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Scope Setting Report
Instrument : MIRACLES

SUMMARY

The purpose of this document is to describe the possible baseline options (scenarios) for the MIRACLES project. The document also includes potential upgrade actions to improve the instrument performance will be developed over time after the construction project. The main idea is to describe a roadmap on how progressively transform the day one scoped instrument to the full scope as envisaged in the instrument proposal.

Three possible baseline options are presented. MIRACLES has been assigned to cost category B (12 M€). After detailed analysis of the costs estimation, it is concluded that a substantial reduction of the budget will result in a poor day-1 performance. On the other hand, cost estimations labelled as Option 2 and Option 3 offer solutions for delivering a world leading performance instrument. These ought to be carefully considered.

TABLE OF CONTENT **PAGE**

SUMMARY ... 2
1. OVERVIEW ... 4
1.1. Science Case ... 4
1.2. Requirements ... 5
1.3. Configuration options ... 6
2. TIMELINE ... 7
3.1 OPTION 1: SCOPE WITHIN COST CATEGORY B (12M€) ... 7
3.1. Scope ... 7
3.2. Costing ... 8
3.3. Upgrade/Staging plan ... 9
4. OPTION 2: WORLD CLASS SCOPE REQUIREMENTS (15.9 M€) ... 9
4.1. Scope ... 9
4.2. Costing ... 10
4.3. Upgrade/Staging plan ... 11
5. OPTION 3: FULL SCOPE (17.7 M€) ... 12
5.1. Scope ... 12
5.2. Costing ... 12
6. RISK ... 14
7. REFERENCES ... 15

1. OVERVIEW

1.1. Science Case

MIRACLES is a ToF-Backscattering spectrometer, aiming to optimize the full ESS pulse (3 ms) to achieve a sample flux larger than any other backscattering spectrometer. To reach a state-of-the art performance, high values of energy and momentum resolution and wide dynamic (Q,E) range are aimed, along with a trade-off between flexible energy resolution and gain in flux.

Moreover, MIRACLES is pointed to address connection of quasielastic signal (QENS) to the inelastic response (INS) of a neutron spectroscopy study, based in, for instance, the capability provided by the chopper cascade to select wavelengths from 2 to 20 Å and working in offset mode. This allows access to incoherent scattering in a wide time range in a single instrument at longer timescales and with simultaneous access to high Q, not achievable by direct TOF. This is important for many complex systems, where there is a variety of dynamical processes taking place. Also, it is expected that the time-space domain covered by QENS in MIRACLES could overlap for efficient relationship with molecular dynamics simulations. These features will provide insight into the study of the dynamics of complex systems, ranging from biological organisms to energy devices and in the future novel magnetic materials.

The primary spectrometer comprises a chopper system providing a tuneable energy bandwidth with the following components: (i) Guide configuration according to "High-level technical description"; (ii) Pulse-Width Definition (PWD) chopper pair (7.0 m and 7.01 m from the moderator); (iii) Pulse-Suppression (PS) chopper pair (7.5 m and 7.51 m from the moderator); and (iv) Wavelength-Band Definition and Frame Overlap (WBD/FO) choppers: (22.5 m, 56.25 m, 80.5 m from the moderator).

The secondary spectrometer consists of a circular array of Si crystals working as analyzers plus 2 arrays of ^{3}He tube detectors surrounding the sample area. Additional devices necessary for a high quality experiments ensuring for a low background signal performance are a radial collimator and a Beryllium filter.

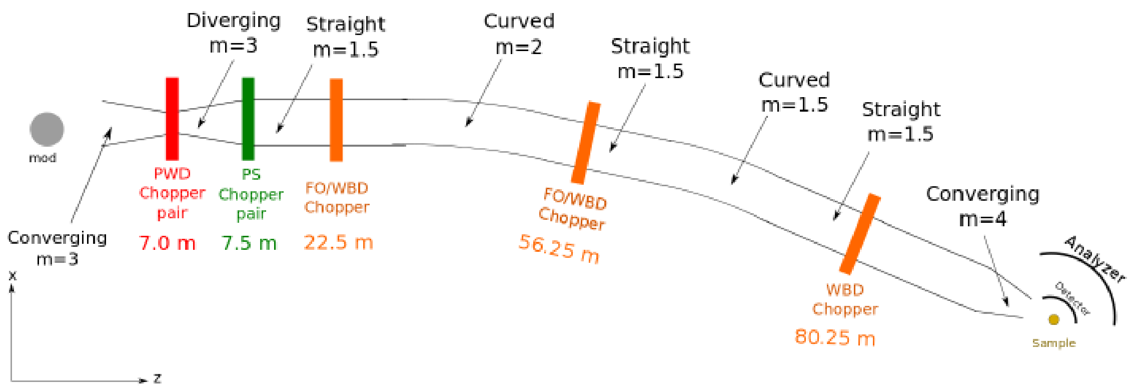

Fig. 1. Miracles conceptual layout

The science scope for MIRACLES is primarily, but not only, focused on the following cases:

- Life sciences: MIRACLES is aimed to the study of dynamics of proteins and nucleic acids, with high statistical accuracy preventing from biological degradation, as well as enzymatic selectivity and biomolecule functionality (applied to e.g. biotech and pharmaceutical topics, like drug delivery,…). In all these cases fast dynamics in the picosecond scale can be explored with the simultaneous elastic and quasielastic responses offered by MIRACLES.

- Energy sciences: direct information about the diffusional processes of hydrogen and interatomic interactions in fuel cell devices can be studied by QENS. For this, a high flux and tuneable energy resolution is required. Also, the study of nanoporous materials, such as clathatre hydrates and metal-organic frameworks (MOFs) for the storage of catalytic molecules, as well as the study of fast-time resolved catalytic processes require a high flux for time resolved studies. All requirements can be offered by MIRACLES.

- Climate change: The ToF backscattering spectrometer MIRACLES can easily cover hydration and water dynamics, such as ice-cloud nucleation processes (important to modulate Earth's radiation and water balances), or alternative fine-grained cements that yield a reduced of greenhouse gas emissions during fabrication.

- Polymer science and soft matter: polymer dynamics typically extends over a very broad spectral range, from slow viscous processes to fast picosecond methyl-group rotations. MIRACLES can contribute to carry out, in a single experiment, a detailed characterization study within the range of molecular processes and relaxation time distributions. Moreover, high resolution with wide dynamic range is ideal to study long-chain molecules with complex molecular structure.

- Next-generation magnetic sensors and storage: inelastic neutron scattering is an ideal tool for the study of spin dynamics of molecular nanomagnets, one of the main subjects for applications in quantum information processing. Intramolecular dynamics require an energy range of 0.1-10 meV. Finally, magnetic fluctuations in frustrated magnets and superconductors could be analysed to low energy transfers, providing estimated length scale associated with the magnetic fluctuations.

1.2. Requirements

The top level requirements for MIRACLES [1] define the target scope for the instrument construction project. They have been formulated to capture the key aspects of the instrument proposal science case and are:

1. MIRACLES shall provide exceptional flux.
2. MIRACLES shall be capable of covering a wavelength range between 2 and 20 Å. These are key parameters to allow for flexibility of the elastic resolution, wide Q-range

coverage and extension of the energy range covered by the instrument well beyond the quasielastic regime.

3. MIRACLES shall allow for a variable elastic energy resolution between 2 and 32 μeV, when using a wavelength of 6.267 Å (Si(111) reflection), with an energy transfer range centered at the elastic line from -600 to +600 μeV. In addition, when selecting λ=2.08 Å (Si333 reflection), the resolution can be relaxed to 300 μeV, and $\hbar\omega$ from about 10 meV in energy gain to -40 meV in energy loss.
4. MIRACLES shall be capable of spatial Q-resolution in the range of 0.02 $Å^{-1}$ in forward and 0.1 $Å^{-1}$ in backscattering, within the energy transfer window of ± 0.6 meV and allow the measurement of sample areas as small as 1x1 cm^2.
5. MIRACLES chopper cascade design shall allow for the selection of a well-defined wavelength band of approximately 1.7 Å width centered at any wavelength in the range of 2-20 Å, to allow the measurement of low-energy inelastic excitations. All the other pulses produced by the PWD chopper shall be supressed, while a small dead time is foreseen between subsequent frames to ensure no frame overlap is presented as well as to allow instrument background measurements.
6. MIRACLES guide shall provide for upgrade avenues for the continuous development of the instrument include the incorporation of Si(311), which will enable covering an intermediate resolution and momentum transfer.
7. MIRACLES' secondary spectrometer design shall facilitate the coverage of all surfaces with neutron absorbing materials such to allow for background suppression. Moreover, a collimator system shall suppress unwanted neutron scattering from the sample environment and a Be Filter will remove higher order contamination and contribute to a cleaner background and improved signal to noise ratio.
8. MIRACLES sample environment capabilities shall provide for the wide range of scientific cases covered by MIRACLES that range from magnetic systems to life science.
9. The system's design shall provide the space and flexibility necessary to host and drive future developments in the neutron backscattering field.
10. MIRACLES should serve the user and science and instrumental development program without interruptions during source operations.

1.3. Configuration options

Three configuration options are presented:

1. Option 1: 12.9 M€ or within cost category B. This option definitely fails to provide an adequate level of performance and potential future upgrade will require additional difficult and costly work.

2. Option 2: 15.9 M€. A configuration that manages to meet a majority of scientific requirements at reasonable performance. A suitable day one instrument.

3. Option 3: 17.7 M€. A configuration that is the full technical scope and "converts" MIRACLES into the world leading neutron backscattering spectroscopy instrument.

2. TIMELINE

The project timeline of the instrument from preliminary design to user operation serves as a template to evaluate the three budget configurations including the full scope.

Table 1 Timeline for the development of MIRACLES

	Start	Finish	Duration
Preliminary Design	-	Jun 2017	-
Detailed Design	Jun 2017	Jan 2020	2.5 year
Manufacturing and Procurement	Jan 2020	Dec 2021	2 year
Installation and Integration	Dec 2021	Dec 2023	2 year
Hot commissioning and early science	Dec 2023	Jul 2025	1.5 year
Operation	Jul 2025	-	-

3. OPTION 1: SCOPE WITHIN COST CATEGORY B (12M€)

3.1. Scope

- Primary spectrometer
- Secondary spectrometer:
    - Analyzers covering an angular arc of 30º (2 panels)
    - 30 ^{3}He tube detectors (2×15 ^{3}He PSD detectors).
- Reduced vacuum tank dimensions
- 1 beam monitor between the guide end and the sample. No motorized (manual) slits. No radial Collimation. No Be filter.
- No owned sample environment (everything from SAD pool)
- All necessary associated infrastructure (shielding, cabling, cabins, reduced MC&A,…)

This scope does **not** meet the top level requirements for any of the topics covered by the science case of MIRACLES.

This option has a considerable reduction of analyser angle, as well as detector area, compared to the accepted instrument proposal. This reduction results in a critical loss of detection flux, with a subsequent significant increase of the measurement time. Moreover the lack of the collimator and Be-filter will result in a reduced efficiency of signal detection. All these points are main drawbacks in the study of life science and energy science samples, which are the main targets of MIRACLES.

The nonexistence of an adequate set of sample environment will make MIRACLES' operation fully dependent on the availability of sample environmental pool equipment, this can jeopardize the success of the early experiments and create a bad feeling in the community towards the instrument.

As can be deduced, the science case of MIRACLES will be severely affected. Requirements to carry out, for instance, biological experiments involving protein include access to a large Q-range and excellent signal to noise ratio. In addition, the significant reduction of flux on the detectors will be the main drawback for breakthrough experiments, which will mostly focus in fast measurements or in the use of diluted samples.

One additional issue is that, due to budgetary constraints in this option, a reduced dimension of the tank (and shielding), compared with options 2 and 3, was introduced here. However, this leaves the instrument without room for any upgrade. The future upgrade of this instrument option (addition of a more extended analyser angle, beam monitors, radial collimator, Be filter) is envisioned as difficult and expensive, and would imply the replacement of the vessel, with the subsequent idle status during a long period in the user operation time.

Finally, the recommendation from STAP committee (STAP report, p. 2) remarks: "We would like to stress that **the current budget will result in serious damage** to the user program as the instruments will not be able to take full advantage of the ESS source."

For all these reasons, this scope **does not fulfil** the science case for MIRACLES.

3.2. Costing

The costing is based on bottom-up calculation of the procurement costs and manpower required for the tasks needed to deliver the higher level PBS items.

Table 2 Costing for MIRACLES within Cost Category B

	Phase 1	Design	Procurement & Fabrication	Installation	Commissioning	LABOR BUDGET	NON LABOR BUDGET	Total k€
Primary Shielding	0	200	809	100	0	300	809	1109
Secondary shielding (cave + vacuum tank shielding)	0	200	600	20	0	220	600	820
Neutron Optics without vacuum pumps	0	0	3558	100	0	100	3558	3658
Choppers	0	0	1100.75	65.56	19.14	65.56	1119.89	1185.45
Sample Environment	0	0	0	0	76.5	0	76.5	76.5
Detector and Beam Monitors	0	0	310.69	76.65	0	76.65	310.69	387.34

Motion Control and Automation	0	48.757	27.424	3.413	23.599	52.17	51.023	103.193
Analyzer	0	60	178.04	20	0	80	178.04	258.04
Radial collimator	0	0	0	0	0	0	0	0
Beryllium filter	0	0	0	0	0	0	0	0
Beam Stop	0	50	100	20	0	70	100	170
Slit	0	0	60	10	0	10	60	70
Vacuum tank	0	200	600	70	0	270	600	870
Instrument Infrastructure	0	0	637	0	0	0	637	637
Management & Science	480	600	480	480	360	2400		2400
Contingency	0	75.875	798.090	48.562	11.924	124.438	810.014	1174.452
Total	480	1434.6	9258.994	1014.185	491.162	2928.82	8910.16	**12918.97**
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Labor included in above (Person-Years)	4.1	13.65	7.6	6.1	2.7	34.15		34.15

3.3. Upgrade/Staging plan

The staging plan for this option would consist of replacing the vacuum tank, and later implementing analysers covering a higher angle of the secondary spectrometer tank, addition of ^{3}He tube detectors as a first priority. The second priority will include installation of a radial collimator and the sample positioning motors. A third upgrade package will include installation and commissioning of basic sample environment equipment to fulfil the scientific requirements above proposed (cryofurnace, furnace, humidity and in-situ cell chamber,…). Addition of beam monitors and Be filter are envisioned in a final stage.

4. OPTION 2: WORLD CLASS SCOPE MEETING MOST HIGH LEVEL REQUIREMENTS (15.9 M€)

4.1. Scope

The scope within this cost category is:

- Primary spectrometer
- Angular coverage of secondary spectrometer analyzers: 120º
- 120 ^{3}He tube detectors.
- Full vacuum tank allowing 360º analyzer.
- Radial Collimation to achieve a better signal-to-noise ratio.

- 3 position-sensitive beam monitors installed at the second guide curve, guide end and before the beam stop (transmitted beam); also space allocated (designed and installed) to implement monitors after every chopper set exit in the future.
- Diffraction detector.
- Sample environment (from Day 1):
    - Sample holders
    - Cryofurnace (4-600 K) and furnace (<1600ºC)
    - Cryogen-free CCR (closed-cycle refrigerator): 10-400 K
    - Gas pressure cell and Humidity chamber.

This scope meets most of the high level requirements. Also, it is anticipated to be upgradeable according to future configuration to provide the full scope.

The Option 2 would be a world-class backscattering spectrometer from day one; minimizing the chances of problems and increasing likelihood of success. The science case described in the proposal and mentioned above can be largely covered by this configuration. A larger Q-range with better Q-resolution and improved flux at the detectors, required for studies of protein dynamics, water dynamics, energy devices (catalysis) and magnetic excitations, will be available.

Here it is important to point out the advices from the STAP committee in relation to the secondary spectrometer (p. 7): "The STAP recommends starting with an analyzer crystal **coverage of one full side**. This will save cost and allow testing the Si(311) upgrade option on the empty side."

With respect to detectors, the STAP report states: "Spectroscopy detectors: PSD's are essential on day 1 for good E and Q resolution. Diffraction detectors: due to a relatively small price, it is advised to have them on day 1."

Also, to improve the signal to noise ratio, the STAP report recommends (p. 7): "As a minimum, a radial collimator should be installed for day 1."

In relation with the sample environment equipment (SEE), this scenario follows the recommendations of the STAP report (p. 3): "The STAP recommends that **each spectroscopy instrument should have its own cryofurnace** as a minimum". Also (p. 6): "Day 1 sample environment requirements are a **cryofurnace (2-600K)** and a **sample changer**". The absence of a full suite of sample environment equipment can be partially mitigated with close collaboration with the SAD group, SEE pool and with future collaborations with other groups, including university groups.

4.2. Costing

The costing is based on bottom-up calculation of the procurement costs and manpower required for the tasks needed to deliver the higher level PBS items.

It should be remarked that the secondary cave costs have been analyzed and broke down into its parts including concrete shielding, cabling-housing, vacuum tank,…

Date 2016-10-21

Table 3 Costing for MIRACLES Option 2

	Phase 1	Design	Procurement & Fabrication	Installation	Commissioning	LABOR BUDGET	NON LABOR BUDGET	Total k€
Primary Shielding	0	200	809	100	0	300	809	1109
Secondary shielding (cave + vacuum tank shielding)	0	200	860	20	0	220	860	1080
Neutron Optics without vacuum pumps	0	0	3558	100	0	100	3558	3658
Choppers	0	0	1100.75	65.56	19.14	65.56	1119.89	1185.45
Sample Environment	0	0	0	180	431	180	431	611
Detector and Beam Monitors	0	0	758	76.65	0	76.65	758	834.65
Motion Control and Automation	0	53.712	29.373	4.65	28.578	58.362	57.951	116.313
Analyzer	0	215	712.16	70	0	285	712.16	997.16
Radial collimator	0	50	105	20	0	70	105	175
Beryllium filter	0	0	0	0	0	0	0	0
Beam Stop	0	50	100	20	0	70	100	170
Slit	0	0	60	10	0	10	60	70
Vacuum tank	0	300	940	100	0	400	940	1340
Instrument Infrastructure	0	0	637	0	0	0	637	637
Management & Science	480	600	480	480	480	2520		2520
Contingency	0	106.87	966.928	76.686	47.872	183.557	1014.800	1450.357
Total	480	1775.6	11116.211	1323.546	1006.590	3579.129	11162.801	**15953.93**
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Labor included in above (Person-Years)	4.1	14.65	7.6	6.1	2.7	35.15		35.15

4.3. Upgrade/Staging plan

Upgrades from STAP report:

- Analyzer and detector coverage, up to minimum 150º
- Space for the installation of a Be filter
- Si(111) and full coverage on the other half with Si(311) analyser option depending on neutron tests during commissioning.

The implementation of the remaining analyser Si(111) crystals (with additional ^3He detector tubes) to cover the full scope requirements would cost approximately 500 k€. Moreover, implementation of Si(311) crystals would add extra workload and cost for the upgrade. The use of most of the man power expected for the full scope might help to mitigate the upgrade workload.

Also, additional sample environment equipment is anticipated either by means of sharing costs between other spectroscopy instruments (Minipool) or to be implemented by collaborations with users and other research groups and/or funding from external grants.

Space will be allocated to, in the upgrade plan, implement the needed Be filter. The cost of the filter, required to cut-off contributions from higher wavelengths to the useful signal, is 450 k€.

5. OPTION 3: FULL SCOPE (17.7 M€)

5.1. Scope

The full instrument scope consists of:

- Primary spectrometer.
- Position-sensitive beam monitors at the exit of every chopper set (5) and before (guide end/slits) and after (beam stop, transmitted beam) the sample (2).
- Radial collimator to improve detection signal and Beryllium filter to remove higher frequency background.
- Half coverage secondary spectrometer Si(111) analyzers and 150 ^3He tube detectors (2 arrays of 75)
- Full suite of sample environment, including:
    - Clamped pressure cell through SAD pool and collaborations
    - High magnetic field (up to 9 T) through SAD pool
    - Dilution (down to 4 mK) through SAD pool

Future upgrade envisioned will include full coverage with Si(311) and subsequent addition of ^3He tube detector arrays.

This scope meets all the high level requirements and fulfils the science case.

5.2. Costing

The costing is based on bottom-up calculation of the procurement costs and manpower required for the tasks needed to deliver the higher level PBS items.

It should be highlighted that, in all the options, the costs for some items like vacuum pumps to evacuate the guides (which can reach about 200 k€, and may not be included in the ESS Vacuum System section), or the total sum of the electronics of the detector (that may reach ~600 k€) can be subject for discussion in the Scope Setting Meeting.

Table 4 Costing for MIRACLES Full Scope

	Phase 1	Design	Procurement & Fabrication	Installation	Commissioning	LABORAL BUDGET	NON LABORAL BUDGET	Total k€
Primary Shielding	0	200	809	100	0	300	809	1109
Secondary shielding (cave + vacuum tank shielding)	0	200	860	20	0	220	860	1080
Neutron Optics without vacuum pumps	0	0	3558	100	0	100	3558	3658
Choppers	0	0	1100.75	65.56	19.14	65.56	1119.89	1185.45
Sample Environment	0	0	0	300	808	300	808	1108
Detector and Beam Monitors	0	0	1024.95	76.65	0	76.65	1024.95	1101.6
Motion Control and Automation	0	62.1	39.494	5.995	33.984	68.095	73.478	141.573
Analyser	0	300	890	100	0	400	890	1290
Radial collimator	0	50	105	20	0	70	105	175
Berylium filter	0	0	450	20	0	20	450	470
Beam Stop	0	50	100	20	0	70	100	170
Slit	0	0	60	10	0	10	60	70
Vacuum tank	0	300	940	100	0	400	940	1340
Instrument Infrastructure	0	0	637	0	0	0	637	637
Management & Science	480	600	480	480	480	2520		2520
Contingency	0	116.21	1057.419	93.821	86.112	210.031	1143.532	1605.562
Total	480	1878.31	12111.613	1512.026	1427.244	3870.345	12578.850	**17661.19**
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Labour included in above (Person-Years)	4.1	15.65	7.6	6.1	2.7	36.15		36,15

6. RISK

Using ESS risk measure: impact x likelihood:

Risk level	Risk event	Risk impact	Treatment	Category	Treatment plan
5 x 5 (Option 1) Very high	Failure to deliver science case and not fulfilling scientific community expectations	Instrument will not be world class; users will not wish to use it	Mitigate	Budget, quality, function	Communicate with stakeholders the lowered expectations. Start planning for upgrade, incl. seeking funding. Responsible: MIRACLES team and ESS management
4 x 4 High	CF delay	MIRACLES construction will be delayed, risk to starting user programme on schedule	Observe	Schedule, budget	Access to Hall 2 is on the critical path for MIRACLES. Mitigate by using external areas (incl. ESS BILBAO) to start pre-installation Responsible: CF and MIRACLES team.
3 x 5 High	Improper design according to instrument requirements and delay in monolith insert design	Schedule for external milestone TARGET LEVEL ESS-0019533	Observe	Schedule, budget, quality, function	Follow progress of design and project schedule. Responsible: Target and MIRACLES team
3 x 3 High	Inadequate shielding design	High background levels. Instrument cannot measure as expected.	Observe	Budget, quality, function	Follow progress of design. Contingency to improve shielding once instrument is in construction. Responsible: MIRACLES, Optics & Shielding group
5 x 2 High	Failure of choppers within bunker during operation	Unable to perform: - cannot adapt flux/resolution - cannot ensure single frame per source period	Mitigate	Budget, quality, function	Mitigate through use of commercial supplier and careful design/specification. If continuous, choppers to be replaced, either within bunker (cost, delay) or outside bunker (cost, delay, major impact on scientific performance). Continuous monitoring of all chopper parameters needed. Responsible: MIRACLES team, chopper group
5 x 2 High	Late delivery of components	MIRACLES construction will be delayed, risk to starting user programme on	Mitigate	Schedule, budget	Properly assess the delivery time and transportation, incl. time for installation and arrival at site. Define the critical path for all

		schedule			components. Responsible: MIRACLES team
2 x 5 High	Weak integration process	Integration plan, checklist of activities, work package documentation, interface control document	Mitigate	Schedule, budget, quality, function	Consider integration plan in work package documentation, provide detailed description of interfaces, schedule and list of activities. Responsible: MIRACLES team

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Option 1

- Within this budget, due to the lack of analyser/detector coverage, the team will not be able to deliver the science case.

- This configuration would lead to lead to an extremely reduced Q-range coverage and low flux at detector (due to the reduced analyser coverage) as well as poor signal to noise ratio (due to lack of collimation and Be filters).

Option 2

- The main risk is the delay in delivery of the ESS, CF and some of MIRACLES components.

- Minor risks are the lack of full analyser/detector coverage and the Be filter, meaning that the full science case cannot be delivered on Day 1. Would need to upgrade as soon as possible

Option 3

- The main risk is the delay in delivery of the ESS and the MIRACLES components

7. REFERENCES

1. ESS-0053465: Concepts of Operations for the MIRACLES instrument

2. ESS Spectroscopy STAP Meeting report