

Magnetic Ordering in $\text{Ce}_{1-x}\text{Yb}_x\text{RhIn}_5$ Heavy Fermions as a Function of Doping

NIST August 5, 2015

JOHN CALIFF COLLINI¹

MENTOR: DR. STEVE DISSELER²

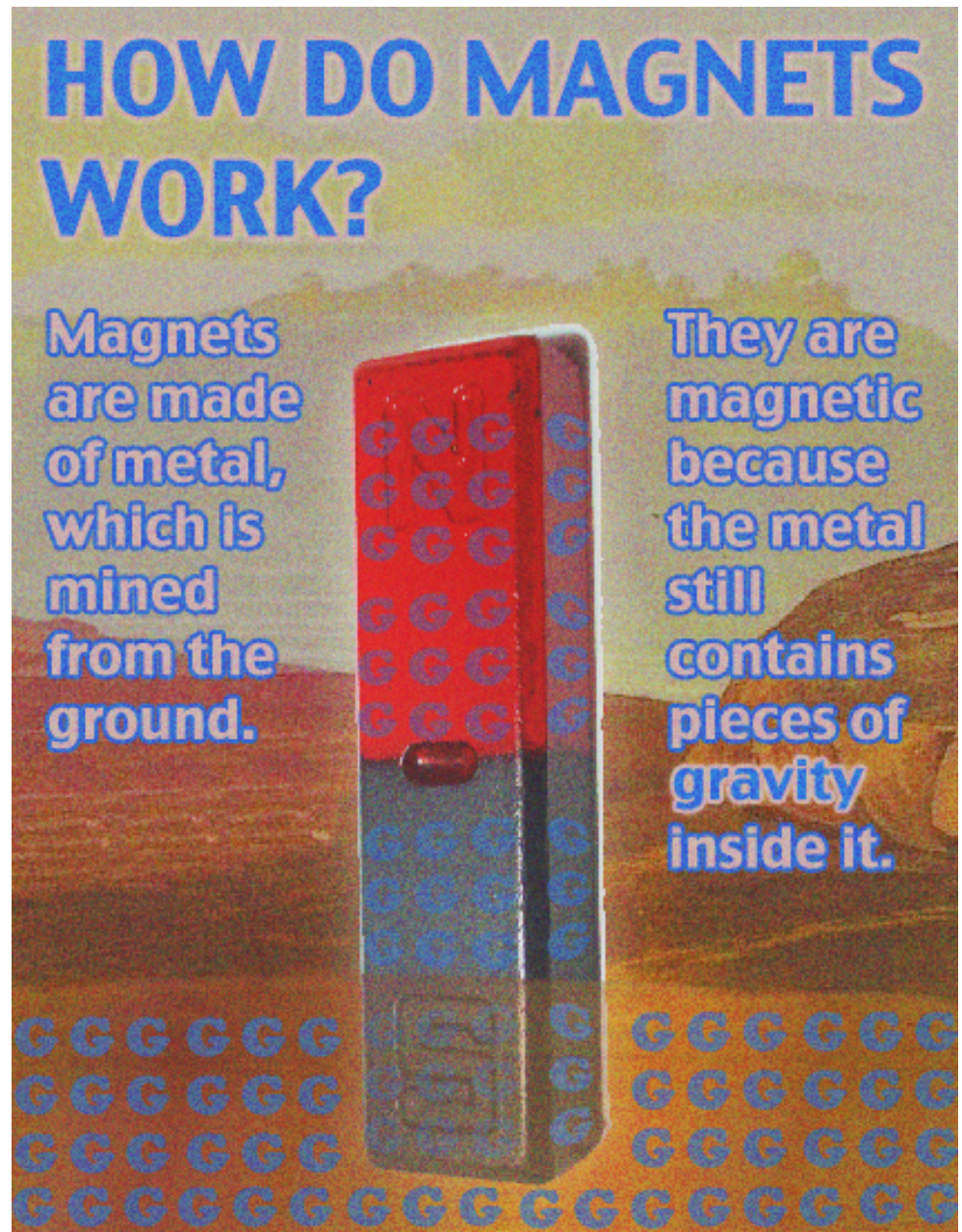
NCNR SURF GROUP AT NIST

¹ROCHESTER INSTITUTE OF TECHNOLOGY

²NCNR CONDENSED MATTER SCIENCE GROUP



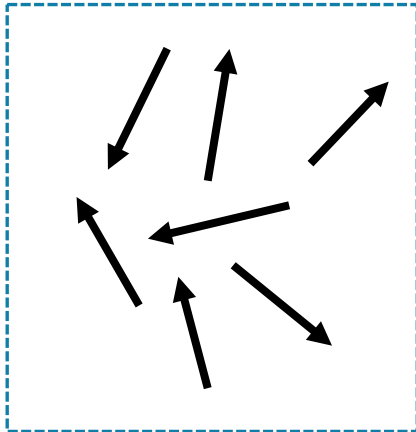
One Definition:



Types of Magnetic States (only 3 shown)

$T > T_c$: DISORDERED

Paramagnetic



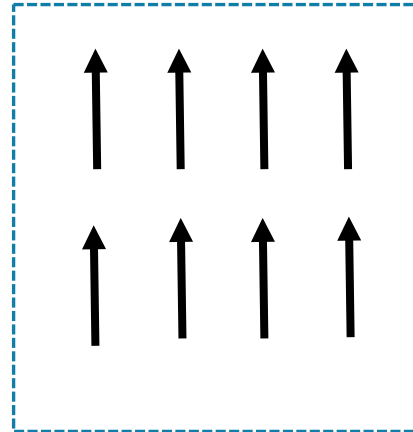
$$\langle \vec{M} \rangle = 0$$

$$\vec{M} = \chi_m \vec{H}$$



$T < T_c$: ORDERED

Ferromagnetic



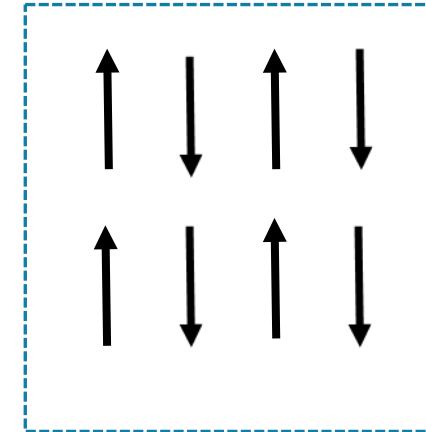
$$\langle \vec{M} \rangle \neq 0$$

$$H = -J \sum_{i,j} \vec{s}_i \cdot \vec{s}_j$$

$$J > 0$$

Ex: Iron and Cobalt

Antiferromagnetic



$$\langle \vec{M} \rangle = 0$$

$$H = -J \sum_{i,j} \vec{s}_i \cdot \vec{s}_j$$

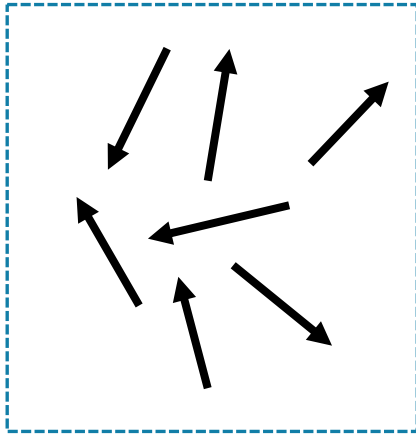
$$J < 0$$

Ex: Common Metal-Oxides

Types of Magnetic States (only 3 shown)

$T > T_c$: DISORDERED

Paramagnetic

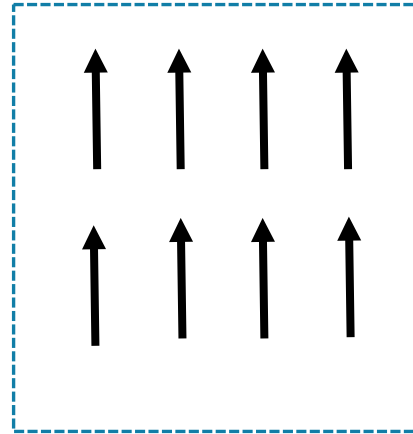


$$\langle \vec{M} \rangle = 0$$

$$\vec{M} = \chi_m \vec{H}$$

$T < T_c$: ORDERED

Ferromagnetic



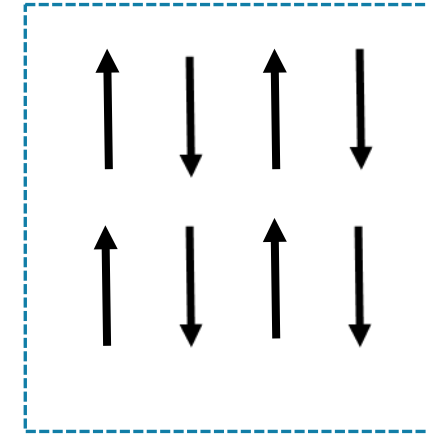
$$\langle \vec{M} \rangle \neq 0$$

$$H = -J \sum_{i,j} \vec{s}_i \cdot \vec{s}_j$$

$$J > 0$$

Ex: Iron and Cobalt

Antiferromagnetic



$$\langle \vec{M} \rangle = 0$$

$$H = -J \sum_{i,j} \vec{s}_i \cdot \vec{s}_j$$

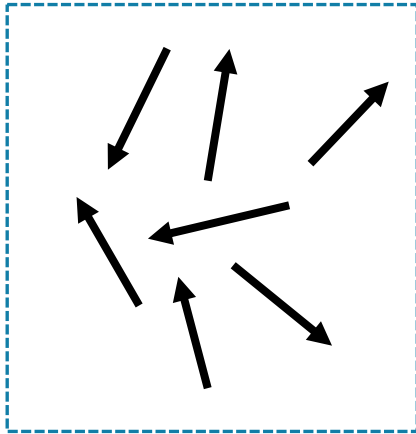
$$J < 0$$

Ex: Common Metal-Oxides

Types of Magnetic States (only 3 shown)

$T > T_c$: DISORDERED

Paramagnetic



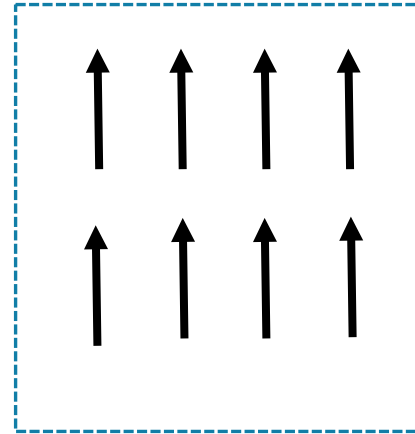
$$\langle \vec{M} \rangle = 0$$

$$\vec{M} = \chi_m \vec{H}$$



$T < T_c$: ORDERED

Ferromagnetic



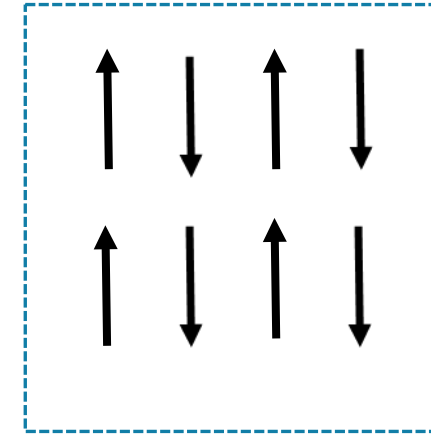
$$\langle \vec{M} \rangle \neq 0$$

$$H = -J \sum_{i,j} \vec{s}_i \cdot \vec{s}_j$$

$$J > 0$$

Ex: Iron and Cobalt

Antiferromagnetic



$$\langle \vec{M} \rangle = 0$$

$$H = -J \sum_{i,j} \vec{s}_i \cdot \vec{s}_j$$

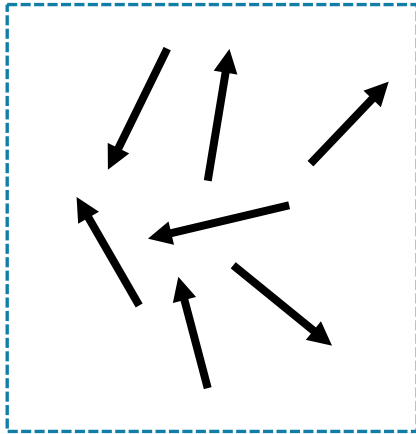
$$J < 0$$

Ex: Common Metal-Oxides

Types of Magnetic States (only 3 shown)

$T > T_c$: DISORDERED

Paramagnetic



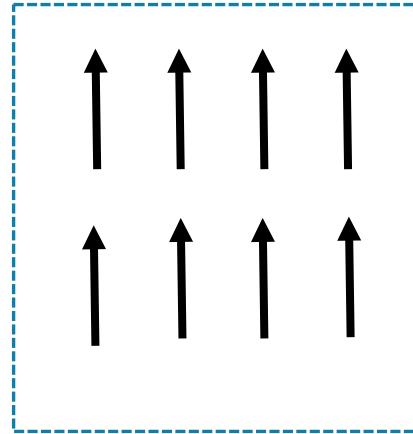
$$\langle \vec{M} \rangle = 0$$

$$\vec{M} = \chi_m \vec{H}$$



$T < T_c$: ORDERED

Ferromagnetic



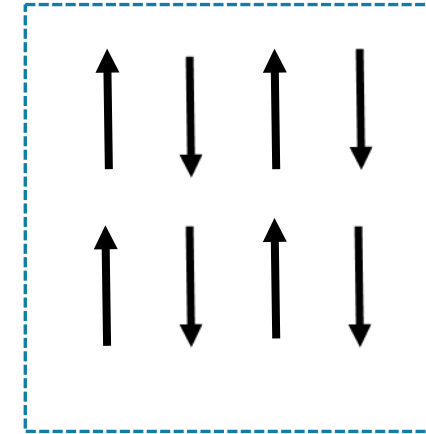
$$\langle \vec{M} \rangle \neq 0$$

$$H = -J \sum_{i,j} \vec{s}_i \cdot \vec{s}_j$$

$$J > 0$$

Ex: Iron and Cobalt

Antiferromagnetic



$$\langle \vec{M} \rangle = 0$$

$$H = -J \sum_{i,j} \vec{s}_i \cdot \vec{s}_j$$

$$J < 0$$

Ex: Common Metal-Oxides

What are Heavy Fermions?

Kondo Interactions

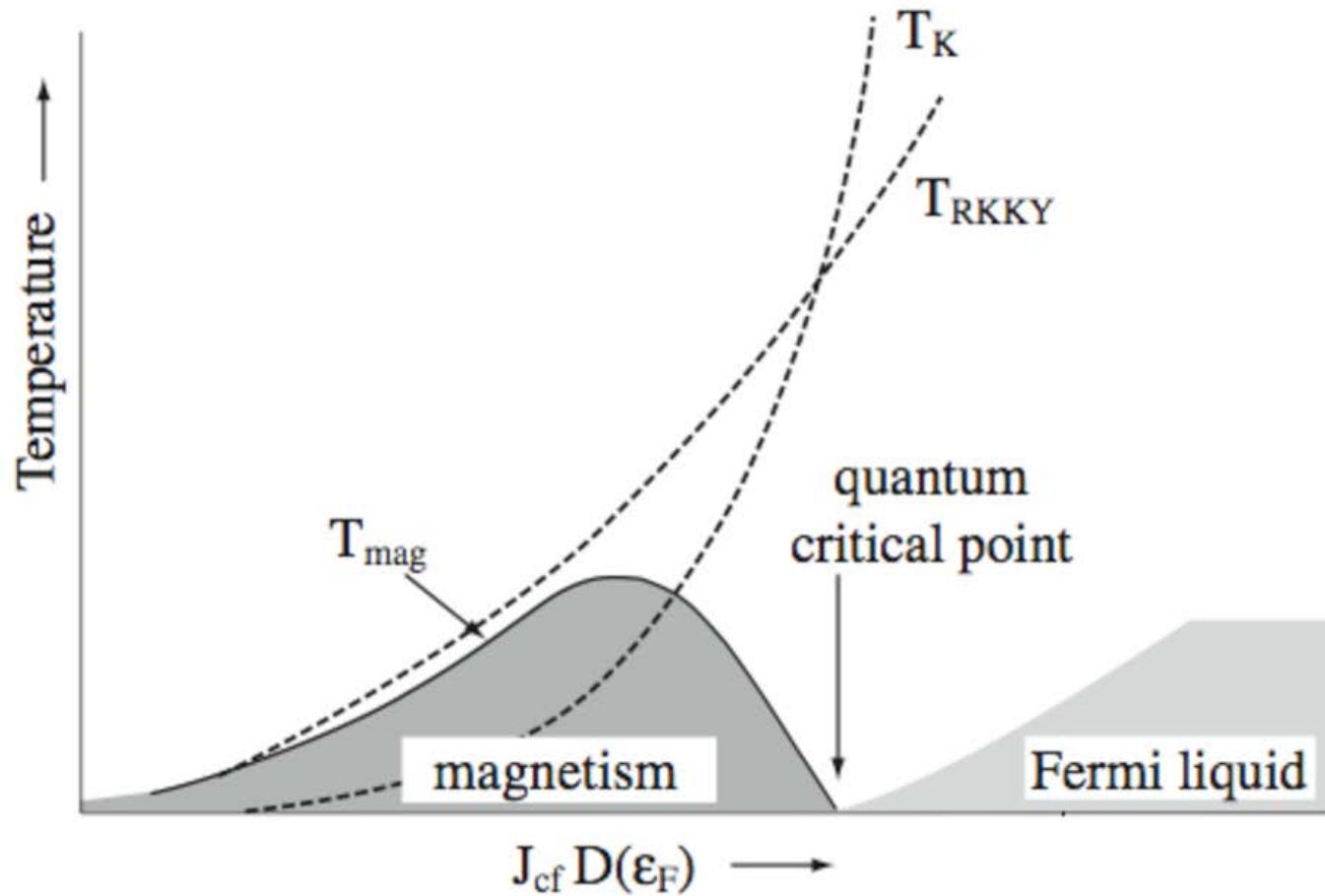
- Conduction spin screening
- Suppresses magnetic ordering

RKKY Interactions

- Coupled moments dependent on distance
- Enhances magnetic ordering

Combining Both

- Huge increase in effective mass.
- Kondo and RKKY interactions co-exist
- Possible unconventional superconductivity near QCP



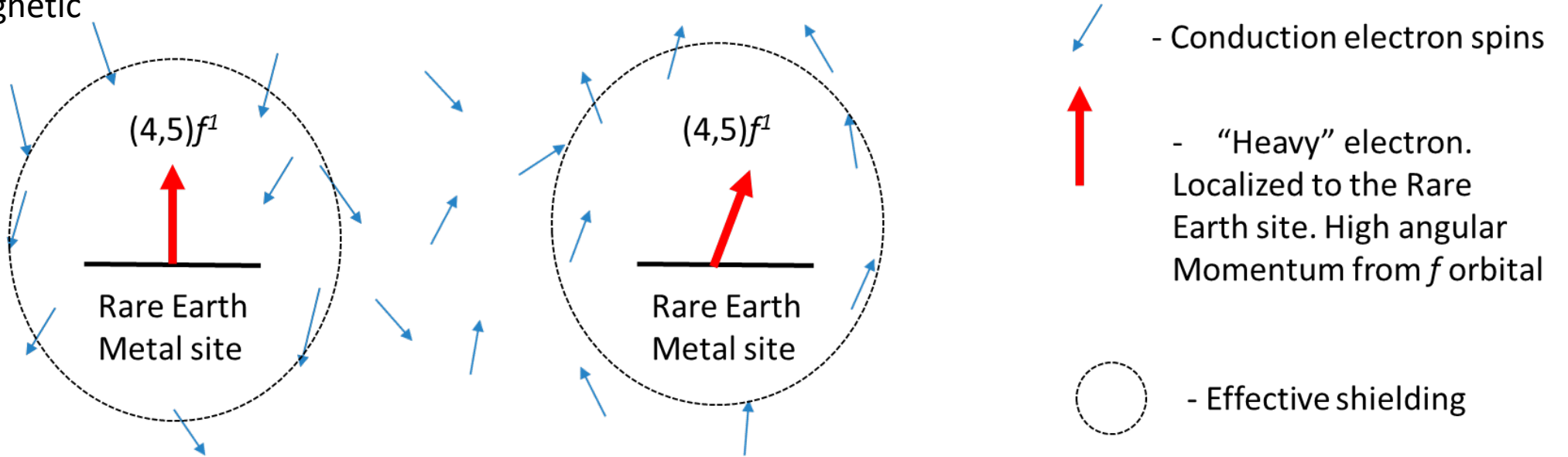
Also, increasing H , P , doping, ect.

from UNLP

What are Heavy Fermions?

Kondo Effect

- Electron spin screening
- Suppresses magnetic ordering



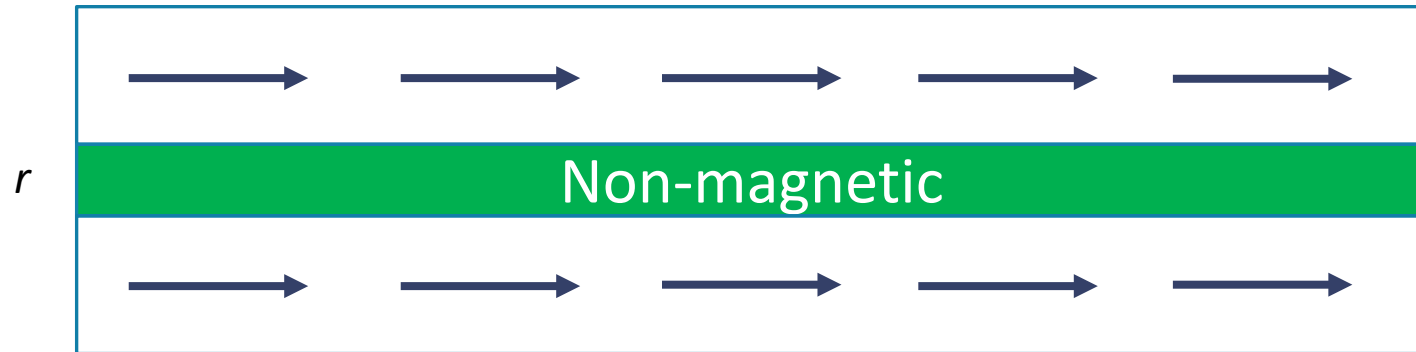
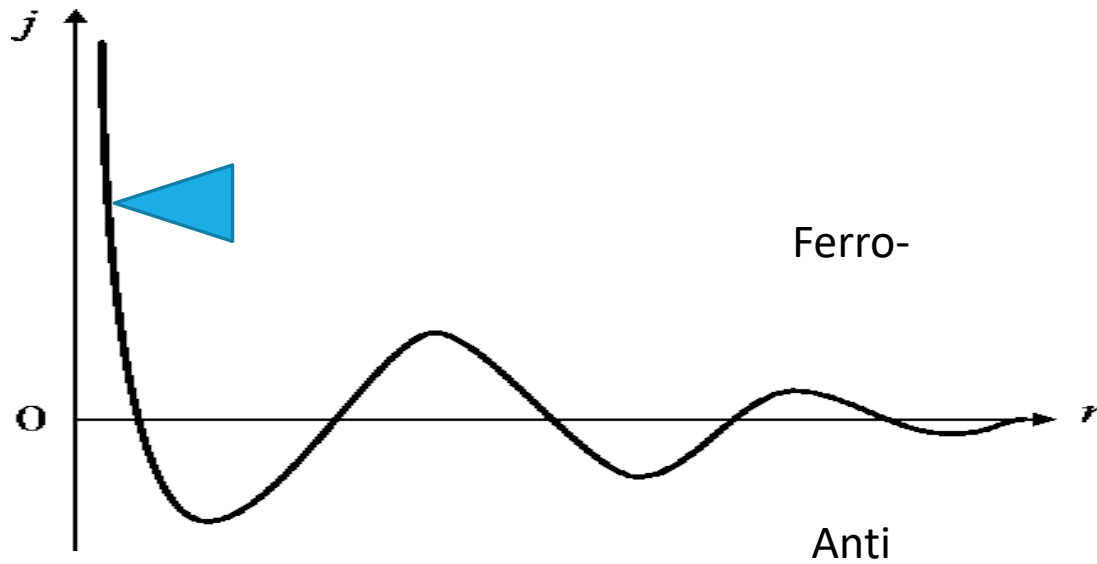
What are Heavy Fermions?

Kondo Effect

- Conduction spin screening
- Suppresses magnetic ordering

RKKY Interactions

- Coupled moments dependent on distance
- Enhances magnetic ordering



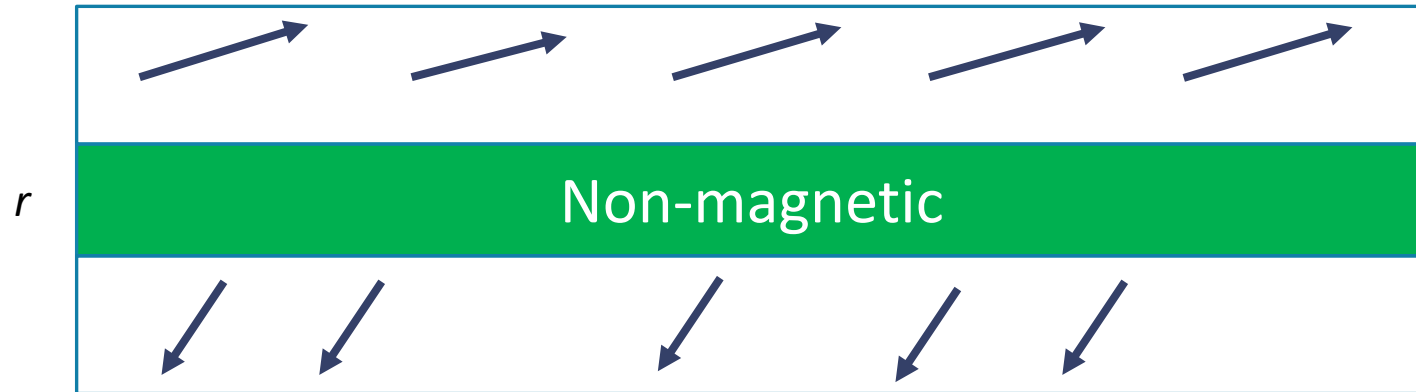
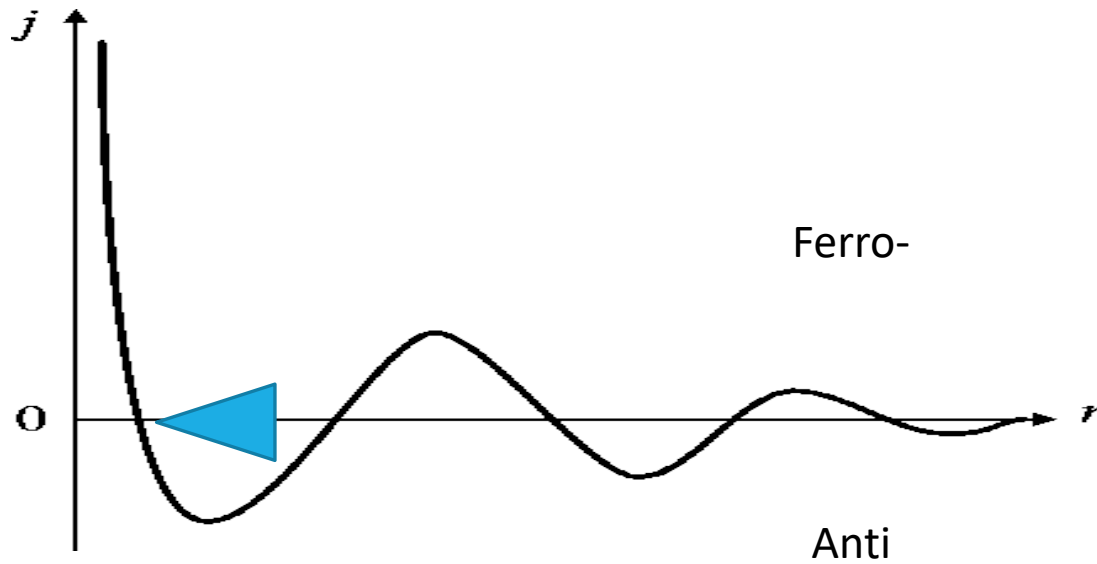
What are Heavy Fermions?

Kondo Effect

- Conduction spin screening
- Suppresses magnetic ordering

RKKY Interactions

- Coupled moments dependent on distance
- Enhances magnetic ordering



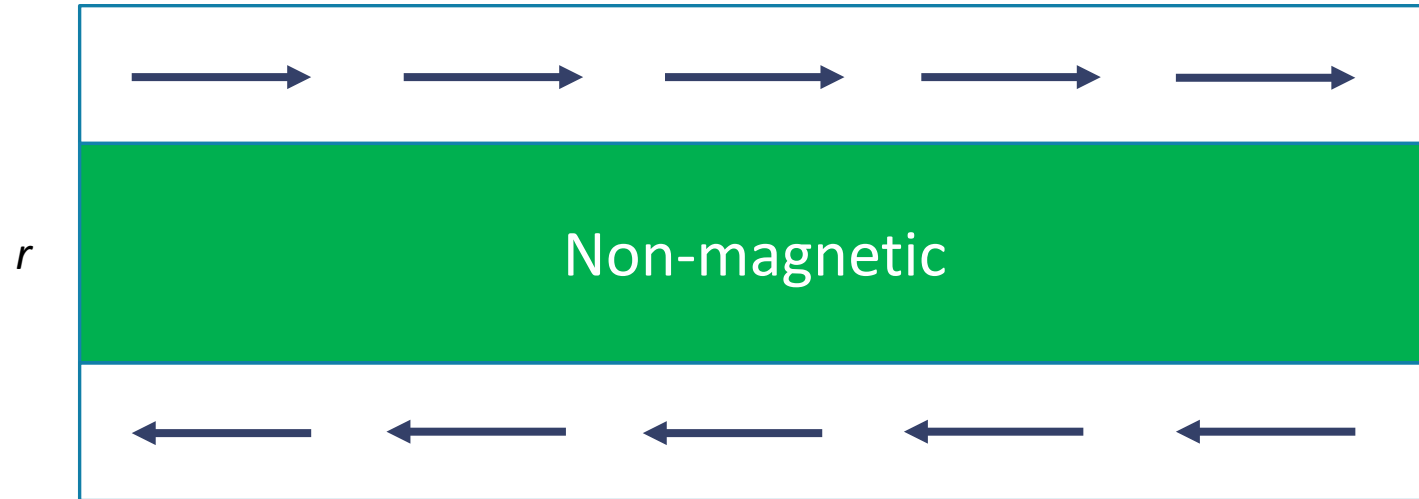
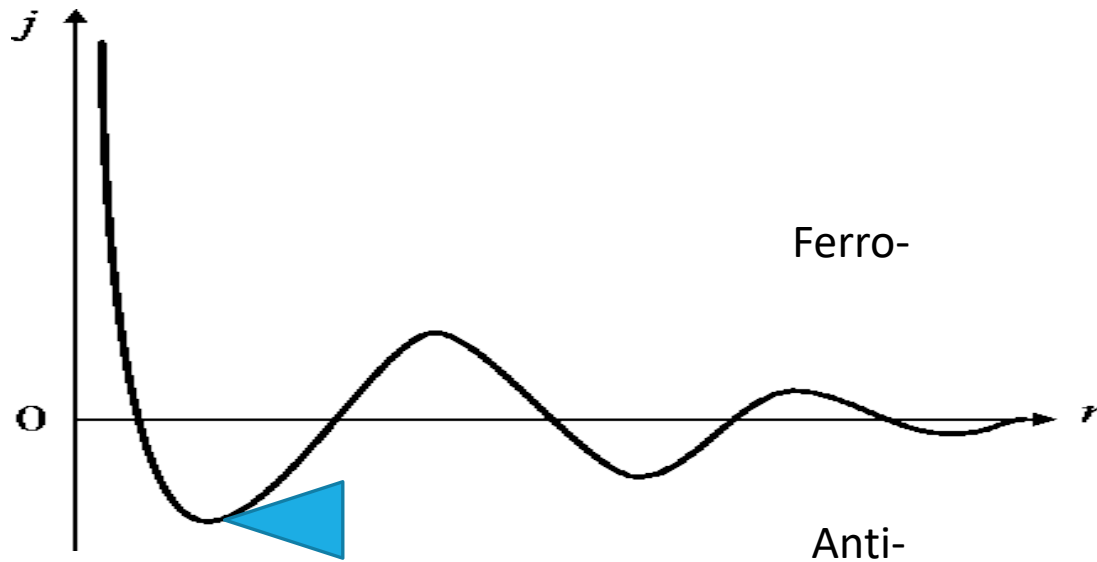
What are Heavy Fermions?

Kondo Effect

- Conduction spin screening
- Suppresses magnetic ordering

RKKY Interactions

- Coupled moments dependent on distance
- Enhances magnetic ordering



What are Heavy Fermions?

Kondo Interactions

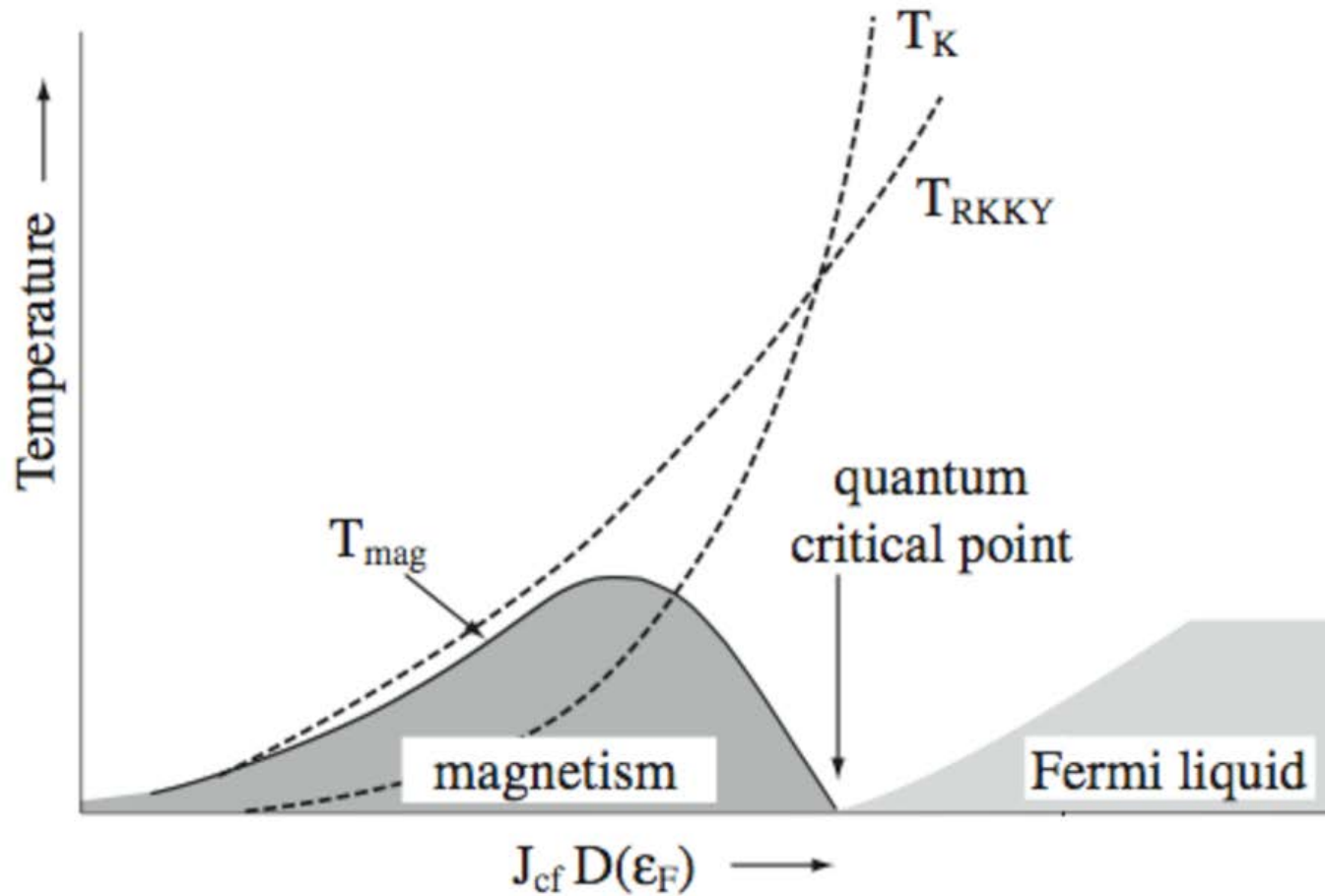
- Conduction spin screening
- Suppresses magnetic ordering

RKKY Interactions

- Coupled moments dependent on distance
- Enhances magnetic ordering

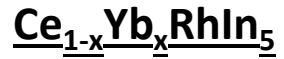
Combining Both

- Huge increase in effective mass.
- Kondo and RKKY interactions co-exist
- Possible unconventional superconductivity near QCP



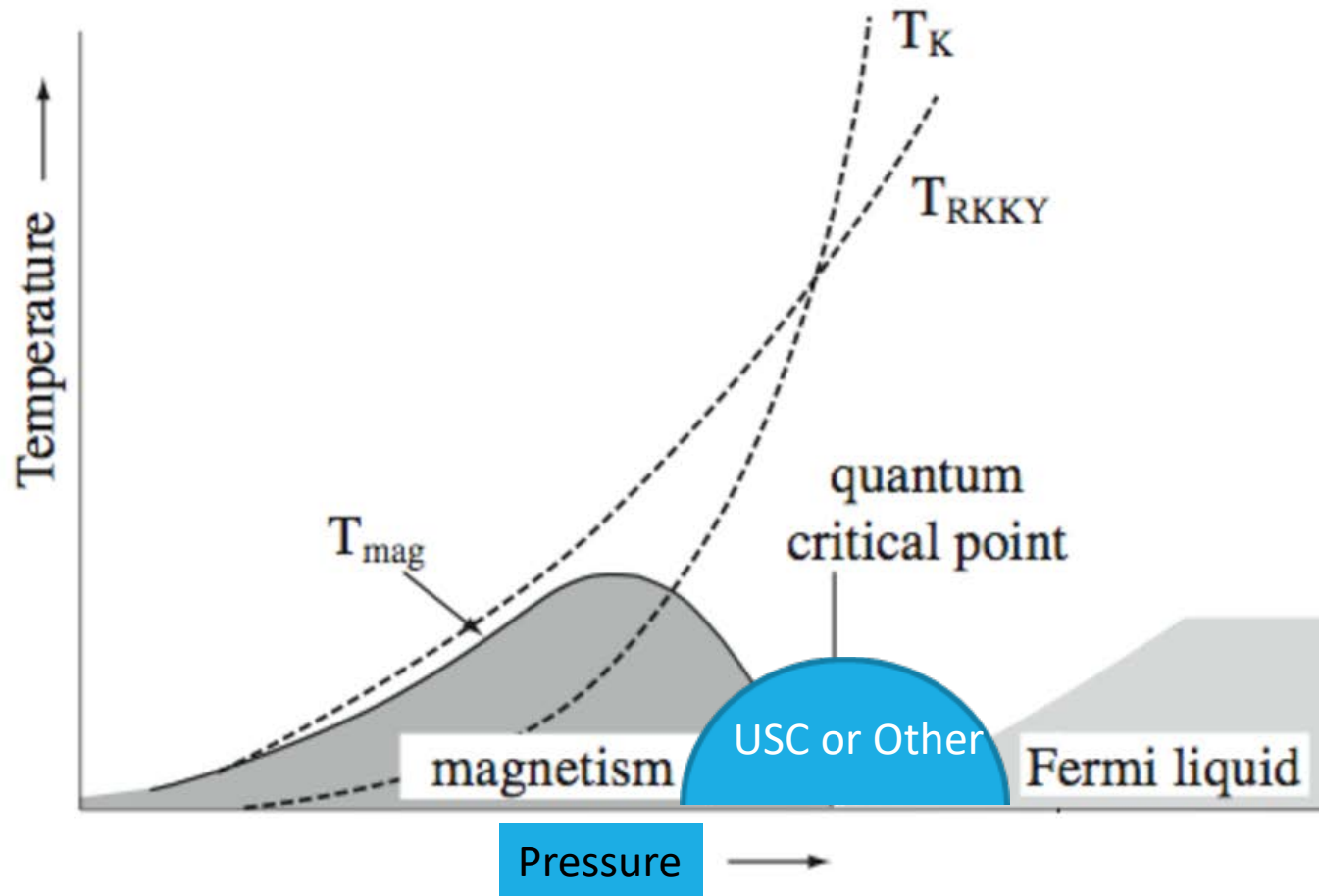
Also, increasing H , P , doping, ect.

from UNLP



QCP

- Kondo and RKKY on equal footing.
- Material can go superconducting under pressure.
- USC is similar to High Temp SC in copperates.



CeRhIn₅ goes superconducting under applied pressure

$\text{Ce}_{(1-x)}\text{Yb}_x\text{RhIn}_5$ (Heavy Fermion Material)

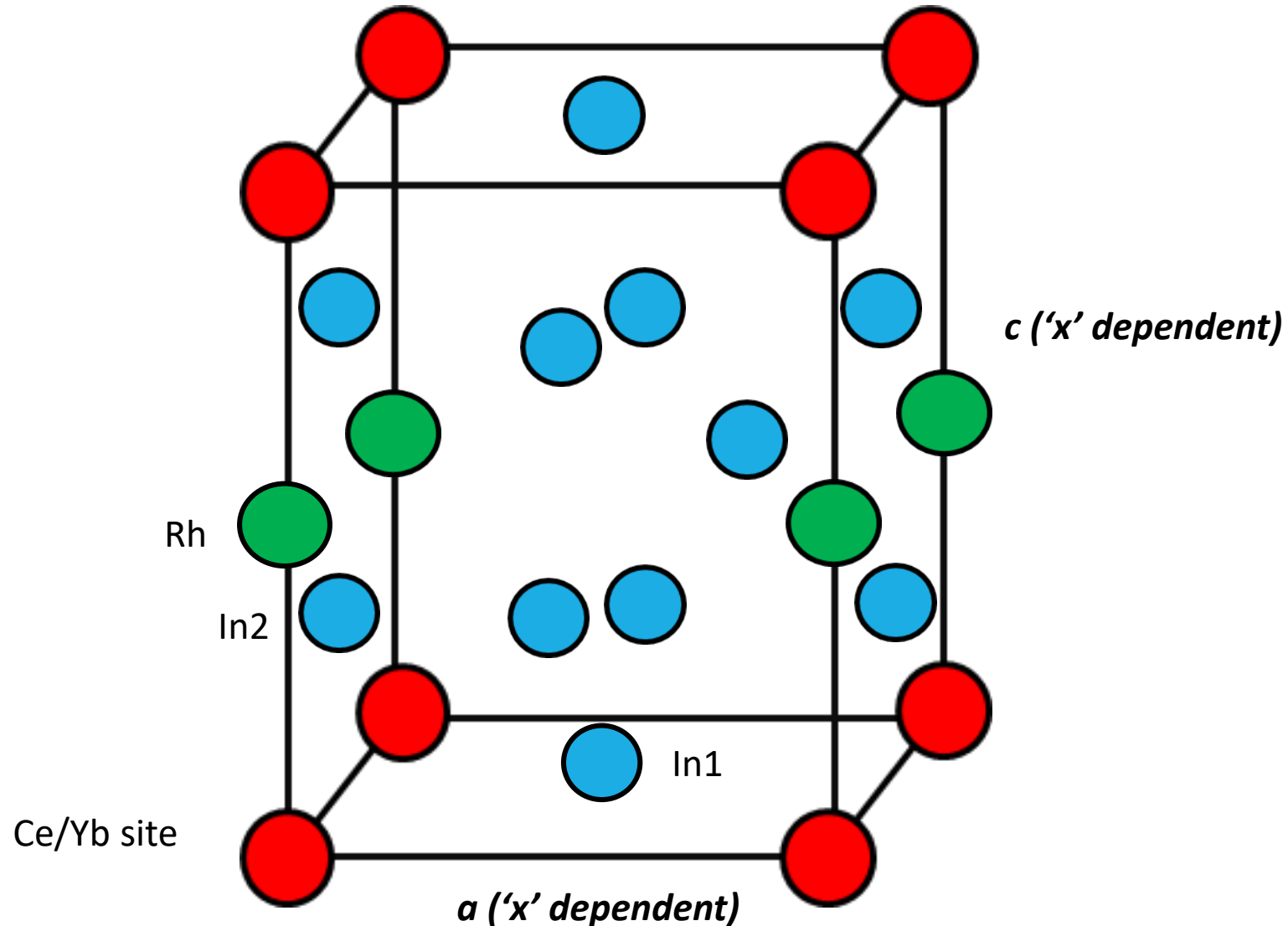
Tetragonal:

$a=b \neq c$

$\alpha=\beta=\gamma=90^\circ$

Space group:

$P 4/m m m$



Goal: $\text{Ce}_{1-x}\text{Yb}_x\text{RhIn}_5$ Magnetic Transitions

Finding the transition
(in terms of T and x)

For change to commensurate structure



Increasing x



Metallic Paramagnet ⁴

Turns antiferromagnetic

$\mathbf{k}=(\frac{1}{2},\frac{1}{2},0.297)$ ³

T=3.8 K

(incommensurate structure)

Finding

the transition

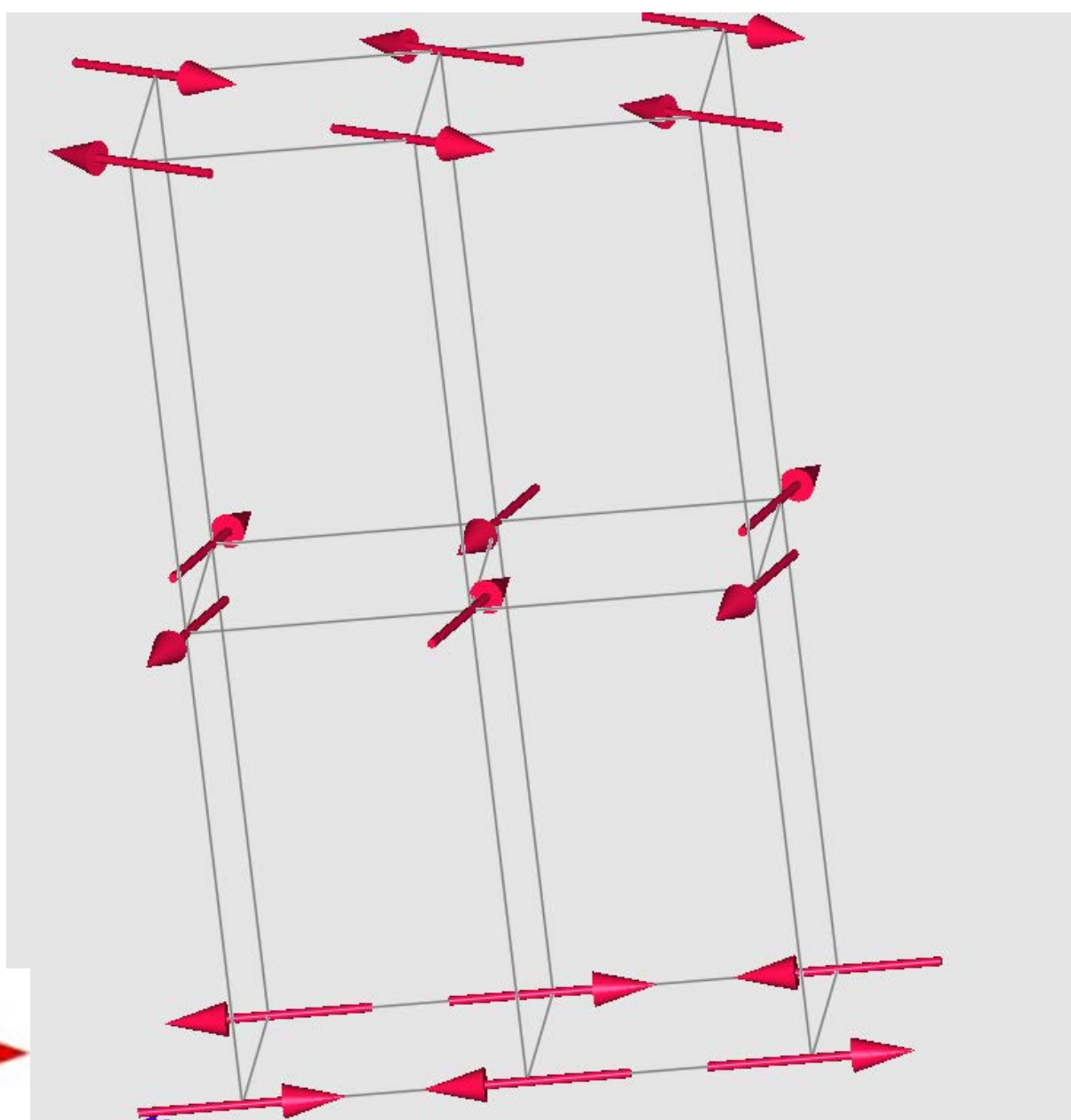
(in terms of T and x)

For magnetic ordering



³Wei Bao, P. G. Pagliuso, J. L. Sarrao, J. D. Thompson, Z. Fisk, J.W. Lynn, and R.W Erwin. *Incommensurate magnetic structure of CeRhIn5*. Phys. B 62-22

⁴Z. Bukowski, , K. Gofryk, D. Kaczorowski. *Magnetic and transport properties of YbRhIn5 and YbIn5 single crystals* . Solid State Communications 134-7.



³Wei Bao, P. G. Pagliuso, J. L. Sarrao, J. D. Thompson, Z. Fisk, J.W. Lynn, and R.W Erwin. *Incommensurate magnetic structure of CeRhIn5*. Phys. B 62-22

Goal: $\text{Ce}_{1-x}\text{Yb}_x\text{RhIn}_5$ Magnetic Transitions

Finding the transition
(in terms of T and x)

For change to commensurate structure

CeRhIn_5

Increasing x

YbRhIn_5

Metallic Paramagnet ⁴

Turns antiferromagnetic

$\mathbf{k}=(\frac{1}{2},\frac{1}{2},0.297)$ ³

T=3.8 K

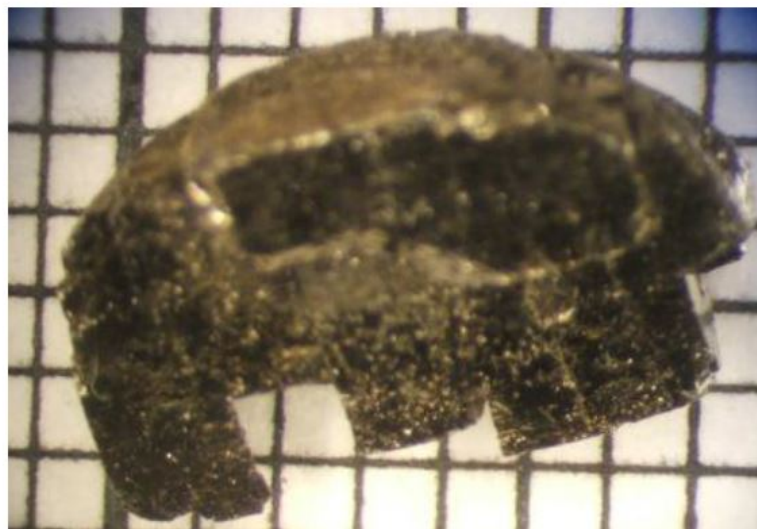
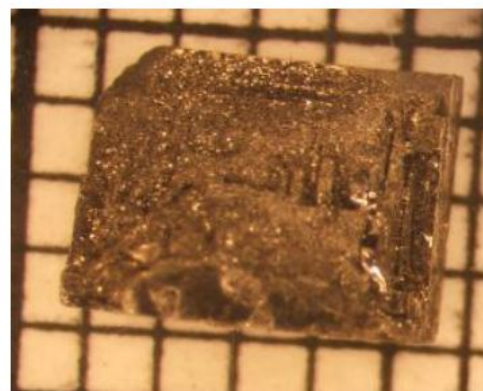
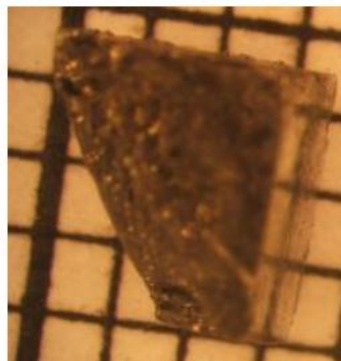
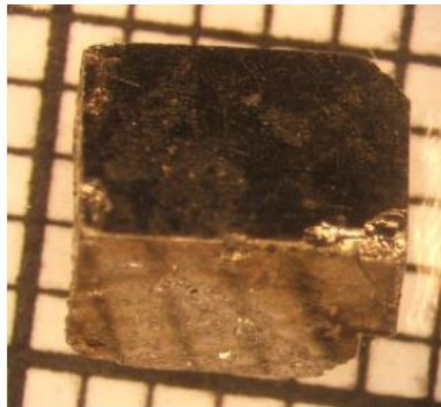
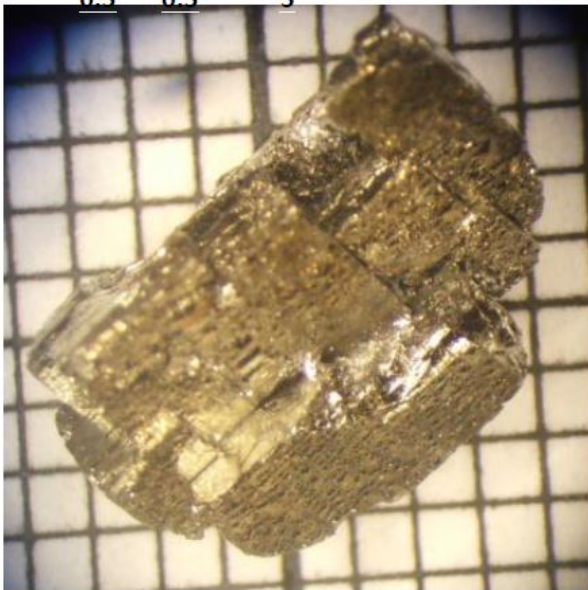
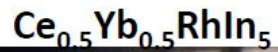
(incommensurate structure)

Finding

the transition

(in terms of T and x)

For magnetic ordering



Actual sample concentrations were not matching with the concentrations used to make these samples.

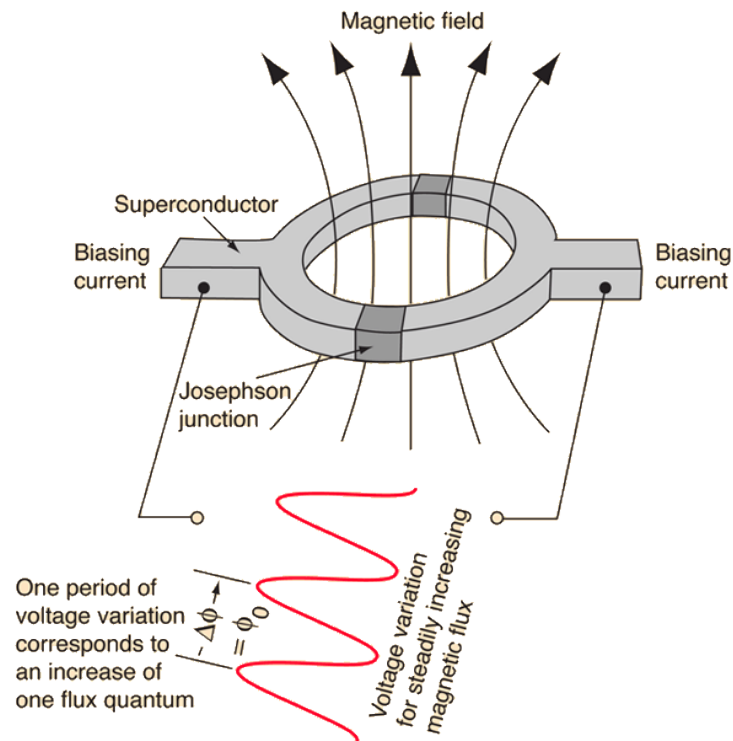
Needed a way to measure concentrations.

Made powders and headed to UMD for SQUID measurements.

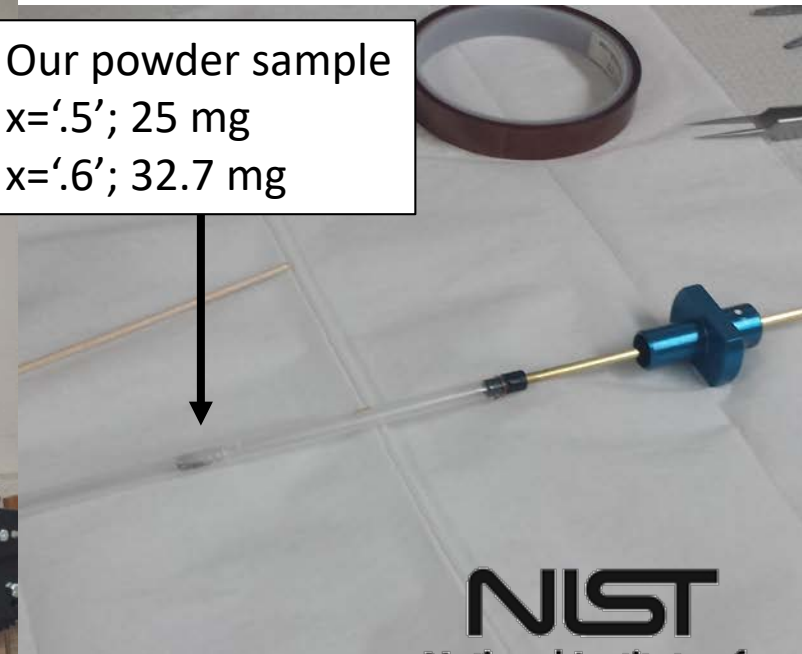
SQUID Magnetometry for measuring μ_{eff} (superconducting quantum interference device)

SENSITIVE LOW TEMP MAGNETOMETER

SQUID AT U MARYLAND COLLEGE PARK



Our powder sample
 $x=.5$; 25 mg
 $x=.6$; 32.7 mg



NIST
National Institute of
Standards and Technology
U.S. Department of Commerce

Sample reported as x='.5'

$C = 0.967 \pm 0.004$ [(emu K)/or]

Curie Temp = -43.2 ± 0.4 [K]

$\mu_{\text{eff}} = 2.7814 \pm 0.0009 \mu_B$

$x = 0.090 \pm 0.001$

$$\chi(T) = \frac{\mu_{\text{bulk}}(T)}{H * \text{moles}} = \frac{C}{T - \theta_m} - \chi_0$$

T - Temperature [K]

C - Curie Number [(emu K)/or]

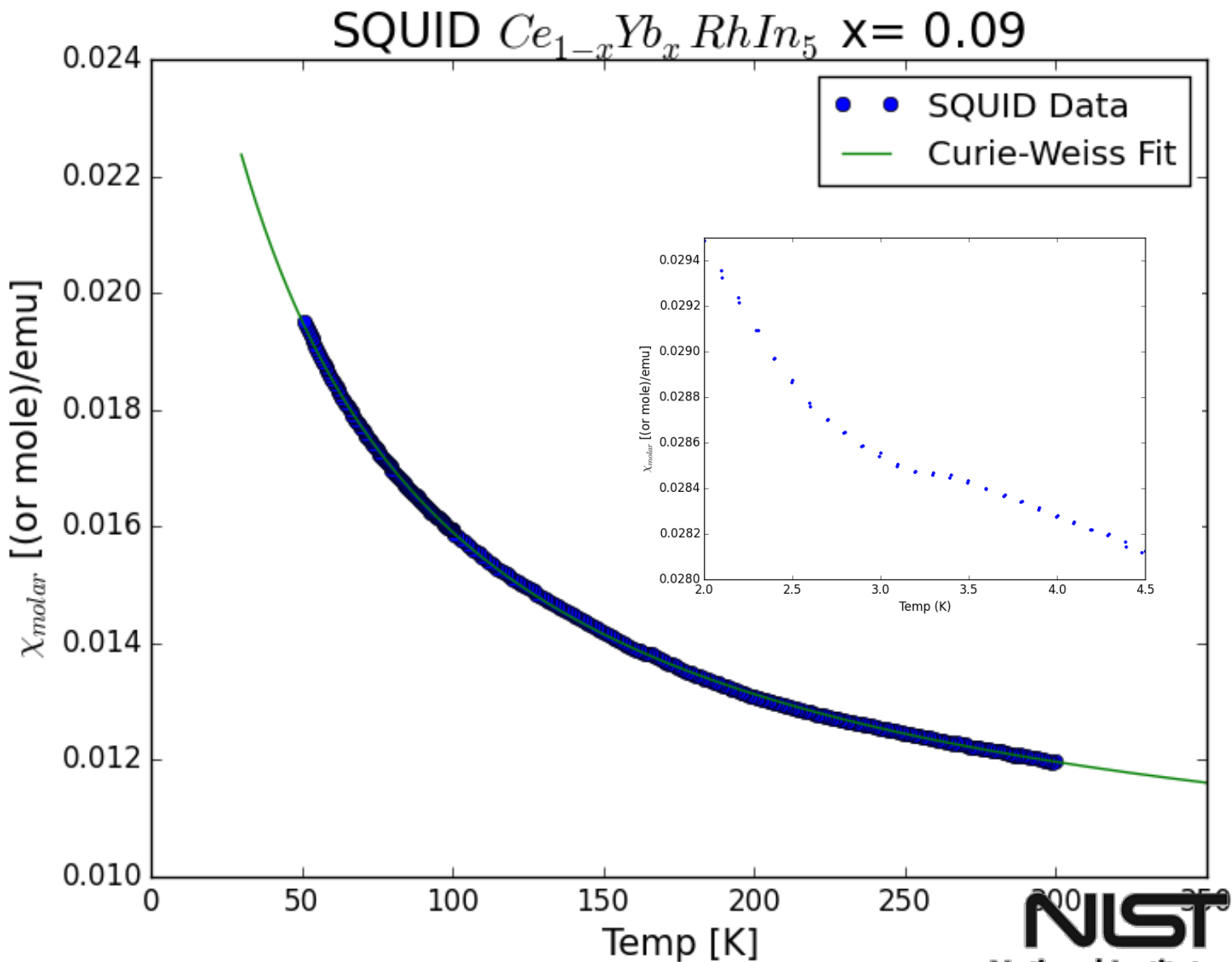
θ_m - Curie Temp. [K] (+ Ferro, - Anti)

$$C_{\text{molar}} = \frac{N_a \mu_{\text{eff}}^2(x)}{3k_B}$$

$$\mu_{\text{eff}}^2(x) = x P_{Yb^{+3}}^2 + (1 - x) P_{Ce^{+2}}^2$$

$$P_{Ce^{+3}} = 2.54 \mu_B$$

$$P_{Yb^{+3}} = 4.54 \mu_B$$



NIST

National Institute of
Standards and Technology
U.S. Department of Commerce

Sample reported as x='.6'

$C = 0.799 \pm 0.002$ [(emu K)/or]

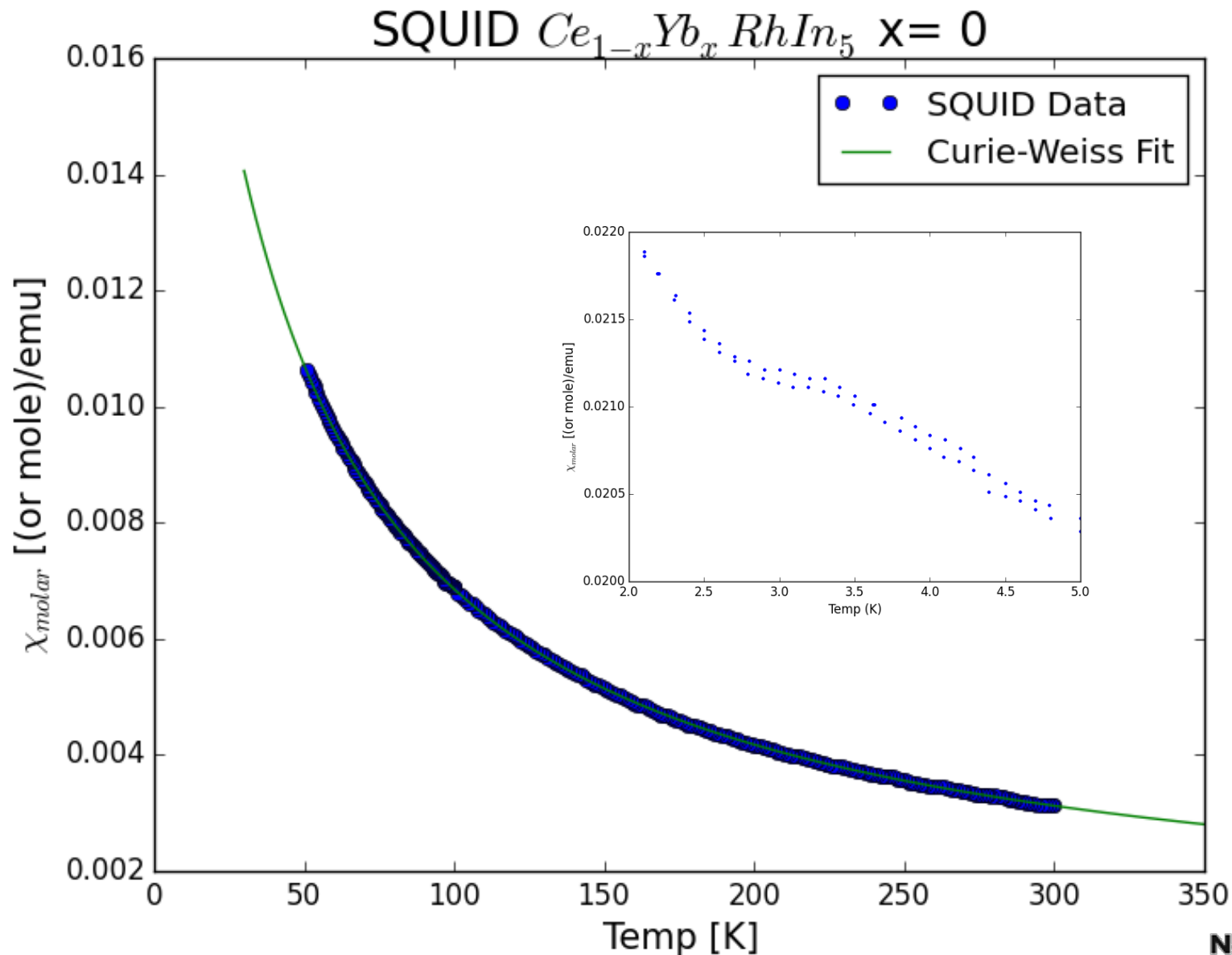
Curie Temp = -29.8 ± 0.4 [K]

$\mu_{\text{eff}} = 2.5280 \pm .0009 \mu_B$

$x = -0.0043 \pm 0.0004$

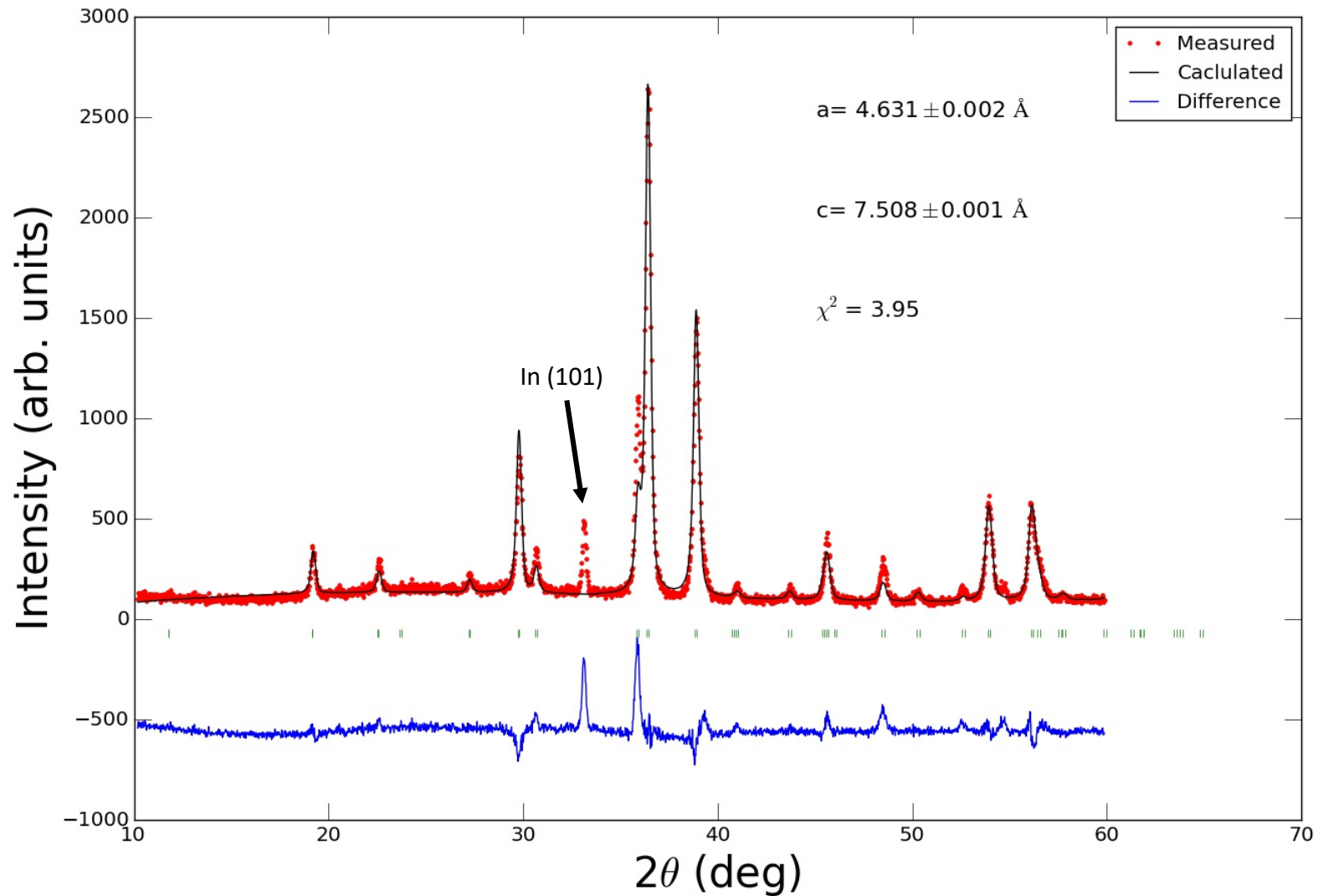


Effectively close to zero:
Only seems to be
 Ce^{+3} moment contributing.
Very small doping on the order
of <1%



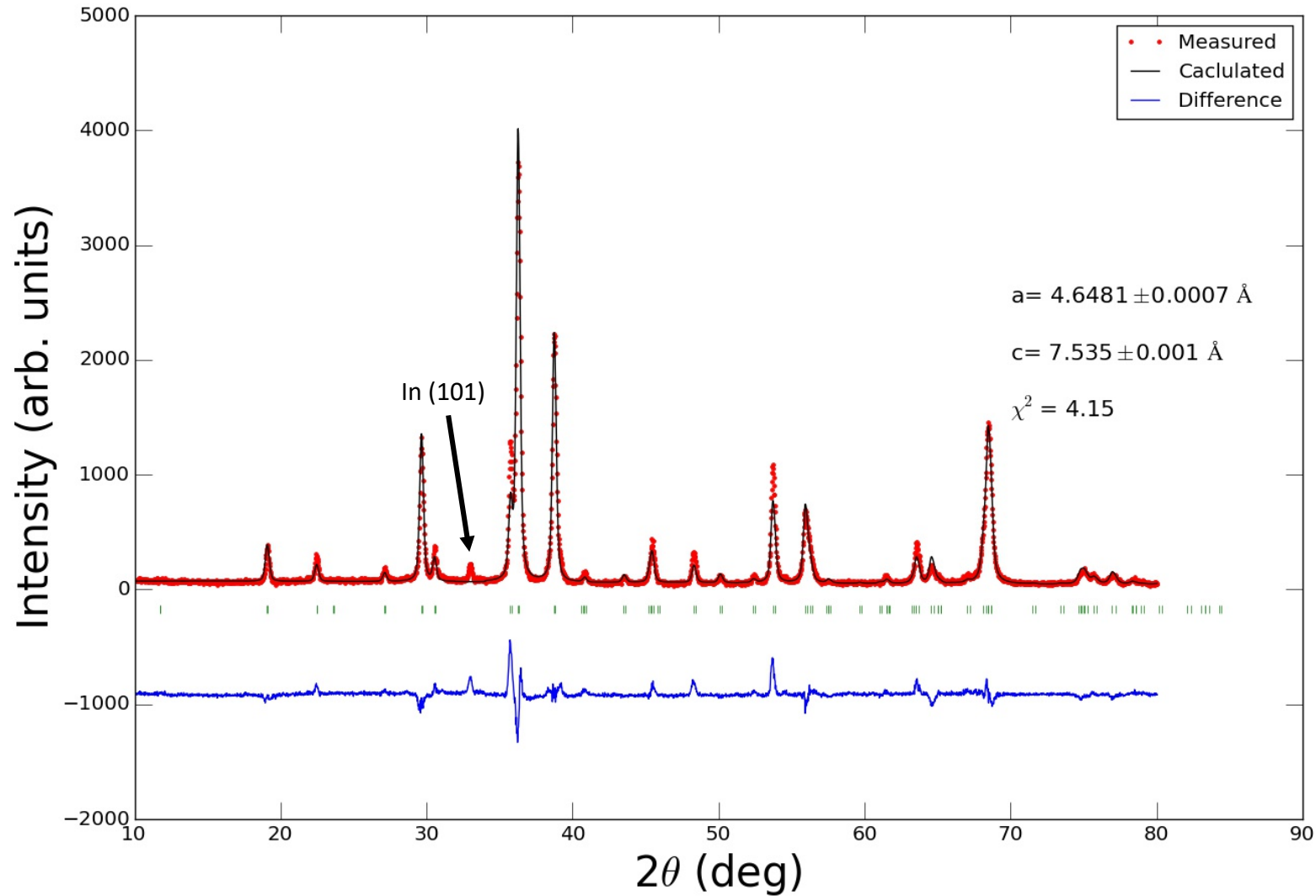
X-ray powder diffraction $\text{Ce}_1\text{Yb}_0\text{RhIn}_5$ ($x < 1\%$)

Rietveld
refinement
done with
FullProf
Software



X-ray powder diffraction $\text{Ce}_{.91}\text{Yb}_{.09}\text{RhIn}_5$ ($x=.09$)

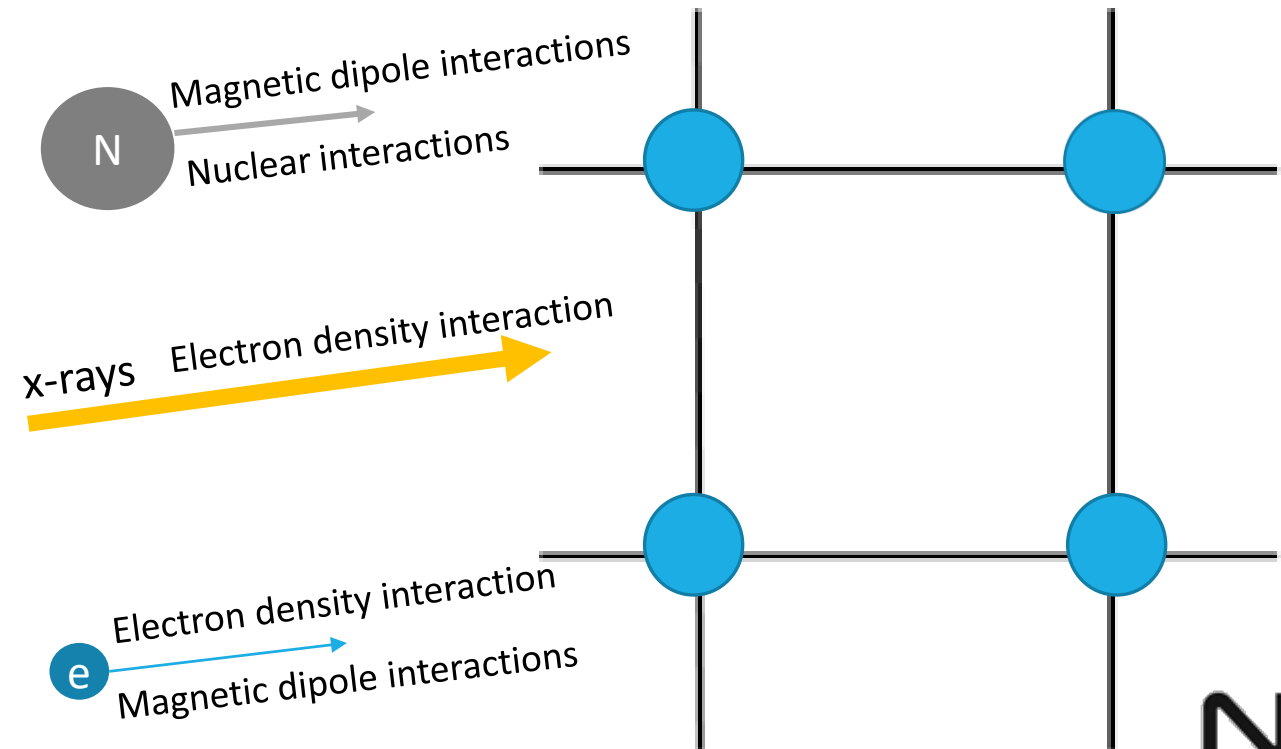
Rietveld
refinement
done with
FullProf
Software



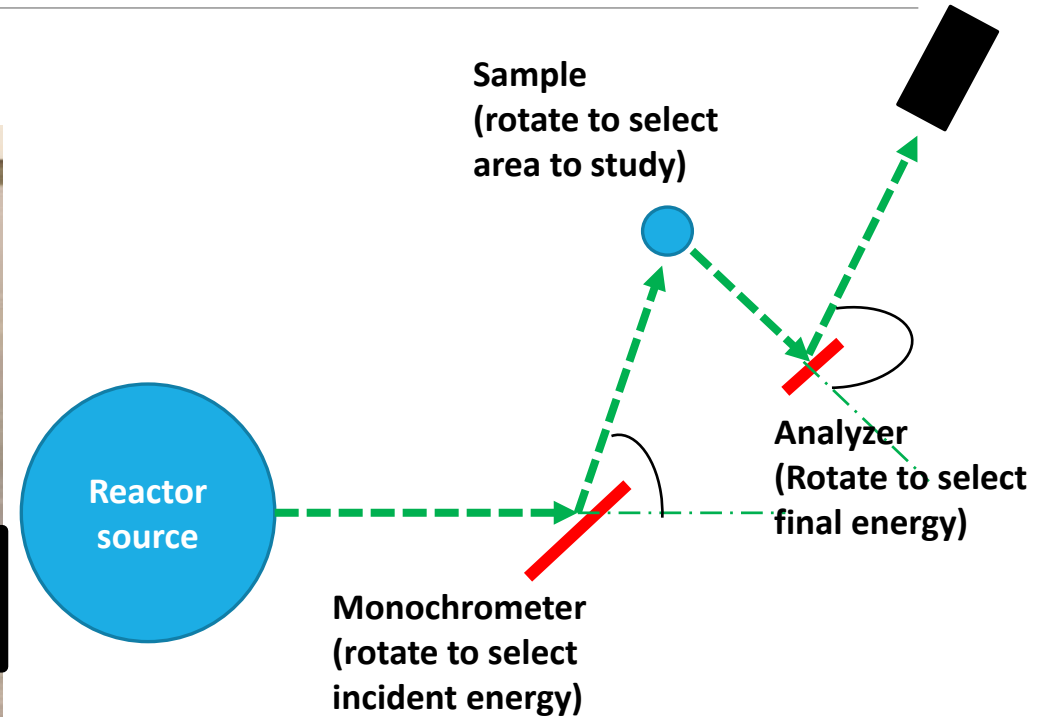
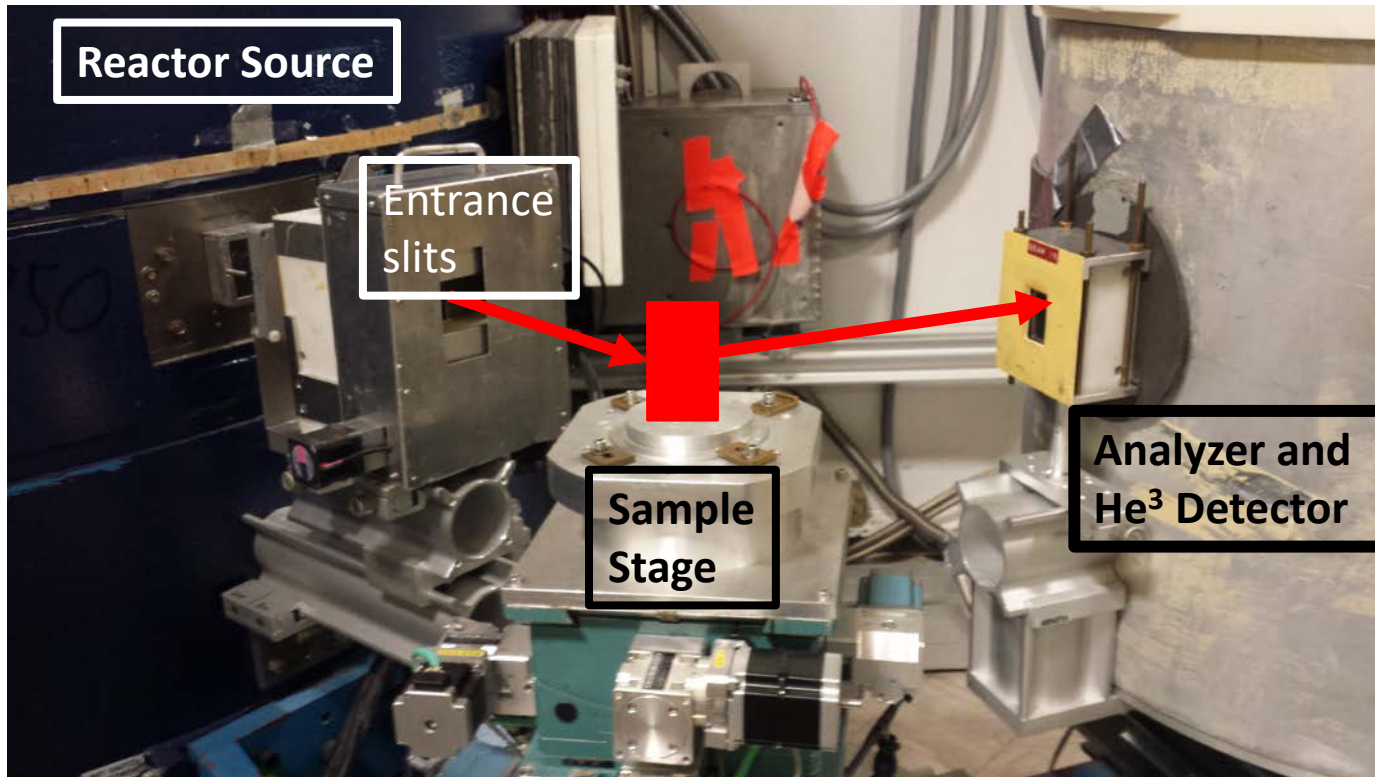
Why Neutrons?

The power of neutron scattering

- Neutrons have spin and zero charge (nuclear and magnetic scattering).
- Large penetration depth (bulk probe).
- Cross-sections good for low Z elements (Nuclear interactions).
- (More easily) Controllable energies.
- Energy scale great for dynamic interactions (inelastic scattering).

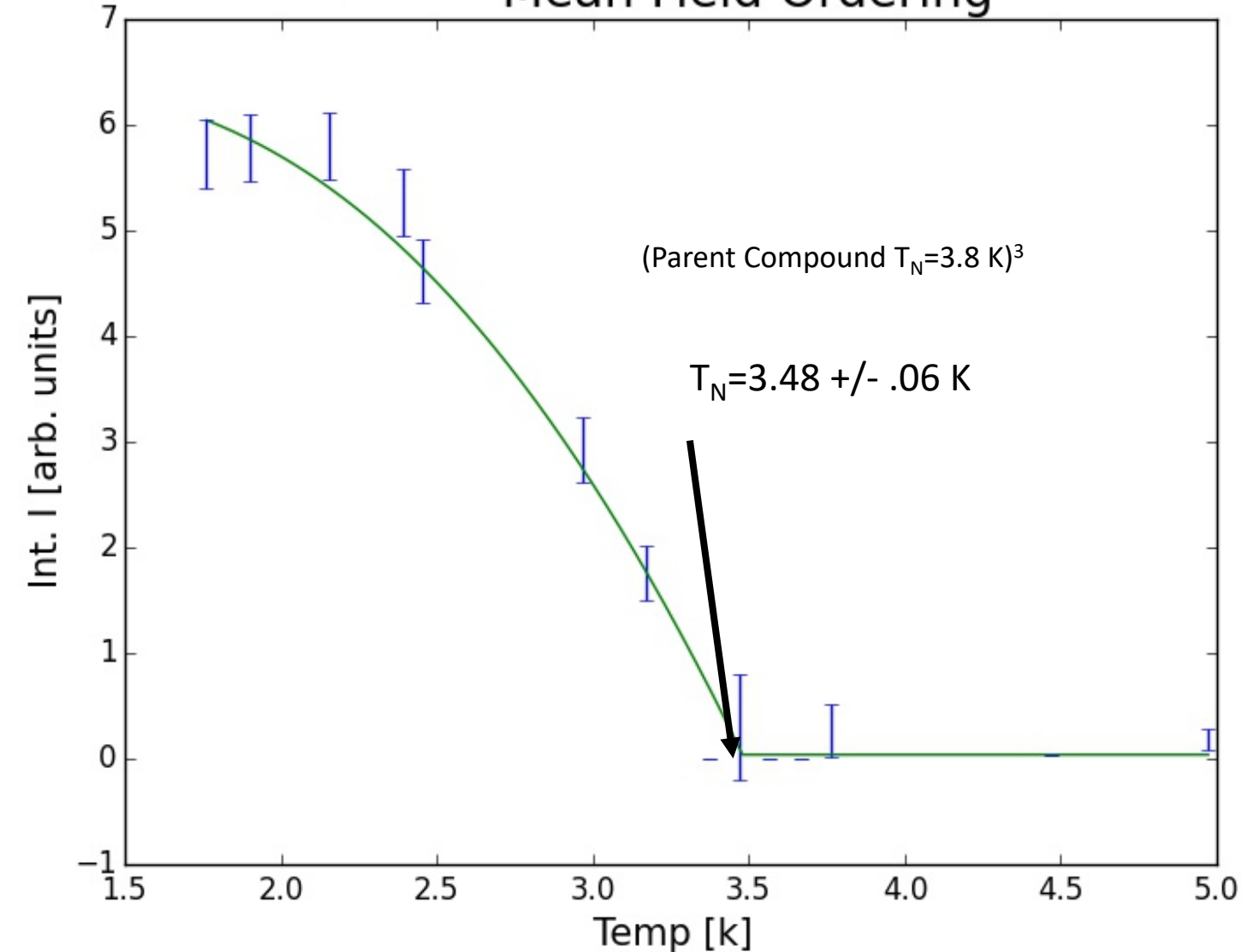


BT4 Triple Axis Spectrometer

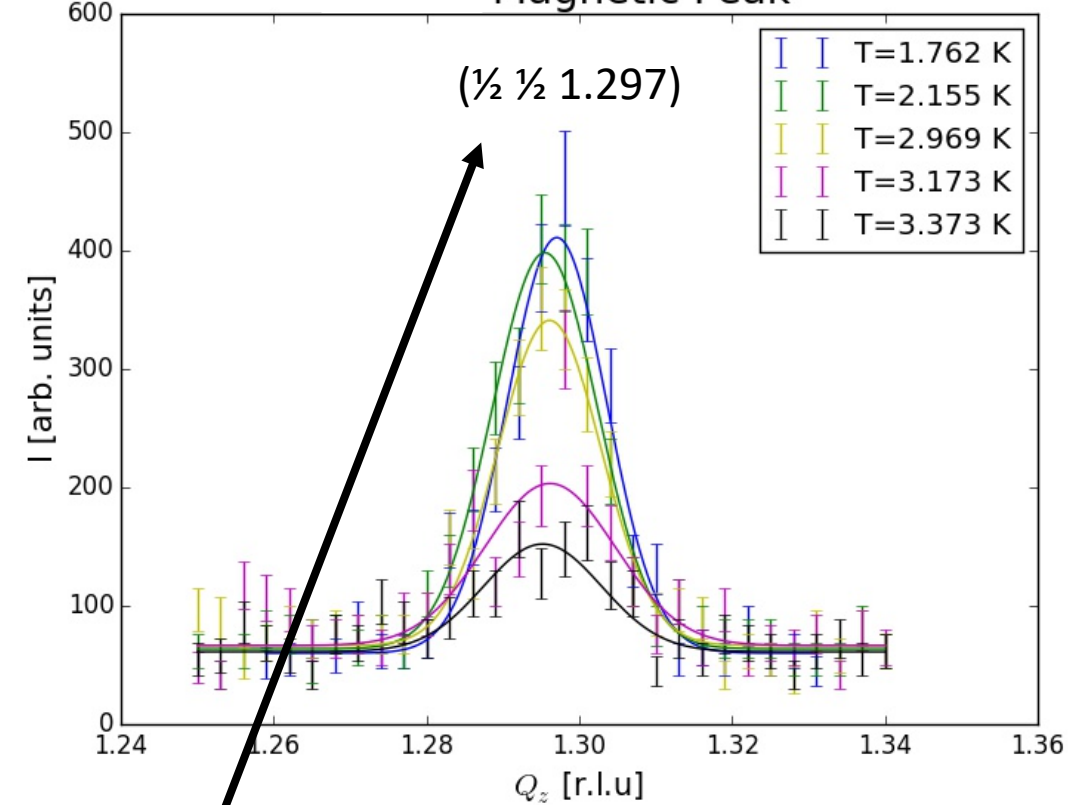


Measuring the Onset of Magnetic Ordering: $x < 1\%$

Mean Field Ordering

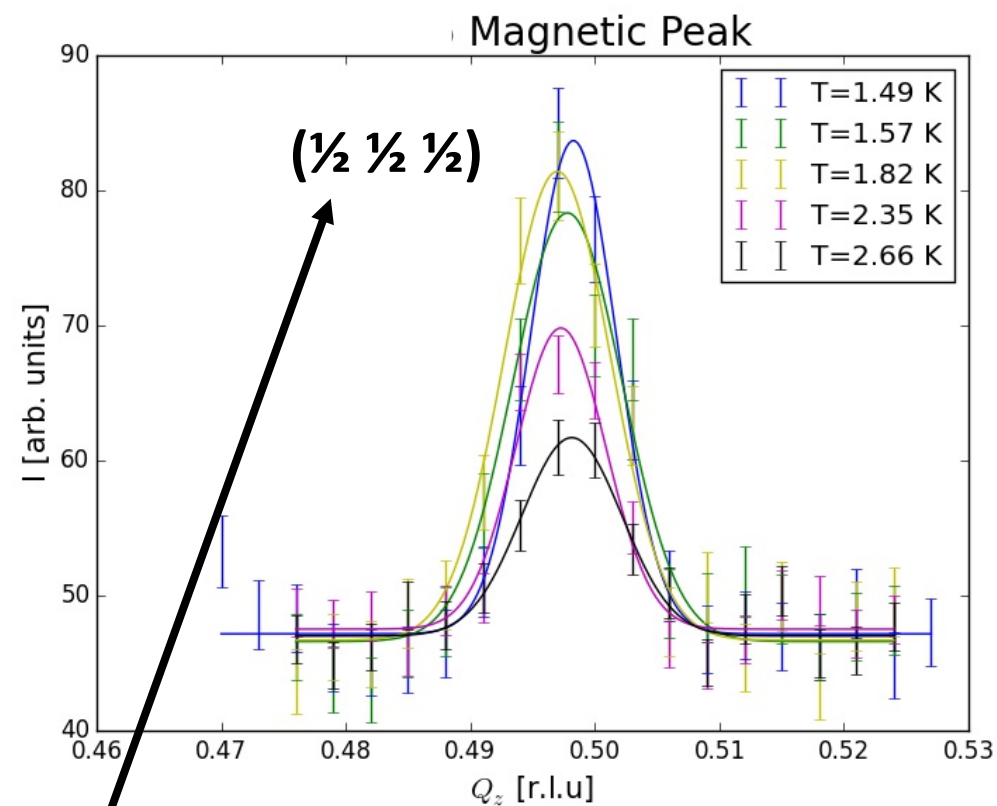
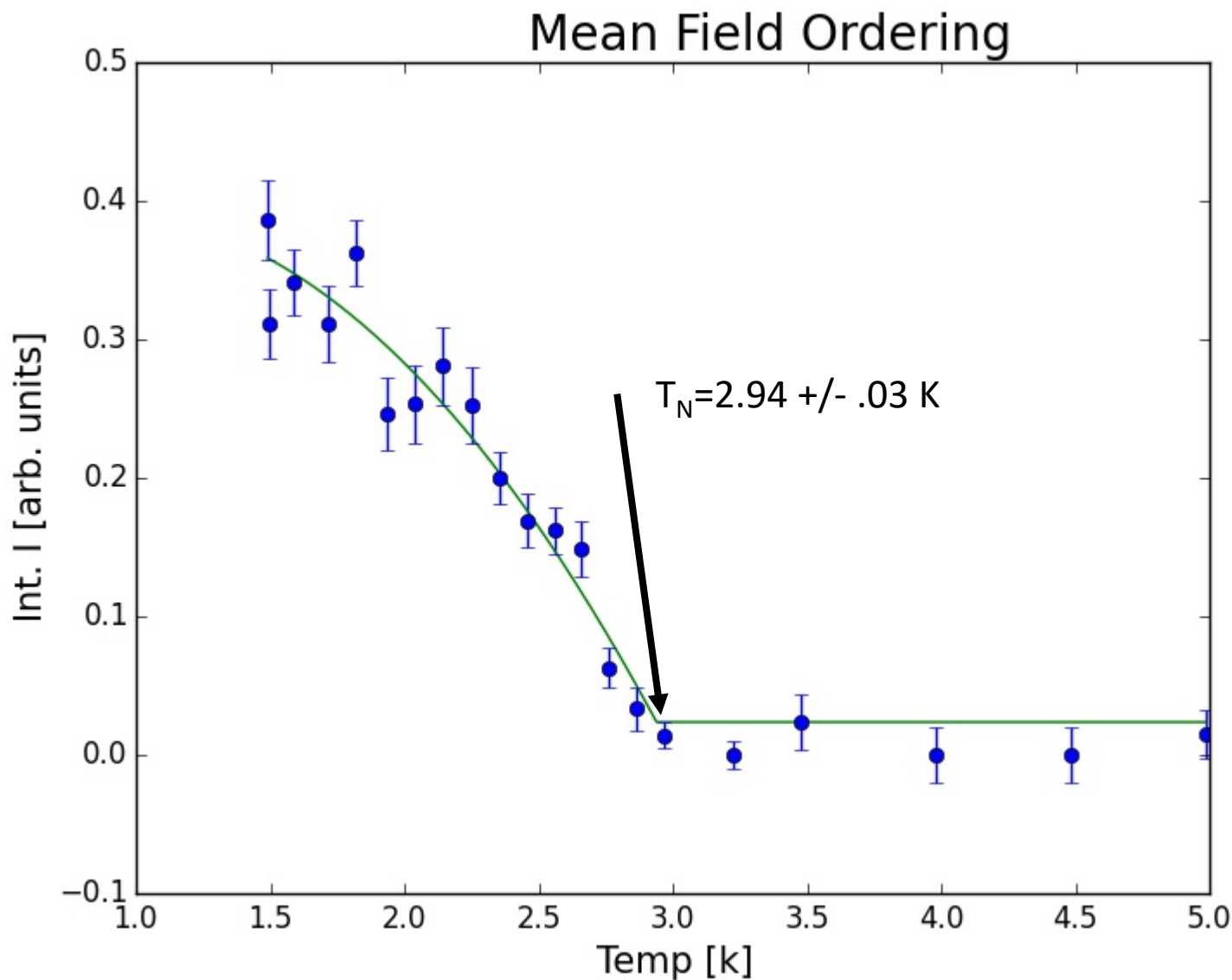


Magnetic Peak



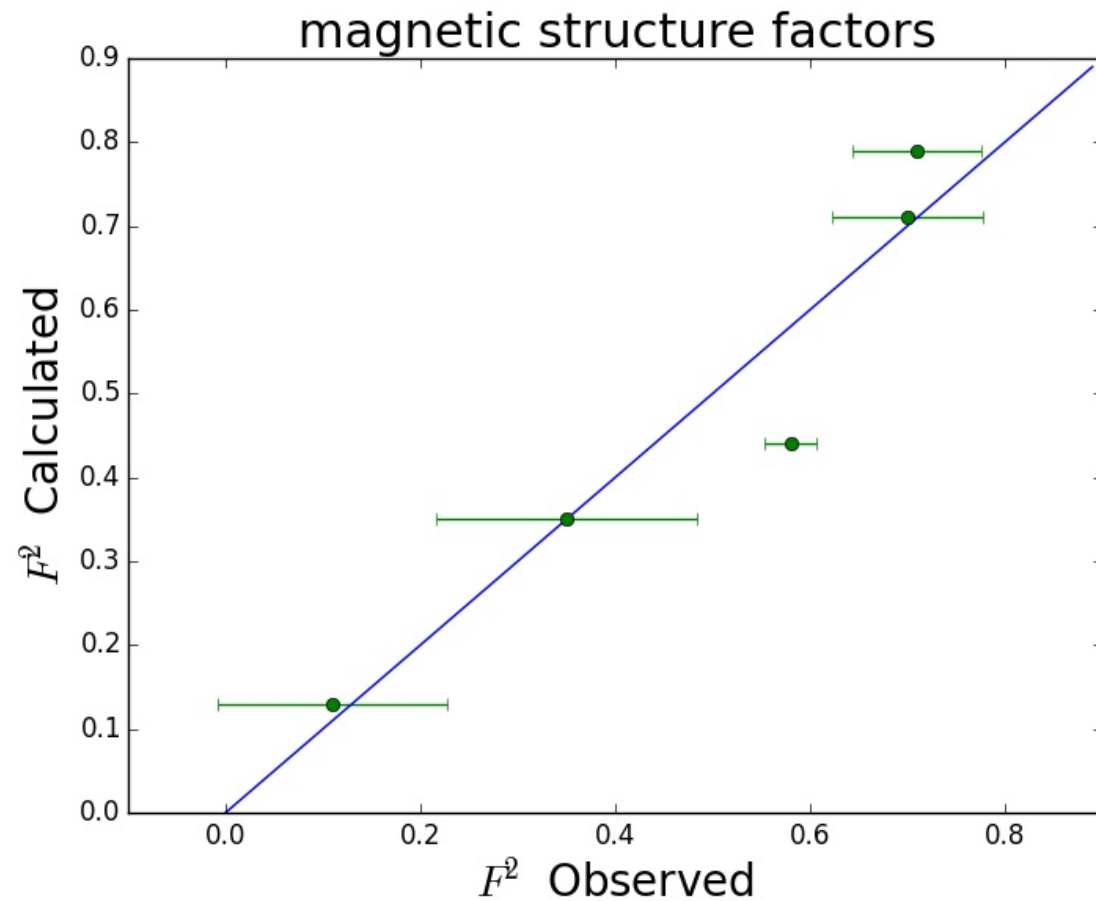
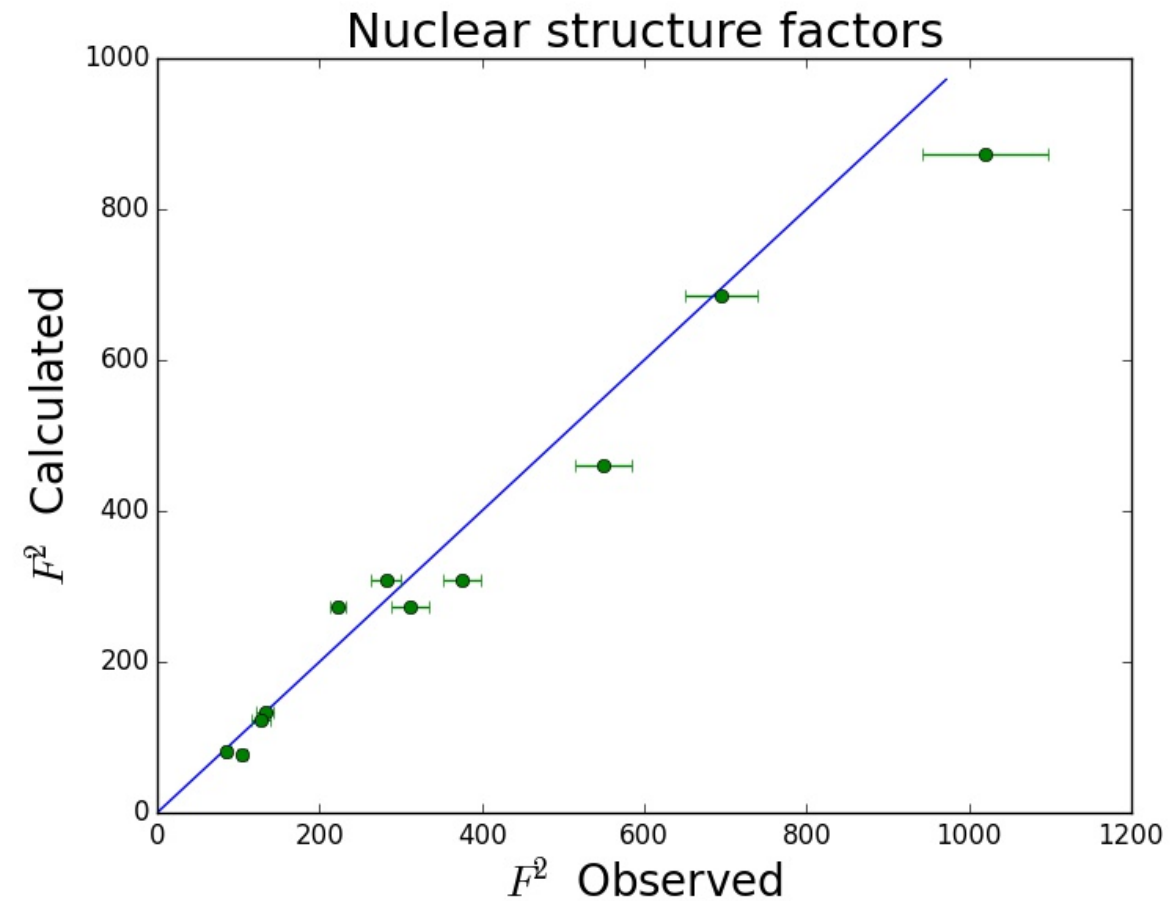
Same structure as parent compound. [(001)+k peak]

Measuring the Onset of Magnetic Ordering: $x \sim 50\%$

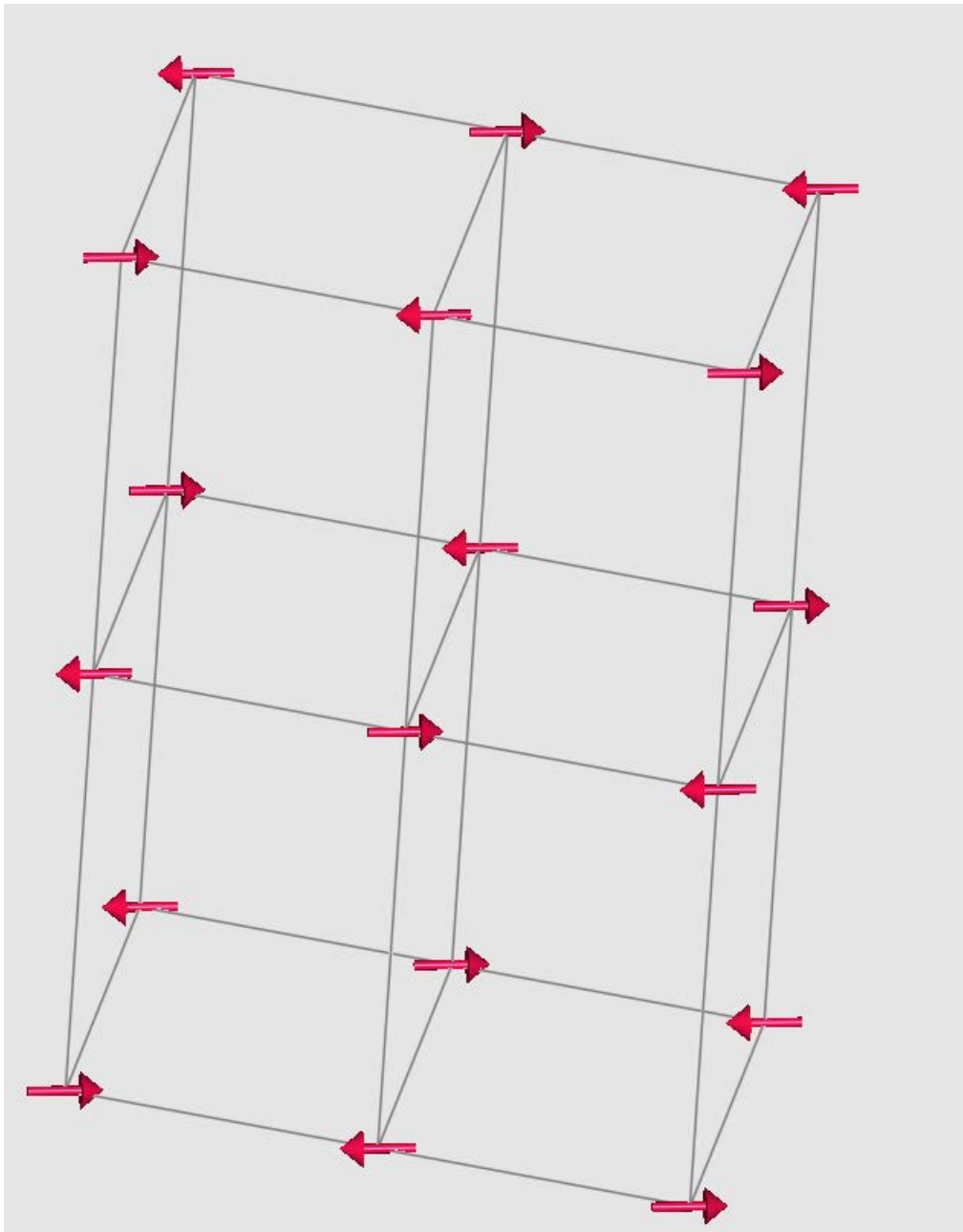


Changes from parent compound. New structure was formed!

Measuring the Magnetic Structure: $x \sim 50\%$



Each point represents the structure factor of a single diffraction peak



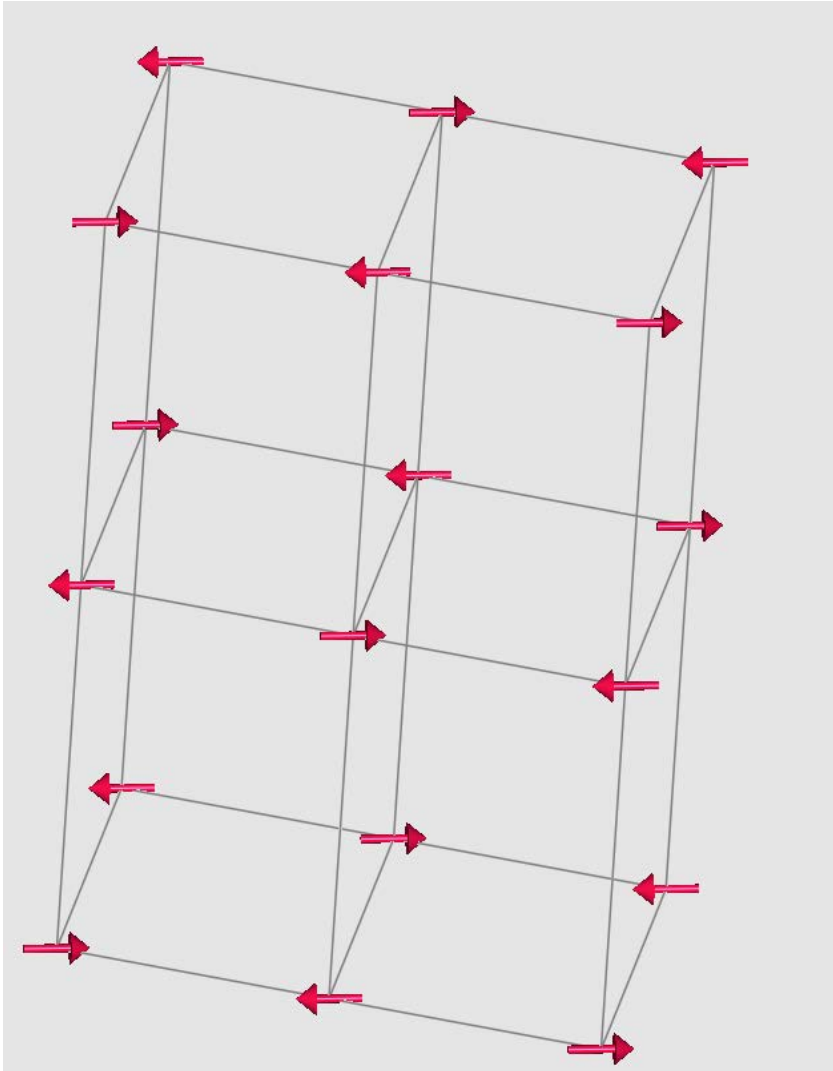
$\text{Ce}_{1-x}\text{Yb}_x\text{RhIn}_5$ $\mathbf{k}=(\frac{1}{2} \frac{1}{2} \frac{1}{2})$ structure

$$\mu_{eff} = \begin{pmatrix} .345 \pm .017 \\ 0 \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ .119 \pm .030 \\ 0 \end{pmatrix}$$

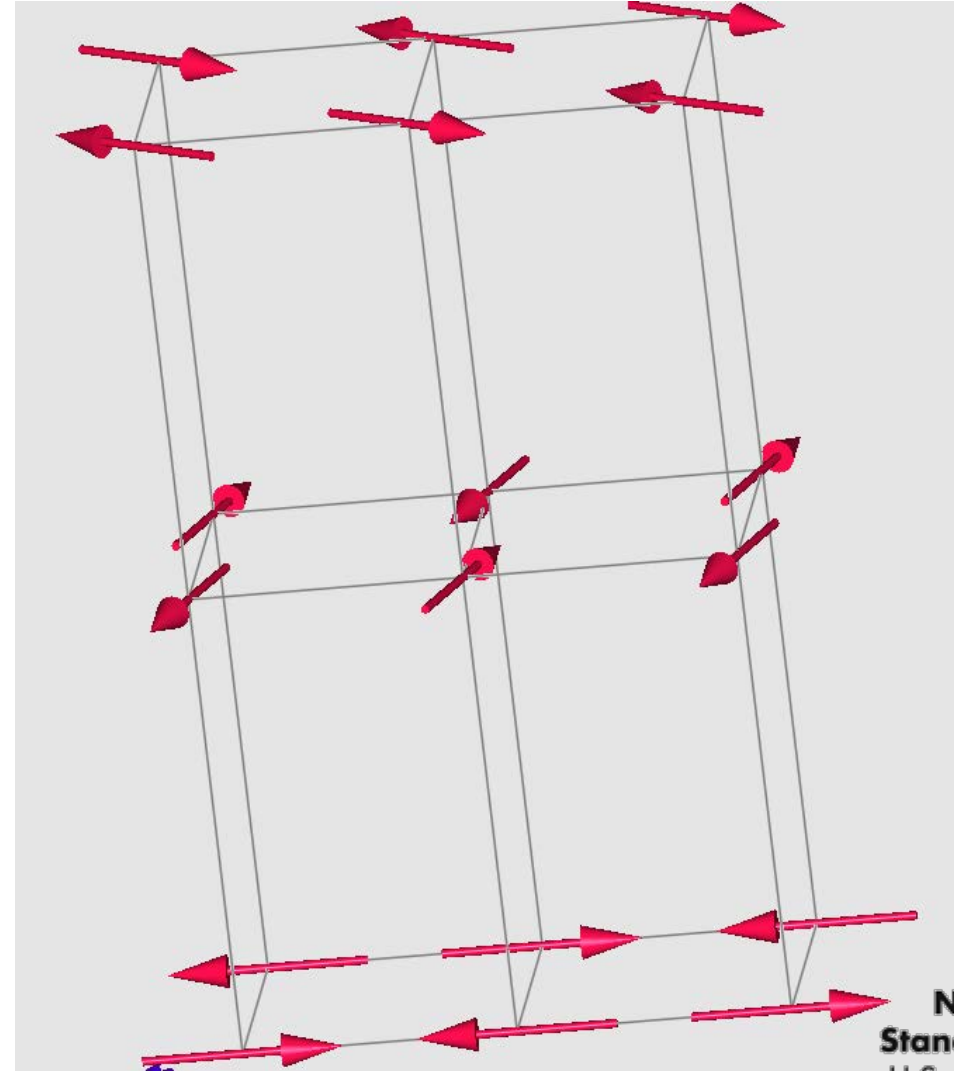
$$\mu_{eff} = .365 \pm .034 \mu_B$$

$$\theta \cong 19 \text{ degrees}$$

$\mathbf{k}=(\frac{1}{2} \frac{1}{2} \frac{1}{2})$ structure [commensurate]
Intermediate Yb concentration



$\mathbf{k}=(\frac{1}{2} \frac{1}{2} .297)$ structure [spiral]
Low Yb concentration



Conclusion of $\text{Ce}_{1-x}\text{Yb}_x\text{RhIn}_5$

- We measured properties of $\text{Ce}_{1-x}\text{Yb}_x\text{RhIn}_5$ using a combination SQUID, XRD, and Neutron Scattering
- We found a limited solubility of Yb into CeRhIn_5 , which needs to be better understood to continue this study.
- Results:
 1. At low Yb concentrations, these compounds have a lower ordering temperature.
 2. At intermediate Yb concentrations, the magnetic structure changes from incommensurate to commensurate.
 3. A new magnetic structure was solved for these intermediate concentration.
- Future work :
 1. Apply pressure and magnetic field at low temperatures to induce new interesting phase transitions.
 2. Better measurements of the concentrations in these samples.
 3. Study why the magnetic structure changes with Yb concentration.
 4. Start to form a complete phase diagram from experiments to make better theories on how unconventional superconductivity works

A big thanks to:

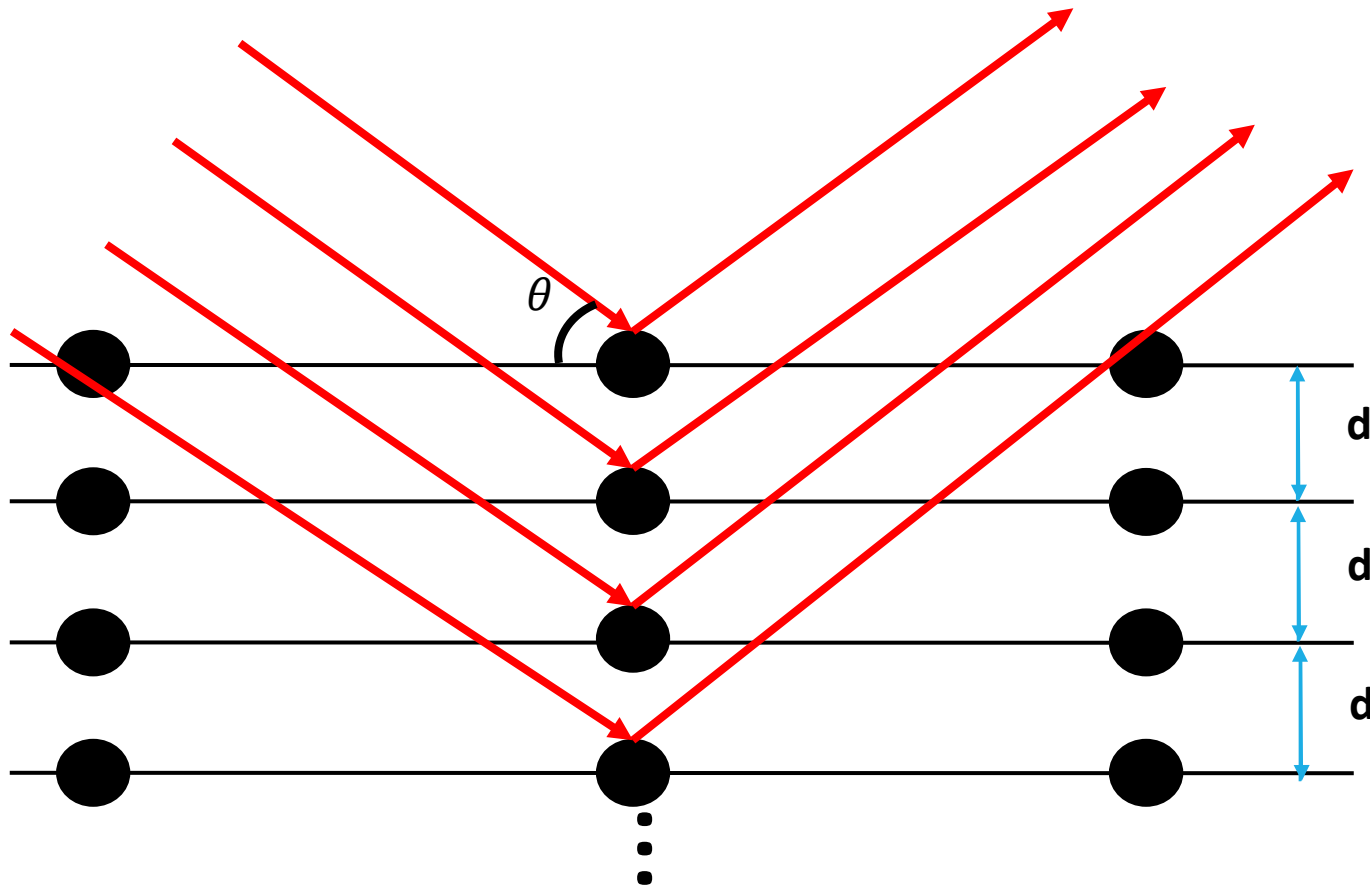
- NSF
- Steve Disseler
- William Ratcliff
- Julie Borchers
- Joseph Lesniewski
- Arnold Rubinshtein (MML)
- Shanta Ranjan Saha (UMD)
- Brian Maple (UC San Diego)
- Sooyoung Jang (UC San Diego)

References and Citations

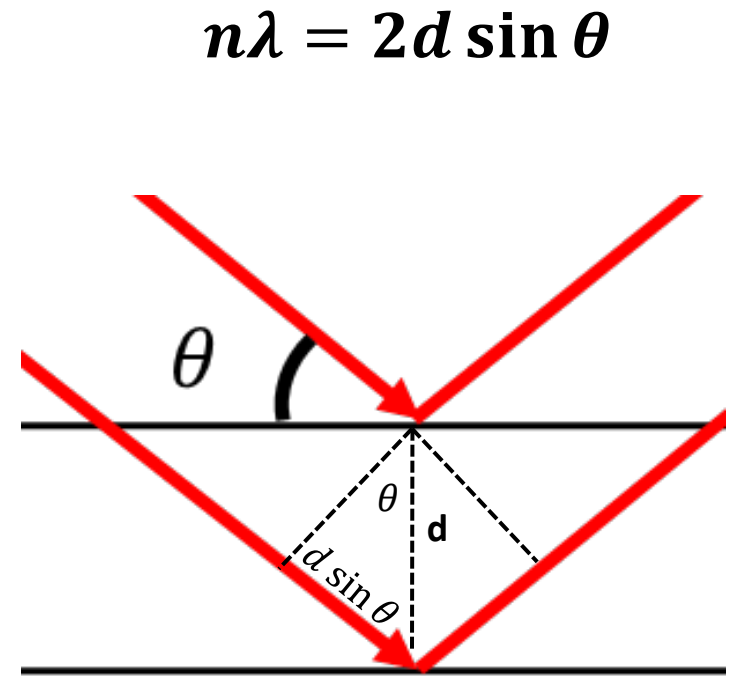
- Wei Bao, P. G. Pagliuso, J. L. Sarrao, J. D. Thompson, Z. Fisk, J. W. Lynn, and R. W. Erwin. *Incommensurate magnetic structure of CeRhIn5*. **Phys. B** **62-22**
- Z. Bukowski, K. Gofryk, D. Kaczorowski. *Magnetic and transport properties of YbRhIn5 and YbIrIn5 single crystals*. **Solid State Communications** **134-7**
- Tuson Park, F. Ronning, H. Q. Yuan, M. B. Salamon, R. Movshovich, J. L. Sarrao & J. D. Thompson. *Hidden magnetism and quantum criticality in the heavy fermion superconductor CeRhIn5*. **Nature** **440**
- P. Coleman. *Heavy Fermions: electrons at the edge of magnetism*. Rutgers.
- Gen Shirane, Stephen M. Shapiro, John M. Tranquada. *Neutron Scattering with a Triple-Axis Spectrometer*. Cambridge.
- Neil W. Ashcroft, N. David Mermin. *Solid State Physics*. Brooks/Cole.



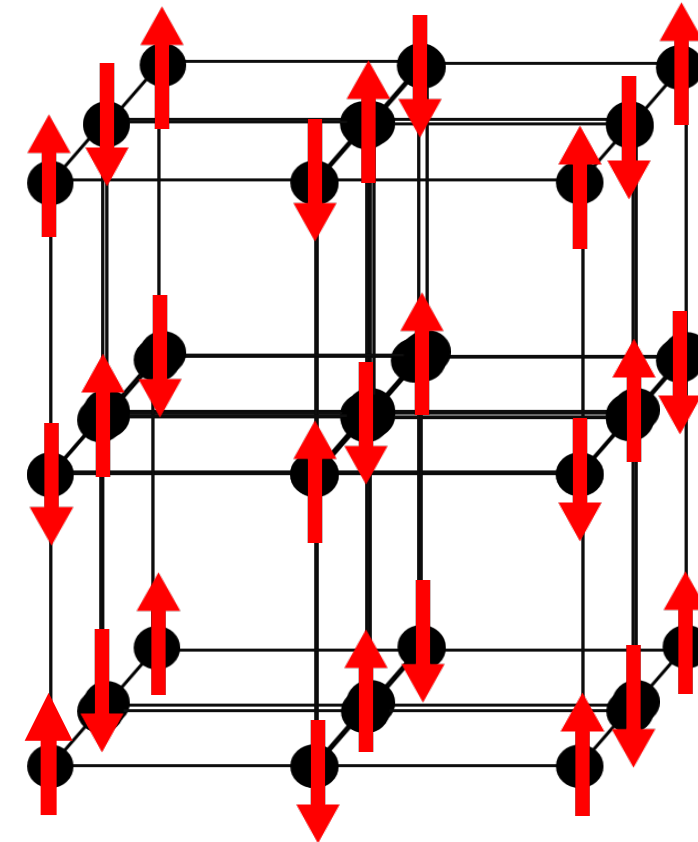
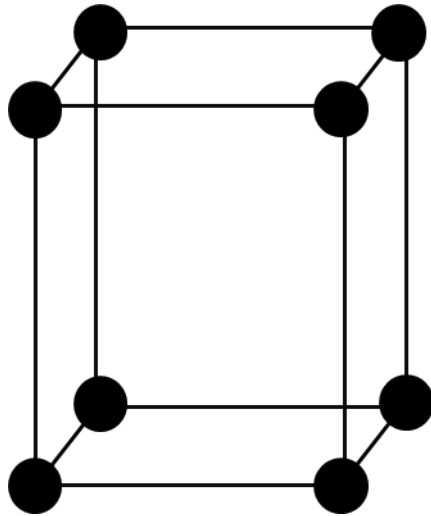
Bragg's Law for Crystal Diffraction



...



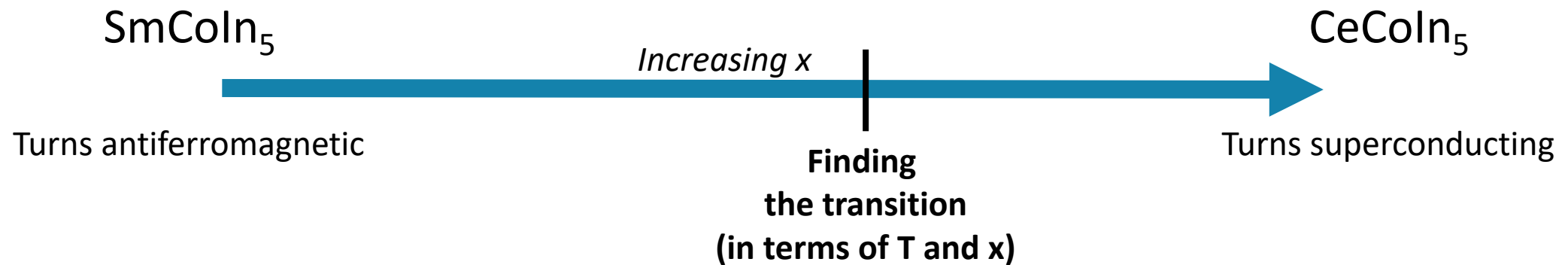
Nuclear vs. Magnetic Unit Cell in Neutron Scattering



$$\mathbf{k} = (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$$

(repeats every $2a, 2b,$ and $2c$)

Original Goal: $\text{Sm}_{1-x}\text{Ce}_x\text{CoIn}_5$



$\text{Sm}_{(1-x)}\text{Ce}_x\text{CoIn}_5$ (Heavy Fermion Material)

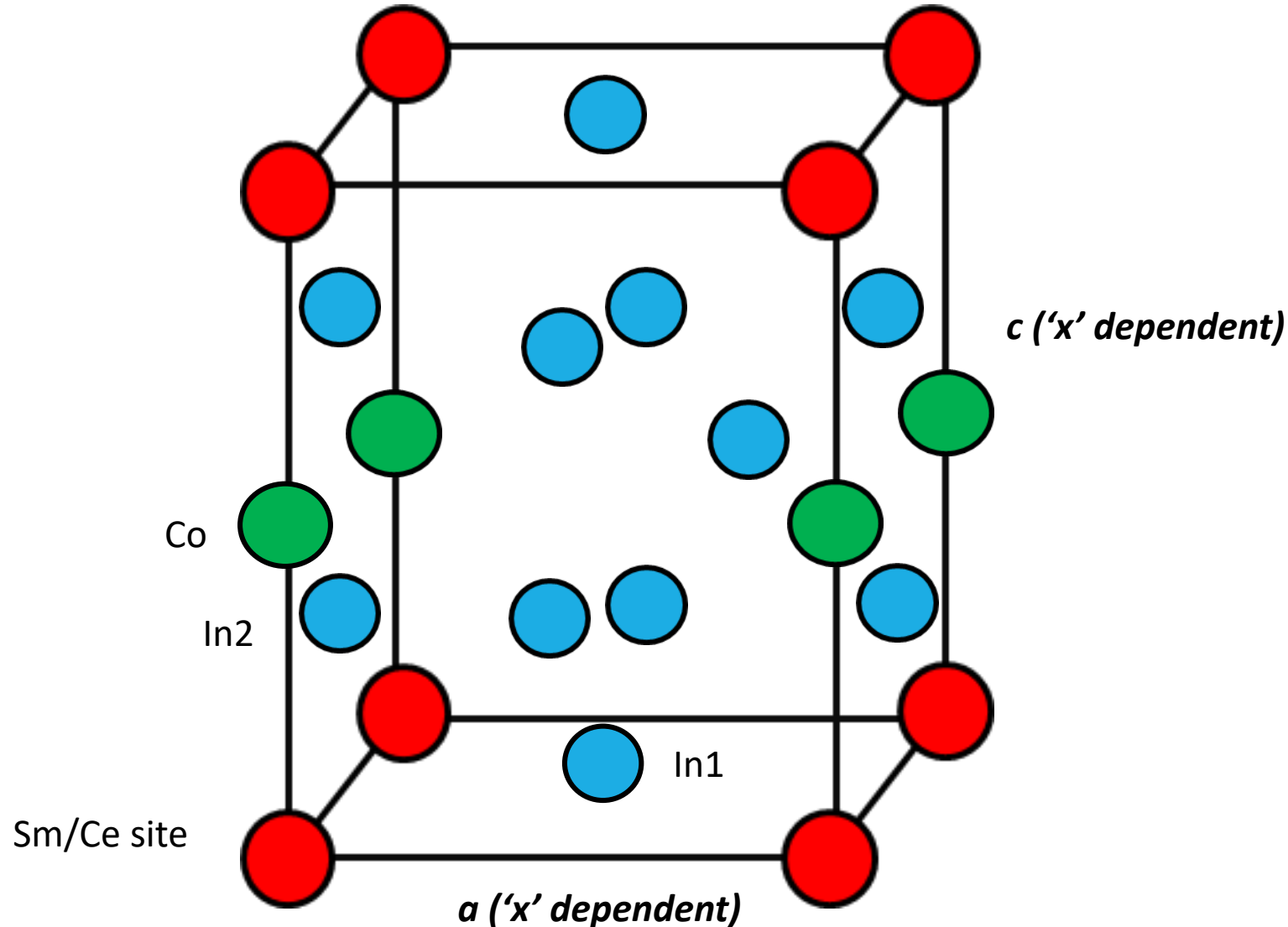
Tetragonal:

$a=b \neq c$

$\alpha=\beta=\gamma=90^\circ$

Space group:

$P 4/m m m$

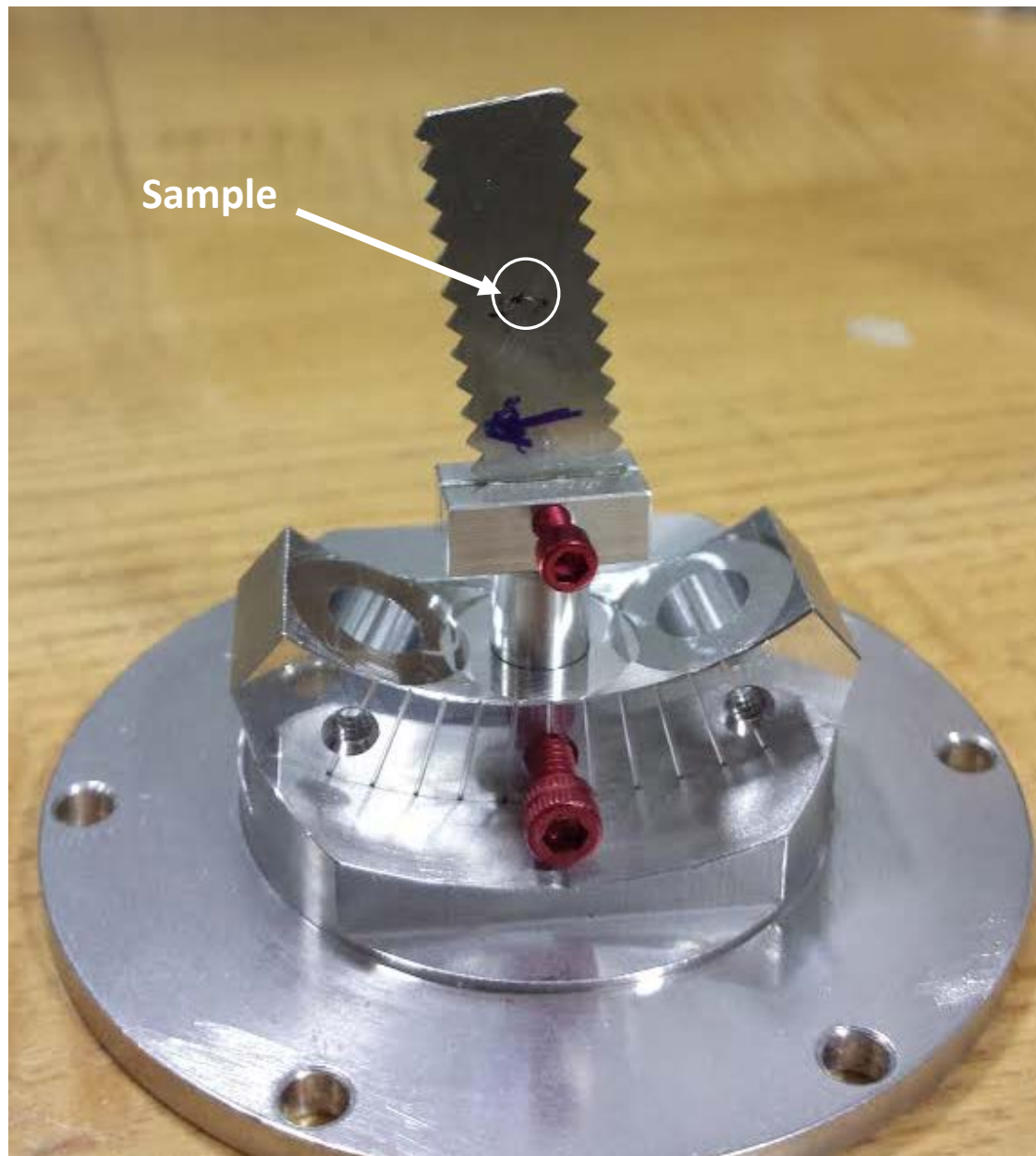


Measured Parameters (x-ray)

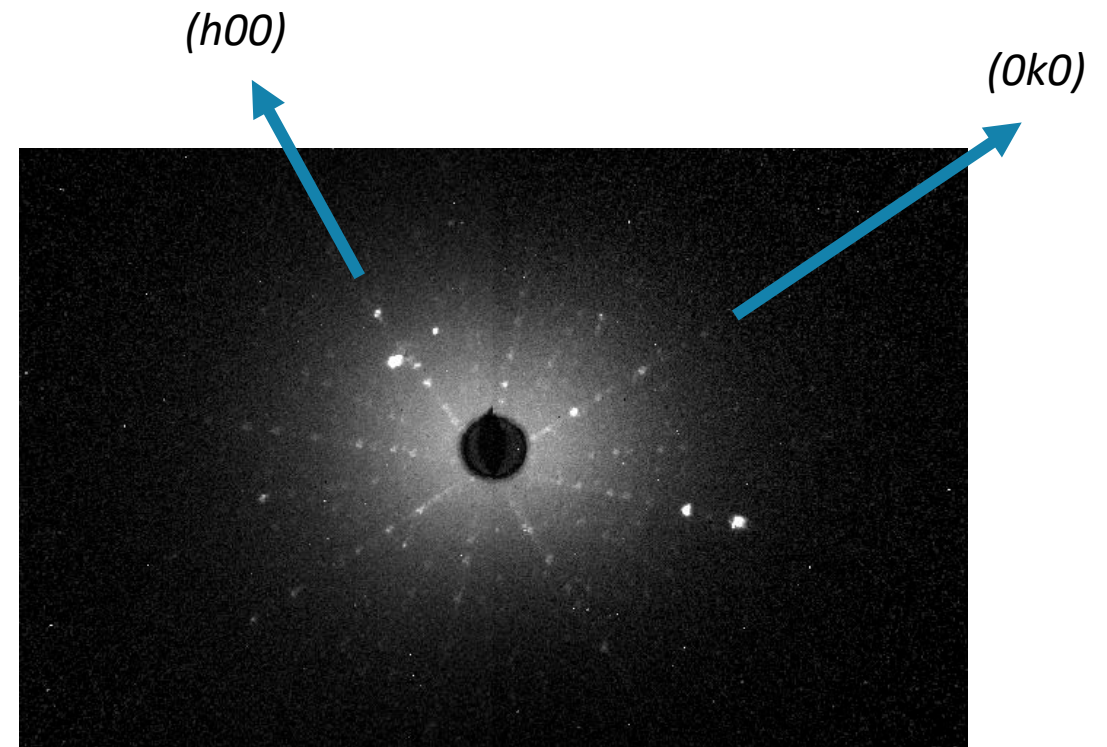
($x=0$ powder)

$a = 4.5798 \pm .0001 \text{ \AA}$

$c = 7.4708 \pm .0002 \text{ \AA}$

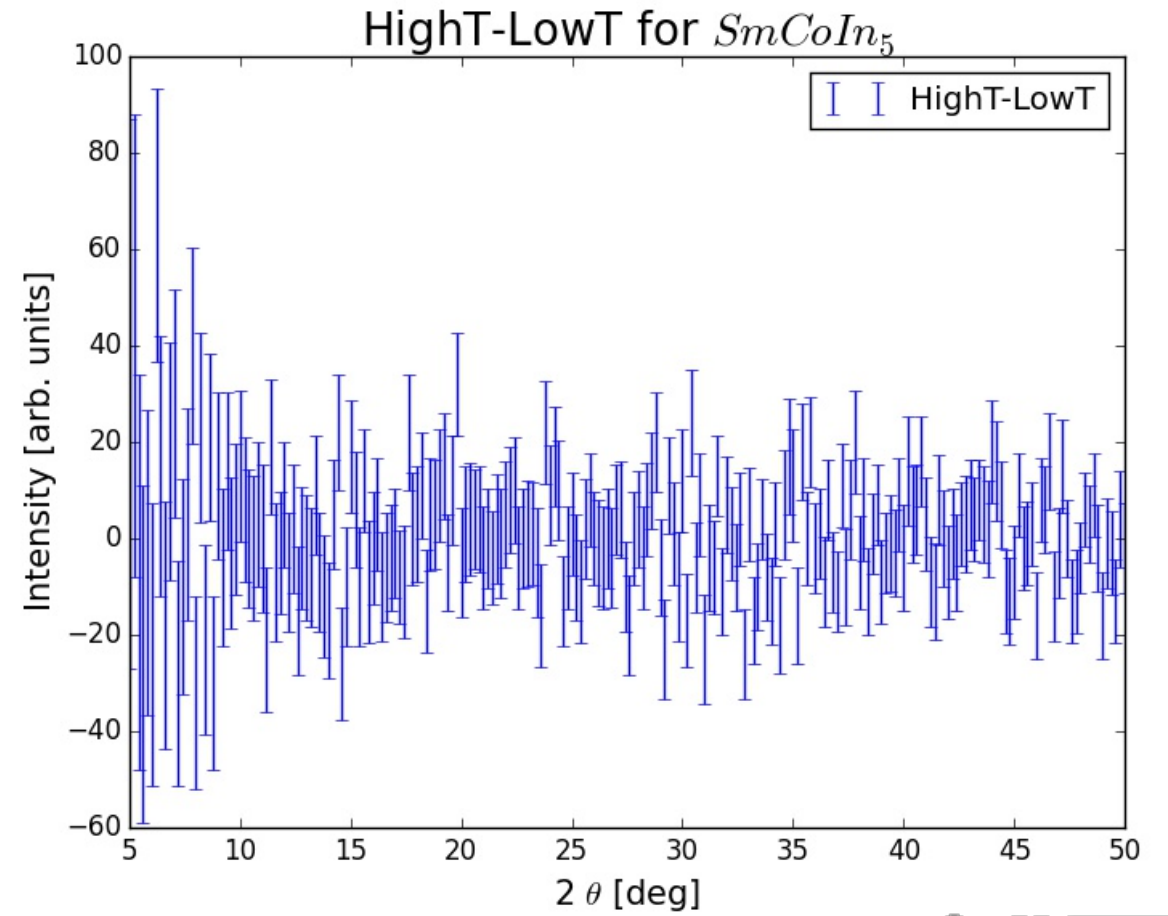
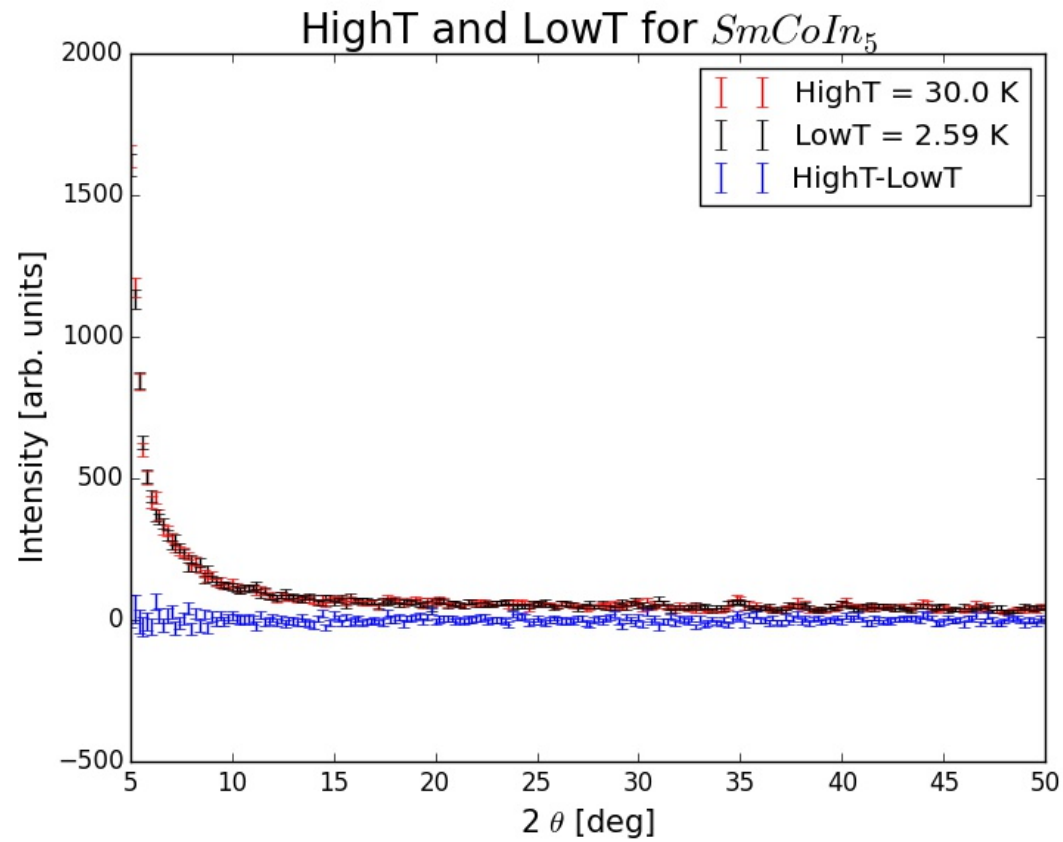


Laue x-ray diffraction

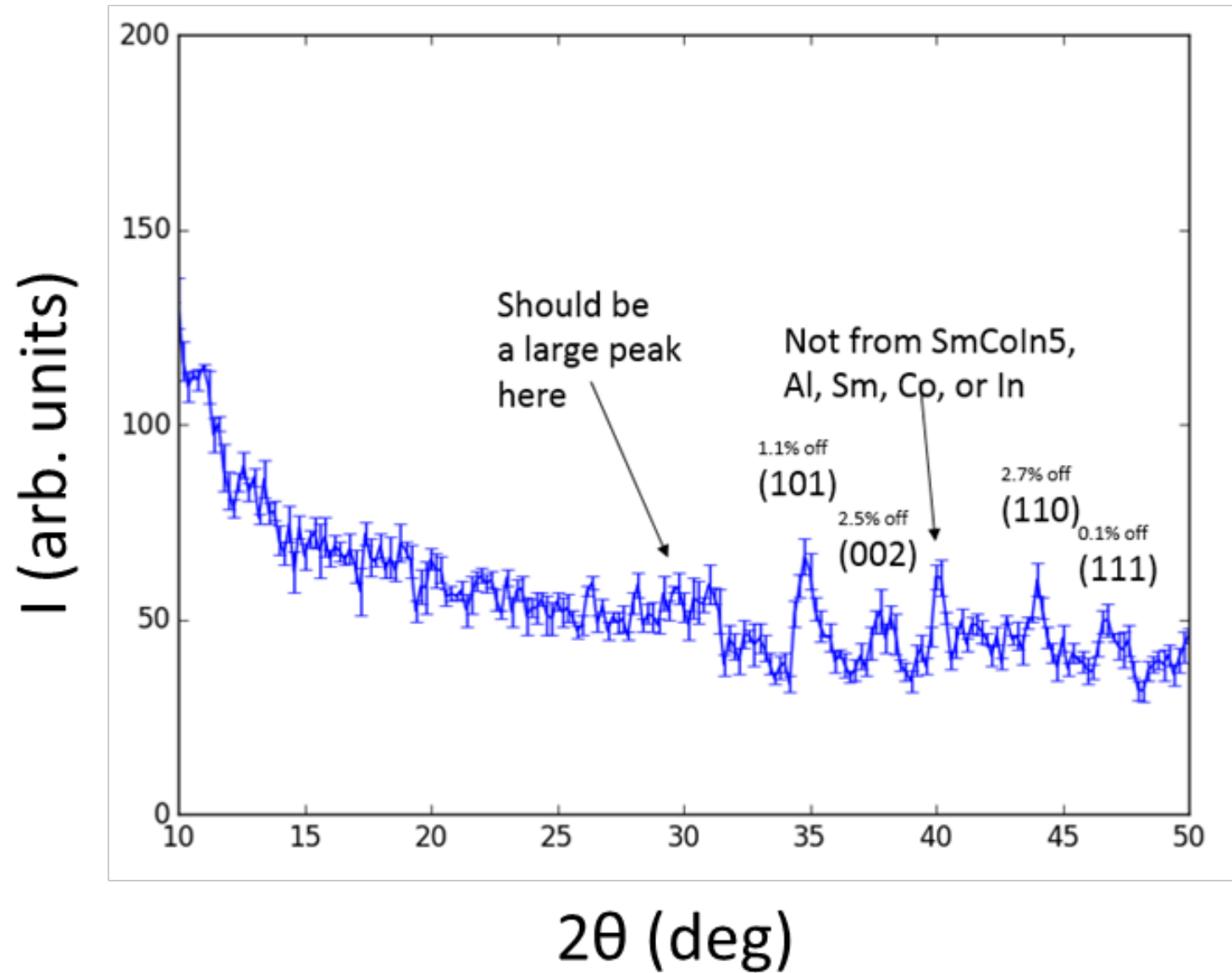


$(00l)$ face

No Magnetic Peaks found for SmCoIn_5



4 scans averaged together (powder) $E=14.7\text{meV}$



Why?

E=35 meV

Element	Formula Unit	Atomic Weight (g/m)	Cross Sections ($1 \times 10^{-24} \text{ cm}^2$)		
			Coherent	Incoherent	Absorption
Sm	1	105.360	0.422	39.000	5072.236
Co	1	58.933	0.779	4.800	31.845
In	5	114.820	2.080	0.540	165.991

Data from NCNR Scattering and Activation Database

Determining μ_{eff} and x using the SQUID

Curie-Weiss Law for Paramagnetism

$$\chi(T) = \frac{\mu_{\text{bulk}}(T)}{H * \text{moles}} = \frac{C}{T - \theta_m} - \chi_0$$

T - Temperature [K]

C - Curie Number [(emu K)/or]

θ_m - Curie Temp. [K] (+ Ferro, - Anti)

Fit using:

$$\frac{\mu_{\text{bulk}}(T)}{H} = \frac{a}{T - \theta_m} - b$$

$$C_{\text{molar}} = \frac{N_a \mu_{\text{eff}}^2(x)}{3k_B}$$

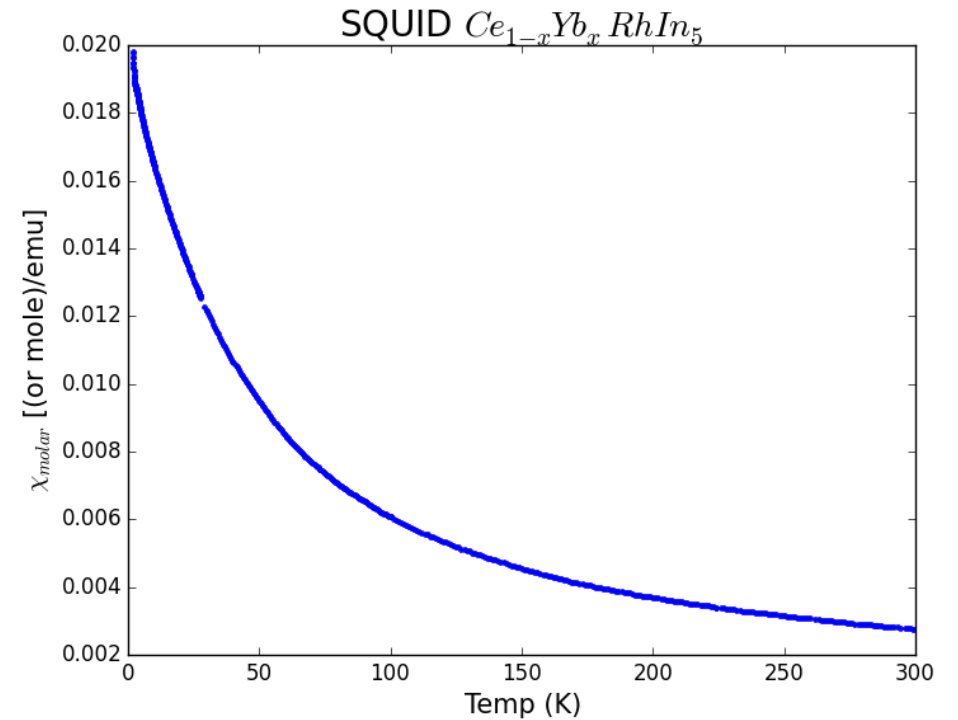
$$a = \text{moles}(x) * C(x)$$

$$b = \text{moles}(x) * \chi_0$$

$$\mu_{\text{eff}}^2(x) = xP_{Yb^{+3}}^2 + (1 - x)P_{Ce^{+2}}^2$$

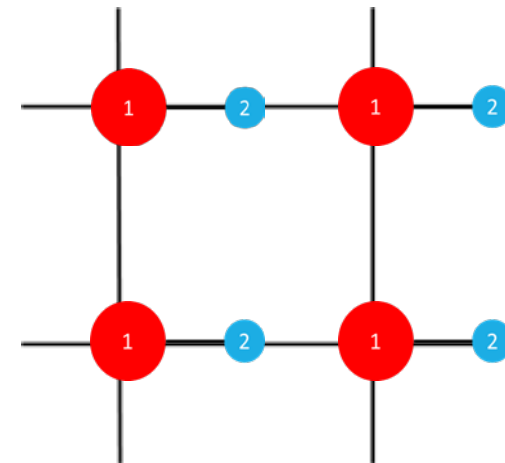
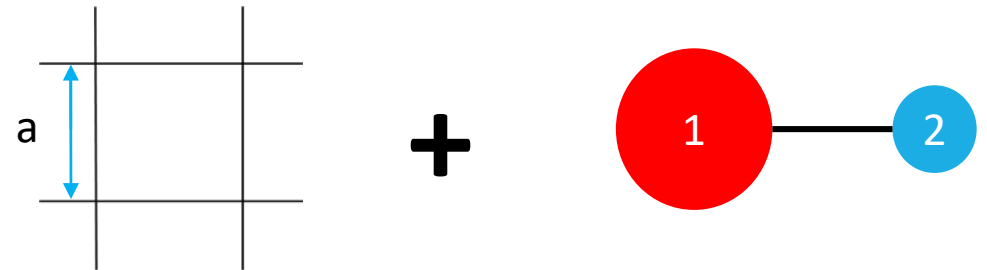
$$P_{Ce^{+3}} = 2.54 \mu_B$$

$$P_{Yb^{+3}} = 4.54 \mu_B$$



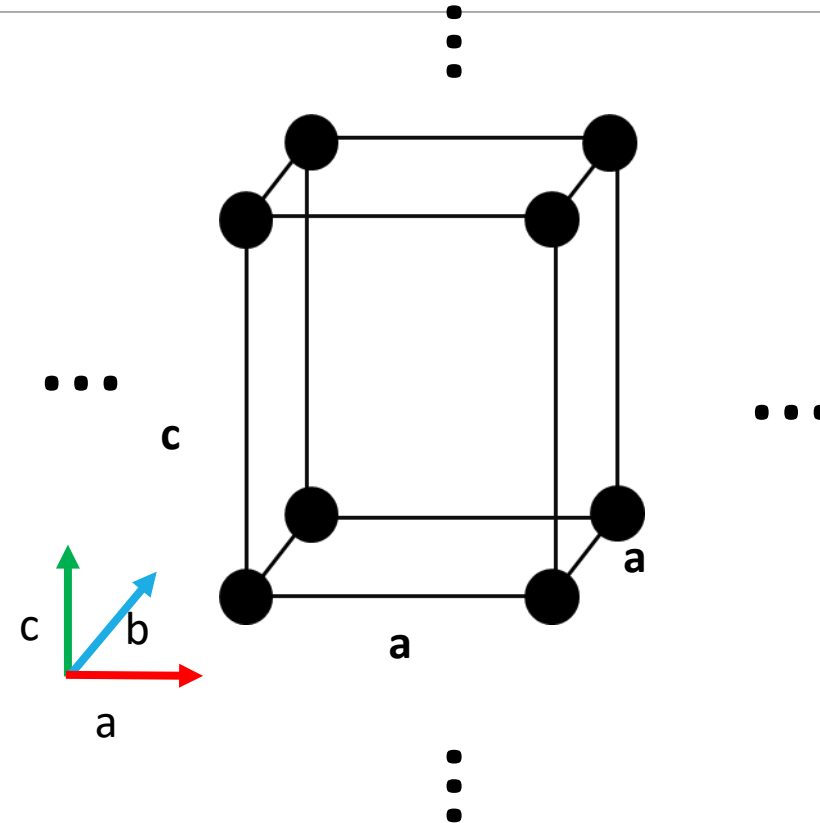
Crash course in crystallography

- Lattice + Atomic Basis = Crystal



Crash course in crystallography

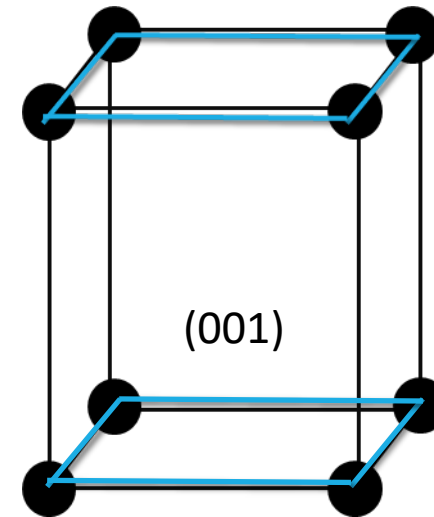
- Lattice + Atomic Basis = Crystal
- Unit cell



Crash course in crystallography

- Lattice + Atomic Basis = Crystal
- Unit cell
- Reciprocal space and the Miller indices

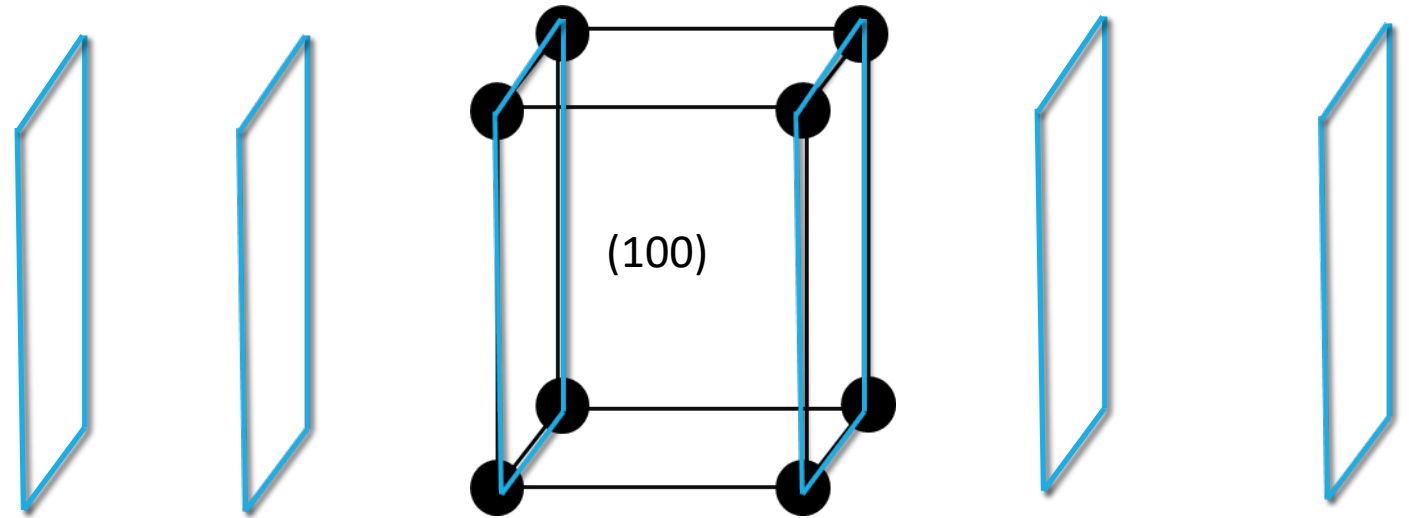
A measure of frequency.



Crash course in crystallography

- Lattice + Atomic Basis = Crystal
- Unit cell
- Reciprocal space and the Miller indices

A measure of frequency.



Crash course in crystallography

- Lattice + Atomic Basis = Crystal
- Unit cell
- Reciprocal space and the Miller indices

A measure of frequency.

