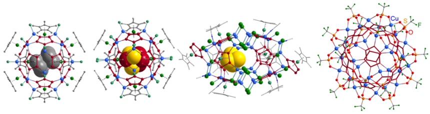

Figure 1. (left to right) Copper haide-based supramolecules encapsulating molecules of ferrocene, P_4S_3, and As_4. Inorganic core of a supramolecule based on copper triflate.

Keywords: giant supramolecule, pentaphosphaferrocene, inclusion compound, host-guest interaction, intermolecular interaction, single-crystal X-ray diffraction

MS33-P7 Small Angle Neutron Diffraction on the Vortex Lattice of Type II Superconductors

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In type II superconductors in magnetic fields $H_{c1}<H<H_{c2}$ the flux form a Vortex Lattice VL, whose geometry represents a delicate balance of the electronic Fermi surface features and pinning. This provides a very sensitive probe of some microscopic electronic properties which can be measured using small angle neutron scattering technique SANS. Below we describe selected results.

i) $YBa_2Cu_3O_{7-\delta}$ with δ=0, 0.15 at 2 K and for fields of up to 16 T applied parallel to the crystal c-axis, we observe in the SANS data (see Fig. 1) a sequence of field-driven and first-order transitions between different VL structures. By rotating the field away from the c-axis, we observe each structure transition to shift to either higher or lower field dependent on whether the field is rotated towards the [100] or [010] direction. We argue that these transitions are determined by the Fermi Surface Morphology [1].

(ii) KFe_2As_2, and related materials. We find an intrinsic anisotropy of the superconducting state in this material. With the SANS technique we monitor the vortex and find a field dependent anisotropy, indicating multiband superconductivity. These results support that KFe_2As_2 is Pauli limited for field applied in the basal plane.

iii) The flux-line lattice in CaAlSi has been studied by small-angle neutron scattering. A well-defined hexagonal flux-line lattice is seen just above Hc1 in an applied field of only 54 Oe. A 30_ reorientation of this vortex lattice has been observed in a very low field of 200 Oe. This reorientation transition is first-order and reflect nonlocal effects [3].

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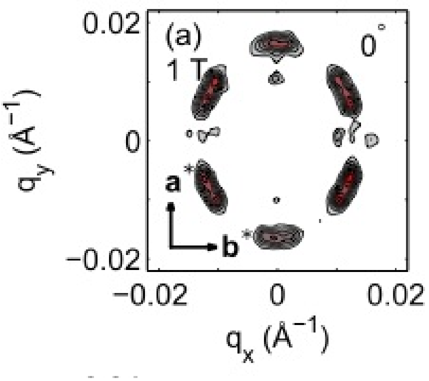

Figure 1. SANS diffraction pattern from a VL on $YBa_2Cu_3O_{7-d}$ at 2K and an external field of 1T parallel to c

Keywords: SANS, Vortex Lattice, superconductors

MS33-P8 Alien Features: In Superspace, No One Can Hear You Scream…

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Single-crystal diffraction is the foremost technique used to give the definitive answer to how atoms and molecules pack in the crystalline solid state. As a maturing technique, data collections have been getting faster and faster, and structure determination is becoming more routine, with an increasing number of non-expert users collecting data, solving and refining structures, and publishing their results. However, with the advent of higher intensity laboratory X-ray sources, easier access to synchrotron radiation and more sensitive detectors, more and more molecular structures are showing alien features beyond the realms of conventional crystallography. These include, super-lattice reflections, incommensurate satellite peaks and diffuse features. These can affect everything from the smallest molecules to large macrocycles to frameworks. [1-3]

Here we present a selection of the data that have made us want to scream when working in collaboration with the Chemists in Oxford.

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[3] C. B. Pinheiro, *et. al.*, IUCrJ (2015), 2, 137-154.

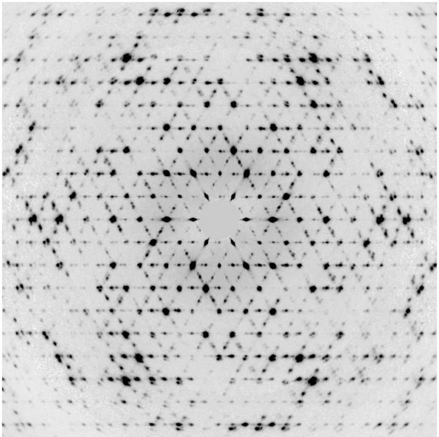

Figure 1. Can you hear us scream?

Keywords: modulated structures, diffuse scattering, non-Bragg