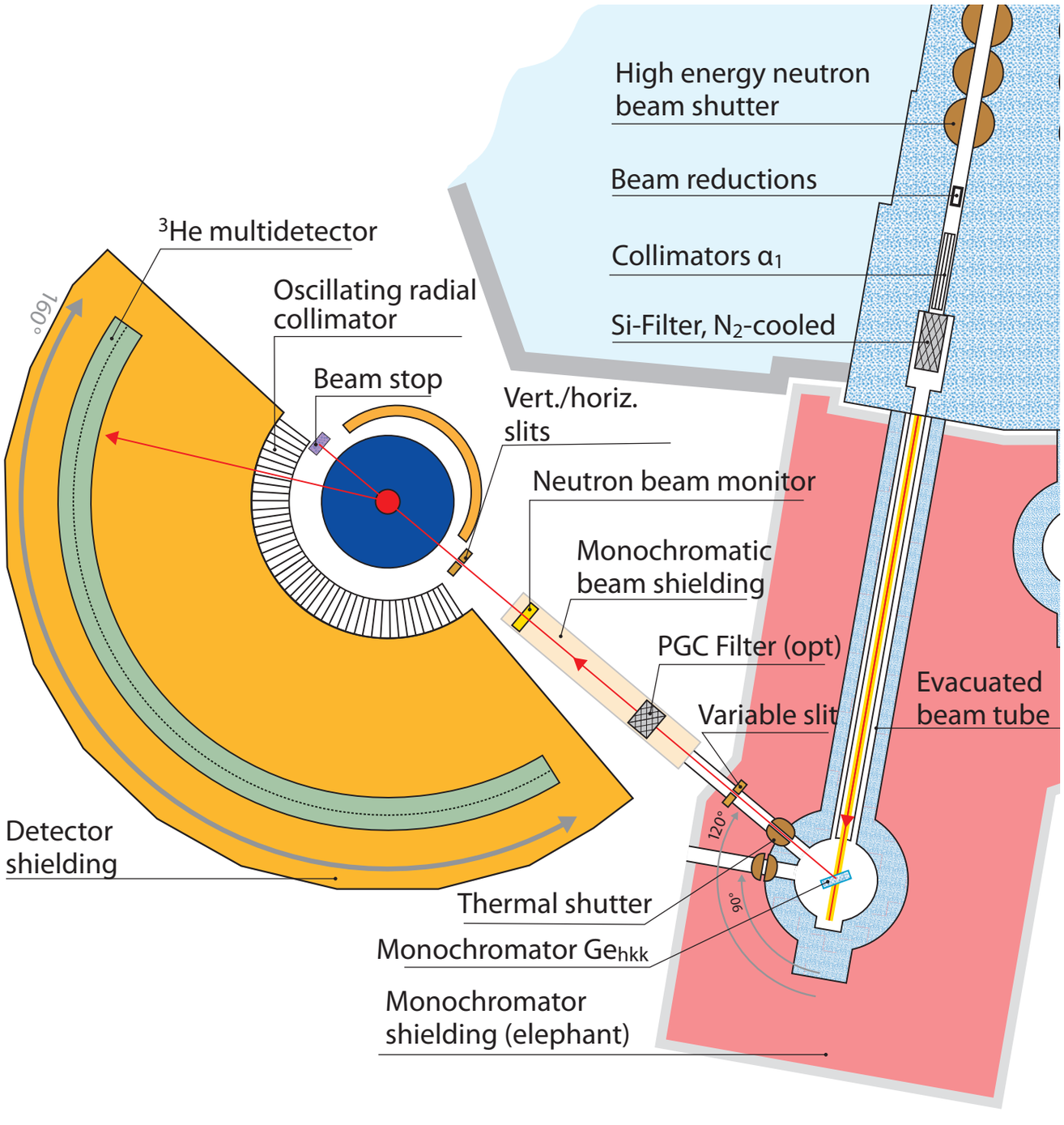
High Resolution Powder Diffractometer for Thermal Neutrons

Vladimir Pomjakushin and Denis Sheptyakov



Guidelines from Marc Janoschek

- Which parts of your instrument do have frequent technical problems?
- What parts of your instrument are outdated compared to other facilities?
- What is the percentage of user days you are not able to deliver due to …?

- Which components result in additional work for you that could be avoided by upgrading aspects of the instrument.
- When you report on components that need to be exchanged/repaired due to technical difficulties, please also consider how this change could be additionally used to improve your instruments scientific capabilities.
- Are there quick wins to technically improve your instrument or extend its science case?
- Are there scientific questions for which your type of instrument is ideal but technical difficulties prevent such measurements?

- Please consider budget and procurement of items above.
- possible internal and external funding avenues. For example, which parts could be covered from internal LNS/LMU investment budget, which parts need additional funding.

HRPT schedule for one cycle 20-30 experiments

HRPT Schedule Sep – Dec 2022 DUO SINQ Website Instrument: HRPT Change settings

W			September	October	November	December
35	Th	1	**Lampronti** (-1) Summary 2021 2893 (4d)	39 Sa 1	44 Tu 1	48 Th 1
	Fr	2	Internal developments **Sheptyakov** Summary 2022 0314 (2d) ORI4	Su 2 Magnetic ordering of the... **Král** Summary 2022 1012 (3d) (Pomjakushin) p20346 ORI4	**Vayer** Summary 2022 1032 (2d)	High Field Powder Diffraction Study of Magnetoelectric Coupling Phase of TbTaO4 **Saxena** Summary 2022 0980 (5d) (Sheptyakov) p20342 MA6
	Sa	3		40 Mo 3	We 2	Fr 2
	Su	4	**Paunovic** Summary 2022 1165 (1d)	Tu 4 Determination of magnetic structure in Ce2Ni5C3 **Kulbakov** Summary 2022 0757 (3d) (Pomjakushin) p20335 ORI4	Th 3 Magnetic ordering of high-entropy garnet Dy3(ScGaInMgZr)2Ga3O12 **Damay** Summary 2022 0909 (3d) (Sheptyakov) p20339 Variox/Dil	Sa 3
36	Mo	5	Instrument and internal **Pomjakushin** Summary 2022 1424 (3d) ORI4	We 5	Fr 4	Su 4
	Tu	6		Th 6	Sa 5	49 Mo 5 Discerning the coke formati... (-1) in the micropores of zeolite catalysts during methanol to-hydrocarbons reaction by... **Paunovic** Summary 2022 1165 (2d) (Sheptyakov) p20352 Furnace FT
	We	7		Fr 7 Crystal and Magnetic Structure of CuSn(OD)6 **Peets** Summary 2022 1210 (3d) (Pomjakushin) p20354 ORI4	Su 6	Tu 6
	Th	8	Magnetic structures of topological semimetals, LnSbTe (Ln = Nd, Dy, Tb, Ho) **Plokhikh** Summary 2022 0904 (4d) (Pomjakushin) p20338 ORI4	Sa 8	45 Mo 7 (-1) Effect of cation disorder induced by substitution in the high-temperature multiferroics YBa(Cu,Co,Ni)FeO5 **Aurelio** Summary 2022 1004 (4d) (Sheptyakov) p20345 Cryofurnace	We 7
	Fr	9		Su 9	Tu 8	Th 8 Structure determination of a substitution series of... **Kronbo** Summary 2022 0930 (2d) (Sheptyakov) p20341
	Sa	10		41 Mo 10 Magnetic Ground State of... **Mannathanath Chakkingal** Summary 2022 1057 (2d) (Pomjakushin) p20348 ORI4	We 9	Fr 9
	Su	11		Tu 11	Th 10	Sa 10 Neutron scattering study on the magnetic and lattice structures of EuCo2Al9 **Mingfang** Summary 2022 1122 (3d) (Sheptyakov) p20351
37	Mo	12		We 12 Hydrogen induced magnetic... **Cedervall** Summary 2022 0823 (2d) (Pomjakushin) p20337 ORI4	Fr 11	Su 11
	Tu	13		Th 13	Sa 12 Study of the magnetic structures of the novel room temperature magnetocaloric compounds R6(Fe,Mn)Bi2 (R = Tb, Dy) **Aurelio** Summary 2022 0928 (4d) (Sheptyakov) p20340 Cryofurnace	50 Mo 12
	We	14		Fr 14 Instrument and internal **Pomjakushin** Summary 2022 1424 (3d) ORI4	46 Mo 14	Tu 13 Internal developments **Sheptyakov** Summary 2022 0314 (2d) ORI4
	Th	15		Sa 15	Tu 15	We 14
	Fr	16		Su 16	We 16 Instrument and internal **Pomjakushin** Summary 2022 1424 (5d) (Sheptyakov, Pomjakushin) ORI4	Th 15 Instrument and internal **Pomjakushin** Summary 2022 1424 (4d) (Sheptyakov, Pomjakushin) ORI4
	Sa	17	Negative thermal expansion of the spin-1/2 1D magnet Pauflerite **Quintero Castro** Summary 2022 0971 (5d) (Sheptyakov) p20334 ORI4	42 Mo 17	Th 17	Fr 16
	Su	18		Tu 18	Fr 18	Sa 17
38	Mo	19		We 19	Sa 19	Su 18
	Tu	20		Th 20	Su 20	51 Mo 19 Instrument and internal **Pomjakushin** Summary 2022 1424 (4d) (Sheptyakov, Pomjakushin) ORI4
	We	21	**Crosnier-Lopez** (-1) Summary 2022 0815 (0d)	Fr 21 (-1) Two-dimensional antiferromagnetism in a fluoride FeTiF_6 . 6H_2O **Dubrovskiy** Summary 2022 1068 (3d) (Sheptyakov) p20349 ORI4	47 Mo 21	Tu 20
	Th	22	Accurate b(coh) values of... **Gehlhaar** Summary 2022 1470 (2d) (Sheptyakov) ORI4	Sa 22	Tu 22	We 21
	Fr	23		Su 23	We 23	Th 22
	Sa	24	Internal developments **Sheptyakov** Summary 2022 0314 (2d) ORI4	43 Mo 24	Th 24	Fr 23
	Su	25		Tu 25 Magnetic structures and... **Sharma** Summary 2022 1070 (2d) (Sheptyakov) p20350 ORI4	Fr 25 Magnetic ground state of the Na2Co2TeO6 honeycomb **Guo** Summary 2022 0989 (3d) (Pomjakushin) p20343 ORI4	Sa 24
39	Mo	26	Magnetic structure of non-centrosymmetric antiferromagnet Ce2PtAl7Ge4 **Shin** Summary 2022 1205 (3d) (Pomjakushin) p20353 ORI4	We 26	Sa 26	Su 25
	Tu	27		Th 27	Su 27	52 Mo 26
	We	28		Fr 28 Instrument and internal **Pomjakushin** Summary 2022 1424 (4d) (Sheptyakov, Pomjakushin) ORI4	48 Mo 28 Magnetic field induced... **Guo** Summary 2022 0990 (2d) (Pomjakushin) p20344 MA6	Tu 27
	Th	29		Sa 29	Tu 29	We 28
	Fr	30	**Král** Summary 2022 1012 (3d)	Su 30	We 30 **Saxena** Summary 2022 0980 (5d)	Th 29
				44 **Vayer**		Fr 30

https://www.psi.ch/en/sinq/hrpt/examples-of-results-and-publication-statistics

Publication Statistics about 20 publications /year

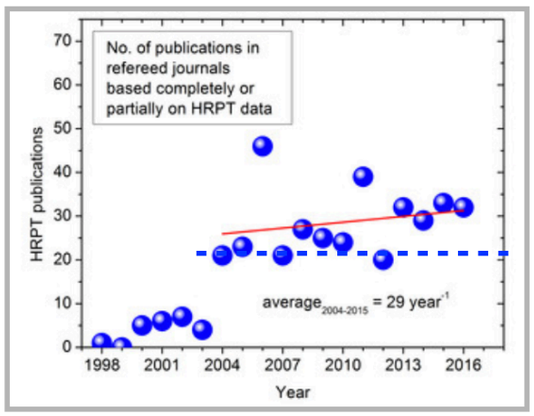
- Statistics of HRPT publications
- Examples of results
- References

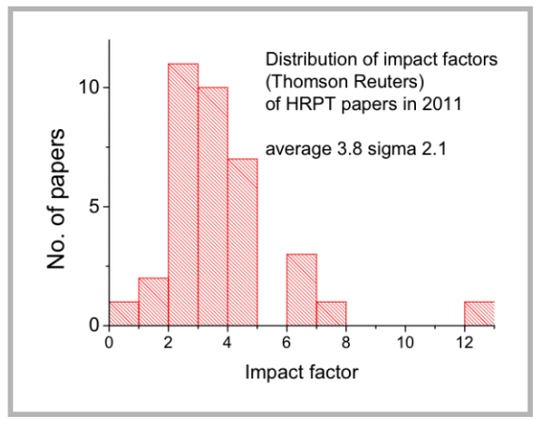
Statistics of HRPT publications

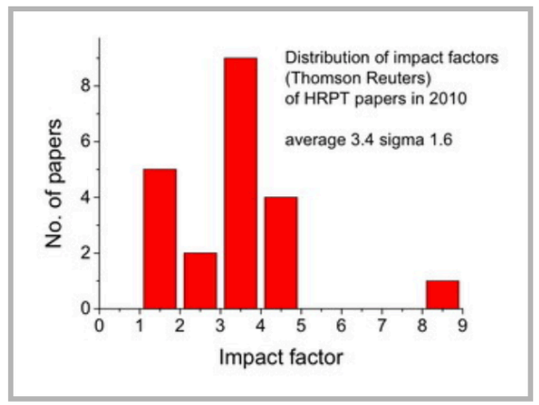
22, 18 publications in 2020, 2021

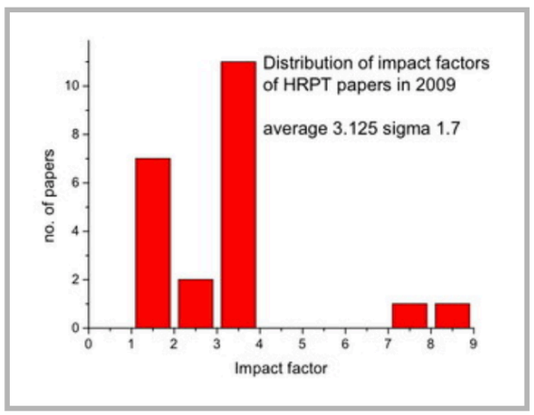
HRPT publications (automatically updated from DORA)

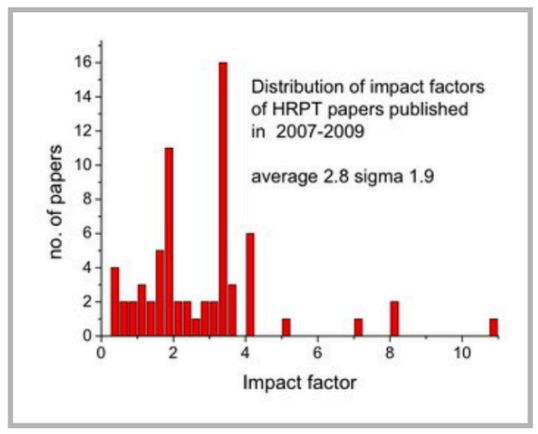
TOTAL SINQ: 118, 83 publications in 2020, 2021



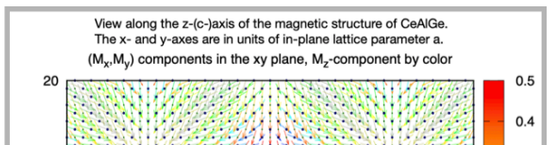


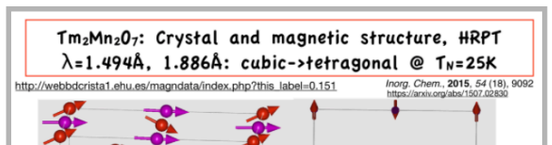


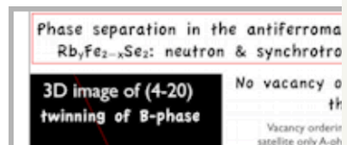


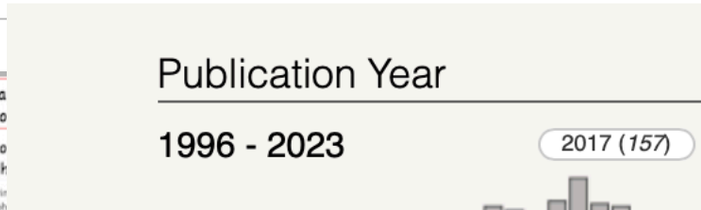


Examples of results





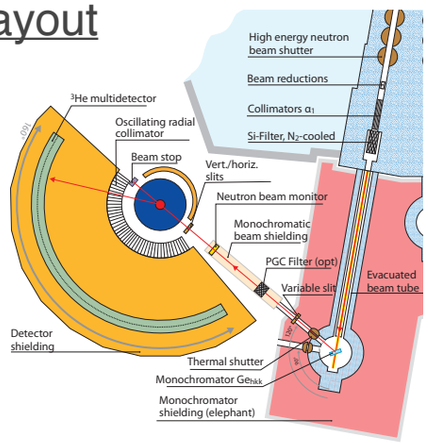




V. Pomjakushin, HF

Technical Specifications

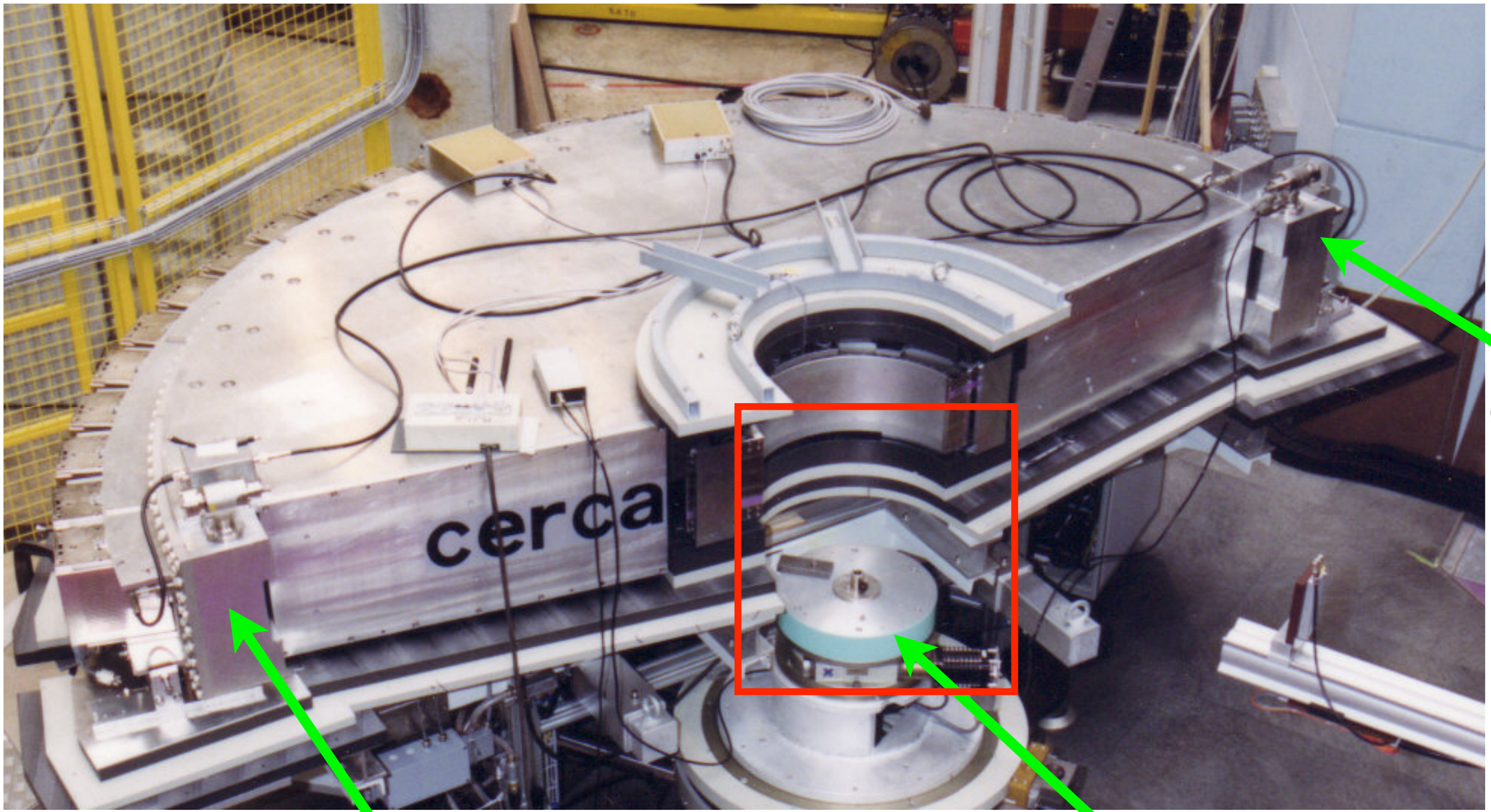
HRPT layout



https://www.psi.ch/en/sinq/hrpt/specifications

Neutrons:	thermal (0.84-2.954Å) beam 1RNS41 from a water scatterer close to the SINQ target. Neutron flux measured by gold foil activation
Primary collimation:	Gd-O Soller collimators with primary white beam collimations α1 = 6', 12', 24' (high resolution), - = approx. 40' (high intensity)
Liquid N_2 cooled Si	20 cm length
Monochromator	Ge (hkk) of wafer type, 28 cm high, variable vertical focusing, total mosaic halfwidth 15'
Secondary collimation:	variable computer controlled slit system for monochromatic beam
Radial collimators:	Oscillating mylar-Gd-O collimators to eliminate Bragg peaks from sample environment such as from cryostat or furnace tails. FWFM are 14mm and 28mm
PSD detector: (LCP1600 from Cerca, F-26104 Romans)	^{3}He (3.6 bar + 1.1 bar CF_4), 25 x 64 = 1600 counters, step 0.1°, 15 cm high, radius 1.5 m, effective detection length 3.5 cm
HRPT gas mixture cleaning/adding system (more pictures)	cleaning of the gas mixture from (O2, H2O, etc) by a circulation of the gas mixture through the appropriate filters without pumping out the mixture.
Sample temperature:	50 mK - 1800 K
Magnetic field:	superconducting magnet MAO6, field H vertical to scattering plane, H up to 6 T.
Zero matrix pressure cells:	up to 8, 15 kbar for full scattering angle range. Example of pattern,
Sample changers:	Room temperature sample changer for eight (8) samples, low temperature sample changer for four (4) samples (more pictures) , low temperature sample changer for five (5) samples with sample rotation

HRPT Detector and sample table



HRPT short work list 2023-

HRPT 2017-18 to do list.

6.12.2017

1. • xyz sample table.

3. • Encoder on sample rotation for lt5, (2 kEur)
Feasibility is OK from Alex B. low-temperature sample changer

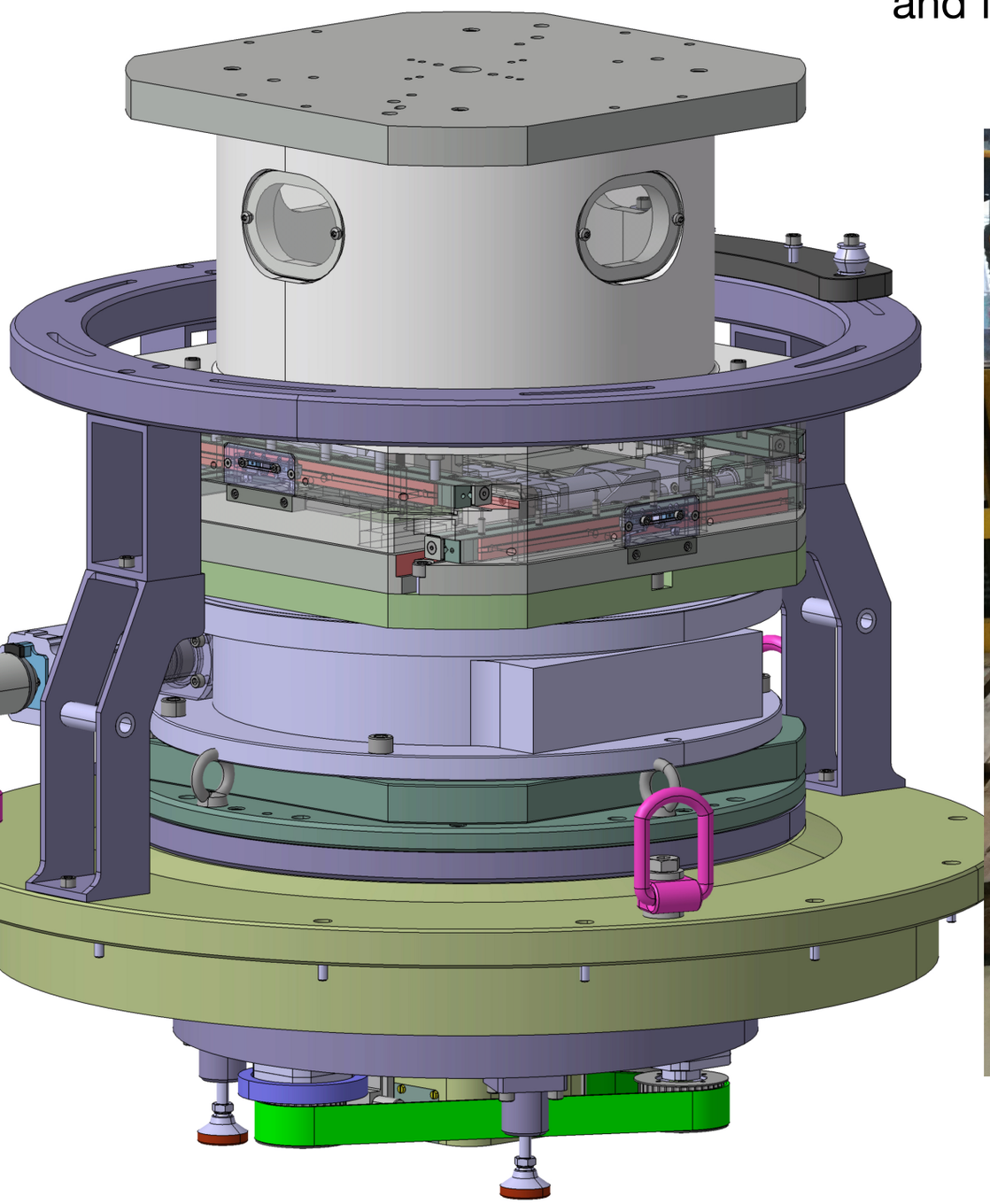
• Some channels in the detector are dying
by 2023: 15 ch. in total are bad. +8 (practically sequential) in 2023

Study: production of new analog cards/chan. for detector electronics. ? This is a long term project.

2. • motorised beam stop.

“new” xyz sample table -hardware was ready and tested in 2017: Installation is still pending.

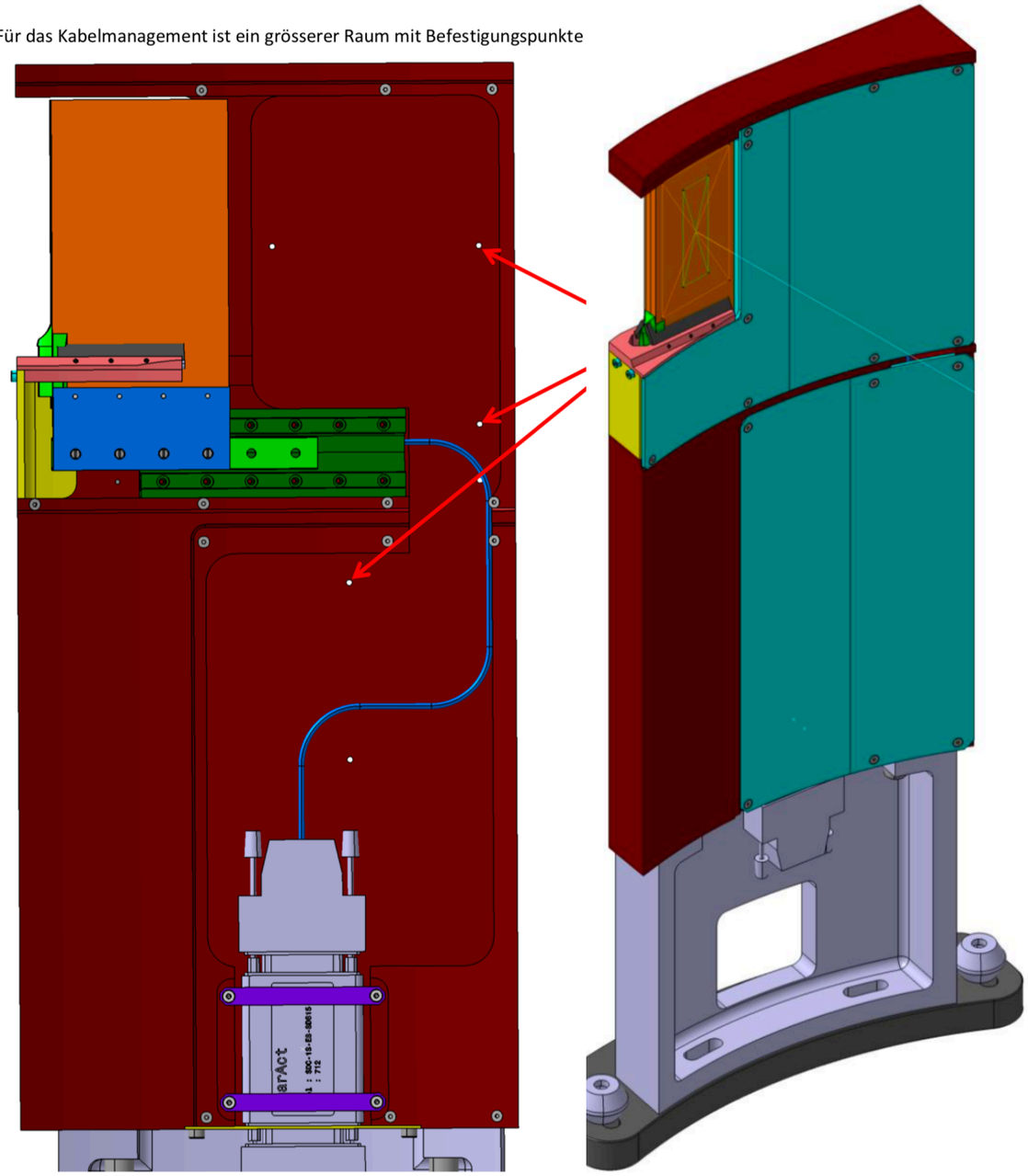
- The old sample table does not allow precise positioning along x,y-directions for some experiments, which is crucial to avoid aberration of diffraction patterns.
- Positioning along z-axis is needed for new low-T sample changer, and for some other special setups



motorised beam-stop - ready
2018: Installation is still pending.

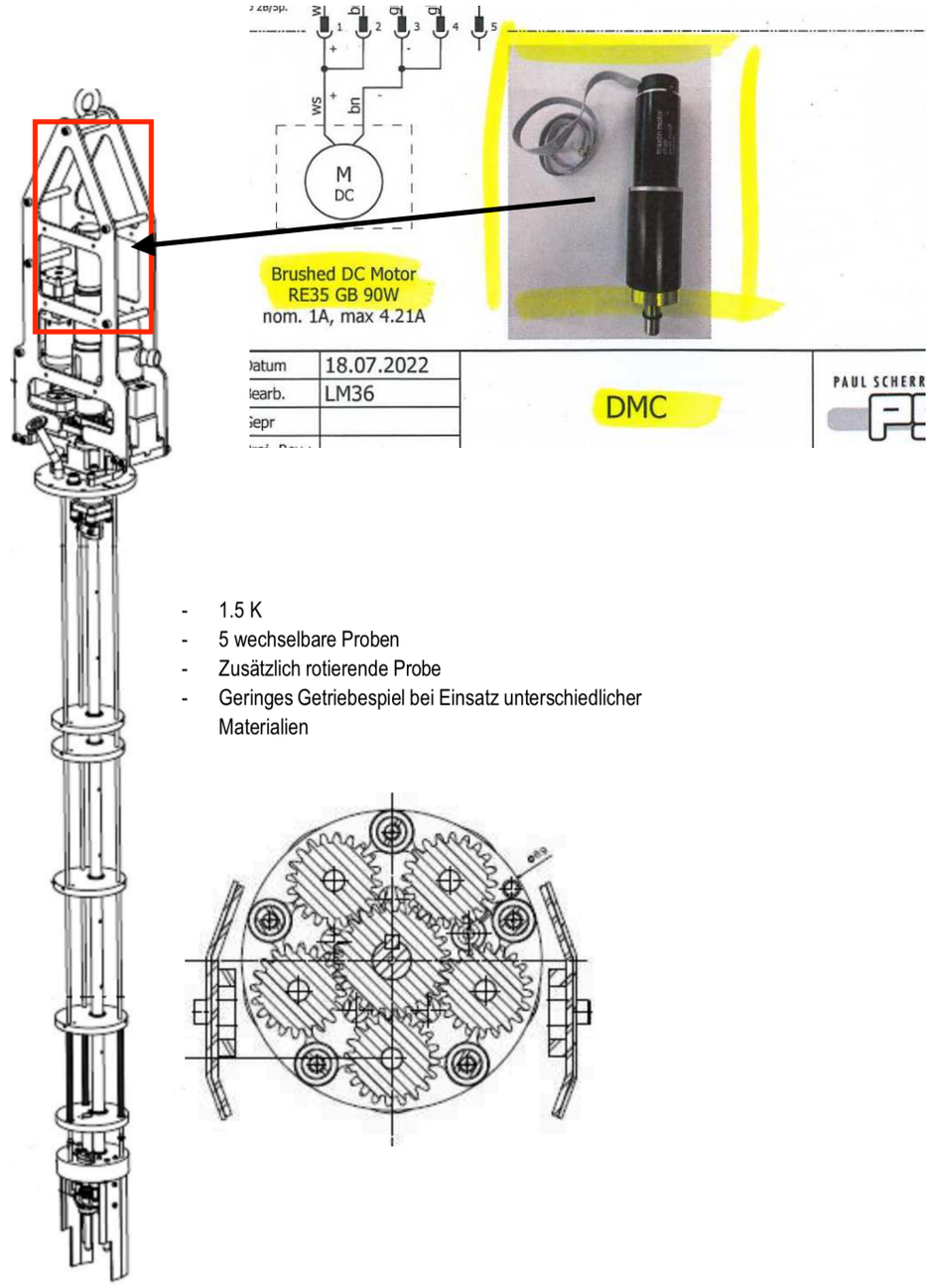
4) Kabelfreiheit

Für das Kabelmanagement ist ein grösserer Raum mit Befestigungspunkte



- fine position adjustment for SANS signals
- automatic measurements of muR absorption
- …

encoder on sample rotation motor - design is done, Installation is still pending.



- measurements of single crystals in sample changer
- computer controlled rotation frequency

Summary of the planned HRPT maintenance/ development for 2023-...

New xyz-sample table. Hardware, including electronics on the table, was ready in 2017. Installation is still pending.

Motorised, computer controlled beam stop with adjustable position. Hardware, including electronics on the table, was ready in 2018. It is in the finished state, installation is still pending.

Absolute encoder for the sample rotation axis for the LT5 cryogenic sample changer. This extension of the LT5's functions has already been designed by Alex B. It requires either no or only extremely minor mechanical adjustments, but the installation of an additional encoder and corresponding commissioning of an additional axis.

The front-end analog electronics of the detector. Some modules are already misbehaving, but at the moment we can live with this problem by software tricks/recalibrations. Some preliminary study of the problem is foreseen in 2024. By 2023: 15 ch. in total are bad. +8 (practically sequential) in 2023.

————————————————————————————————

After the above list is done:

Power supply/UPS for the controls of resolvers (electronics cabinet at the elephant). - This is partially done. Otherwise, one day we risk losing the actual positions of very important motors that move our monochromator.

Controller of the refilling of the liquid nitrogen into the silicone filter. It fails from time to time.

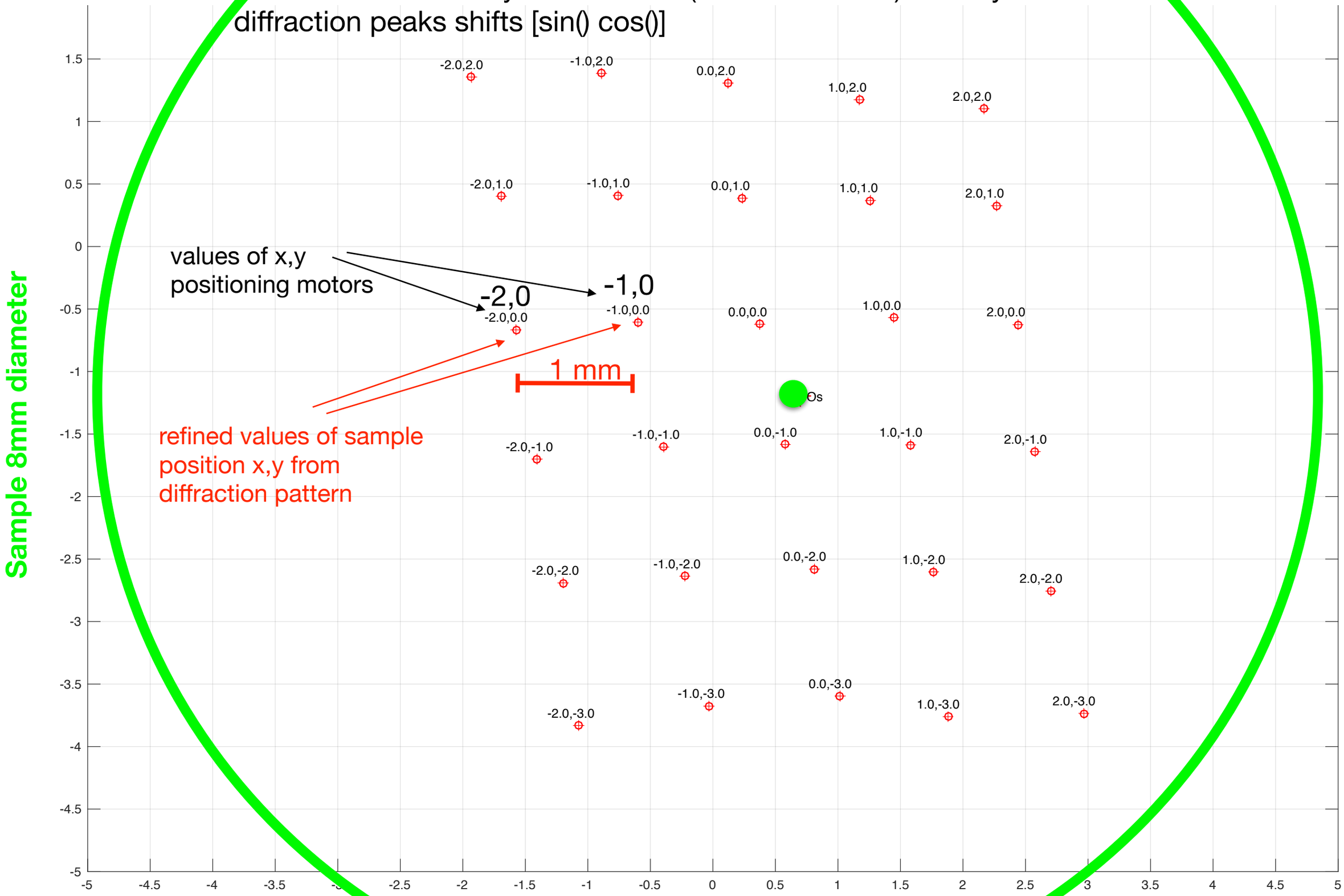
Check the electronics of the 3He cleaning system pump. Repeat the cleaning, and maybe pressurising.

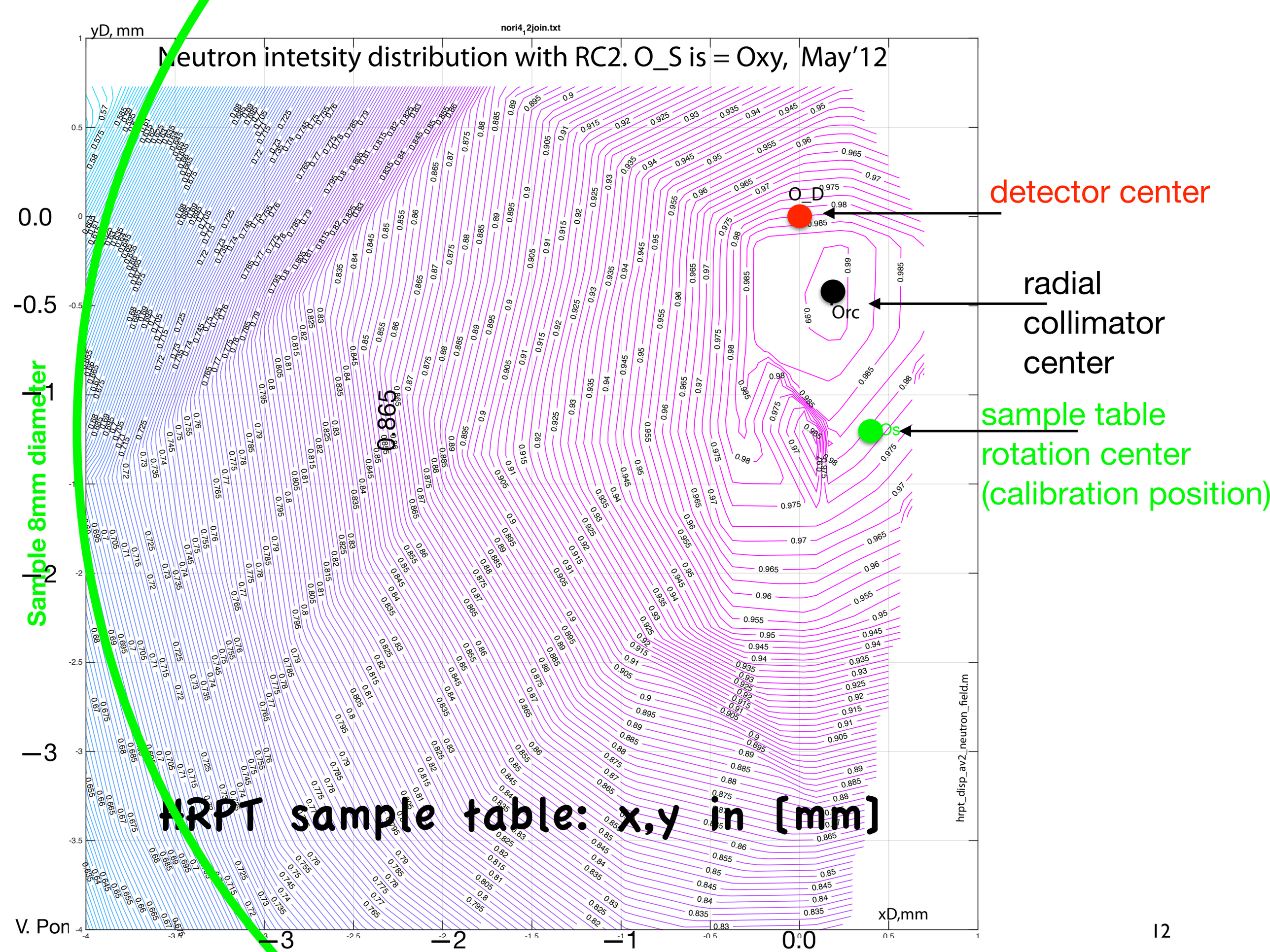
Further study of the decrease in the gas amplification ratio after cleaning and pressurising the gas mixture in the detector.

Thank you

precise sample positioning with respect to calibration

We can determine by diffraction the (x,y) position of sample with the accuracy better than 0.1mm! by the detector (radius 1500mm) from systematic diffraction peaks shifts [sin() cos()]




Neutron intetsity distribution with RC2. O_S is = Oxy, May'12
nori4_12join.txt
yD, mm
xD,mm
hrpt_disp_av2_neutron_field.m
O_D
Orc
Os
Sample 8mm diameter
HRPT sample table: x,y in [mm]
detector center
radial collimator center
sample table rotation center (calibration position)

average Debay-Waller ADP(x,y) of Na2Ca3Al2F14 at 1.9A