Installation and Commissioning for cold chopper spectrometer: CSPEC. (Very Preliminary)

Will work in conjunction with ESS Generic Commissioning Plan.

*Requested by STAP:*
*(1) a clear commissioning plan that shows the path for early experiments and (2) a set of first day bench-mark experiments including necessary provisions such as sample environment and software for reduction and analysis, with urgency for CSPEC and BIFROST.*

Assume a team of 2 scientists + 0.5 data scientist
Cold commissioning prior to BOT will be performed during installation phase.

Prior to BOT
Facility verification

(1) Timing signal / accuracy /
(2) Pulse line shape verification
(3) Power information / fluctuations?
(4) Moderator info (temperature)

Instrument verification
(1) Vacuum verification along guide/ gauges.
(2) Electrical installation verification.
(3) MCA verification of all motorised components (monitors, slits)
(4) Monitors reading/display.
(5) Chopper opening verification (lasers).
(6) Detector commissioning : electrical grounding, voltage control, gas system, pulse height spectrum, electronic background level verification, voxel resolution, VMM electronics to data acquisition.
(7) Verification that data acquisition will receive data from all components (monitors, choppers, instrument shutter, slits, radial collimator, detectors, sample environment)
(8) Instrument control verification (NICOS).
(9) Data acquisition and visualisation
SCIPP (Replacement to Mantid). We are working towards a suitable data acquisition and visualisation process.
(10) Data analysis MSlice, Dave, Horace.
Simulations: Packages
Molecular Dynamics simulations i.e. VASP (DFT): Working with Chalmers University on MDMC project: Molecular dynamics Tillväxtverket grant(Jan Swenson). Will test MDMC software on liquid water/ further real data with a first version.
SpinW
McPhase
SPINVERT
McStas simulation of sample environment.

Machine-learning-assisted insight into spin ice $Dy_2Ti_2O_7$
AI processing (see Nature Communications volume 11, Article number: 892 (2020))

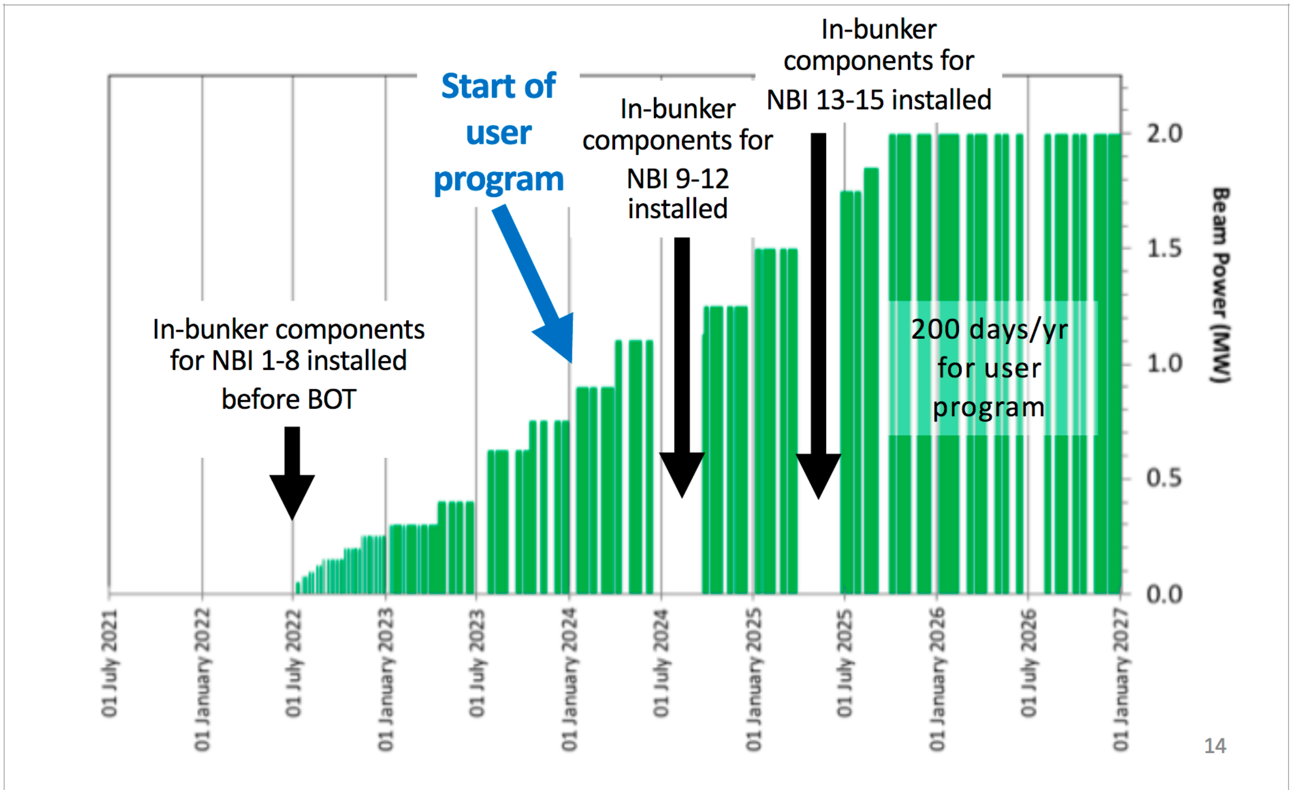



Figure 1: Beampower of ESS. Baseline 2020.

Instrument verification after BOT (Consider ESS Power: day 1: 110 kW, day 1 + 1 year = 1.2 MW)

(1) Shielding effectiveness/ safety of instrument / verification of PSS.
(2) Guide verification.
(3) Monitor verification across wavelength band. Characterise guide transmission. Beam profile at sample. Measurement of flux (position, divergence) as a function of wavelength, stability.
(4) Chopper verification. Transmission. Check beam profile parameters in time as a function of wavelength and frequency. Resolution/ bandwidth. Detector T0 as a function of wavelength (Source offset as a function of wavelength.). Check of RRM mode.
(5) Signal to noise
    - Detector Vane calibration
    - Background verification: Check efficiency of radial collimator (H20) / range of λ.
(6) Detector calibration
    - Incident wavelength determination (Via chopper verification)
    - Detector characterisation
    - TOF determination (Vanadium): Cryofurnace
    - Position determination (Na2Ca3Al2F14, $Y_3Fe_5O_{12}$): Cryofurnace.
    - Data acquisition
        - S(Tof, x,y,z, omega.) for 860 160 voxels, (subdivided into 16 detector slices.)
        - S(Q, omega)
        - Event recording (x,y,z, tof, rotation, sample environment).
(7) Instrument verification (First day bench mark experiment) - sample environment requirements.

(1) Quasielastic scattering profile (H20): Cryofurnace

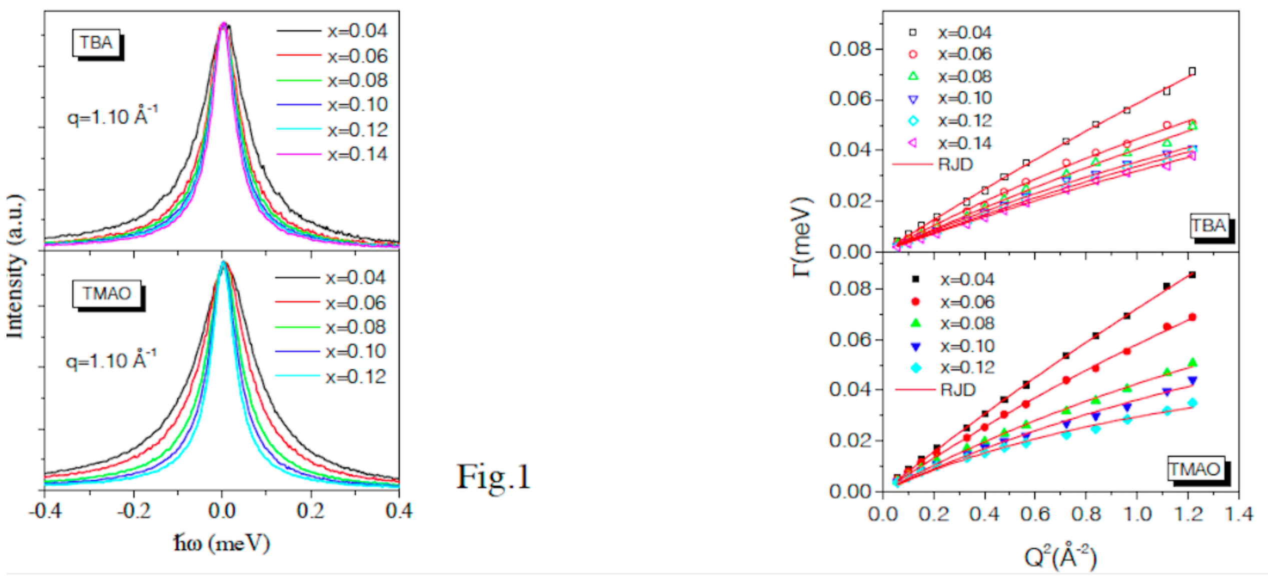



Figure 2: ILL experimental report 30498

(2) Diffusive dynamics of water in aqueous solutions of tert-butyl alcohol and trimethylamine-n-oxide. High resolution QENS, previously measured at IN5 with lambda_i=10 Å energy resolution DeltaE=15 mueV (FWHM), Q-range 0.3-1.1 Å-1). Cryofurnace.

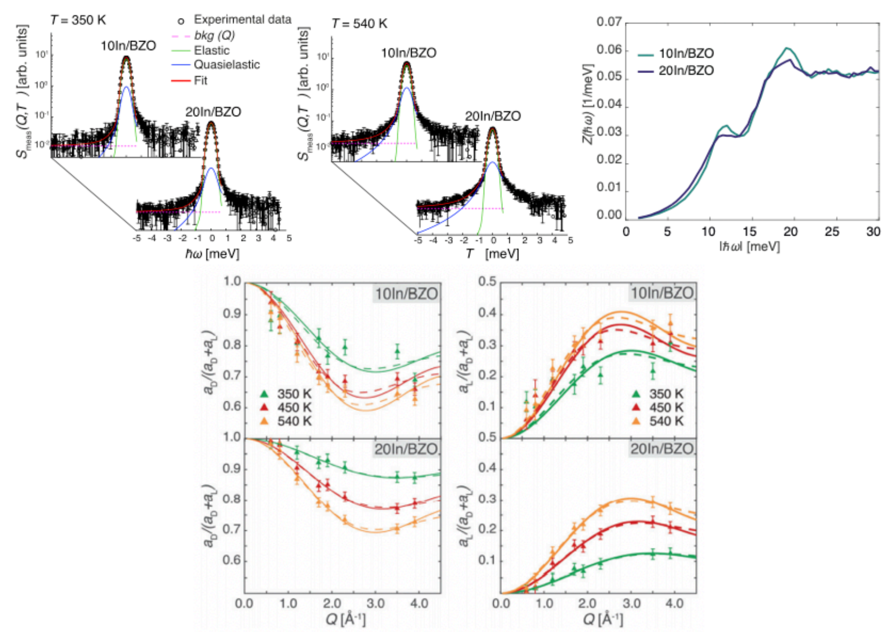
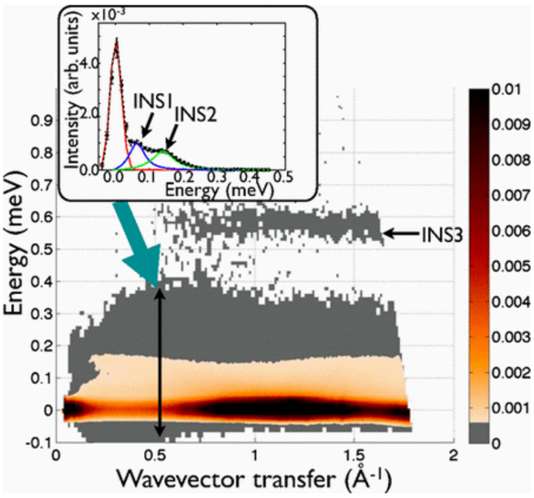
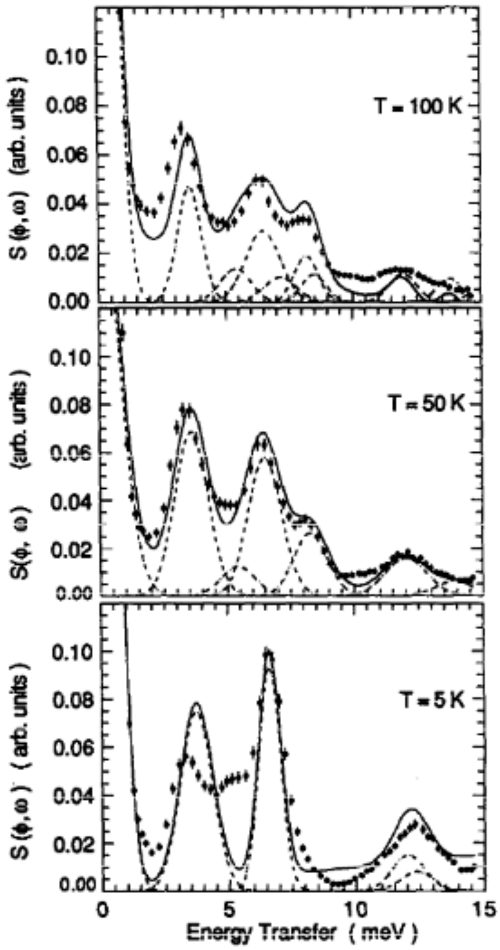



Figure 3: https://doi.org/10.1039/C7CP07340B

(3) Quasielastic signal and gdos of $BaZr_{1-x}In_xO_{3-x/2}$ with $x$ = 0.10 and 0.20. Cryofurnace. https://doi.org/10.1039/C7CP07340B

(4) Inelastic scattering Powder (Soft modes/Crystal field): Soft modes: Gd3Ga5O12 (Dilution insert) soft modes at 0.1 and 0.5 meV: Crystal Fields ErCu4Al8 (Cryofurnace).

| | |
|---|---|
|  |  Fig. 1. Inelastic magnetic scattering spectra obtained at different temperatures for $ErCu_4Al_8$. The phonon contributions have been subtracted by scaling similar measurements on the isostructural non-magnetic $YMn_4Al_8$ compound. The full lines are the fits to the model Hamiltonian, as described in the text. The single excitations contributing to the spectra are shown by dashed lines. At $T = 5$ K the compound is magnetically ordered. |
| Figure 4(a):Phys. Rev. B 82, 174408 | Figure 4(b): https://doi.org/10.1016/0038-1098(94)00912-0 Paci et al. |

(5) Inelastic single crystal Yb3Ga5O12 (Dilution insert/ rotation stage) soft modes at 0.1 and 0.5 meV - previously measured on CNCS and IN5. Molecular nano magnets (Mn12) - Q dependence across a range of Ei - RRM / Q dependence. CuSO4·5D2O: Stringent test of signal to noise.

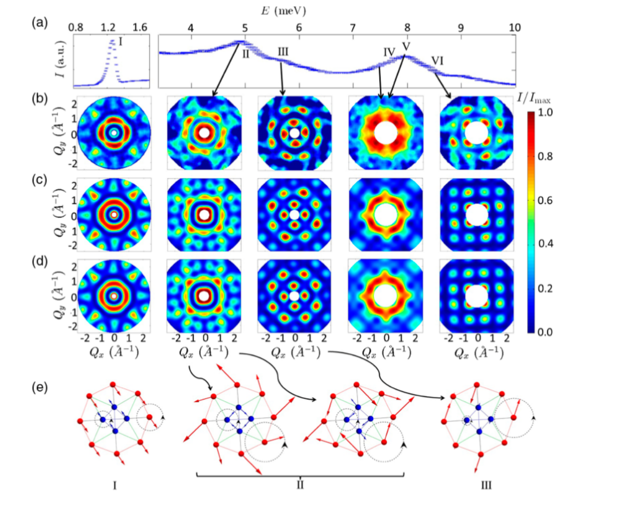



Figure 5(a) : PRL 2017 119, 217202, T = 1.5 K.

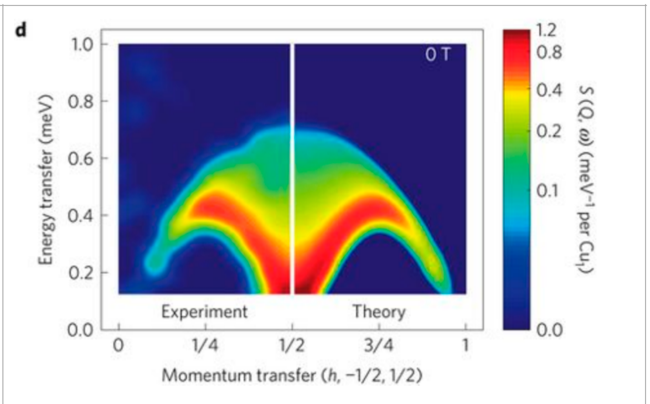



Figure 5(b) Nature Physics 9, 435-441 (2013)
Neutron scattering results for CuSO4·5D2O, Spin-1/2 (Heisenberg) antiferromagnetic chain.

(6) Inelastic single crystal - magnetic field dependence (dilution/6.5 T magnet/ rotation stage).

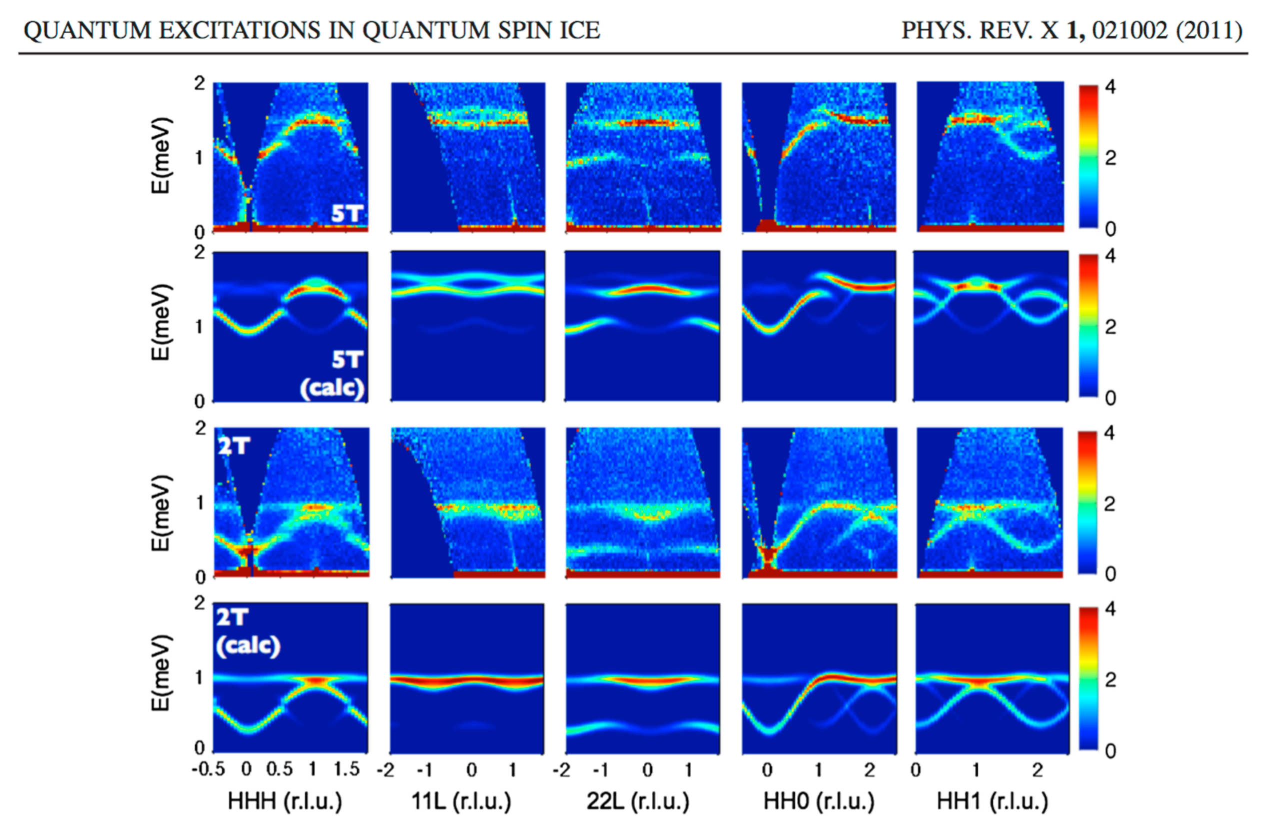



Figure 6: Quantum excitations in Yb2Ti2O7:PRX 1, 021002 (2011)

Early experiments.
High pressure not until 1.5 MW.
In operando studies (later)
Early experiments must consider the weak power of the ESS 110 KW at BOT.