y, z	$x-y, x, z+\frac{1}{2}$	$\bar{y}, x-y, z$	$\bar{x}, \bar{y}, z+\frac{1}{2}$	$\bar{x}+y, \bar{x}, z$	$y, \bar{x}+y, z+\frac{1}{2}$	$x, x-y, z+\frac{1}{2}$	y, x, z	$\bar{x}+y, y, z+\frac{1}{2}$	$\bar{x}, \bar{x}+y, z$	$\bar{y}, \bar{x}, z+\frac{1}{2}$	$x-y, \bar{y}, z$
Γ_1	1	1	1	1	1	1	1	1	1	1	1	1
Γ_2	1	1	1	1	1	1	−1	−1	−1	−1	−1	−1
Γ_3	1	−1	1	−1	1	−1	1	−1	1	−1	1	−1
Γ_4	1	−1	1	−1	1	−1	−1	1	−1	1	−1	1

Note that magnetic moments are axial vector. After mirror operation, it needs to be reversed.



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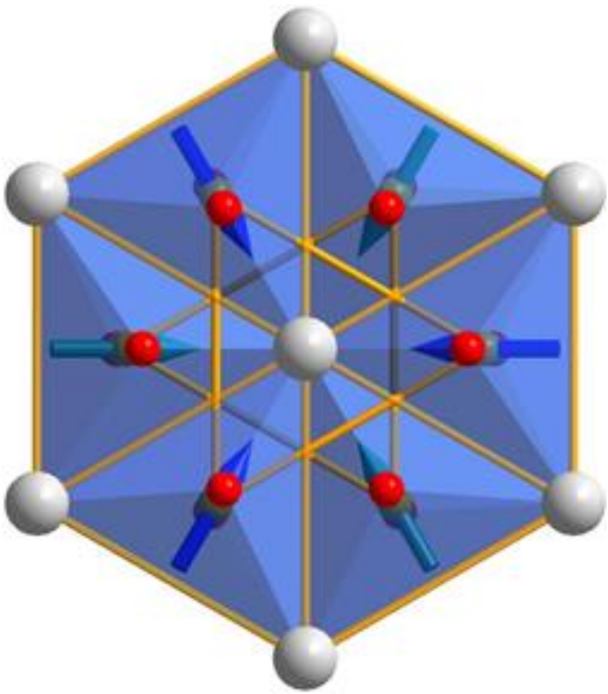
2.6 Representations and decomposition

- For LuFeO3, there are six magnetic moments in each unit cell.



	h_1	h_{20}
	1	$m(x,x,z)$
	x	y
	y	x
	z	z
(x_1,y_1,z_1)	(x_1,y_1,z_1)	(y_1,x_1,z_1)
(x_2,y_2,z_2)	(x_2,y_2,z_2)	(y_2,x_2,z_2)
(x_3,y_3,z_3)	(x_3,y_3,z_3)	(y_3,x_3,z_3)
(x_4,y_4,z_4)	(x_4,y_4,z_4)	(y_4,x_4,z_4)
(x_5,y_5,z_5)	(x_5,y_5,z_5)	(y_5,x_5,z_5)
(x_6,y_6,z_6)	(x_6,y_6,z_6)	(y_6,x_6,z_6)
Character	18	6

$$\Gamma = 1\Gamma_1 + 2\Gamma_2+2\Gamma_3+1\Gamma_4+3\Gamma_5+3\Gamma_6$$

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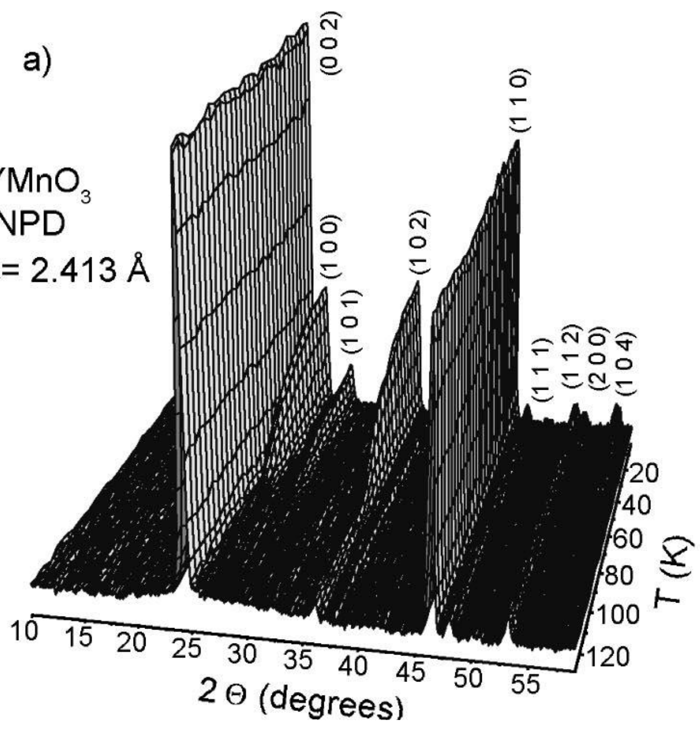
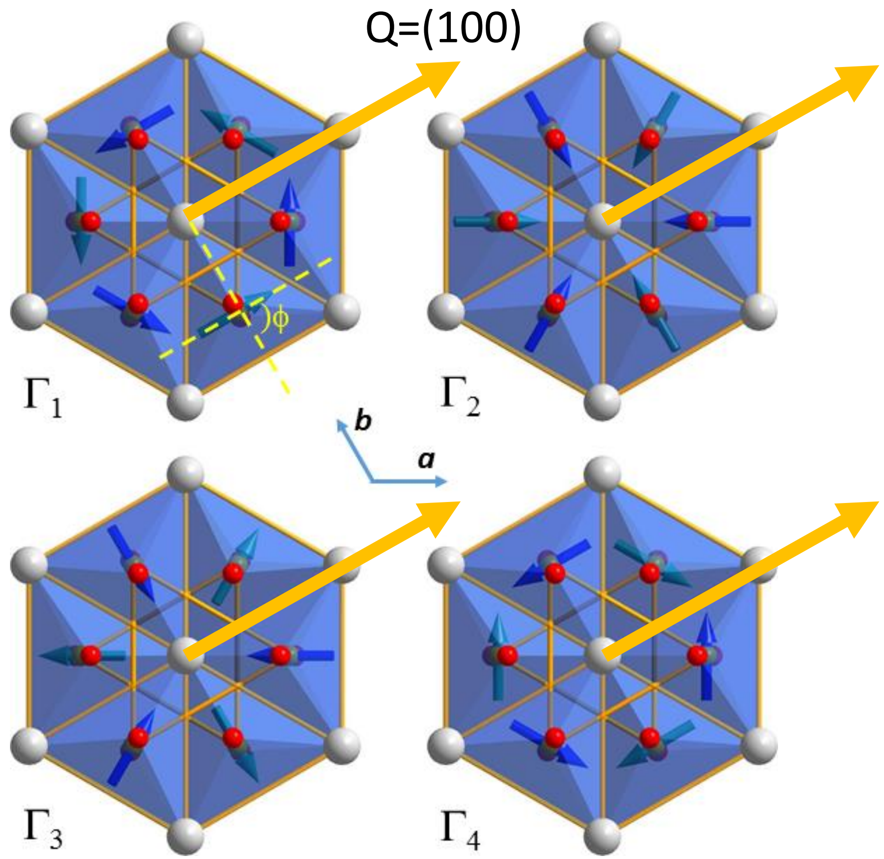
Normally, we can rule out the IR if it does not occur.
In this case, all of them occurs.
So this actually does not help much.
We need other ways to narrow down the possibilities.

Final determination of magnetic structure

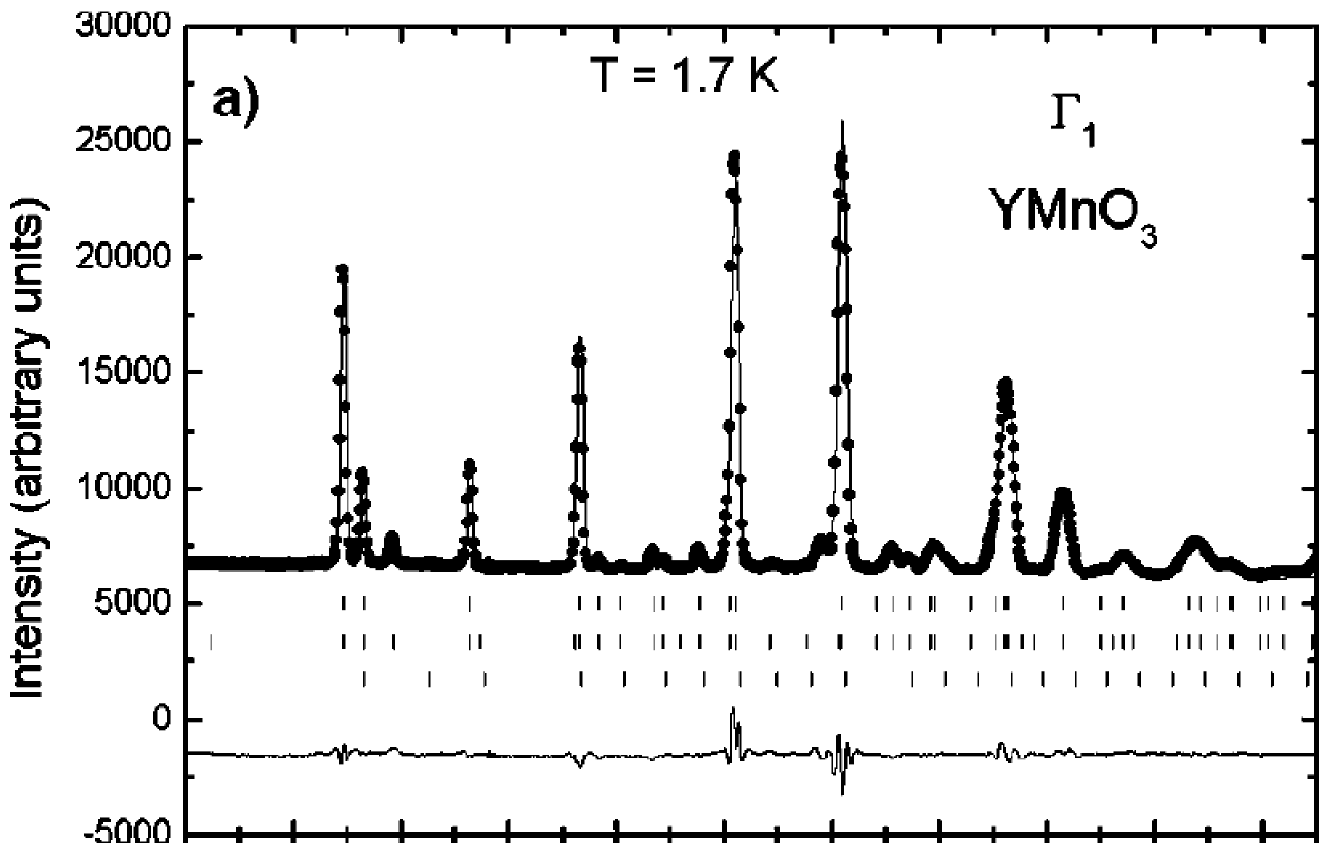
1. Quick look: None-zero (100) peaks means the existence of Γ_1 and Γ_3





$I \propto e^{i\boldsymbol{Q}\cdot\boldsymbol{r}}\boldsymbol{Q} \times (\boldsymbol{Q} \times \boldsymbol{M})$ Neutron beam only detects $\mathbf{M} \perp \boldsymbol{Q}$

2. Fit the diffraction spectra using all IRs, the best fit should corresponds to the real magnetic structure



Conclusion

- Magnetic structure can be analyzed using the group theory according to the symmetry.
- The determination will rely on the comparison with the neutron diffraction.