The beginnings of Magnetic Structure Analysis

1948: First demonstration of the neutron diffraction

1949: the first direct evidence of Antiferromagnetism (in MnO)

AFM: Louis Néel – 1930
The beginnings of Magnetic Structure Analysis

1951: the Néel model of ferrimagnetism was confirmed

Magnetic Structure of Magnetite and Its Use in Studying the Neutron Magnetic Interaction
C. G. Shull, E. O. Wollan, and W. A. Strausser
Oak Ridge National Laboratory, Oak Ridge, Tennessee
December 8, 1939

Phys. Rev. 81, 483 (1951)

1953: Review articles on magnetic structures began appearing

Neutron Diffraction Studies of Various Transition Elements
C. G. Shull and M. K. Wilkinson
Oak Ridge National Laboratory, Oak Ridge, Tennessee

Recent Magnetic Structure Studies by Neutron Diffraction
By C. G. Shull,
Massachusetts Institute of Technology, Cambridge, Massachusetts, U. S. A.

Fe$_3$O$_4$, MnO, FeO, CoO, NiO, Cr, α-Mn, Ni, Fe
(powder and single crystal data & unpolarized and polarized neutrons)
The beginnings of Magnetic Structure Analysis

1955: Scheme of magnetic structures of the perovskite cited over 1900 times
The discovery of novel magnetic structures is unceasing, driven by their relationships to ferroelectricity, thermo-electricity, superconductivity, improved permanent magnets, and spintronic technologies.
Classifications of magnetic structures

**k-vector criteria**

- ferromagnet
- antiferromagnet
- reciprocal space
- magnetic peaks
- reciprocal space
- antiferromagnet
- reciprocal space
- circular helix
- circular cycloid
- transverse spin density wave
- longitudinal spin density wave

\[ \mu_{ij} = \sum_k S_{kj} e^{i k \cdot R_i} \]
Classifications of magnetic structures

“spin-reversal” 1’ operator (aka anti-symmetry or time-inversion) criteria

Four types of magnetic space groups (total of 1651):

**Type I**: $M = G$, made by point groups identical to the 32 crystallographic point groups, not involving the 1' operation. These are termed “single-color” or “colorless” (230 groups)

**Type II**: $M = G + G'$, consist of the 32 groups containing symmetry elements in both pure and prime forms. These are named “grey” groups, or “paramagnetic” groups (230 groups)

**Type III**: $M = D + (G - D)1'$, involves unprimed elements of the subgroup $D$ of index 2 of $G$, and the remaining operators $G$ that are being primed. These are called “black-white” (674 groups)

**Type IV**: $M = D + (G - D)1'$, same as Type III but $D = klassengleiche$, take account of the loss of translations (“anti-translats”) (517 groups). Correspond to those defined by the propagation vector $k = \tau/n, n=even \rightarrow$ do not allow ferromagnetism

$k = (\frac{1}{3},0,0)$

Type I or III MSG

$k = (\frac{1}{2},0,0)$

Type IV MSG
Classifications of magnetic structures

The lack of uniform description has made it impossible to organize the existing magnetic structures into a database.

A Commission on Magnetic Structures of the International Union of Crystallography was established in 2011. The commission’s mandate covers the following:

- establish standards for the description and dissemination of magnetic structures; (magCIF dictionary proposed by H. Stokes and B. Campbell was formally approved in Oct 2016; J. M. Perez-Mato and colleagues have started an online database of magnetic structures based on this new magnetic mCIF standard at the Bilbao Crystallographic Server)
- cooperate with other IUCr Commissions in establishing and maintaining standards of common interest, such as magnetic symmetry-group tables, magnetic nomenclature and magnetic form factor data
- Encourage communication and cultivate consensus among research communities that have independently developed diverse approaches to describing magnetic structures.
- Promote the sponsorship and organization of magnetic-structure sessions, symposia, and schools

Current members: B. Campbell (Chair, USA), M. Avdeev (Australia), M.T. Fernandez-Diaz (France), O. Garlea (USA), M. Henriques (Czech Republic), J.M. Perez-Mato (Spain), J. Rodriguez-Carvajal (France), T. Sato (Japan), A. Wills (UK), O. Zaharko (Switzerland)
A Hierarchy of Magnetic Structures based on Lattice Dimensionality

A magnetic state in a solid is the net result of the competing influences, thermal energy tending to randomize moments versus some quantum mechanical coupling tending to order moments.

Spin-Hamiltonian:

- **isotropic or anisotropic exchange interactions**
  \[ \mathcal{H}_{\text{ex}} = - \sum_{ij} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j \]
  \[ \mathcal{H}_{\text{an-ex}} = - \sum_{ij} J_{ij}^{xy} (\mathbf{S}_{ix} \cdot \mathbf{S}_{jx} + \mathbf{S}_{iy} \cdot \mathbf{S}_{jy}) + J_{ij}^z (\mathbf{S}_{iz} \cdot \mathbf{S}_{jz}) \]

- **antisymmetric Dzyaloshinskii-Moriya**
  \[ \mathcal{H}_{\text{DM}} = - \sum_{ij} D_{ij} \mathbf{S}_i \times \mathbf{S}_j \]

- **dipolar interactions**
  \[ \mathcal{H}_{\text{dip}} = \sum_{ij} \frac{(g \mu_B)^2}{r_{ij}^3} [3(\mathbf{r}_{ij} \cdot \mathbf{S}_i)(\mathbf{r}_{ij} \cdot \mathbf{S}_j) - \mathbf{S}_i \cdot \mathbf{S}_j] \]

- **single-ion anisotropy**
  \[ \mathcal{H}_{\text{ani}} = - \frac{1}{2} \sum_i D_S s_{iz}^2 + \frac{1}{2} \sum_i D'(S_{ix}^2 - S_{iy}^2) \]

- **field coupling**
  \[ \mathcal{H}_H = -H \sum_i g_i \mu_B \mathbf{S}_i \]
A Hierarchy of Magnetic Structures based on Lattice Dimensionality

• most of the magnetic ground states being realized primarily through the competition between *exchange interactions* \( \sum_{ij} J_{ij} S_i \cdot S_j \)

• all magnetic structures are three-dimensional, but …

• the strength of \( J_{ij} \) along different crystal direction, reflected in the velocity of spin-waves propagating in the lattice, can be very different

Example:

3D: \( J_\perp = J_{//}/2, J_z = J_{//}/10 \)

2D: \( J_\perp = J_{//}/4, J_z = J_{//} \times 10^{-3} \)

1D: \( J_\perp = J_{//} \times 10^{-2}, J_z = J_{//} \times 10^{-3} \)
A Hierarchy of Magnetic Structures based on Lattice Dimensionality

→ the effective dimensionality of the lattice plays an important role in the magnetic behavior and selection of magnetic structure

- 3D - networks
  
  perovskite, pyrochlore - corner-sharing tetrahedral, spinels with pyrochlore and diamond lattices, edge-sharing tetrahedra, …

- Layered structures
  
  square-planar, edge-sharing triangles, kagomé, honeycomb lattices, striped-kagomé ...

- Quasi-one-dimensional lattices
  
  simple-chain, ladders, sawtooth chains,…
3D - networks : Perovskites

ABO$_3$

Ordering scheme proposed by:
E. Wollan and W. Koehler, Phys. Rev., 100, 545 (1955)

A-type : antiferro- coupled ferromagnetic planes

B-type: ferromagnetic order (also called F)

C-type: ferromagnetic coupled antiferromagnetic planes

D-type: criss-crossed stripes

E and F-type: antiferromagnetism with ferrimagnetic planes

G-type: antiferromagnetically coupled spins in all directions
3D - networks: Perovskites

Symmetry: \textit{Pnma}

\[ \boldsymbol{k} = (0,0,0), \text{ M in 4b: (0,0,1/2)} \]

\[ \Gamma_{Mag} = 3\Gamma_1^1 + 0\Gamma_2^1 + 3\Gamma_3^1 + 0\Gamma_4^1 + 3\Gamma_5^1 + 0\Gamma_6^1 + 3\Gamma_7^1 + 0\Gamma_8^1 \]

in Kovalev notation

<table>
<thead>
<tr>
<th>IR</th>
<th>BV</th>
<th>Point Group</th>
<th>Shubnikov Group</th>
</tr>
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<tbody>
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<td>( \Gamma_1 )</td>
<td>( \psi_1 )</td>
<td>mmm</td>
<td>\textit{Pnma}, #62.441</td>
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<tr>
<td></td>
<td>( \psi_2 )</td>
<td>mmm</td>
<td>\textit{Pnma}, #62.441</td>
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<tr>
<td></td>
<td>( \psi_3 )</td>
<td>mmm</td>
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<td>( \psi_5 )</td>
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<td>( \psi_6 )</td>
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<td>( \Gamma_5 )</td>
<td>( \psi_7 )</td>
<td>mmm</td>
<td>\textit{Pnm'a'}, #62.448</td>
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<td>( \psi_9 )</td>
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<td>( \Gamma_7 )</td>
<td>( \psi_{10} )</td>
<td>mmm</td>
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<tr>
<td></td>
<td>( \psi_{11} )</td>
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<tr>
<td></td>
<td>( \psi_{12} )</td>
<td>mmm</td>
<td>\textit{Pn'm'a}, #62.446</td>
</tr>
</tbody>
</table>

\( \Gamma_1 \psi_1 \)

\( G_x \)

\( \Gamma_3 \psi_4 \)

\( B_x \)

\( \Gamma_5 \psi_7 \)

\( A_x \)

\( \Gamma_7 \psi_{10} \)

\( C_x \)
3D - networks : Perovskites


$H = - \sum_{i,j} J_{ij}(S_i \cdot S_j) - D \sum_i S_i^{2}$

$J \sim 9.6$ K, $J' \sim -6.7$ K, $D = 1.92$ K

Possible maximal symmetries $\mathbf{k} = (0,0,0)$

<table>
<thead>
<tr>
<th>Multiplicity</th>
<th>Wyckoff letter</th>
<th>Coordinates</th>
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</thead>
<tbody>
<tr>
<td>8</td>
<td>d</td>
<td>$(x,y,z</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$(x-y+1/2,z</td>
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<tr>
<td></td>
<td></td>
<td>$(x-y,z</td>
</tr>
<tr>
<td>4</td>
<td>c</td>
<td>$(x,1/4,z</td>
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<td></td>
<td></td>
<td>$(x-3/4,z</td>
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<tr>
<td>4</td>
<td>b</td>
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<td></td>
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<tr>
<td>4</td>
<td>a</td>
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</tr>
<tr>
<td></td>
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<td>$(0,1/2,0</td>
</tr>
</tbody>
</table>

YbAlO$_3$, Yb $\equiv S_{\text{eff}} = 1/2$ quantum chain material {Podlesnyak et al. Nature Comm. 10, 698 (2019)}
A$^{3+}_{2}$B$^{4+}_{2}$O$_{7}$

- two interpenetrating lattices (A, B) of corner-sharing tetrahedra ($Fd\bar{3}m$, sites 16c and 16d)
- strong geometrically frustrated NN AFM interactions → single-ion anisotropy, dipolar interactions, antisymmetric D-M are relevant

$Fd\bar{3}m$, $\mathbf{k} = (0, 0, 0)$

$\Gamma_{\text{mag}}(A) = 1 \Gamma_{3}^{(1)} + 2 \Gamma_{5}^{(1)} + 3 \Gamma_{7}^{(1)} + 3 \Gamma_{9}^{(2)}$
### 3D - networks : Pyrochlore lattices

<table>
<thead>
<tr>
<th></th>
<th>Anisotropy</th>
<th>Free moment</th>
<th>$\theta_{CW}$</th>
<th>$T_N$, $T_C$, or $T_f$</th>
<th>Ground State</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sm$_2$Ti$_2$O$_7$ [35]</td>
<td>Ising</td>
<td>1.5 $\mu_B$</td>
<td>-0.3 K</td>
<td>0.3 K</td>
<td>All-in/All-out</td>
</tr>
<tr>
<td>Gd$_2$Ti$_2$O$_7$ [53]</td>
<td>Heisenberg</td>
<td>7.9 $\mu_B$</td>
<td>-9 K</td>
<td>1 K</td>
<td>Partial order</td>
</tr>
<tr>
<td>Tb$_2$Ti$_2$O$_7$ [54]</td>
<td>Ising</td>
<td>9.7 $\mu_B$</td>
<td>-19 K</td>
<td>~1 K</td>
<td>Spin liquid?</td>
</tr>
<tr>
<td>Dy$_2$Ti$_2$O$_7$ [39]</td>
<td>Ising</td>
<td>10.6 $\mu_B$</td>
<td>+0.5 K</td>
<td>~1 K</td>
<td>Spin Ice</td>
</tr>
<tr>
<td>Ho$_2$Ti$_2$O$_7$ [38]</td>
<td>Ising</td>
<td>10.4 $\mu_B$</td>
<td>+1.9 K</td>
<td>~1 K</td>
<td>Spin Ice</td>
</tr>
<tr>
<td>Er$_2$Ti$_2$O$_7$ [46]</td>
<td>XY</td>
<td>9.5 $\mu_B$</td>
<td>-22 K</td>
<td>1.2 K</td>
<td>XY AFM</td>
</tr>
<tr>
<td>Yb$_2$Ti$_2$O$_7$ [55]</td>
<td>XY</td>
<td>4.5 $\mu_B$</td>
<td>+0.6 K</td>
<td>0.25 K</td>
<td>Canted FM</td>
</tr>
</tbody>
</table>

A. Hallas et al. Annu. Rev. Cond. Matter Phys. 9, 105, 2018

$\Gamma_3\psi_1$ (Fd-3m$'$)  
Sm$_2$Ti$_2$O$_7$ : Ising all-in/all-out

$\Gamma_9\psi_9$ (I4$_1$/am’d$'$)  
Ho$_2$Ti$_2$O$_7$ and Dy$_2$Ti$_2$O$_7$ : Ising two-in/two-out, spin ice

$\Gamma_5\psi_3$ (I4$_1$/am’d)  
Er$_2$Ti$_2$O$_7$ : AFM- XY pyrochlore

Pr$_2$Hf$_2$O$_7$ – Quantum Spin Ice (Sibille et al, Nat. Physics 14, 2018)  
NaCaNi$_2$F$_7$ – S=1 Heisenberg model- spin liquid (Plumb et al, Nat. Physics 15, 2019)
3D - networks : Spinel

$\text{AB}_2\text{X}_4$: corner-sharing tetrahedra (B) and diamond lattice (A)

chemically versatile: transition metal Oxides, Sulfides and Selenides

- ACr$_2$O$_4$ with non-magnetically A-site exhibit simultaneous lattice distortion and magnetic order due to the spin–lattice coupling

- AV$_2$O$_4$, with V$^{3+}$ ($3d^2$) - model systems for studying orbital order in frustrated lattice. Sequence of phase transitions: structural distortion followed by a magnetic transition.

ZnV$_2$O$_4$ \(F\overline{d}3m \rightarrow I\overline{4}_1/\text{amd}\) (\(T_{S}=50\text{K}\))

\(k = (0, 0, 1), \text{AFM}\) (\(T_{N}=40\text{K}\))

FeV$_2$O$_4$ (\(A = Fe^{2+} (3d^6) S=2\))

\(F\overline{d}3m \rightarrow I4_1/\text{amd} \rightarrow F\overline{ddd} \rightarrow I4_1/\text{amd}\).

collinear FerriM (\(T_{N1}= 110\text{K}\)) \(\rightarrow\) canted FerriM (\(60\text{K}\))

“two-in/two-out”
3D - networks: Diamond-lattice in Spinel systems

Only the A-site of the spinel lattice is occupied by magnetic atoms

• two interpenetrating FCC sublattices: four NN ($J_1$) and twelve NNN ($J_2$) competing exchange interactions

• for $J_2/J_1 > 1/8$ → large ground-state degeneracy and the possibility of spin-liquid behavior. The degeneracy could be lifted by thermal or quantum effects to enable a magnetic ordering via the “order-by-disorder” mechanism (CoAl$_2$O$_4$, MnSc$_2$S$_4$, FeSc$_2$S$_4$ … )

MnSc$_2$S$_4$: Commensurate (C) → IC below $T_{N2} = 1.9$ K, $k = (3/4 \pm 0.02, 3/4 \pm 0.02, 0)$

Spiral spin-liquid state → helical long-range ordered state due to dipolar and $J_3$ perturbations

3D - networks: Double Perovskites with edge-sharing tetrahedra

- **B’ magnetic site** = frustrated FCC lattice.
- **A** = diamagnetic alkaline earth or lanthanide cation
- **spin-orbit coupling** → monoclinic distortion ($I4/m$ or $P2_1/n$, $\sqrt{a_p} \times \sqrt{a_p} \times 2a_p$)

\[ \text{C. Jones and P. D. Battle, J. Solid State Chem. 78, 108, 1989} \]

- **Type I**: dominant (B’-O-O-B’) NN interactions → AFM order between successive (001) ferro planes; $\mathbf{k} = (0, 0, 1)$
- **Type II**: dominant (B’-O-A-O-B’) NNN exchange interactions → spins alternate along two directions
- **Type III**: comparable NN and NNN; $\mathbf{k} = (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
**3D - networks : Double Perovskites**

\[ \text{A}_2\text{BB'}\text{O}_6 \] - when B, B' or A, B' are magnetic: the interplay between intra-lattice frustration and the inter-lattice interaction can lead to a wide variety magnetic states

FM metals (B–O–B’–O–B coupling mediated by itinerant electrons) :
- \( \text{Sr}_2\text{FeMoO}_6 \) \( (T_C = 420 \text{ K}) \)
- \( \text{Sr}_2\text{CrReO}_6 \) \( (T_C = 625 \text{ K}) \)

Ferri insulators :
- \( \text{Sr}_2\text{CrOsO}_6 \) \( (T_C = 725 \text{ K}) \)
- \( \text{Ca}_2\text{FeReO}_6 \) \( (520 \text{ K}) \)
- \( \text{Sr}_2\text{MnReO}_6 \), ...

AFM insulators :
- \( \text{Sr}_2\text{FeOsO}_6 \), \( \text{Sr}_2\text{CoOsO}_6 \), \( \text{Nd}_2\text{NaOsO}_6 \), ...

**Diagram**

- \( \text{Sr}_2\text{CoOsO}_6 \): \( 14/m \to 12/m \)
  - Os: \( T_{N1} = 108 \text{ K}, \mathbf{k}_1 = (\frac{1}{2}, \frac{1}{2}, 0) \)
  - Co: \( T_{N2} = 67 \text{ K}, \mathbf{k}_2 = (\frac{1}{2}, 0, \frac{1}{2}) \)

- \( \text{Nd}_2\text{NaOsO}_6 \): \( P2_1/n \)
  - \( T_N = 16 \text{ K}, \mathbf{k} = (\frac{1}{2}, \frac{1}{2}, 0) \)
2D structures: Square-planar metal-oxygen/halogen

\[ \text{K}_2\text{NiF}_4, \]


Inter-layer exchange smaller than the intra-plane exchange by at least three orders of magnitude \(\Rightarrow\) 2D Heisenberg antiferromagnet. ("Bragg ridges" rather than Bragg peaks)

Layered perovskite - high-Tc Cuprates
Fe - pnictides: ZrCuSiAs-type (1111) or ThCr\(_2\)Si\(_2\)-type (122), Fe(Se,Te) (11)

structure distorts at \(T_N\)

2D structures: Square-planar metal-pnictogen lattices

Co – pnictides containing two magnetic sublattices (Co, RE)

**NdCoAsO**
- $T_c = 69$ K, FM-Co
- $T_{N1} = 14$ K, AFM-Co
- $T_{N2} = 3.5$ K, AFM-Nd/Co
- $\mathbf{k} = (0, 0, \frac{1}{2})$

**NdCo$_{1.7}$As$_2$**
- $T_c = 69$ K, FM-Co
- $T_N = 6$ K, FiM-Nd/Co
- $\mathbf{k} = (0, 0, 0)$

**NdCo$_2$P$_2$**
- $T_{N1} = 309$ K, AFM-Co
- $T_{N2} \sim 100$ K, AFM-Nd/Co
- $\mathbf{k} = (0, 0, \frac{1}{2})$

$m(\text{Nd}) \neq 0$

$m(\text{Nd}) = 0$
2D structure: edge-sharing equilateral triangles

- simplest geometrical frustrated lattice
- planar 120° spin structure or “three-sublattice \(\sqrt{3} \times \sqrt{3}\) state”
- other ordered states can be stabilized by NNN interactions, anisotropy of the orbital configuration, or magnetoelastic coupling.

- \(\text{VX}_2\) and \(\text{AMX}_3\), where \(A = \text{Cs, Rb, X = Cl, Br, I}\)
- \(A^+\text{M}^{3+}\text{O}_2\) series with delafossite or \(\alpha-\text{NaFeO}_2\) structures
- 6H-perovskites \(\text{Ba}_3\text{M}^{'}\text{M}^{''}2\text{O}_9\) with \(M^{'} = \text{Ni, Co, Mn, and M}^{''} = \text{Nb or Sb}\)
- \(\text{RbFe(MoO}_4\text{)}_2, \text{Rb}_4\text{Mn(MoO}_4\text{)}_3, \text{K}_2\text{M}^{2+}_3(\text{VO}_4\text{)}_2\text{CO}_3, \text{Na}_2\text{BaM}^{2+}_3(\text{VO}_4\text{)}_2, \text{K}_3\text{RE}^{3+}(\text{VO}_4\text{)}_2\)

- XY-type anisotropy (\(D \leq 0\))
  - 120° spin structure in \(ab\) plane
- easy-axis anisotropy (\(D > 0\))
  - successive transitions: colinear and canted “Y”

\begin{align*}
\text{Ba}_3\text{NiNb}_2\text{O}_9, k = (\frac{1}{3}, \frac{1}{3}, \frac{1}{2}) \\
\text{K}_2\text{Mn}_3(\text{VO}_4\text{)}_2\text{CO}_3, k = (\frac{1}{3}, \frac{1}{3}, 0)
\end{align*}
2D structure: edge-sharing equilateral triangles

triangular Heisenberg antiferromagnet: rich range of phases in applied field

thermal and quantum fluctuations stabilize:
- coplanar, three-sublattice “Y state,”
- “uud” state - one-third magnetization plateau
- a coplanar 2:1 canted phase

↩ Seabra et al, PRB, 84, 214418 (2011)
2D structure: Kagomé (corner-shared triangular) lattice

- variety of ground states: spin liquid, short-range order, or long-range order that can be stabilized by further-neighbor and D-M interactions
  - classical kagomé lattice orders with planar 120° between NN spins
    - \( q = 0 \): spin arrangement with uniform vector chirality
    - \( q = \sqrt{3} \times \sqrt{3} \): alternative spin arrangement with staggered vector chirality

- volborthite, herbertsmithite, kapellasite and jarosite series

Fe-based jarosites \( \text{AFe}_3\text{(SO}_4\text{)}_2\text{(OH)}_6 \), with A = K, Na, Ag, (R-3m symmetry)

\( k = (0, 0, 3/2) \) order into planar “\( q = 0 \)” type with AFM stacking of the layers

A. Wills, PRB, 63, 064430 (2001)
2D structure: honeycomb lattices

\[ H = J_1 \sum_n S_i \cdot S_j + J_2 \sum_{nn} S_i \cdot S_j + J_3 \sum_{nnn} S_i \cdot S_j + J_z \sum_{nn} S_i \cdot S_j \]

J$_2$/J$_1$ – J$_3$/J$_1$ phase diagrams for AF J$_1$ > 0 and for FM J$_1$ < 0

Lefrançois, PRB B 94, 214416 (2016)

the Kitaev model (S=1/2 interacting via anisotropic bond-dependent coupling → Majorana-like excitations, or Zigzag ordered state (α-RuCl$_3$, Na$_2$IrO$_3$, …)

2D structure: honeycomb lattices

Examples of honeycomb lattice compounds:

- MnTiO3, - Néel order,
- Cu₃M₂SbO₆, Na₃M₂SbO₆ (M=Cu, Mn, Co, Ni) - zigzag order
  - Na₂Co₂TeO₆, Zigzag \( \mathbf{k} = (1/2, 0, 0) \), \( P \overline{C} 2_1 2_1 2_1 \)
- BaM₂(XO₄)₂ (M = Co, Ni, and X = P, As, V),
  - BaCo₂(AsO₄)₂, Helical \( \mathbf{k} = (0.261, 0, -4/3) \)
  - BaNi₂(PO₄)₂, Néel \( \mathbf{k} = (0, 0, 0) \)
  - BaNi₂(AsO₄)₂, Zigzag \( \mathbf{k} = (\frac{1}{2}, 0, \frac{1}{2}) \)
**2D structure: frustrated “bow-tie” lattices**

“bow-tie” or striped kagomé

\[ \text{Ca}_2\text{Mn}^{4+}_3\text{O}_8, \text{K}_2\text{Mn}^{2+}_3(\text{VO}_4)_2(\text{OH})_2 \]

Striped triangular lattice

\[ \text{Mn}^{2+}_5(\text{VO}_4)_2(\text{OH})_4 \]

\[ k = (0, \frac{1}{2}, 0) \]

\[ m(\text{Mn}1) \approx 1.98 \mu_B \]
\[ m(\text{Mn}2) \approx 2.43 \mu_B \]
\[ m(\text{Mn}3) \approx 2.48 \mu_B \]

\[ \text{AFM - NN} \]
\[ \text{Mn}1, 3 \text{ NN} \]
\[ \text{Mn}2, 4 \text{ NN} \]

\[ P_b2/c \]

\[ k = (0, \frac{1}{2}, 0) \]

\[ m(\text{Mn}1) \approx 1.7 \mu_B \]
\[ m(\text{Mn}2) \approx 2.5 \mu_B \]

\[ \text{AFM - NN} \]
\[ \text{Mn}1, 3 \text{ NN} \]
\[ \text{Mn}2, 4 \text{ NN} \]
2D structure: Isosceles triangle lattice ↦ possible Quasi-1D

NaMnO$_2$  Cu$_{1+x}$Mn$_x$O$_2$, Mn$^{3+}$($t_{2g}^3e_g^1$)

$k = (\frac{1}{2}, \frac{1}{2}, 0)$ or $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$

C2/m ↦ P-1, $T_S \approx 65$ K (Cu) and $T_S \approx 45$ K (Na)

$$H = J_{\parallel} \sum_{nn} S_i \cdot S_j + J_{\perp} \sum_{nnn} S_i \cdot S_j + J_z \sum_{nnn} S_i \cdot S_j - D \sum_n (S_n^z)^2$$

1D character of spin dynamics

Dally et al. Nature Comm. 9, 2188 (2018)
2D structure: Shastry-Sutherland lattice \( \rightarrow \) possible 0 D

Interpenetrating planar sublattices of orthogonal dimers

\[ \text{REB}_4 : \text{RE} = \text{Er}, \text{Tm} - \text{strong Ising} \]
\[ \text{RE} = \text{Ho} - \text{XY anisotropy.} \]

\[ \text{HoB}_4 : \]
- \( T_{N1} = 7K, k_1 = (0.02, 0.02, 0.4) \) and \( T_{N2} = 5K, k_2 = (1 0 0) \)
- Fractional magnetization plateaus in applied field

**Yb\(_2\)Pt\(_2\)Pb, Yb -strong Ising anisotropy**

\( k_1 = (1/5,1/5, 0) \) & \( k_2 = (-1/5,1/5, 0) \)

\[ \text{spinon dispersion along the c axis typical of the} \]
\[ S=1/2 \text{ Heisenberg-Ising XXZ spin Hamiltonian} \]

\[ \text{Miiller et al., PRB 93, 104419 (2016)} \]

\[ \text{L. Wu Science 352, 1206 (2016)} \]
\[ \text{Gannon et al. , Nature Comm., 10, 1123 (2019)} \]
Quasi-1D structures

strong exchange coupling between magnetic ions only along one direction

- metal-organic frameworks (MOFs): connected low-dimensional inorganic subnetworks through non-magnetic molecules
- alkali-metal pyroxenes $\text{AMX}_2\text{O}_6$, $A = \text{Li}^+, \text{Na}^+$; $M = \text{Ti}^{3+}, \text{V}^{3+}, \text{Cr}^{3+}, \text{Mn}^{3+}$, and $\text{Fe}^{3+}$; $X = \text{Si}^{4+}, \text{Ge}^{4+}$
- brackebuschite $\text{Ba}_2M^{3+}(\text{VO}_4)_2(\text{OH})$ and descloizite $\text{SrM}^{2+}(\text{VO}_4)(\text{OH})$ transition metal vanadate

$\text{NaMnGe}_2\text{O}_6$ pyroxene

$\mathbf{k} = (0, 0, \frac{1}{2})$

$\text{Co}_4(\text{OH})_2(\text{C}_{10}\text{H}_{16}\text{O}_4)_3$

$\mathbf{k} = (0, 0, 0)$, $d_{\text{interchain}} \sim 12\text{Å}$

$\text{SrCo}^{2+}(\text{VO}_4)(\text{OH})$

$\mathbf{k} = (0, 0, 0)$
Quasi-1D structures: delta or “sawtooth” chains

Prototype example of highly frustrated lattices; can be seen as derived from a kagomé lattice by removing magnetic sites in periodic lines perpendicular to the kagomé spine direction.

- Olivines ($M_2XO_4$, $X = Si$, Ge), oxy-arsenates $A_2Fe_2O(AsO_4)_2$, and alkali Transition Metal Molybdates $CsM_2(MoO_4)_2(OH)$ ($M = Mn$, Fe, Co, Zn), $Rb_2M_3(MoO_4)_3(OH)_2$ ($A = K$, Rb; $M = Mn$, Co).

$Ni_2SiO_4$ 
$k = (\frac{1}{2}, 0, \frac{1}{2})$;

$Rb_2Fe_2O(AsO_4)_2$ 
$k = (0, 0, 0)$;

$CsM_2(MoO_4)_2(OH)$ 
$k = (\frac{1}{2}, 0, 0)$;
Summary

The effective dimensionality & topology of the crystal lattice plays an important role in defining the magnetic ordered state.

A hierarchy of magnetic structures based on lattice dimensionality can be established. Exceptions to this classification can lead to discovery of new physics.

Magnetic structure determination is an important step in understanding materials, as it places your system inside a magnetic phase diagram.

Think of the mechanisms that are responsible for the static order. Consider complementing your findings with spin dynamics studies to answer the “So What?” question.
Thank you!