Spin 1/2 on the kagome lattice: "from theory to experiments and back".

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- B. Bernu
- P. Viot
- J. C. Domenge
- F. Brieuc

Saclay Ipht CEA

- L. Messio
- G. Misguich

Grenoble CNRS

- O. Cepas

Hong Kong

C. M. Fong, P. W. Leung

Grenoble CEA & ILL

- B. Fåk

Orsay LPS

- F. Bert
- E. Kermarrec
- P. Mendels

London (UCL) :

- R. H. Colman
- A. S. Wills

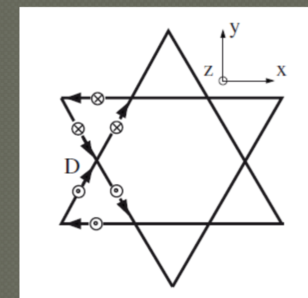
Outline

- A point of view on the properties of herbertsmithite

- Kapellasite:
  A new gapless Spin Liquid.
  B. Fåk, et al. PRL 109, 037208 (2012)
  - Polymorph of herbertsmithite
  - Slightly different crystallography
  - Notably different physics

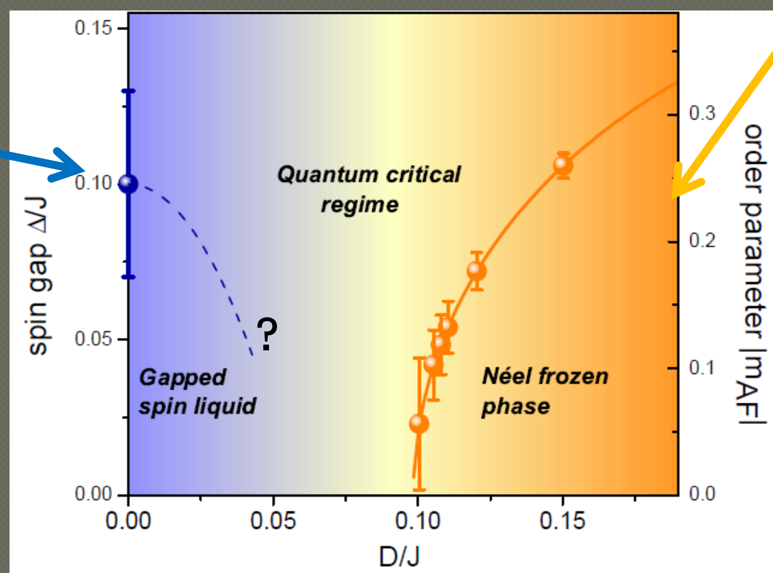
Quantum phase transition induced by Dzyaloshinskii-Moriya interactions

$$H = \sum_{\langle i,j \rangle} [J\mathbf{S}_i \cdot \mathbf{S}_j + \mathbf{D}_{ij} \cdot (\mathbf{S}_i \times \mathbf{S}_j)]$$



O. Cepas… PRB 78 '08

Jiang …, '08
Yan, … '12
Depenbrock '12



Quantum phase transition induced by Dzyaloshinskii-Moriya interactions

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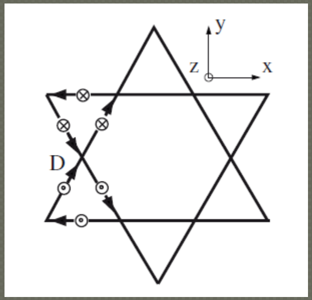

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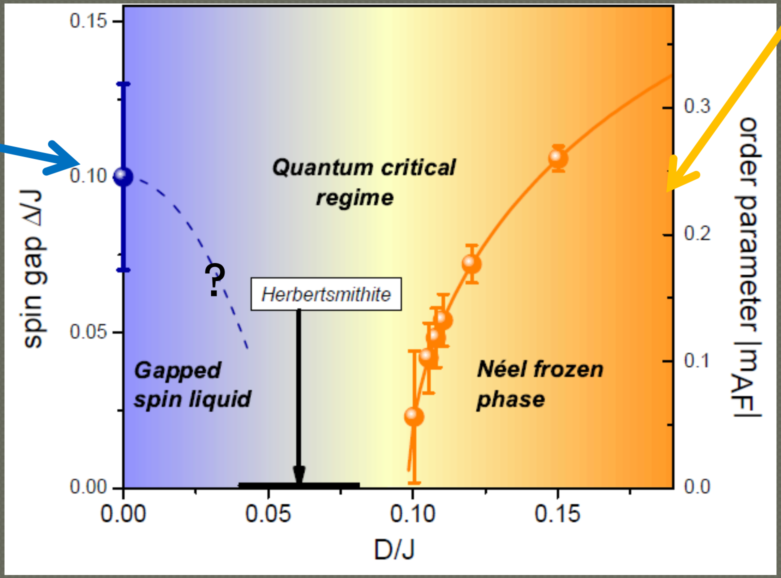
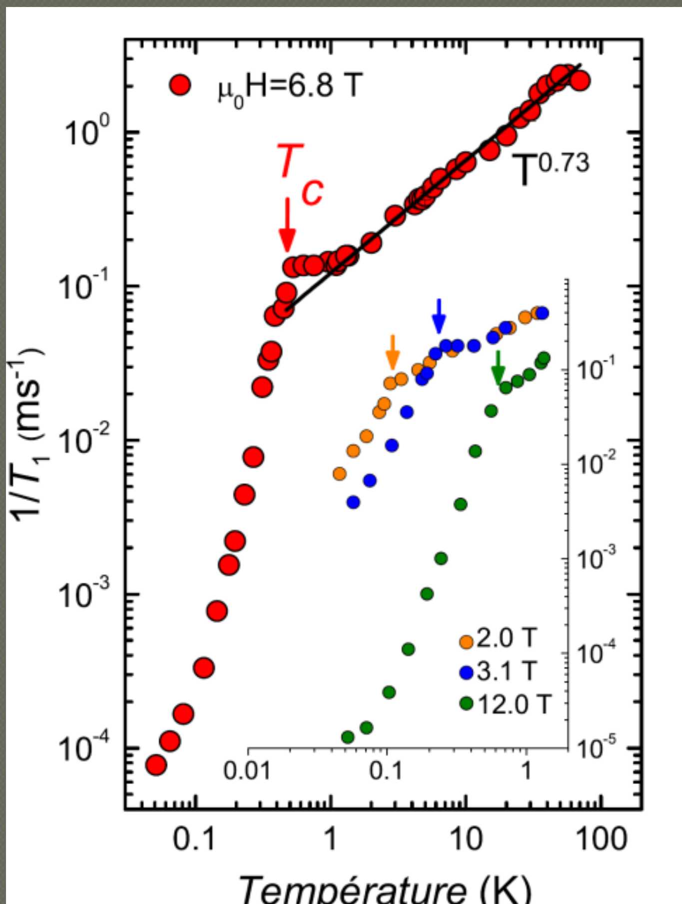
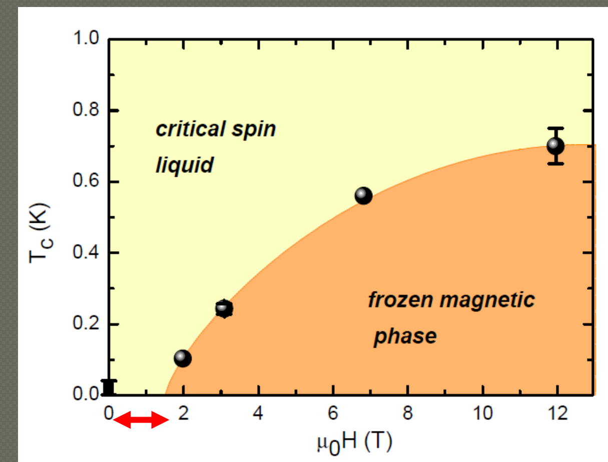


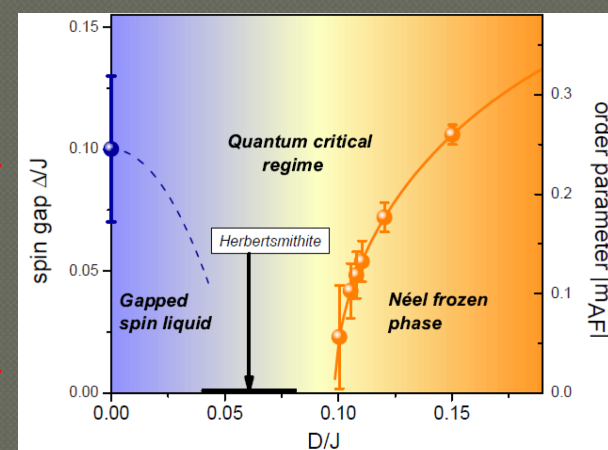
Zorko … PRL 101 '08, El Shawish… PRB 81 '10.

Effect of a magnetic field on Herbertsmithite (1/T1 NMR)





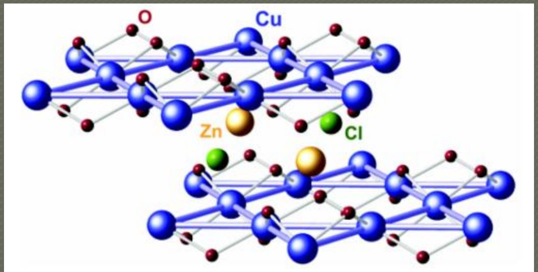
~20K

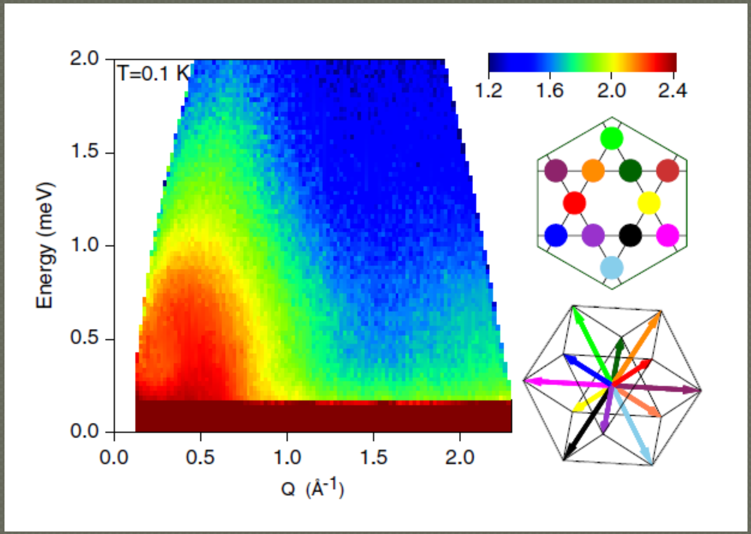


M. Jeong et al: PRL 107, 237201 (2011)

Kapellasite: a new gapless SL

- A metastable polymorph of herbertsmithite
- slightly different crystallography
- Fluctuating down to 20 mK (μSR, INS)

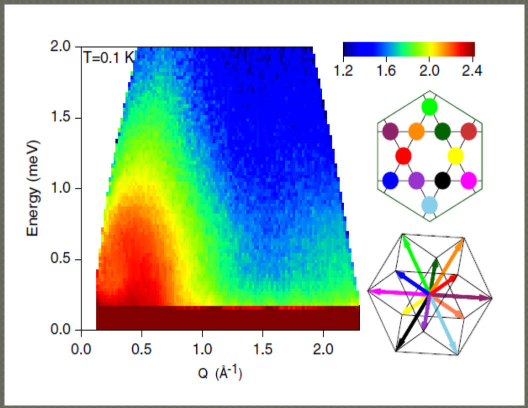


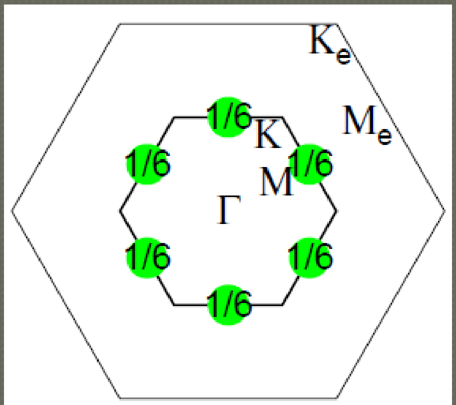


Synthesis:
R. H. Colman, et al., Chem. Mater. 20,6897 (2008) and 22, 5774 (2010).

B. Fåk, et al. PRL 109, 037208 (2012)

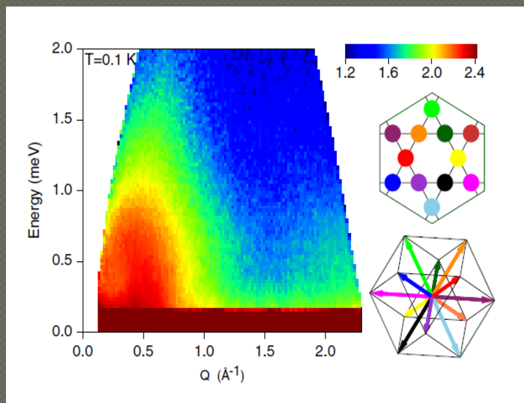
When INS meets PSG analysis

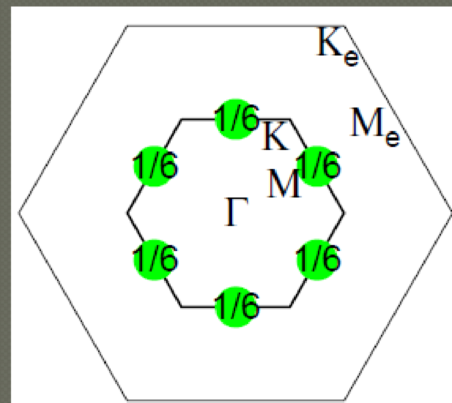




L. Messio PRB 83 (2011)
5 AF "regular "states
on the kagome lattice
Only cuboc2 SRO can fit INS

When INS meets PSG analysis





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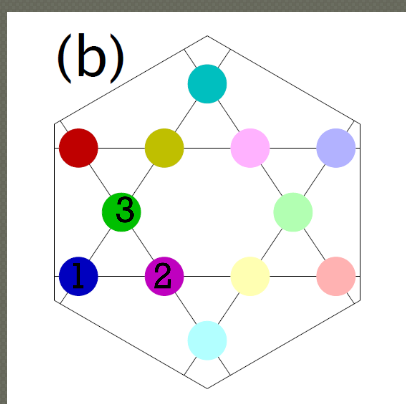
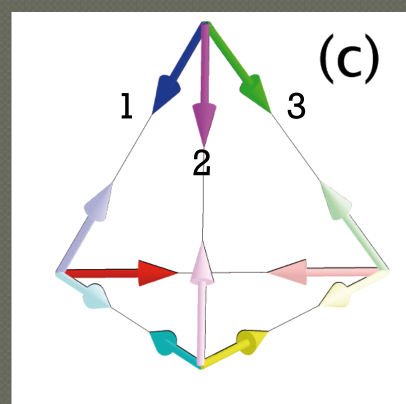
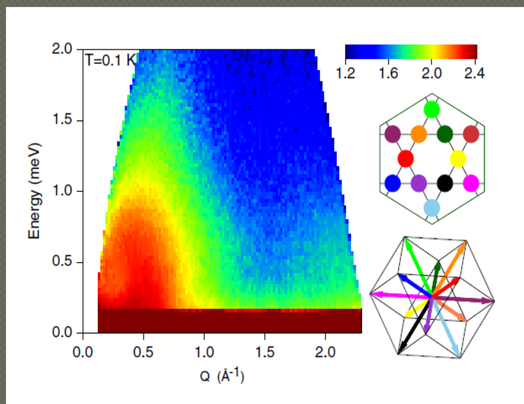


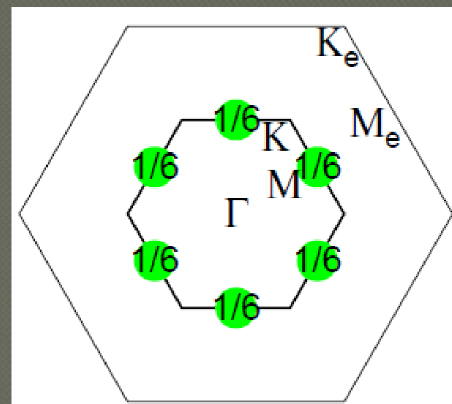
Magnetic unit cell



Short range 3D chiral
disposition of spins

When INS meets PSG analysis





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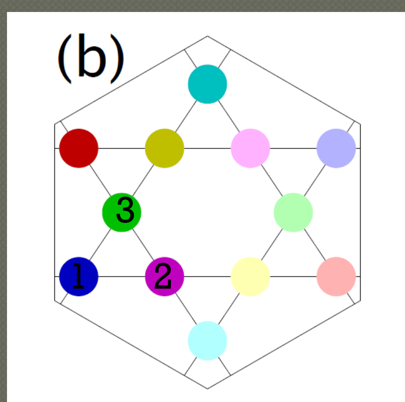
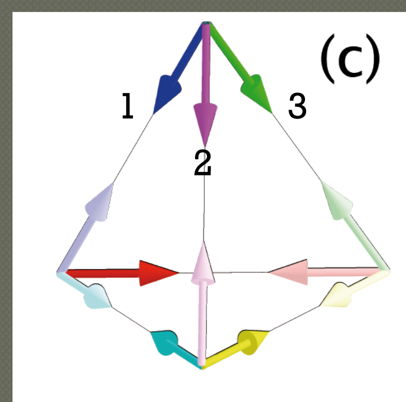


Magnetic unit cell



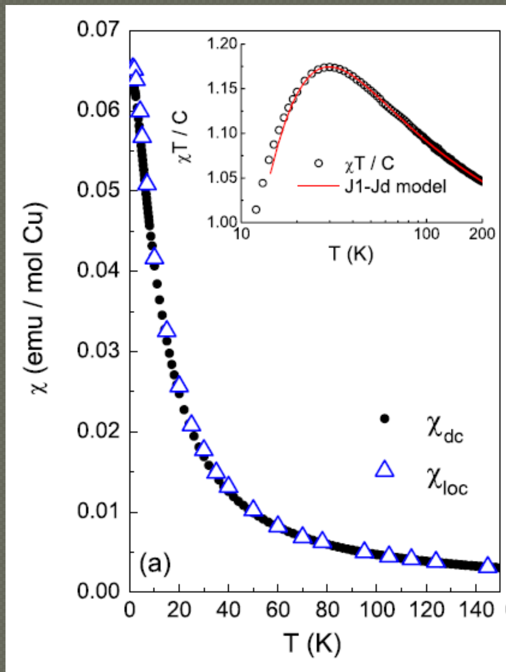
Short range 3D chiral
disposition of spins

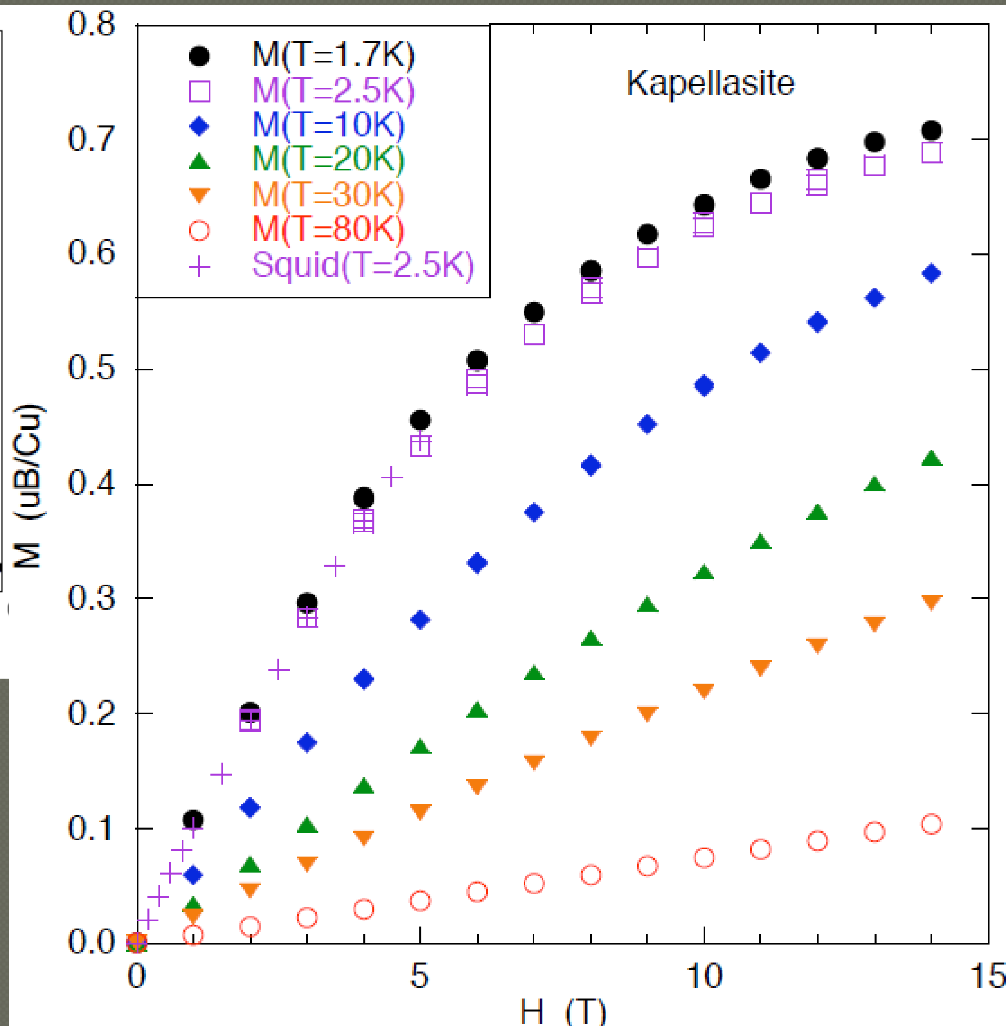
Chirality:

$$\sigma = \frac{S_1.(S_2 \times S_3)}{|S_1.(S_2 \times S_3)|}$$

From experiments to model by HT series

B. Bernu, E. Kermarec, et al.. 2012





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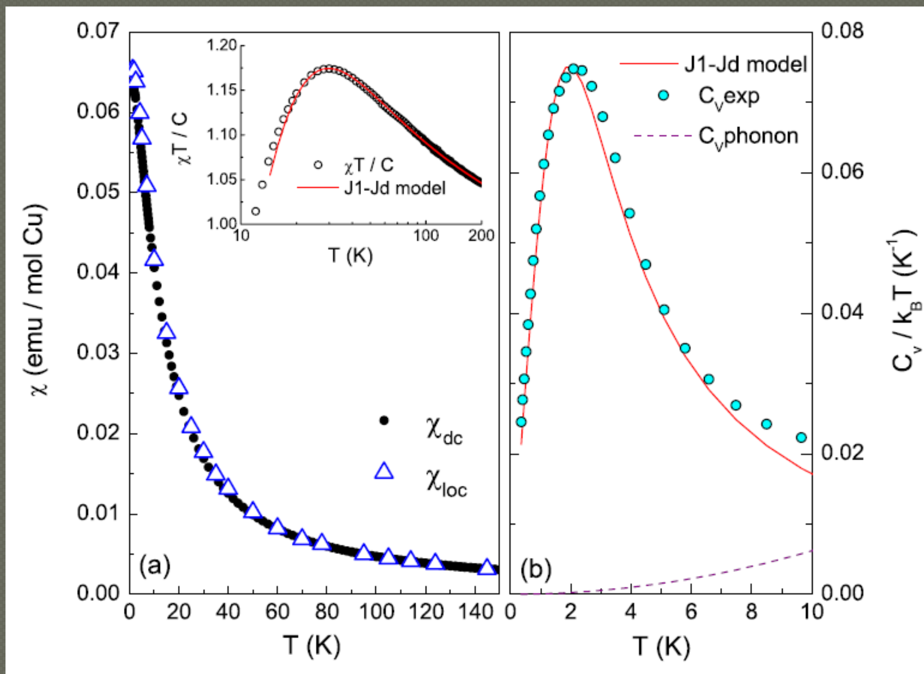
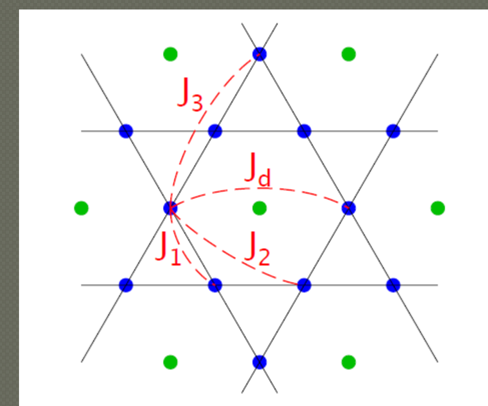


$$H = \sum_{i,j} J_{i,j} S_i . S_j$$

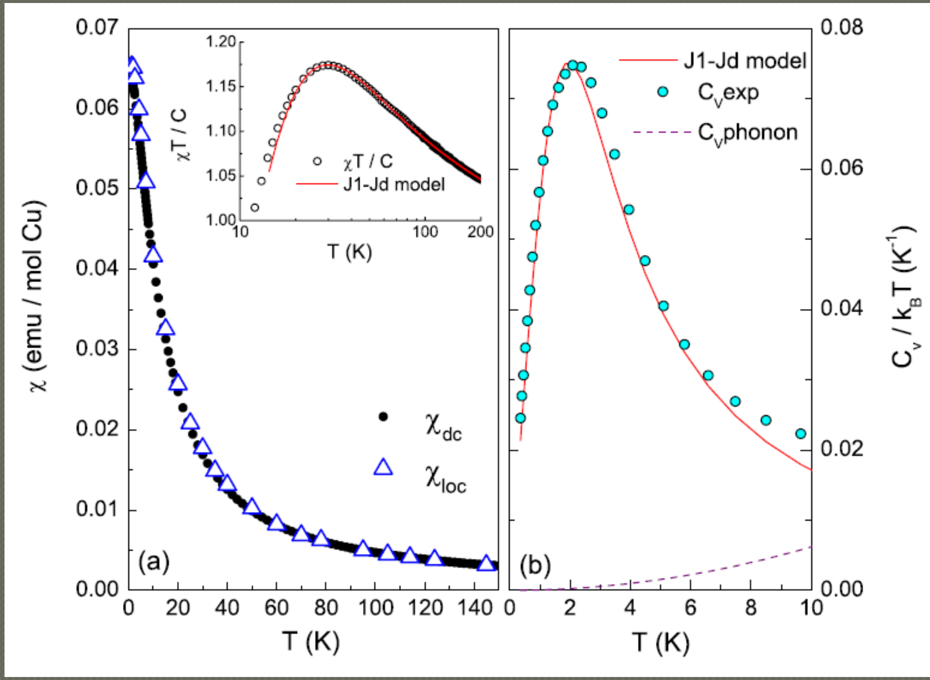


Ferro J_1 competing with AF J_2 or/and J_d

$J_1 = -12.4K$, $J_2 = -3$ K , $J_d = +14.8$ K

From experiments to model by HT series

B. Bernu, E. Kermarec, et al.. 2012



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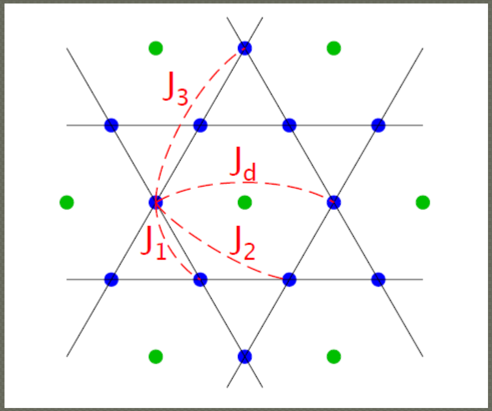
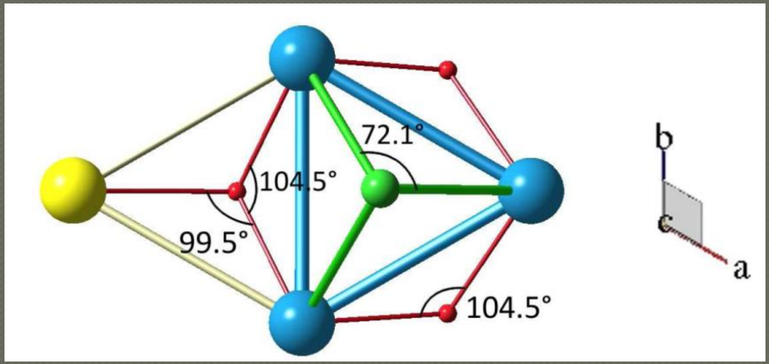
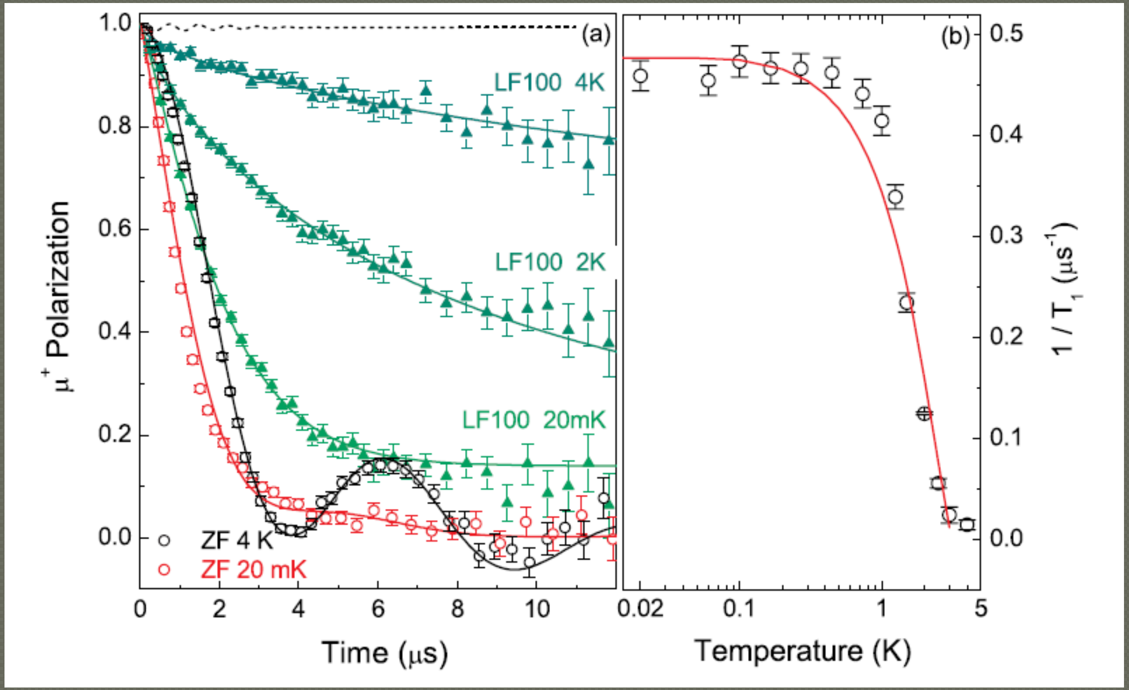




Ferro J_1 competing with AF J_2 or/and J_d

$J_1 = -12.4K,\ J_2 = -3K\ ,\ J_d = +14.8\ K$

μSR relaxation (local low frequency fluctuations)



Right: $1/T_1$ (low temperature plateau)

Experiments (circles) and SBMF calculations (red line).

No adjustable parameters (except the absolute value)

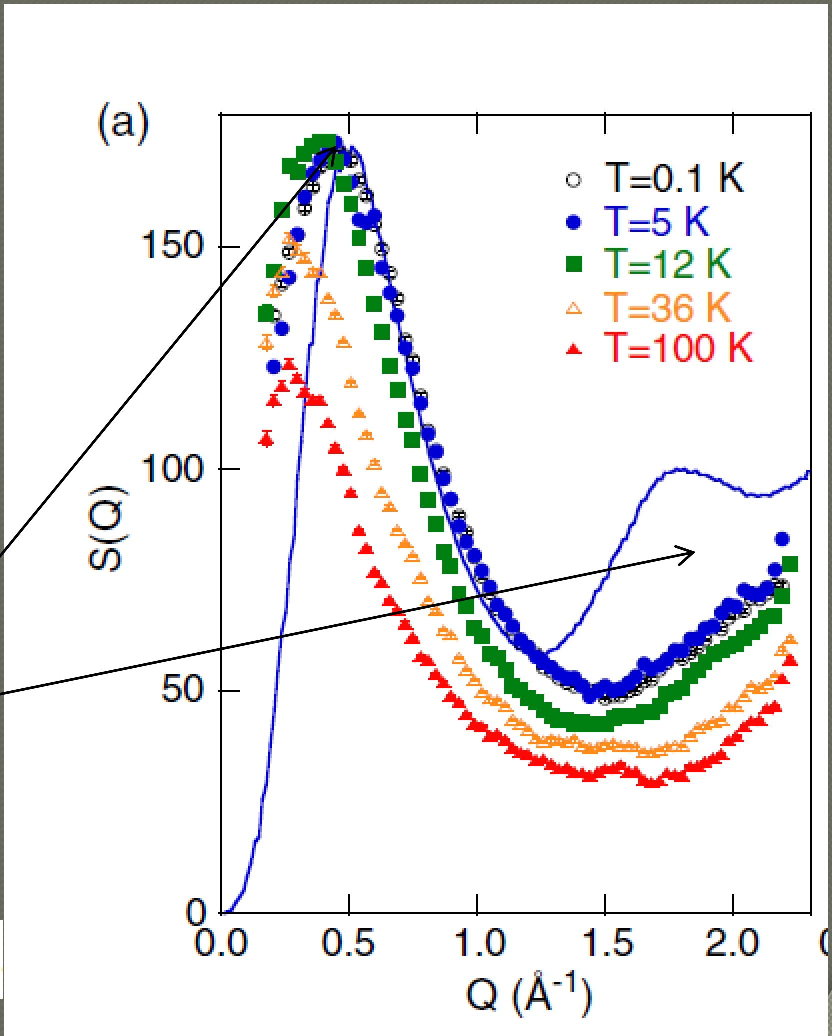
Powder averaged INS

Wave-vector dependence of the inelastic magnetic scattering integrated over the energy range 0.4<E<0.8 meV.

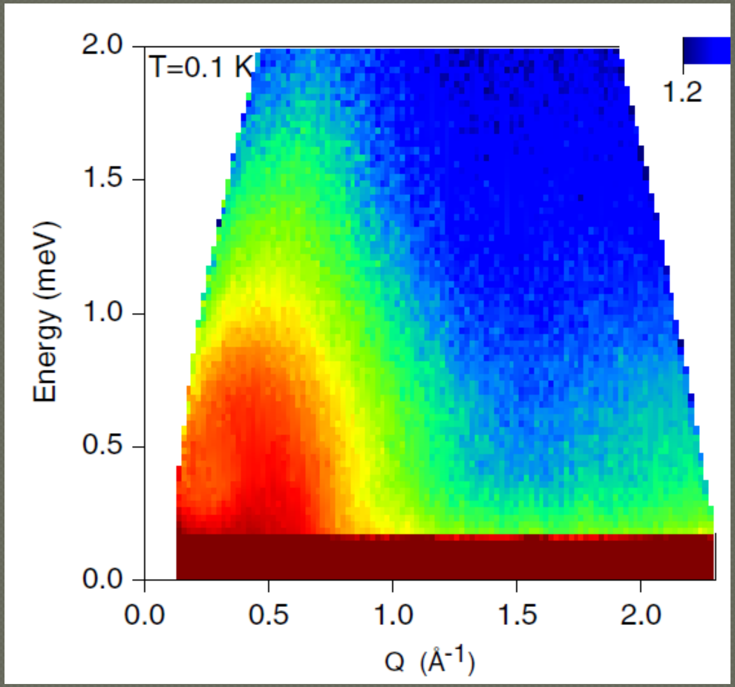
Blue line SBMF calculations. No adjustable parameters

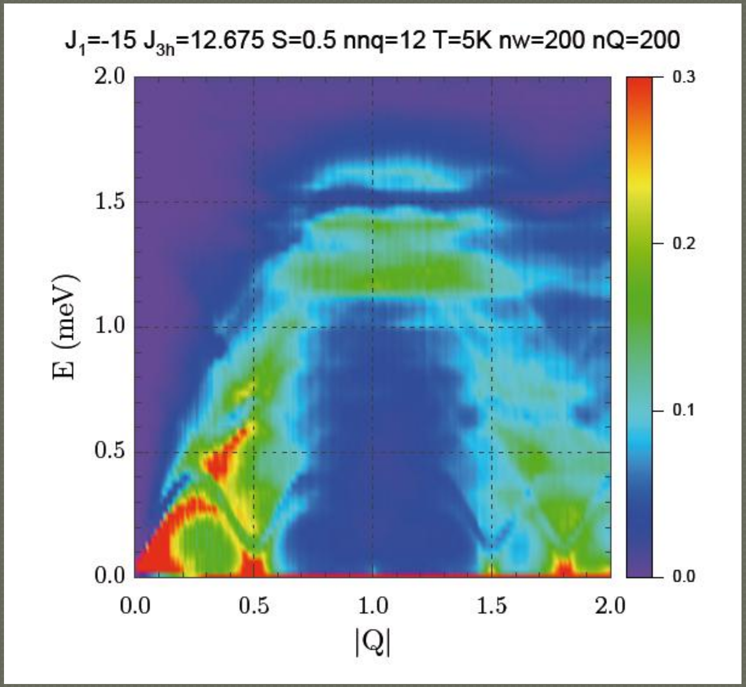
2 features may be due to Zn substitutions on Cu sites ?

$(Cu_{0.73}Zn_{0.27})_3(Zn_{0.88}Cu_{0.12})(OH)_6Cl_2$



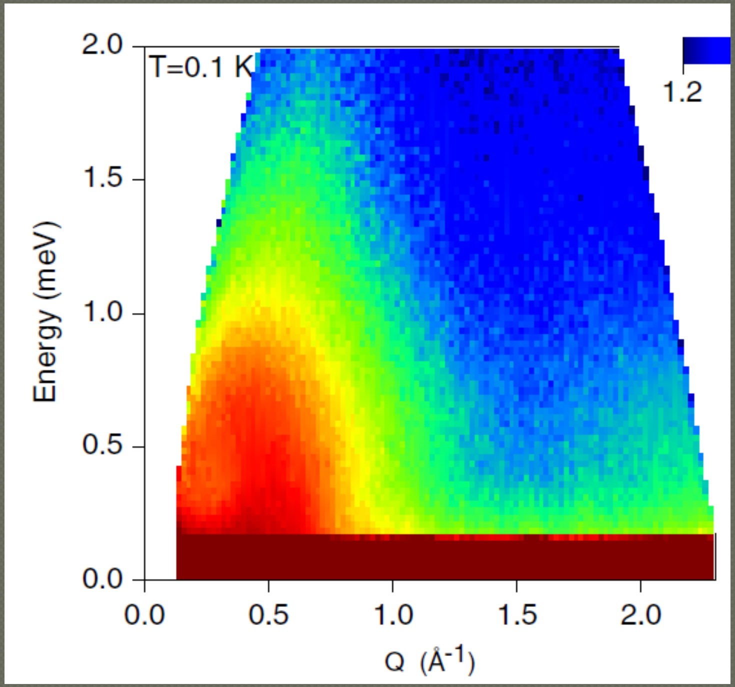
Dynamical correlations

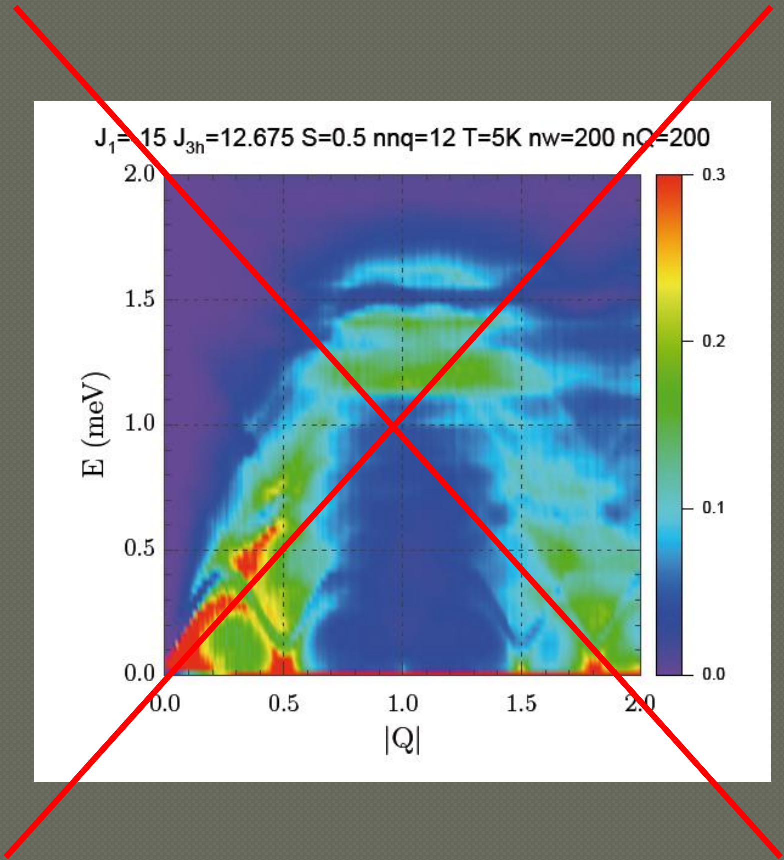




Schwinger bosons calculation

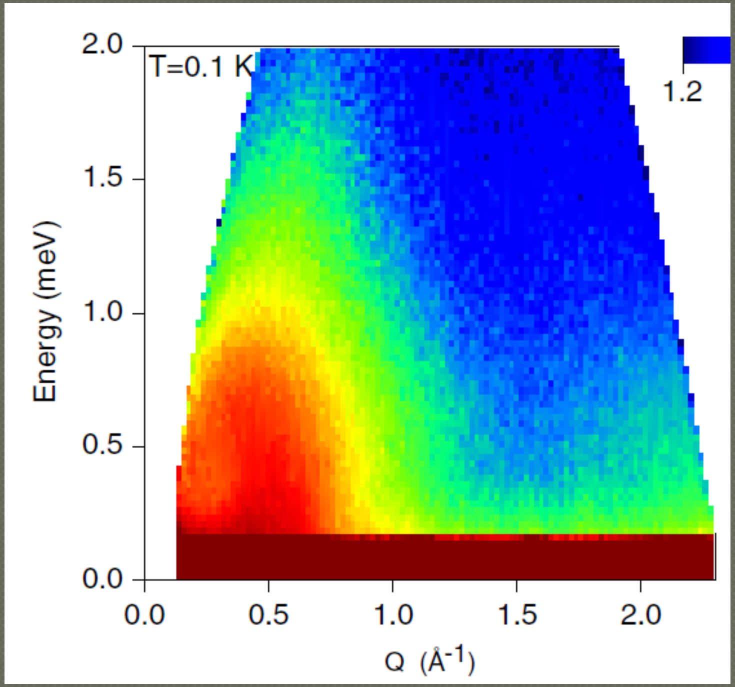
Dynamical correlations





Are not damped spin waves of the SR order!

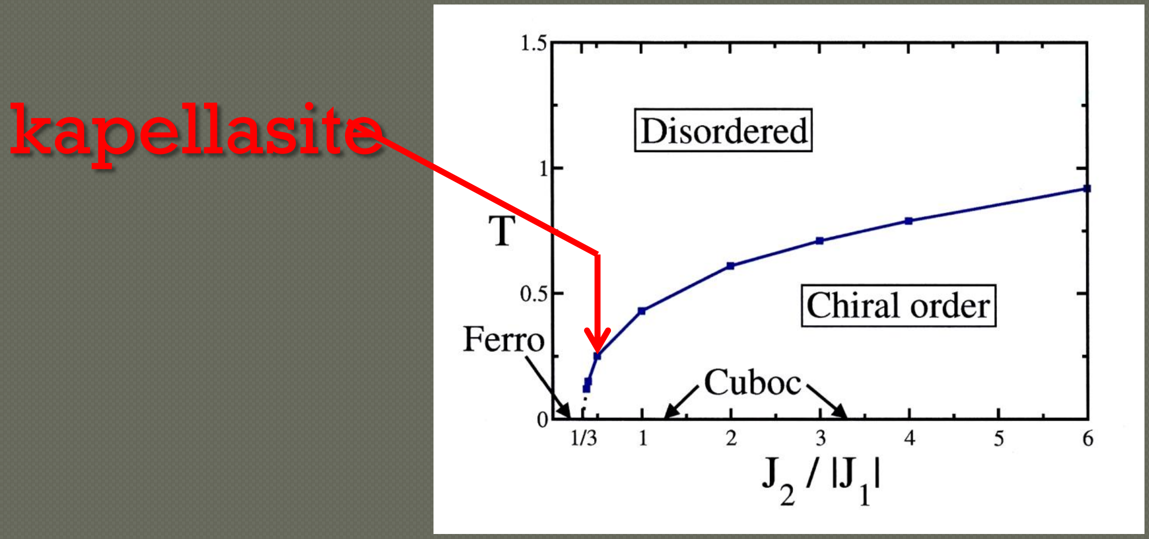
INS



- ✓ Continuum of spinons excitations…
- ✓ Wanted: a fermionic description of spinons!
- ✓ Is it a chiral spin liquid?

The classical cuboc2 phase diagram

- Chiral order parameter -> low temperature time reversal symmetry breaking phase



- Restoration of time reversal symmetry through a (weak) first order thermal phase transition
Domenge et al: PRB 78 2008

Summary of part II

- Kapellasite appears experimentally as a true Spin Liquid: gapless and dynamic down to 20 mK in spite of disorder (J/1000)
- Kapellasite is not in the same spin liquid phase as herbertsmithite. Very far from any critical point.
- A good model with competing interactions has been obtained.
- In the classical limit this model describes a chiral phase. Does the classical chiral phase survive quantum fluctuations? If Yes it might be measured through RIXS *(Ko and Lee PRB 84 2011)*

Outline

- A Quantum phase transition induced by Dzyaloshinskii-Moriya int. *(Cepas PRB 2008)* can explain the critical properties of herbertsmithite.
- Kapellasite: A new, different, gapless Spin Liquid. *B. Fåk, et al. PRL 109, 037208 (2012)*
  - Polymorph of herbertsmithite
  - Dynamical down to 20 mK
  - A good realization of a J1-J2-Jd model on the kagomé lattice with a ferromagnetic J1 *(Bernu 2012)*
- A chiral Spin Liquid?
  - The classical model has a chiral ground state (*Domenge PRB 2008, Messio PRB 2011)* and a weak first order phase transition at non zero temperature.
  - Does the chiral properties of the classical phase survive quantum fluctuations?

Conclusion of this first part

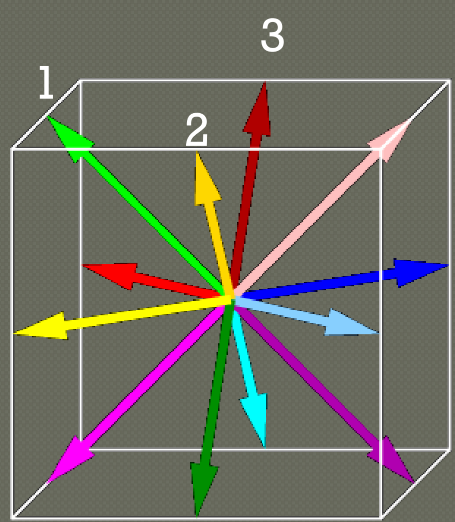
• Critical properties of Herbertsmihtite can be explained by the presence of a near-by Quantum Critical Point induced by Dzyaloshinskii-Moriya interactions.

• This nearby presence also explains why a small magnetic field is enough to push the system to a frozen phase.

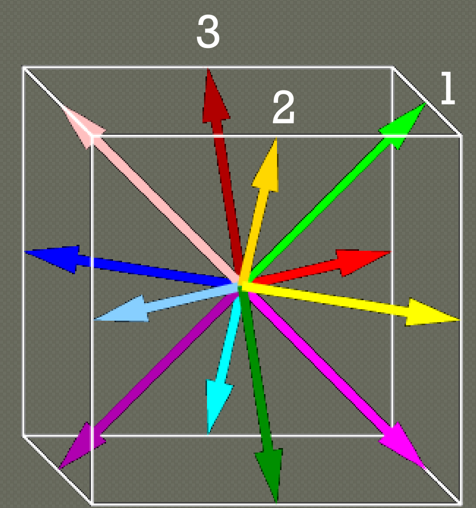
The classical cuboc2 phase

- A chiral order parameter

$$\sigma = \frac{S_1.(S_2 \times S_3)}{|S_1.(S_2 \times S_3)|}$$



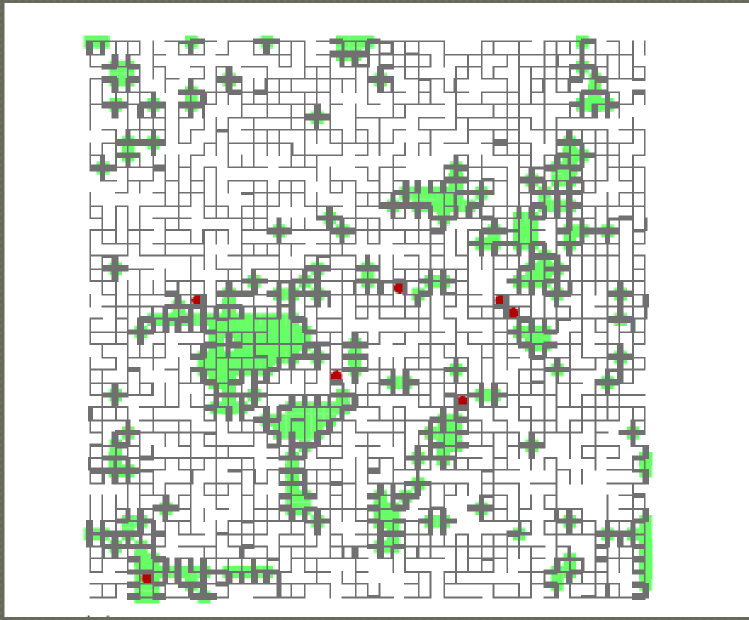
σ = +1



σ = -1

First order phase transition mechanism

Snapshot of a spin chirality configuration near the phase transition:

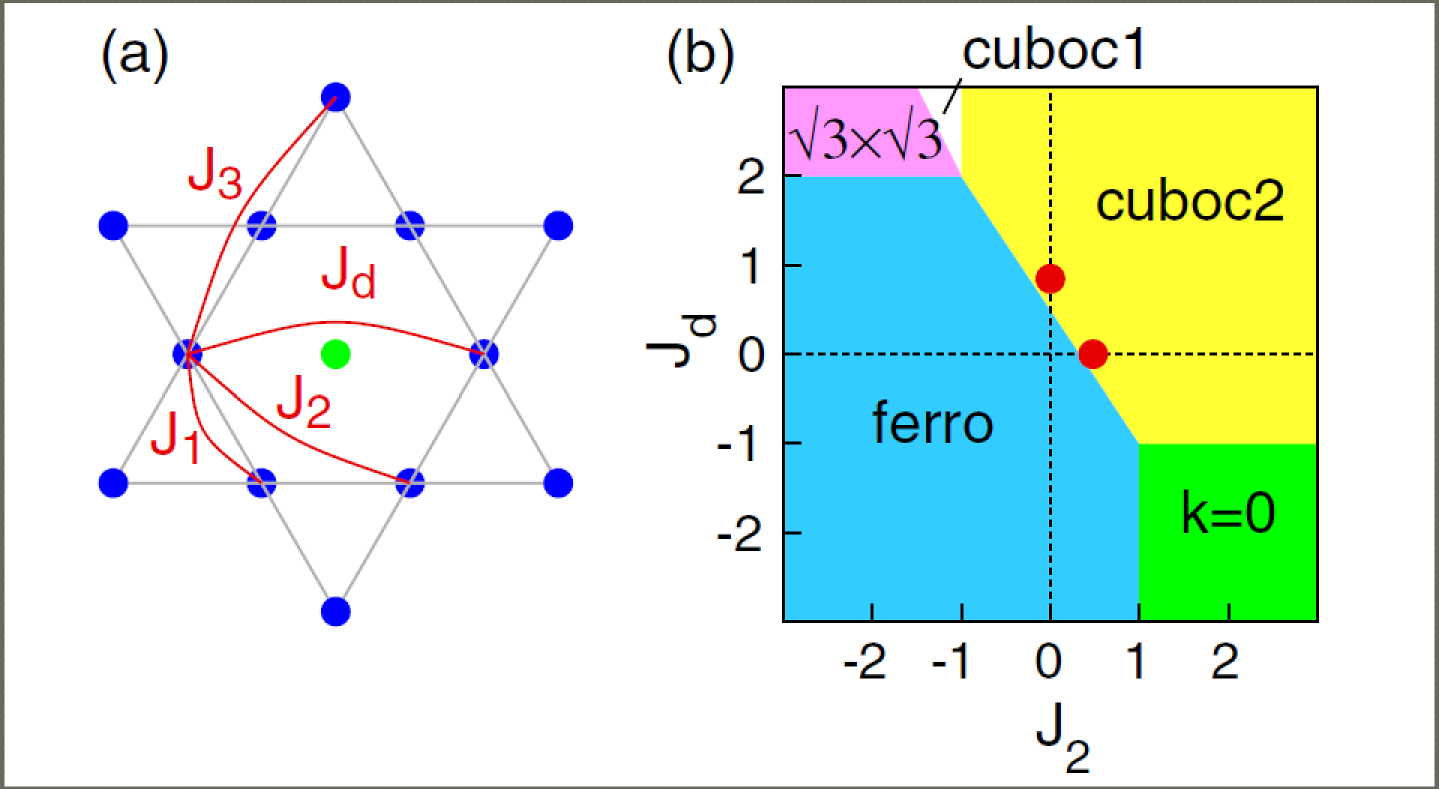


Z2 vortices (brown points) nucleate in the domain walls of chirality (white/green boundaries) and modify the domain wall energy

Messio et al. PRB 78

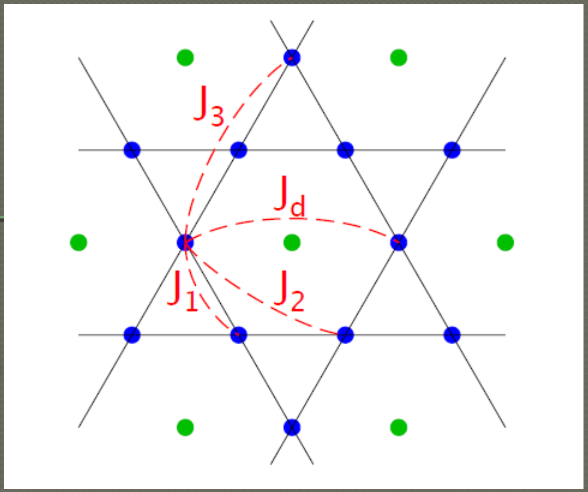
The classical cuboc2 phase

A large range of parameters with J_1 ferro



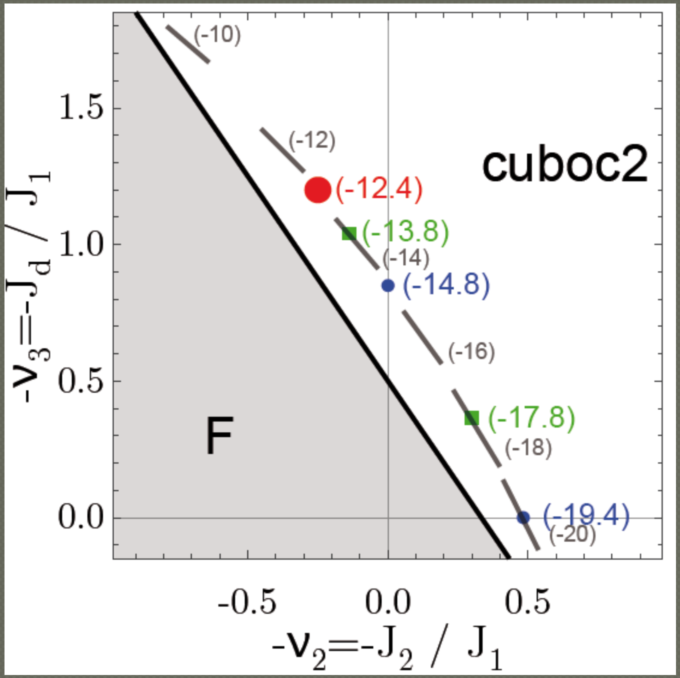
L. Messio Phys. Rev. B 83, 184401 (2011)

HT series (B. Bernu 2012)

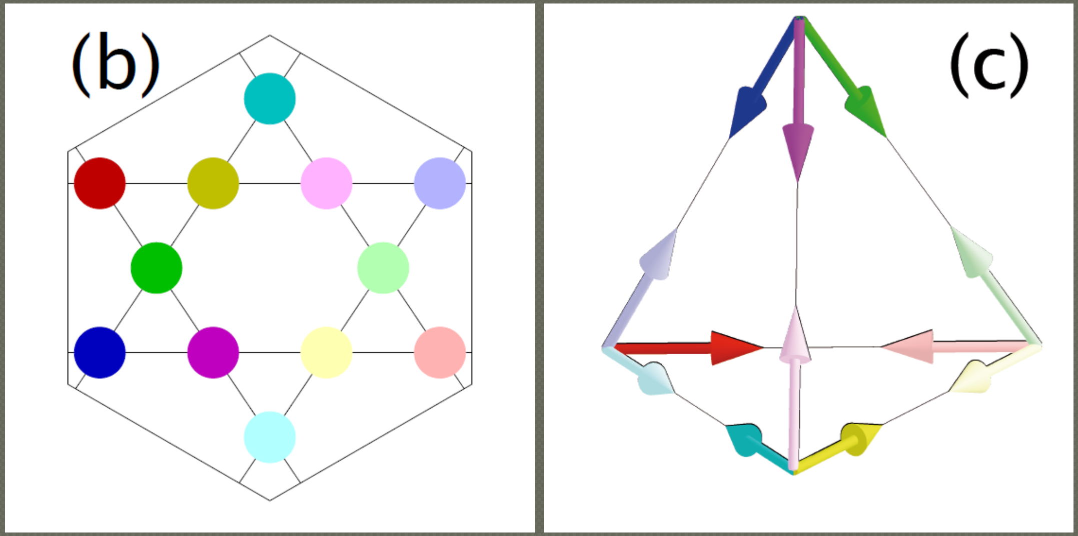


Competing exchange int.

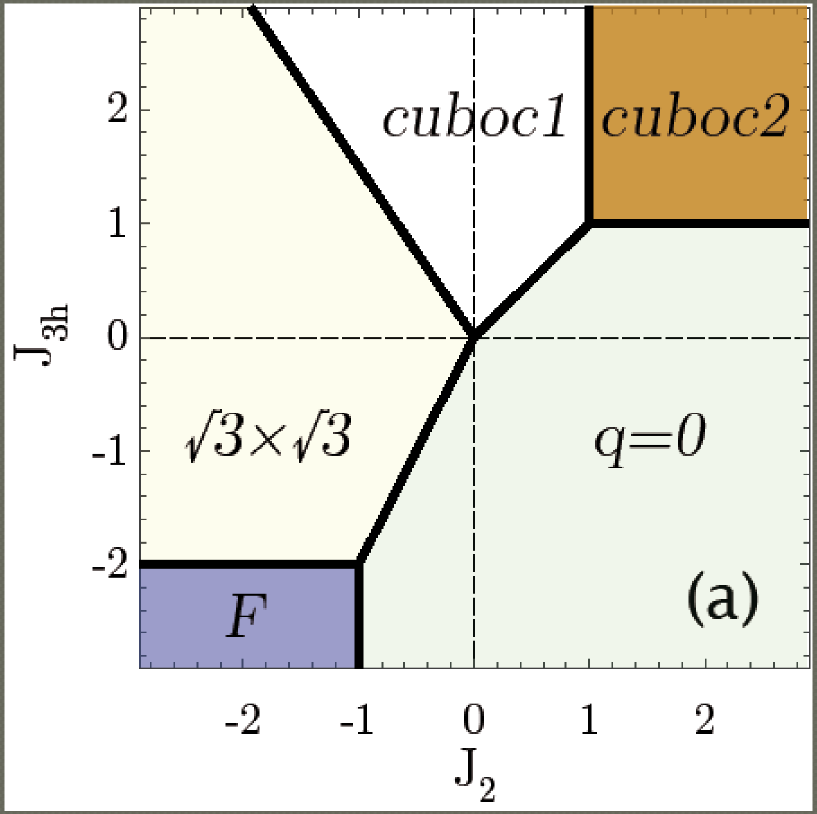
Best set of values J_1 = -12.4K, J_2 = -5K , J_d = +14.8

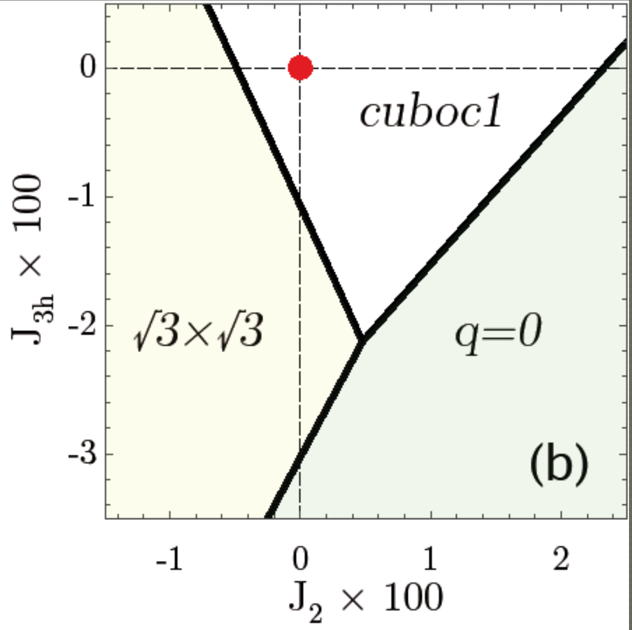


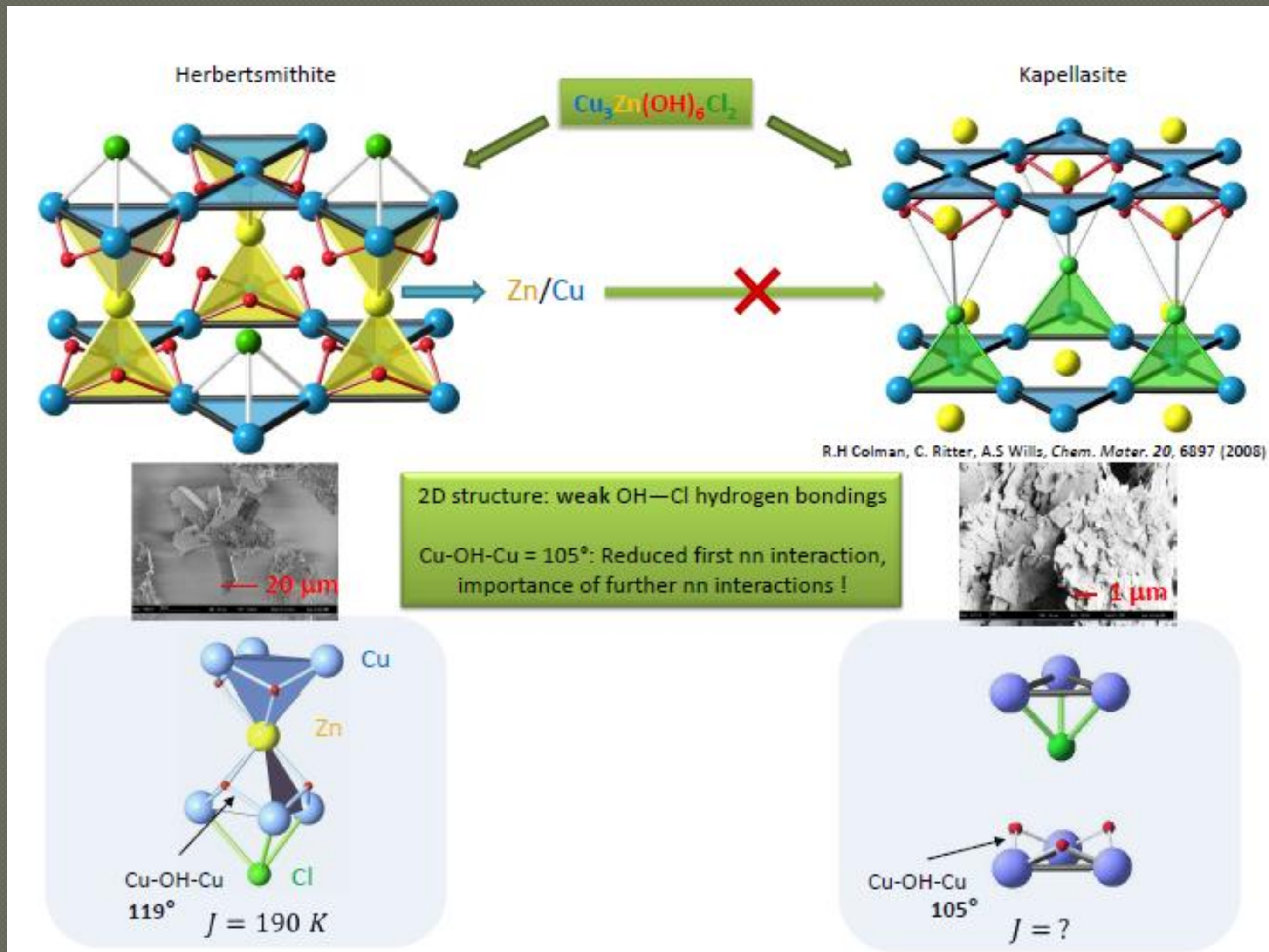
Classical phase diagram



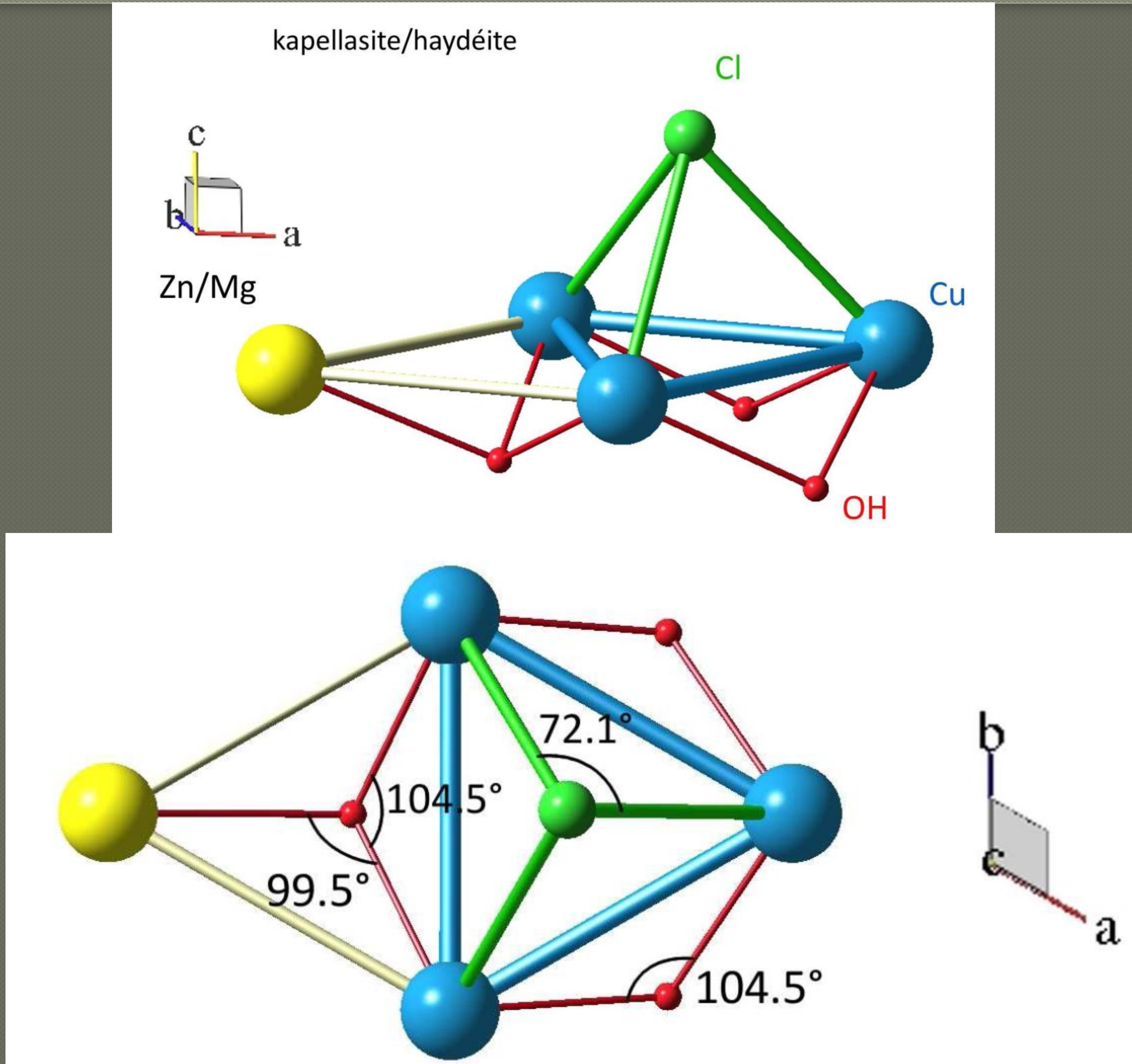
Classical order parameter

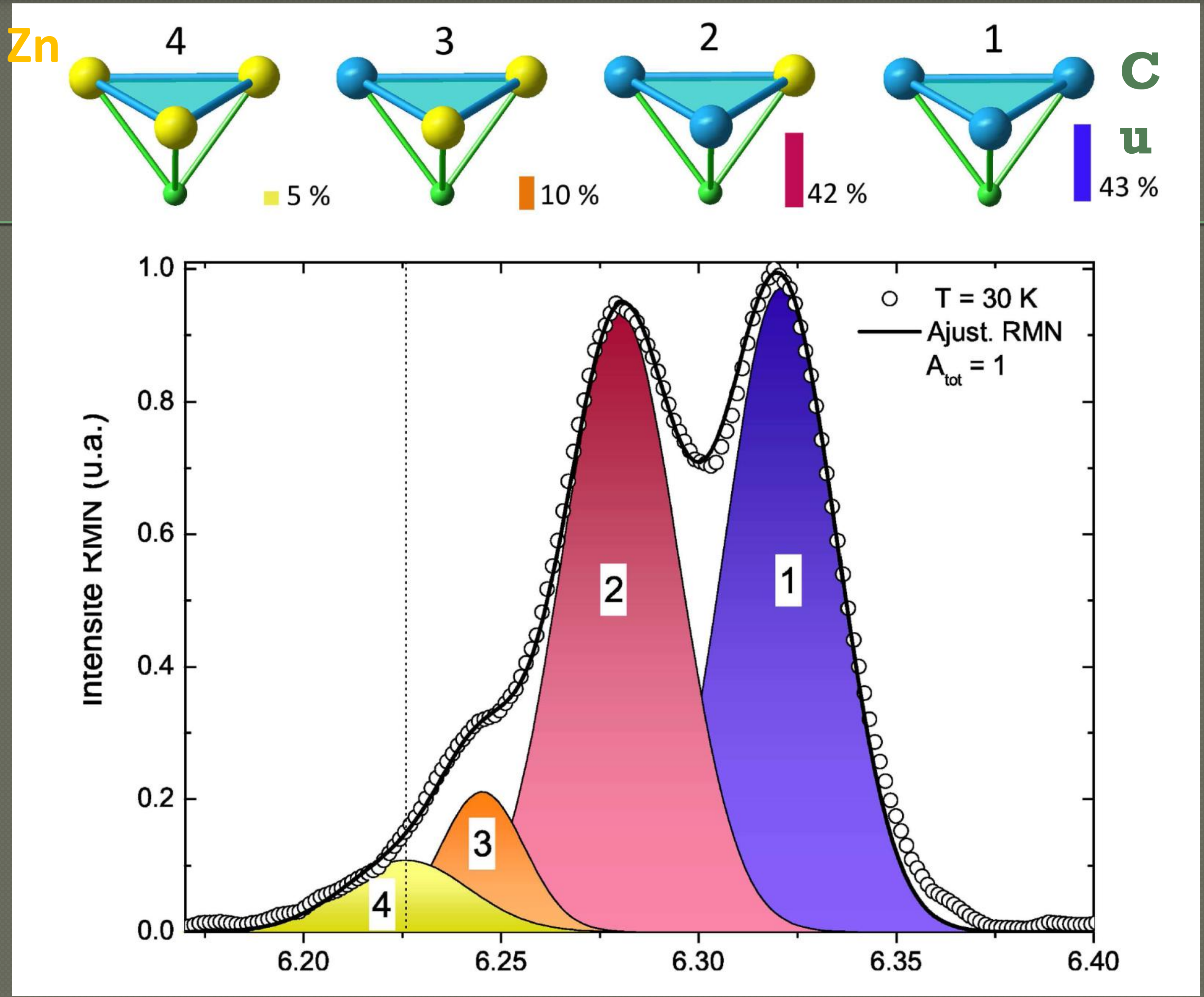

cuboc1
cuboc2
√3×√3
q=0
F
(a)
J3h
J2
-2
-1
0
1
2


cuboc1
√3×√3
q=0
(b)
J3h × 100
J2 × 100
0
-1
-2
-3
1
2



Herbertsmithite
Cu3Zn(OH)6Cl2
Kapellasite
Zn/Cu
R.H Colman, C. Ritter, A.S Wills, Chem. Mater. 20, 6897 (2008)
20 µm
2D structure: weak OH—Cl hydrogen bondings
Cu-OH-Cu = 105°: Reduced first nn interaction, importance of further nn interactions !
1 µm
Cu
Zn
Cl
Cu-OH-Cu
119°
J = 190 K
Cu-OH-Cu
105°
J = ?


kapellasite/haydéite
Cl
c
b
a
Zn/Mg
Cu
OH
72.1°
104.5°
99.5°
104.5°
b
c
a



Zn
4
3
2
1
C
u
5 %
10 %
42 %
43 %
Intensite RMN (u.a.)
T = 30 K
Ajust. RMN
A_{tot} = 1
1.0
0.8
0.6
0.4
0.2
0.0
6.20
6.25
6.30
6.35
6.40

Field (T)