Single Crystal Diffractometer TOPAZ

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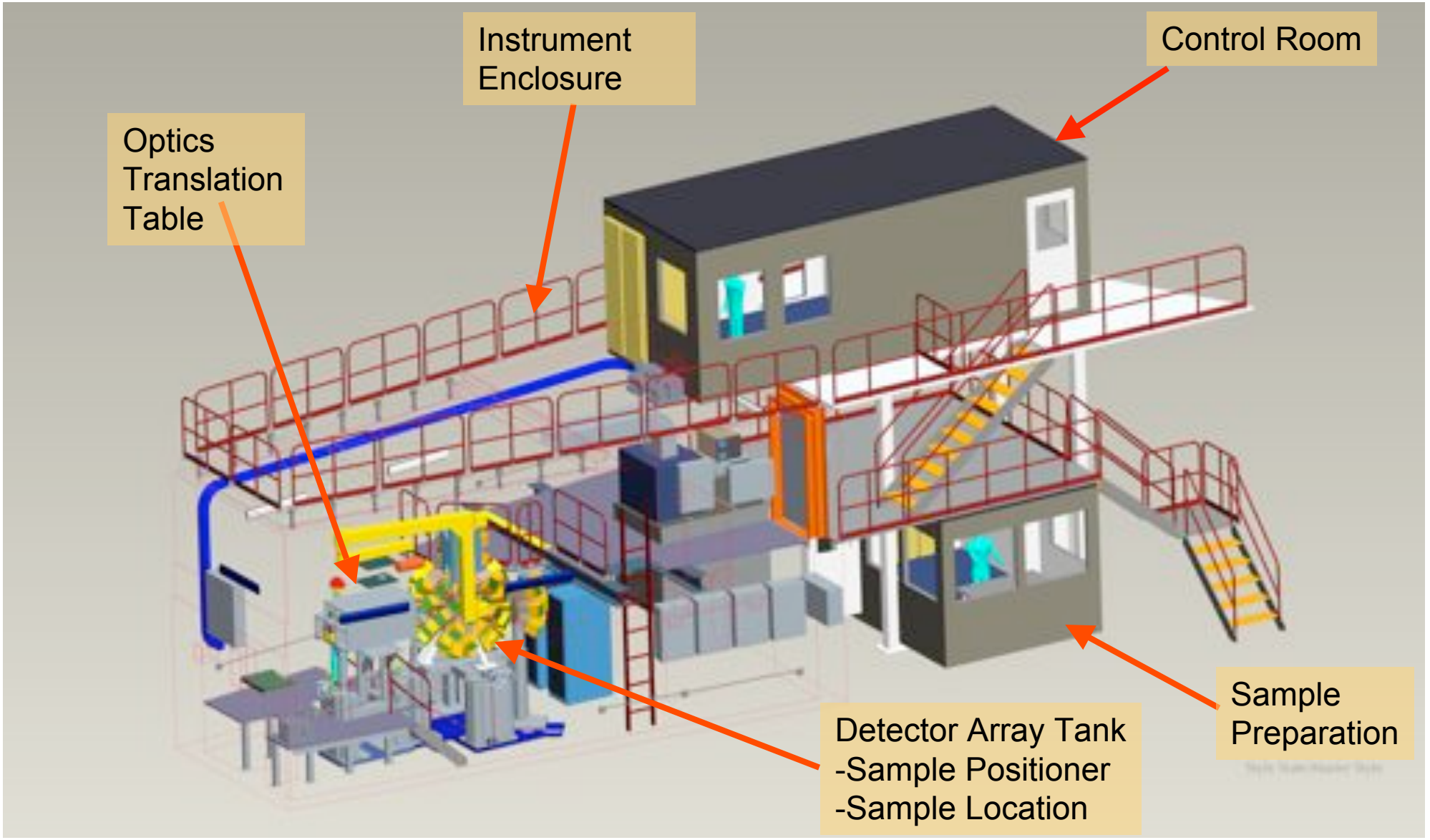
The TOPAZ Single Crystal Beamline



TOPAZ Instrument Installation is in progress

- Installation of various parts of stacked incident beam line shielding
  - Bulk Shield Insert
  - Front End Shielding
  - Base Plates
  - Stacked Shielding Blocks

Bulk Shield

Base Plates

Front End

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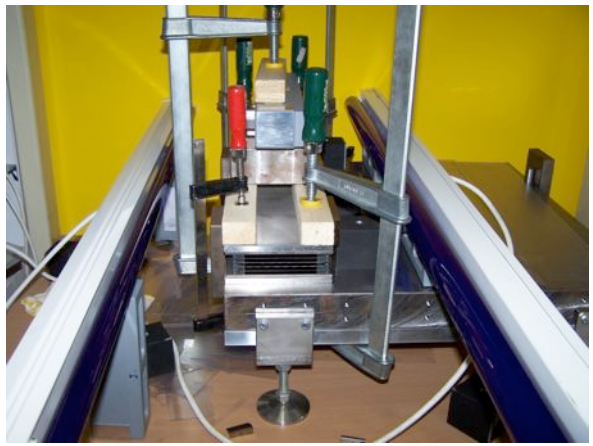
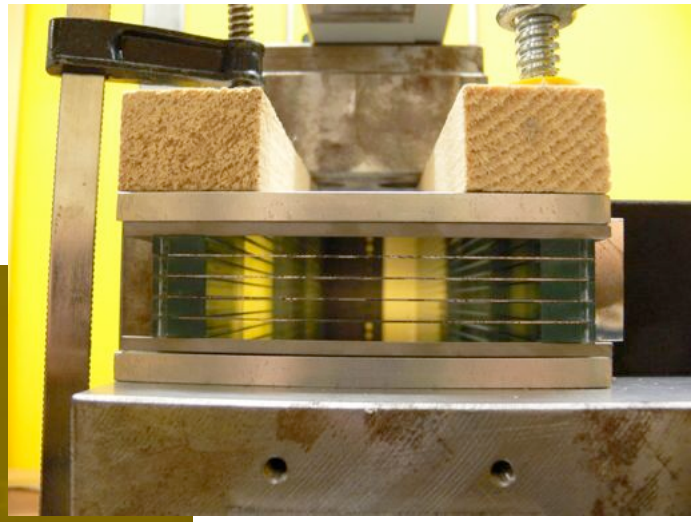
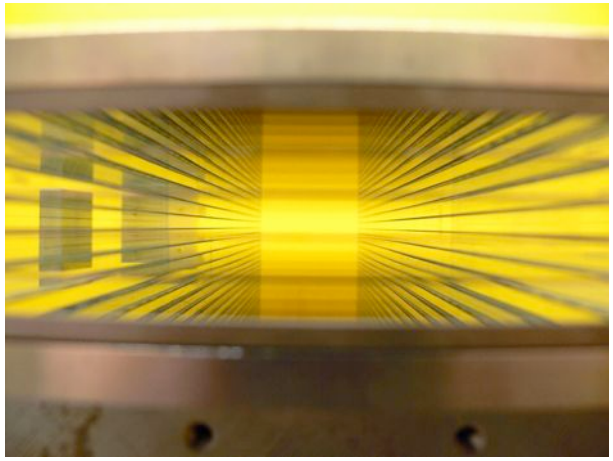
Upcoming Installation of Neutron Guide and Bender System

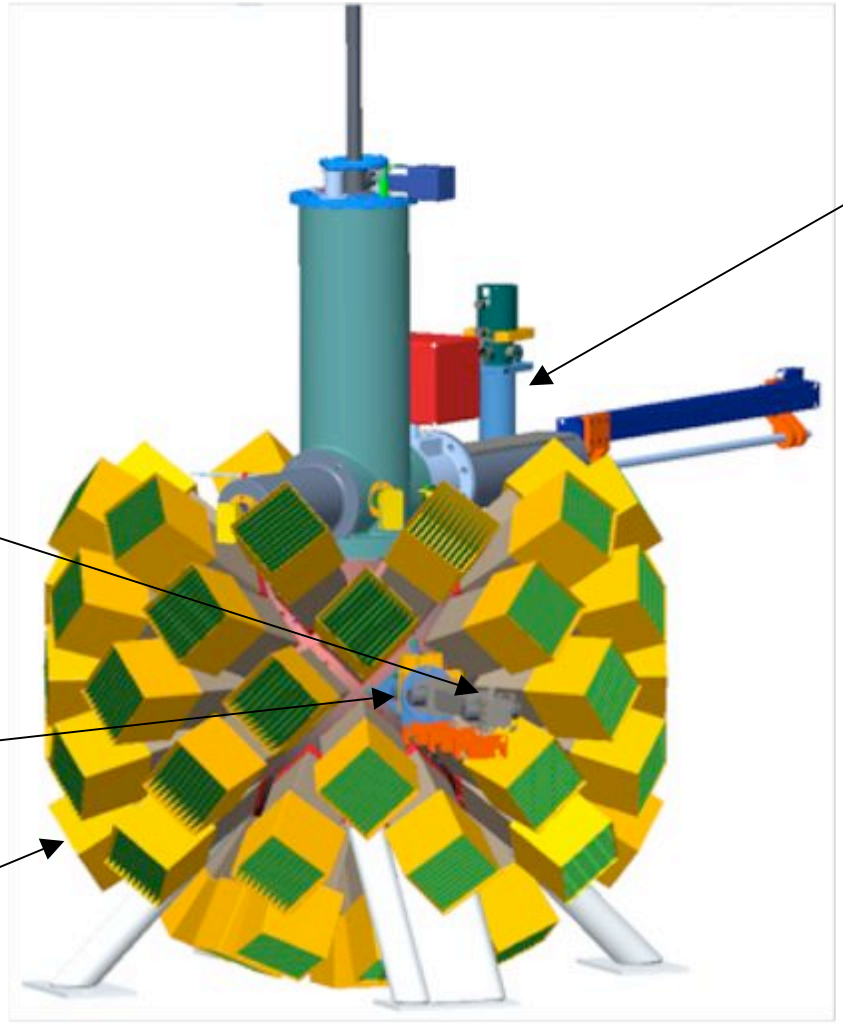
- Neutron Guide (manufacturing pictures of the front segment)
  - Including
  - Guide Supports
  - BW Choppers
  - BW Chopper Supports
  - BW Chopper Base







Topaz Detector Array Tank with Interfacing Sample Positioning and Environment Systems



Sample Changer & Loader, Cooled

Incident Neutron Beam

Incident Beam Focusing Optics

Detector Housing Module

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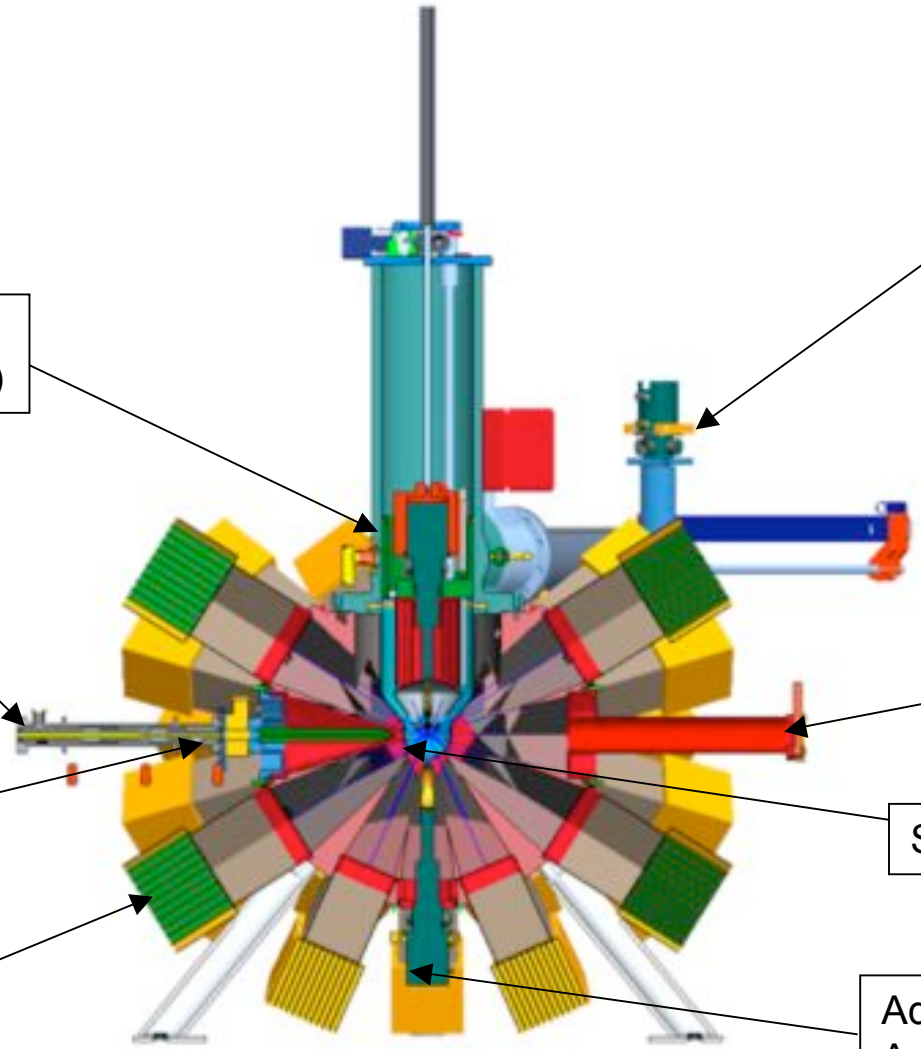

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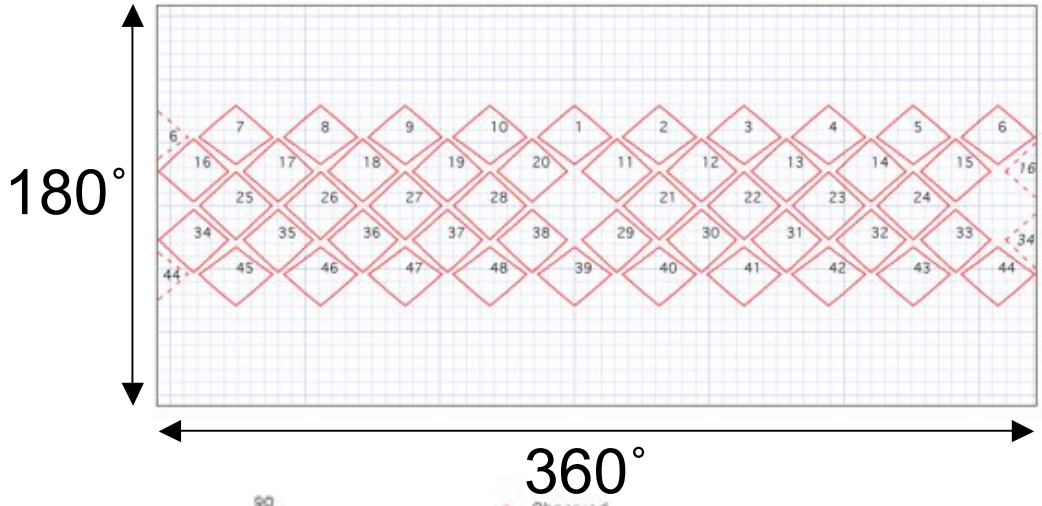
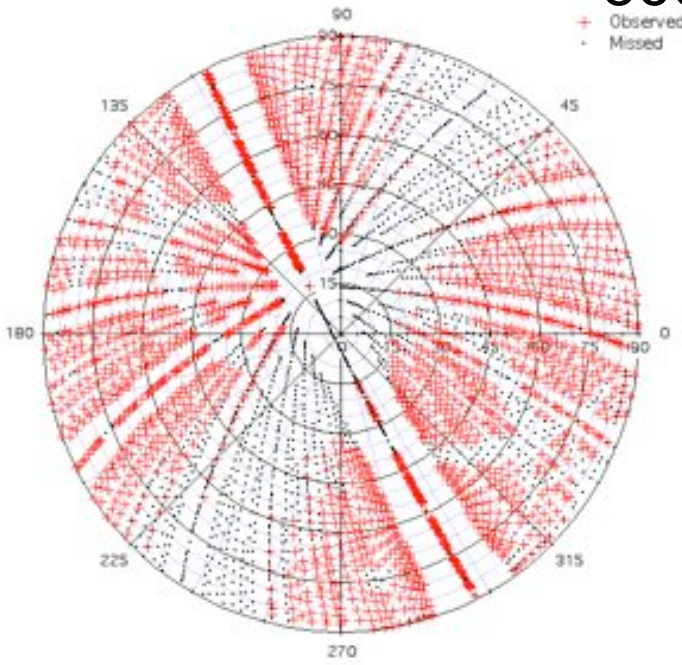
Detector Coverage Simulations

- **In real space:**
  - **Full detector coverage along equatorial axis (48 modules)**
- **In reciprocal space:**
  - **Full detector coverage records approximately 40% of a hemisphere in one crystal setting**
  - **Two settings cover over 80 % of hemisphere**
  - **Multiple crystal positions fill detector gaps with good redundancy**





Red crosses = reflections of oxalic acid collected simultaneously

Pers. Comm. A. Schultz , ANL / IPNS

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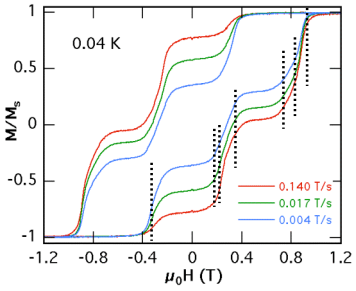
Single Crystal Diffraction Instrument for Reciprocal Space Mapping

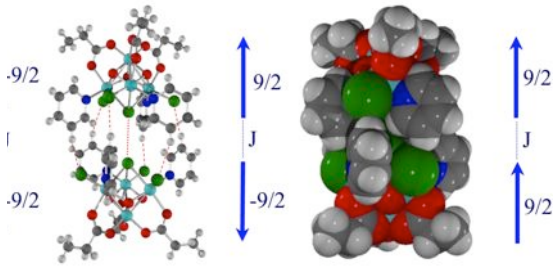
- Neutron Single Crystal Diffractometer (NSCD) for elastic scattering
  - Bragg scattering
  - TDS will be discriminated through data processing and analysis
- Time of flight Laue technique
  - Reciprocal space mapping (wavelength band 0.5 – 4 Å, 4 – 7.2 Å)
    - Probe vast areas of reciprocal space simultaneously
- Collect a full set of elastic diffraction patterns in a matter of minutes > hours @ IPNS
  - Large detector coverage
- Optimized for small sample volumes
  - Measure samples of 0.01 - 0.1 mm^3 [∅=~125μm] -> X-ray diffraction standard
    CURRENT LIMITS ~ 1mm^3 [∅=~1.25mm]
  - Low background
  - High flux on sample

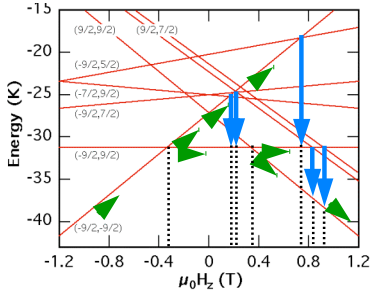
  ==> Well collimated beam
- Investigate single crystalline materials with moderately sized unit cells ~100 Å (<< proteins)
  CURRENT LIMITS ~ 30 Å
- Accommodate various sample environments
  - Cooling
  - Heating
  - Vacuum
  - Polarized neutrons
  - Pressure

Science at TOPAZ

Single Molecule Magnets: Supramolecular Dimers of Mn4 [$[Mn4Pr]_2 \cdot MeCN\ (NA_3)$]: Example of exchange-biased Quantum Tunnelling of Magnetization

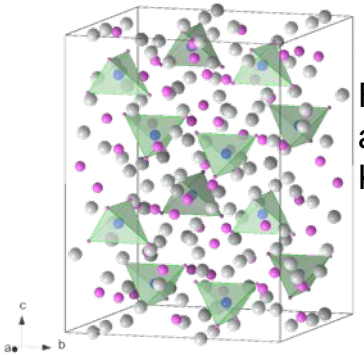






Wernsdorfer, Christou, et al.
***Nature* 2002, *416*, 406**

Science Areas: Chemistry, Physics, Material Science, Geology, Biology



$Yb_{14}MnSb_{11}$

Ferromagnet regarded as a rare example of an underscreened Kondo lattice. (T_C = 53 K)

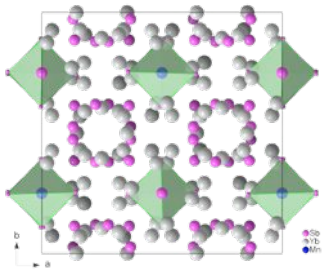
Tetragonal with space group $I4_1/acd$

1 Mn atom

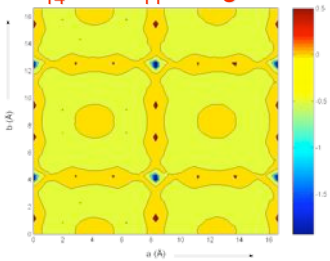
4 inequivalent Sb atoms

Sb (2) involved in Mn-Sb tetrahedra

→ maximum entropy magnetization density reconstruction reveals the presence of a magnetic moment on the Sb site with opposite sign with respect to the Mn moment

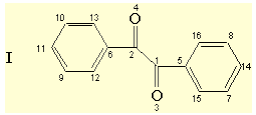


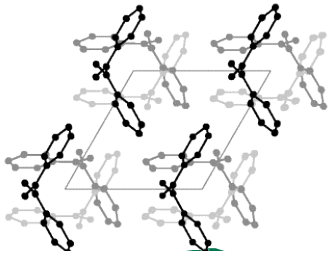
Projection of the spin density in $Yb_{14}MnSb_{11}$ along the *c*-axis.

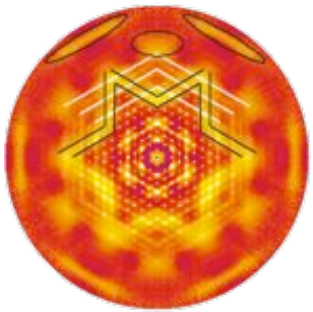


Garlea, et al. *ACNS* 2005, *Pheasant Run, IL.*

- Structure modulations in Benzil exhibit diffuse scattering patterns

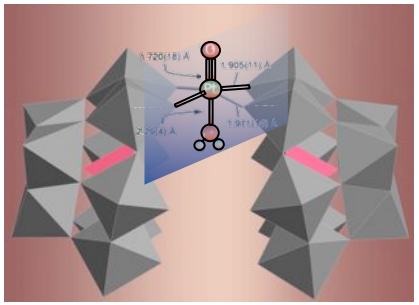


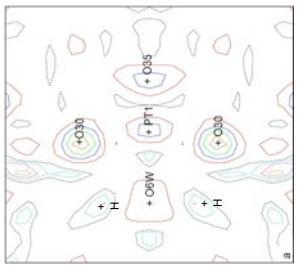




Welberry *et al.*, J. Appl. Cryst., 2003

Terminal hydrogen or water on the Pt in the Late-Transition Metal-Oxo Complex, $O=Pt(H_2O)L_2$, L = $[PW_9O_{34}]^{9-}$





Interesting catalyst

-> Large unit cell [29x32x38]

-> High H content

-> Disordered lattice water

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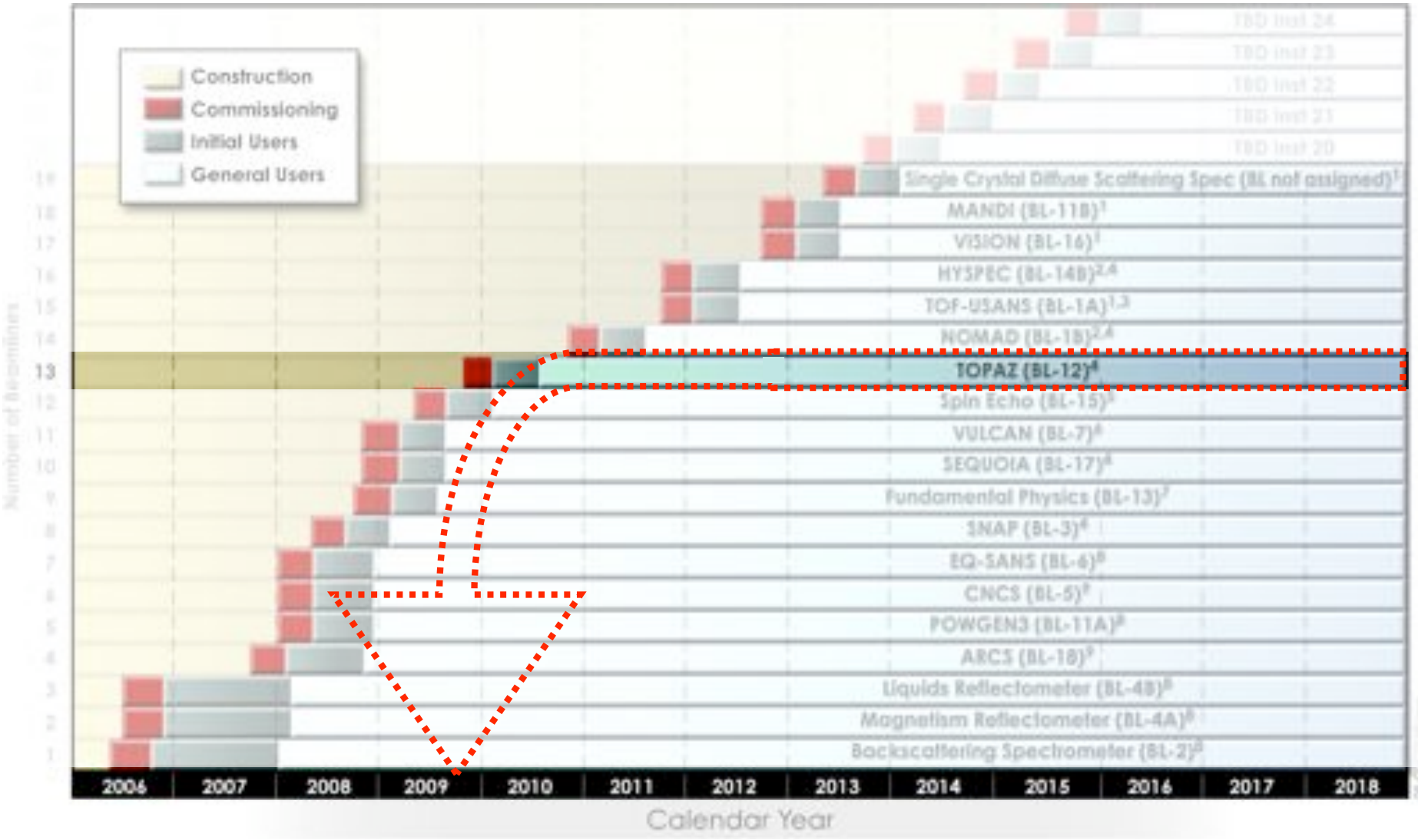
Finally.. When Will Topaz be Completed?

On the SNS Instrument Commissioning Schedule:



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