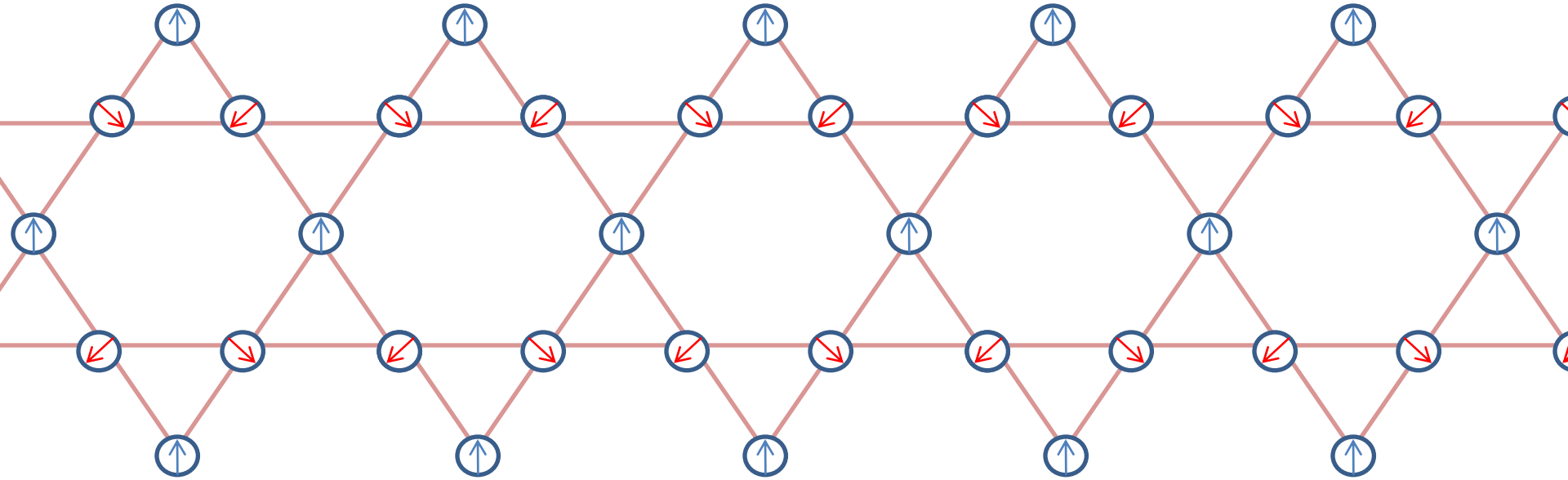
# Synthesis & Characterization of a Spin-1 Kagome Lattice

Ni-Volborthite and Ni-Vesignieite
Frustrated Antiferromagnets




Maggie Lovell
Dr. Jeff Lynn, Dr. Joel Helton

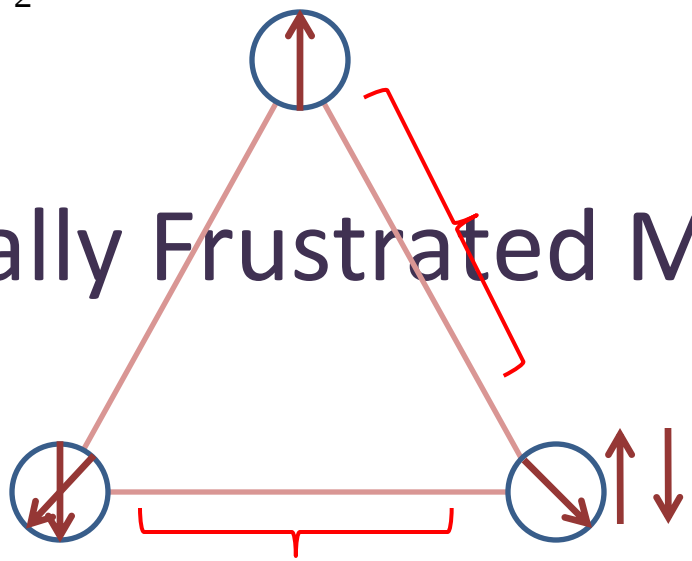
**Frustration:**

When all interactions cannot be simultaneously satisfied.

(Antiferromagnetic when J is positive.)

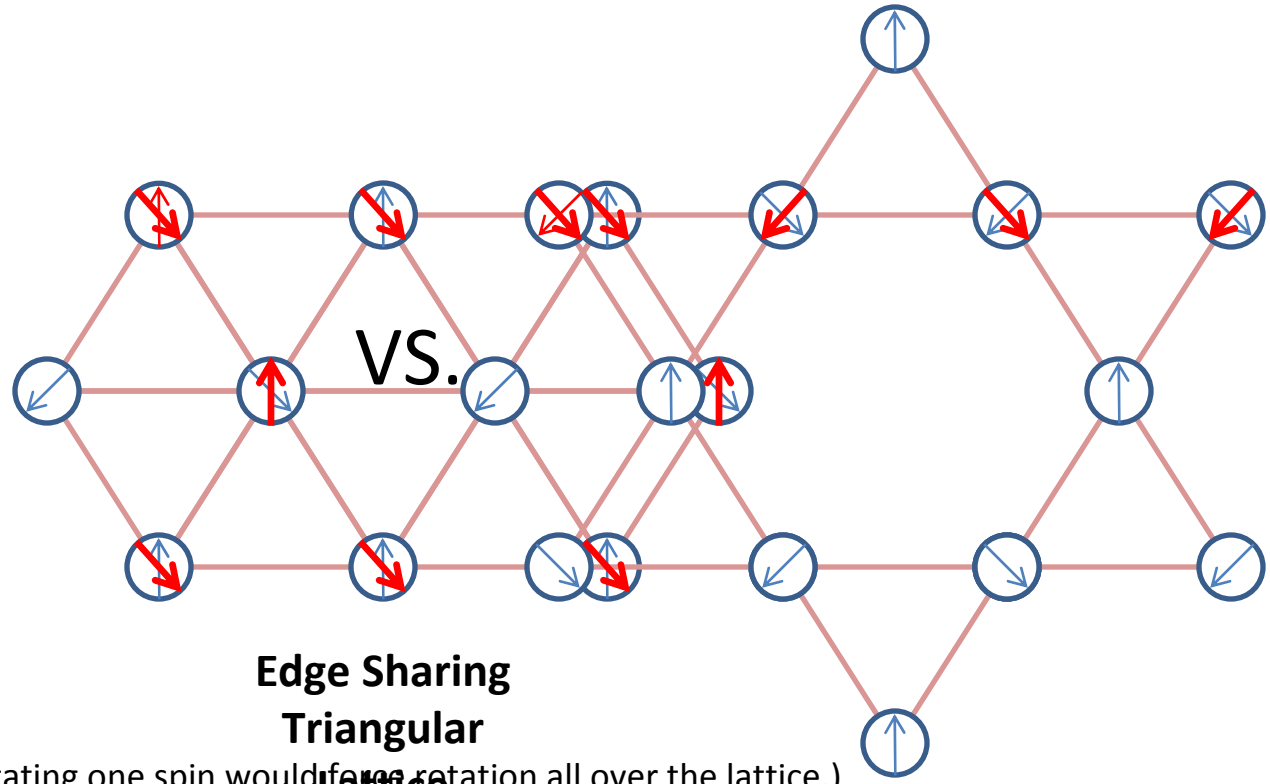
$$\hat{H} = J \sum \vec{S}_1 \cdot \vec{S}_2$$

# Geometrically Frustrated Magnetism



There is no way to satisfy the third spin!

# Frustrated Lattices




**Edge Sharing Triangular Lattice**

(Rotating one spin would force rotation all over the lattice.)

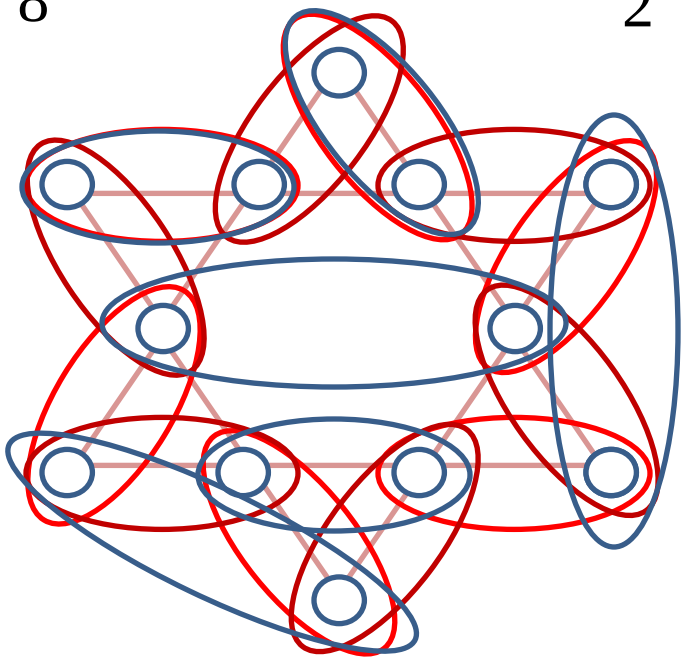
**Corner Sharing Kagome Lattice**

(Lines of spins rotate independently)

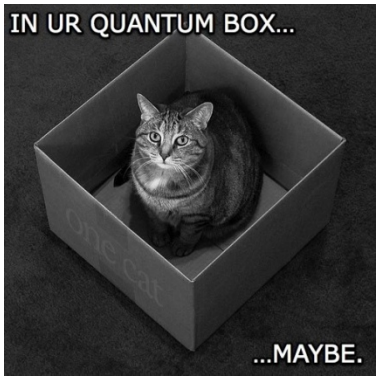
# Spin Liquid

$$E \approx 2JS^2\cos(120) = -\frac{2}{8}J$$

$$E \approx -\frac{1}{2}JS(S+1) \quad = -\frac{3}{8}J$$

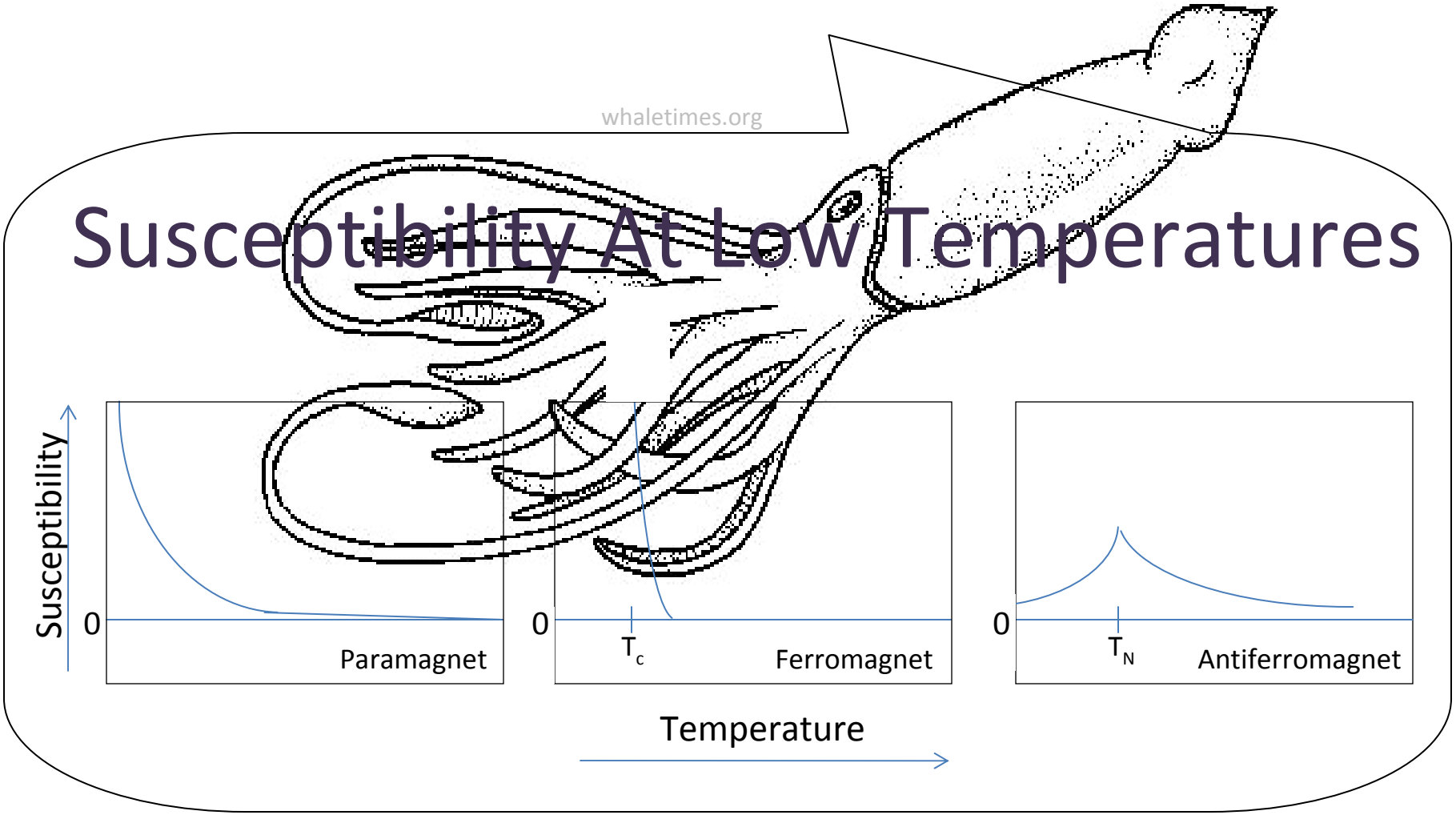


$$\frac{1}{\sqrt{2}}\left|\uparrow\downarrow\right\rangle - \frac{1}{\sqrt{2}}\left|\downarrow\uparrow\right\rangle$$

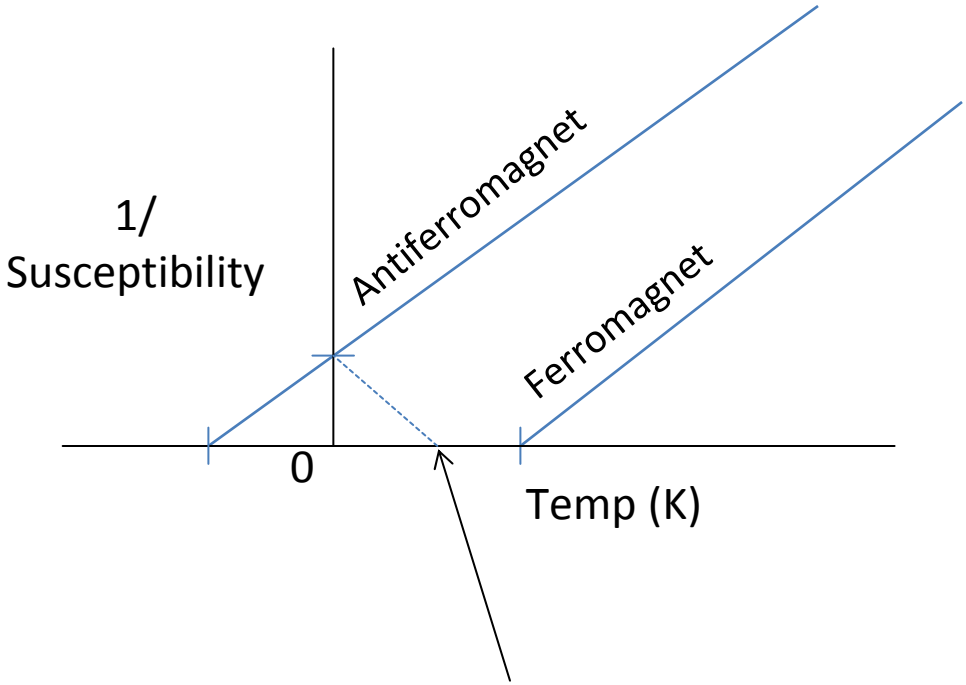



Proposed by P.W. Anderson, *Mat. Res. Bull*. 8, 153 (1973)

# Susceptibility At Low Temperatures



# Curie-Weiss Fit




**Neel temp, $T_N$**
Antiferromagnetic order occurs (near $|\theta_{cw}|$)

**Curie-Weiss Law**:

$$X = \frac{C}{T - \theta_{cw}}$$

Susc. = Curie Constant / (Temp – Cw temp)

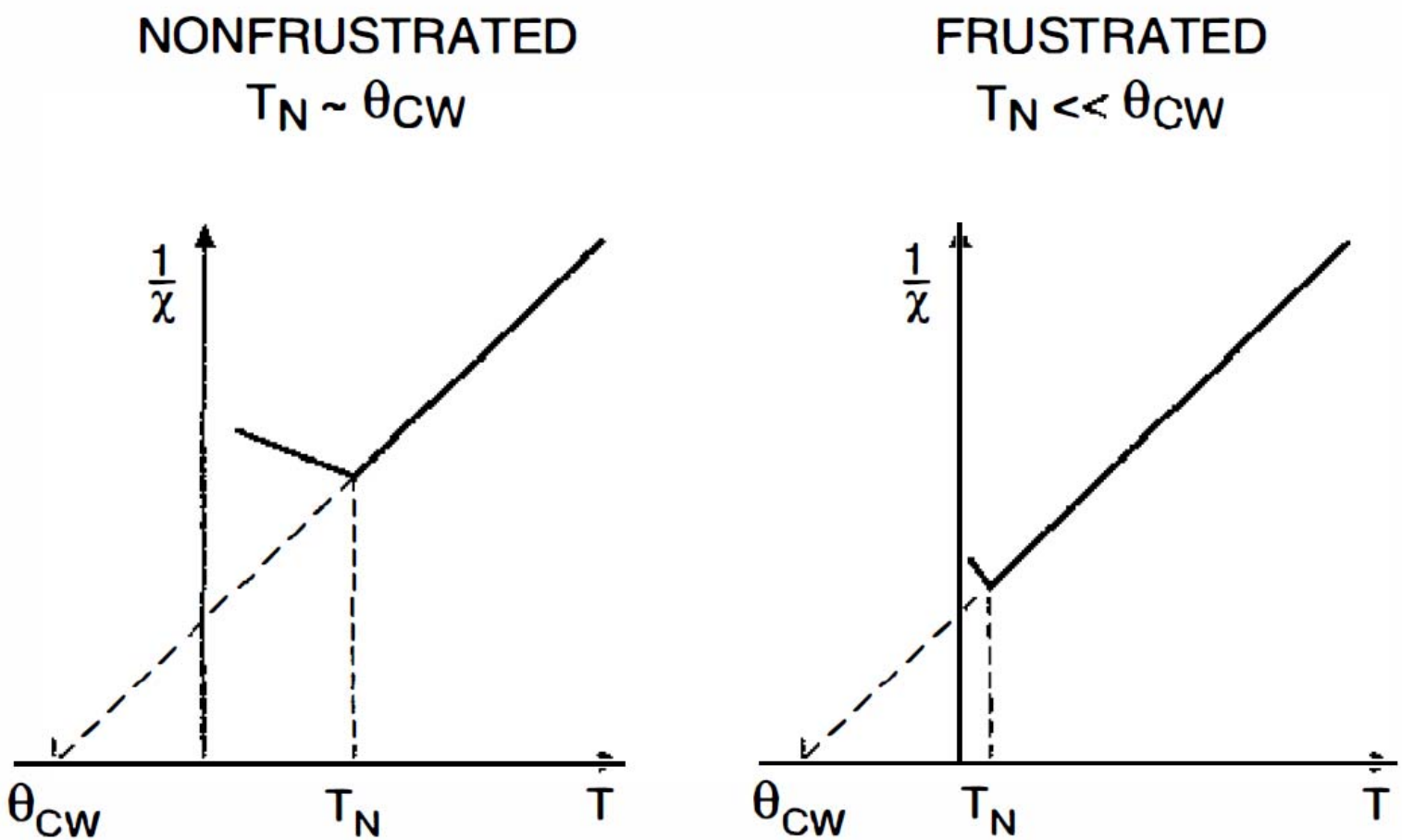
**A Measure of Frustration**

$f = \theta_{cw}/T_N$

>10 = very frustrated

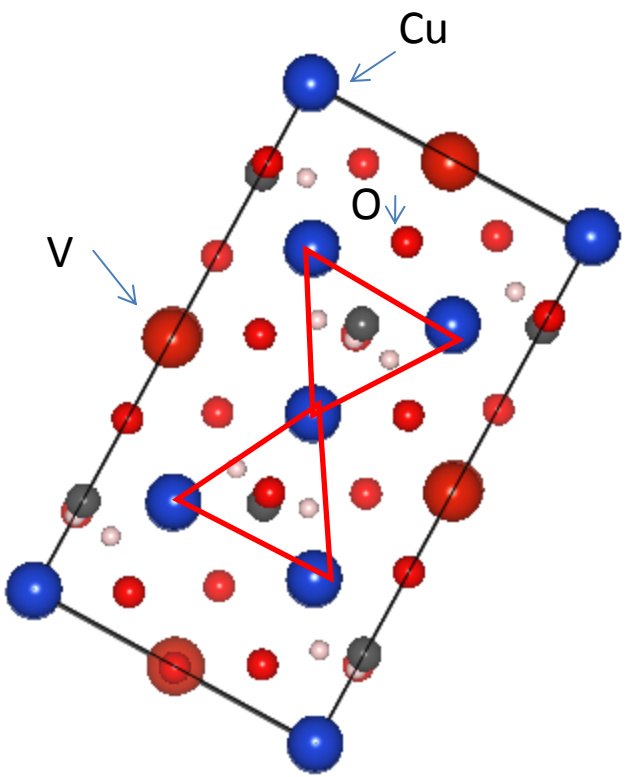
# Evidence of Frustration

$$|\theta_{cw}| \propto |J|$$

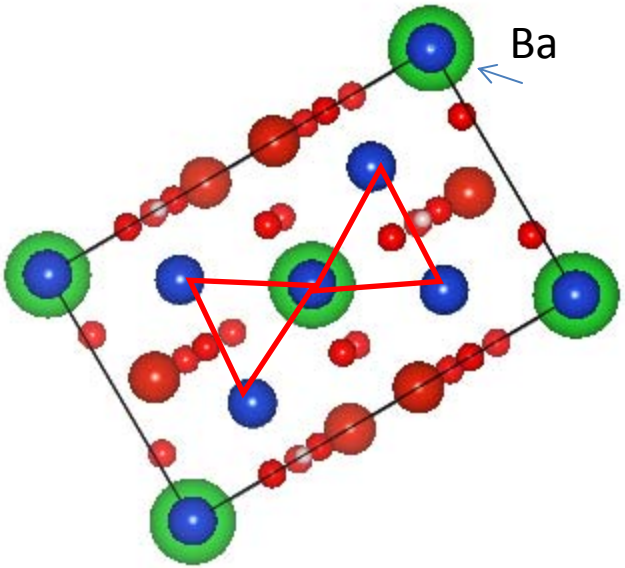



Ramirez, A.P.; Annu. Rev. Mater. Sci. 24:453-80 (1994)

# Distorted Spin-1/2 Kagome Lattices



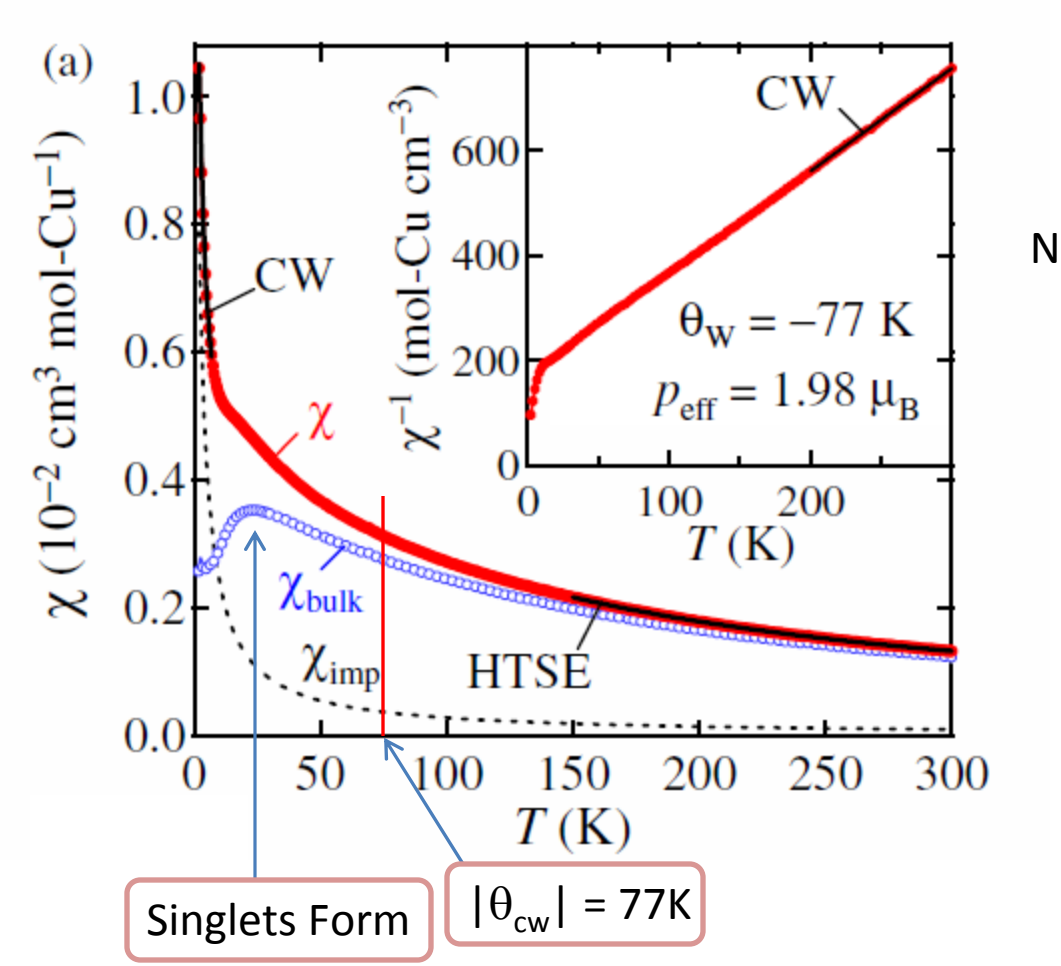

Volborthite
$Cu_3V_2O_7(OH)_2 * 2H_2O$




Vesignieite
$Cu_3Ba(VO_4)_2(OH)_2$

- Very close to ideal kagome. Slightly isosceles.
- Each nearly 2D plane is well separated from the others by the intervening structure.

# Cu-Vesignieite: A Possible Spin Liquid

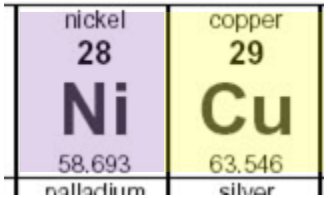



Nothing happens at the projected ordering temperature!
Very frustrated.

Y. Okamoto, H. Yoshida, Z. Hiroi;
*Journal of the Physical Society of Japan* 78,
033701-1 (2009)

# Nickel Vesignieite: A Spin-1 Kagome Lattice

- What is the transition like?
- Bigger spins exhibit less “quantum” behavior.
- Nickel is spin-1…

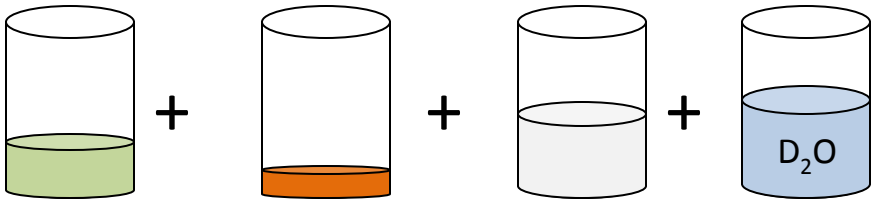


# HUMONGOUS EXPLOSIONS

When all else fails, blow it up real good.

# Making Spin-1 Ni-Vesignieite: $Ni_3Ba(VO_4)_2(OH)_2$

$$3Ni(OH)_2 + V_2O_5 + Ba(CH_3COO)_2 \rightarrow Ni_3Ba(VO_4)_2(OH)_2 + H_2O + 2\ CH_3COOH$$

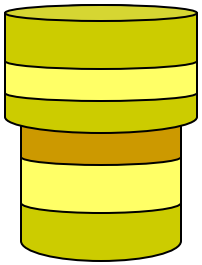



Nickel (II) Hydroxide

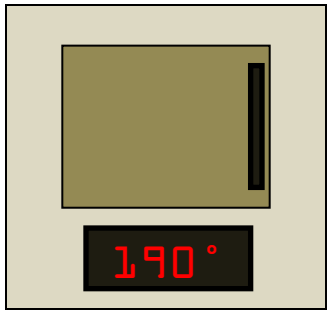
Vanadium (V) Oxide

Barium Acetate

Heavy Water



Screw Top Autoclave

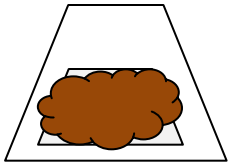



Heated slowly to 190°

Soaked for 40 hours.

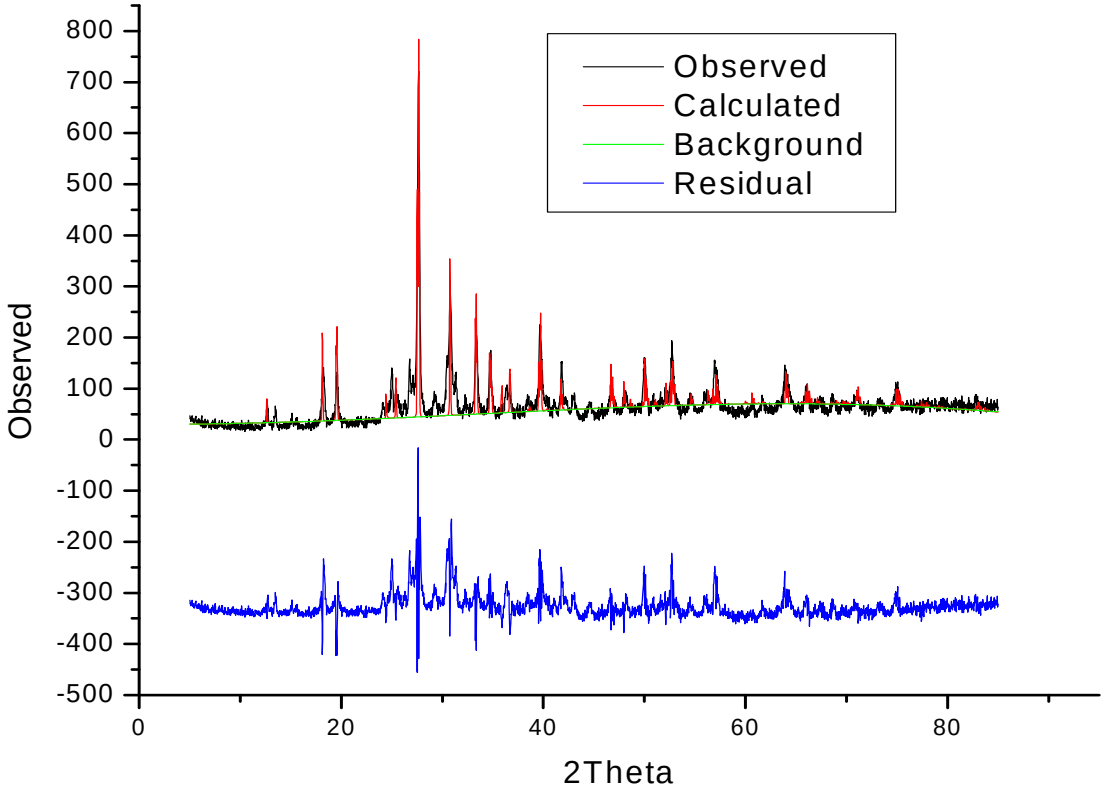
Cooled at 0.1°C per minute.

Washed in $D_2O$



Dried & Crushed To Make Powder

# X-Ray Structural Analysis

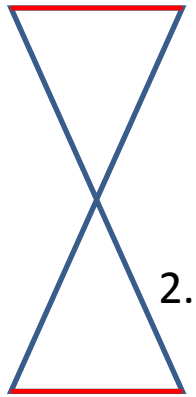



- Compared to Cu-Vesignieite data and theoretical lattice parameters.
- A GSAS fit refined the parameters further.

Space Group: C2/m (Monoclinic)
a= 10.0821 ± 0.001 Å
b= 5.8139 ± 0.0006 Å
c= 7.7613 ± 0.0007 Å
β= 115.286 ± 0.005°

**Calculated Dimensions**

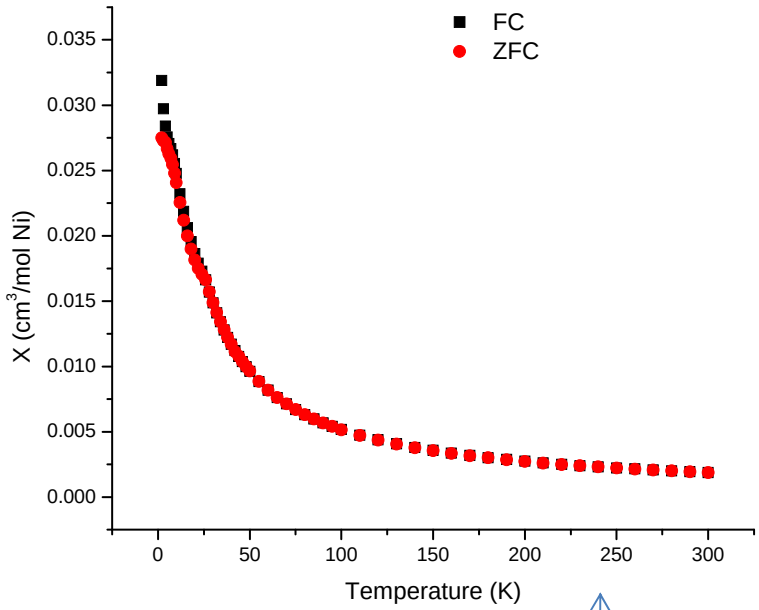
2.9068 ± 0.0003 Å

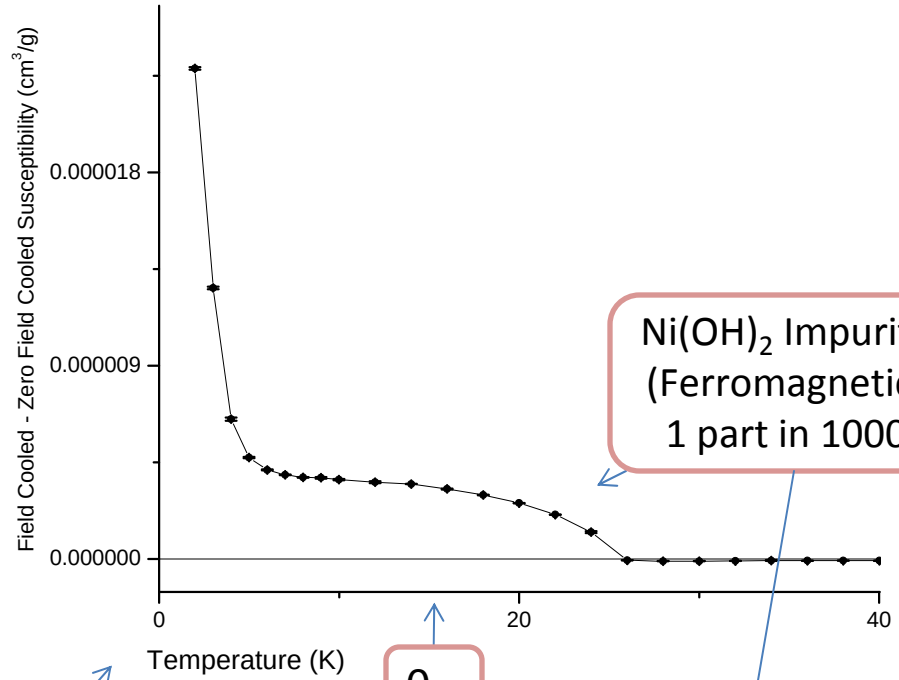


Difference in leg length: ~0.0026 Å

2.9094 ± 0.0003 Å

# Ni-Vesignieite SQUID Data



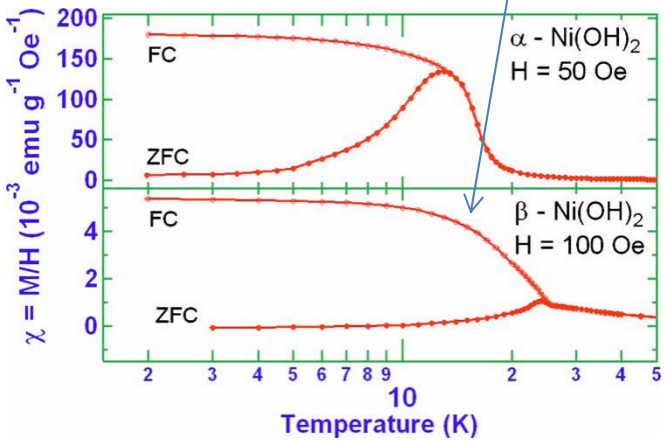

Ni(OH)$_2$ Impurity (Ferromagnetic) 1 part in 1000

$\theta_{cw}$

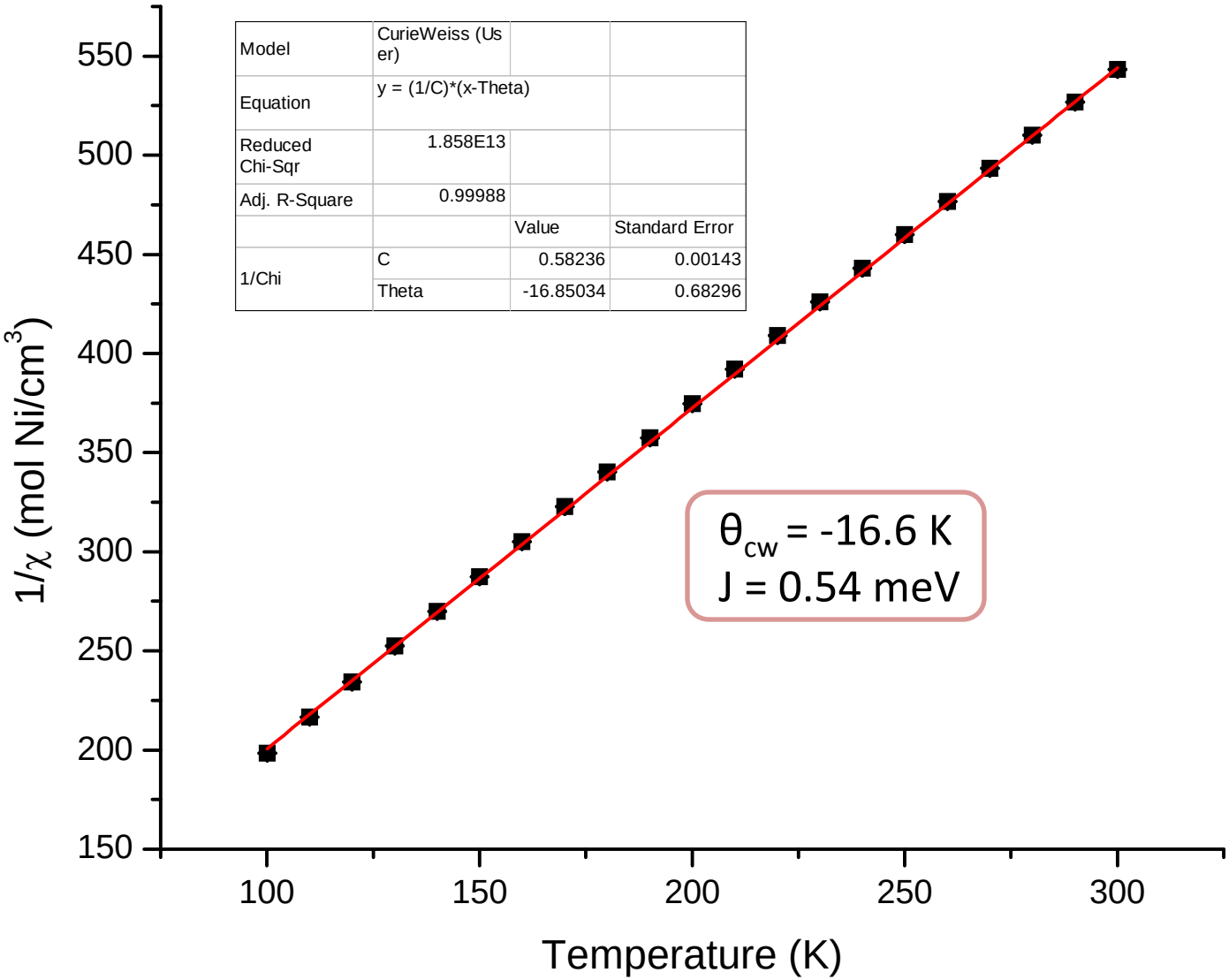
Hard to see what's going on…

FC-ZFC shows a ferromagnetic impurity.

Ni(OH)$_2$ Susceptibility Study by J. Rall, M. Seehra, N. Shah, G. Huffman, *J. App. Phy.* 107, 09B511 (2010)

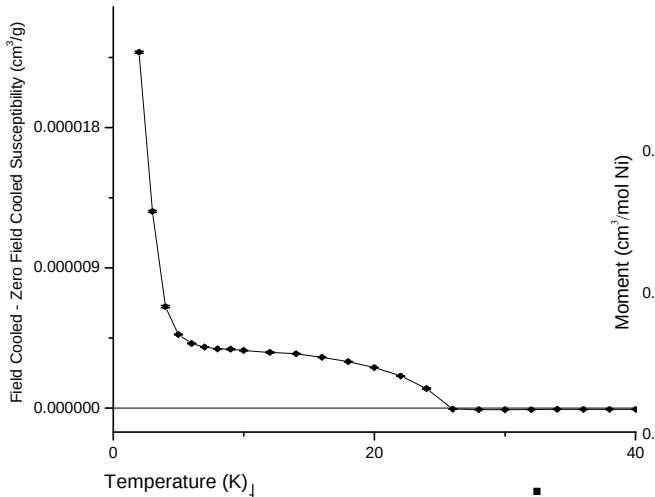


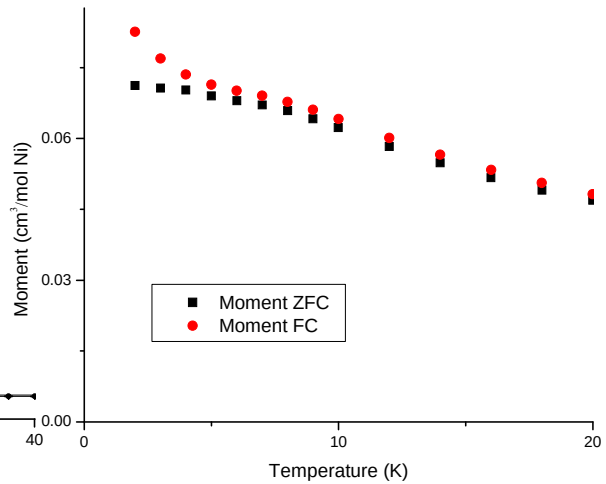
# Antiferromagnetism!

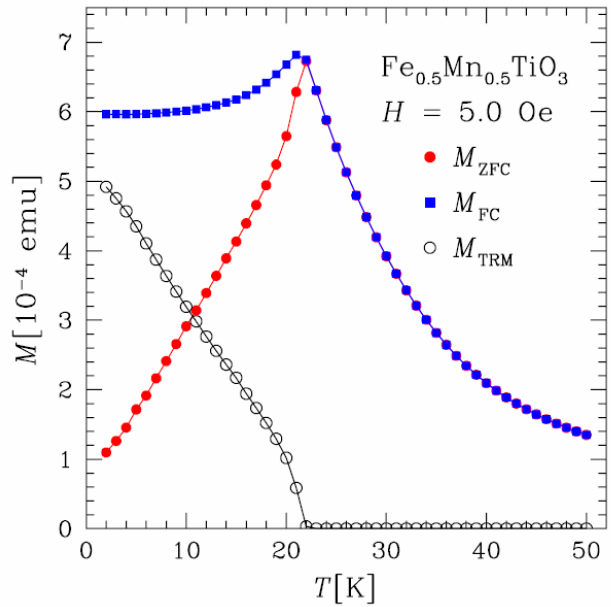



| | | | |
|---|---|---|---|
| Model | CurieWeiss (User) | | |
| Equation | y = (1/C)*(x-Theta) | | |
| Reduced Chi-Sqr | 1.858E13 | | |
| Adj. R-Square | 0.99988 | | |
| | | Value | Standard Error |
| 1/Chi | C | 0.58236 | 0.00143 |
| | Theta | -16.85034 | 0.68296 |

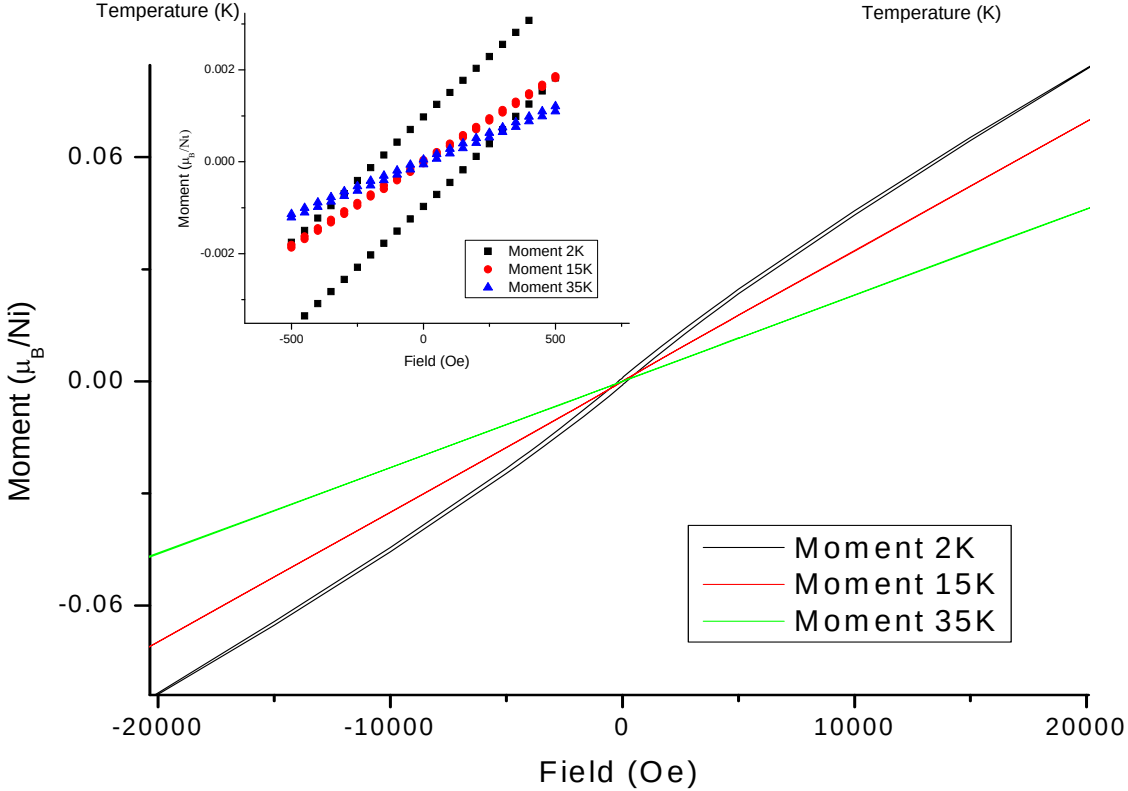
# So what is it?

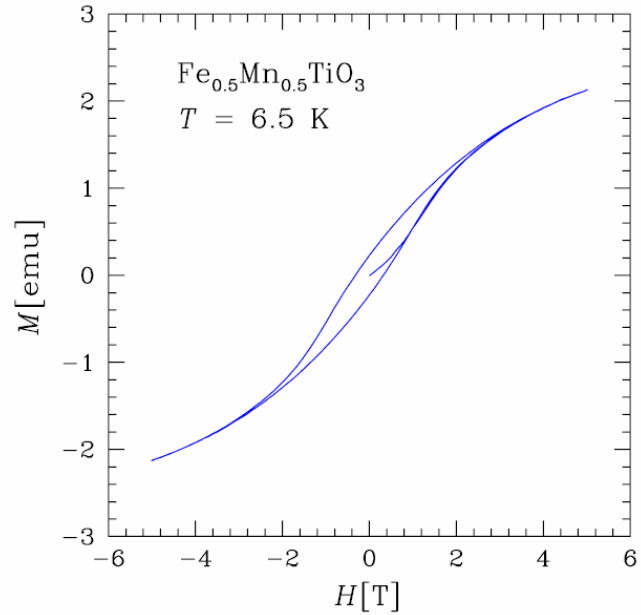



Katzgraber et alia, Phys. Rev. B. 76, 092408 (2007)



# Spin Glass

A spin glass picks one of the many ground states and sticks there.

**It does not fluctuate**.

The term for this is “quenched disorder.”

# Conclusions

We have synthesized Ni-Vesignieite.

It is a slightly distorted kagome lattice.

It shows no order down to $\theta_{cw}/10$ (evidence of frustration).

Likely spin glass transition at about $\theta_{cw}/2$.

# Further Studies

Frequency Dependant SQUID Measurement

Neutron Bragg Scattering

To confirm Spin Glass diagnosis.

Inelastic Neutron Scattering

To explore excitations.

Grow Ni-Volborthite

# Question Time?

Thanks to:
Dr. Cindi Dennis (MSEL) for SQUID Data
Dr. Rick Paul (CSTL/NCNR) for Prompt Gamma Analysis

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Kim Tomasi,
Wendy Queen,
Jason Simmons,
Peng-yen Hsieh,
Efrain Rodriguez,
And Joel Helton
For being totally cool
about that exploding jar.