



# Magnetism and Geometric Frustration

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ILL Clip Session







### Group



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## **Magnetisation Distribution Maps of Powders**



- Molecular Magnets
- Colossal magnetoresistance
- Superconductors







## **Prussian Blue** $\text{Fe}^{\text{III}}_{4}[\text{Fe}^{\text{II}}(\text{CN})_{6}]_{3}.14\text{H}_{2}\text{O}$



Fm-3m

$$Fe_{\downarrow}^{III} - NC - Fe^{II} - CN$$

$$\sim 10.2 \text{\AA}$$

- Origin of colour is CT from Fe II (low spin) to Fe III (high spin)
- Proposed mechanism via spin transfer to the nominally non-magnetic Fe<sup>II</sup>









## **Test Experiment on D1b**

## **Reconstruction**

- Replace any magnetic components
- Polarisation of monochromatic beam using <sup>3</sup>He Spin Filter
- Guide tube with nutator fitted

### Systems

- Prussian Blue
- YNi<sub>3</sub>











## Analysis

- Multipolar refinements
- Spin Patterson Density Distribution Maps
- Maximum Entropy MEMSYS and PRIMA











## **Erbium Titanate Er<sub>2</sub>Ti<sub>2</sub>O<sub>7</sub>**

The model <111> XY Antiferromagnet?

• The Hamiltonian has a macroscopically degenerate set of ground states at T = 0 but MC simulations indicate that thermal fluctuations induce an AF groundstate





Tetrahedral basis with  $\mathbf{k} = 000$ , selected by OBD

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Field dependency from 0 to 9.5 Tesla at 55 mK collected on D3

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## **Future Work**

- Magnetisation density studies of ferromagnetic superconductors that cannot be synthesised as single crystals – D20
- Intermediate and high field magnetic phases of Er<sub>2</sub>Ti<sub>2</sub>O D10
- Determination of AF form factors and AF phase? – CRYOPAD on D3
- Construct Magnetic Phase Diagram for the frustrated itinerant ferromagnetic Iron stannate compound, which displays AH – D20

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