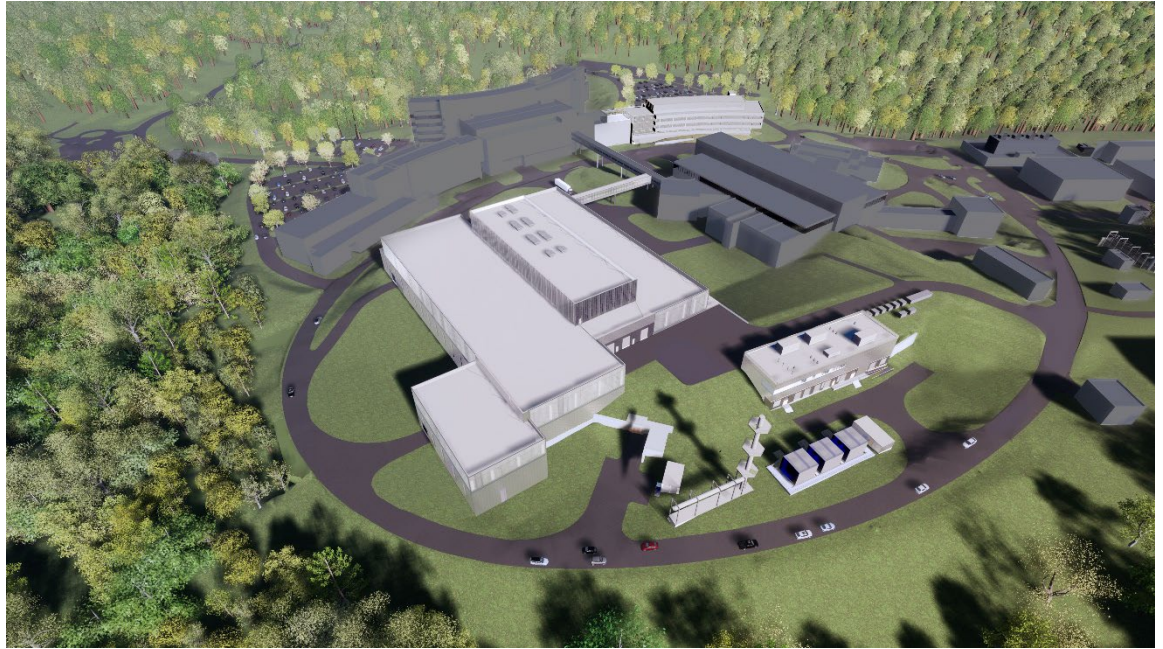


Second Target Station (STS) Project: QIKR Requirements Document



Danielle Wilson
John Ankner

TBD

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reviewed and approved for
public release.**

S04080100-SRD10000-R02

Second Target Station Project

QIKR REQUIREMENTS DOCUMENT

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Revision	Description
00	Initial Release
01	Add specific optics alignment requirements, update sample size in S.04.08.02-R2
02	Reduce min bandwidth (S.04.08.01-R24), update alignment, delete polarization req, update motion & detector req's, delete redundant req's, delete sample env section

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ACRONYMS

FTS	First Target Station
HVAC	Heating, Ventilation, and Air Conditioning
IPPS	Instrument Personnel Protection System
IRR	Instrument Readiness Review
ODH	Oxygen Deficiency Hazard
Q	Wavevector Transfer (change in momentum of scattered neutrons)
RCRA	Resource Conservation and Recovery Act
SiPM	Scintillator Photo Multiplier
SCE	Secondary Confinement Exhaust
STS	Second Target Station
WBS	Work Breakdown Structure

1. INTRODUCTION

This document defines the functional requirements for the subsystems of the QIKR instrument. These requirements are based on the high level scientific requirements derived from science case outlined in the instrument proposal as well as those specified in the *S04010100-SR0001 Second Target Station (STS) Instrument Systems Requirements Document*. These requirements are supported by the *QIKR Technical Report*, S04080100-TRT10000.

2. SCOPE

The project scope includes design, procurement, installation, testing without neutron beam, a Commissioning Plan and Fault Analysis, safety related operating procedures needed to perform commissioning (not user operation), technical support for document preparation (Hazards Analysis, Research Safety Summary, etc.) and completion of an Instrument Readiness Review (IRR).

The QIKR instrument consists of these major level 4 WBS groups:

- Optics
- Choppers
- Shielding
- Detectors
- Motion
- Sample Environment
- Infrastructure & Utilities

The QIKR instrument relies on additional WBS systems with requirements referenced here and defined by the documents indicated in the following sections:

- Section 11: Integrated Controls, WBS S.06.04.08
- Section 12: Scientific Software, WBS S.04.02

3. INSTRUMENT CHARACTERISTICS (S.04.08)

3.1 INSTRUMENT PURPOSE

QIKR will be a general-purpose, horizontal-sample-surface reflectometer. Exploiting the increased brilliance of the Second Target Station (STS), QIKR will collect specular and off-specular reflectivity data faster than the best existing such machines. Utilizing pulse skipping (7.5 Hz), it will often be possible to collect complete specular reflectivity curves using a single instrument setting, enabling “cinematic” operation, wherein the user turns on the instrument and “films” the sample. Samples in time-dependent environments (e.g. temperature, electrochemical, magnetic, or undergoing chemical alteration) will be observed in real time with frame rates as fast as 1 Hz in favorable cases. Cinematic data acquisition promises to make time-dependent measurements routine, with time resolution specified during post-experiment data analysis. This capability will be deployed to observe such processes as *in situ* polymer diffusion, battery electrode charge-discharge cycles, magnetic and other hysteresis loops in real time, and membrane protein insertion into lipid layers.

3.2 INSTRUMENT OVERVIEW

The range of scientific fields served by QIKR is large, requiring specialized sample environments to interrogate solid and free-liquid surfaces, as well as solid/liquid, liquid/liquid and solid/solid internal interfaces. Free liquid and liquid/liquid experiments (and to a lesser extent rheology) are constrained in that the sample surface is defined by gravity, and so cannot be tilted. The incident reflection angle in these cases must be defined by deflecting or sampling the angular divergence of the incident neutron beam. Free liquid surfaces and upper-subphase-transmitting liquid/liquid interfaces require a downward-directed incident beam, while lower-subphase-transmitting liquid/liquid interfaces and rheometers need an upward-directed incident beam. Solid and solid/liquid samples can be tilted and generally are not constrained by the incident-beam direction. Massive sample environments, such as cryogenic magnets, however, may also benefit from a non-tilted sample. Therefore, to address the interests of the entire scientific community, QIKR will feature both downward- and upward directed incident beams, each with its own sample table, detector, and associated beam conditioning.

Collecting data rapidly and accurately is important for all experiments, particularly ones involving kinetic measurements. True kinetic measurements would need to be collected at a single instrument setting covering the full Q range of interest. The 15-Hz STS repetition rate affords a much larger wavelength bandwidth than is available at the 60-Hz FTS, but to achieve true single-setting operation for most samples, QIKR will need to be able to run in frame-skipping mode at 7.5 Hz. Beyond rapid data acquisition, the neutron flux of the STS will enable experiments with unprecedented time resolution. In addition, while optimizing transport of short-wavelength neutrons at peak moderator flux ($\lambda = 2.5 \text{ \AA}$) is essential to maximize Q bandwidth and minimize counting time, the instrument will also be capable of operating at 15 Hz and in different wavelength bands. In such modes, one covers the full Q range with multiple incident beam settings.

As data acquisition time decreases, the proportion of time spent aligning samples or setting up and waiting for sample environments to equilibrate grows. To maximize time spent collecting data, time spent carrying out these support tasks should be minimized.

For further details, refer to the *QIKR Technical Report*, S04080100-TRT10000.

3.3 HIGH LEVEL INSTRUMENT REQUIREMENTS (S.04.08.01)

From the *Instrument Systems Requirements Document*, S04010100-SR0001, the following requirements are derived. The requirements in this table apply to both the upward- and downward-directed beamlines unless otherwise noted. Requirements throughout the remainder of this document refer back to these:

Req. No.	Description	Traceability
S.04.08.01-R1	QIKR components shall be designed for a lifetime of at least 10 years	S.4-R03
S.04.08.01-R2	QIKR shall be designed to support $\geq 95\%$ availability during beam operations <i>Note: Instrument equipment must be capable of operating throughout the 5000 hours of yearly planned STS facility operation.</i>	S.4-R04
S.04.08.01-R3	QIKR shall be capable of operating independently and without negatively impacting the performance of other instruments	S.4-R05
S.04.08.01-R4	QIKR equipment, including shielding, shall be designed to be removable/ replaceable and must use minimal amounts of RCRA-listed materials and materials that activate with long-lived isotopes	S.4-R06
S.04.08.01-R5	QIKR shall be capable of remote operations	S.4-R07
S.04.08.01-R6	QIKR shall be designed to operate safely and efficiently within the context of the user program	S.4-R08
S.04.08.01-R7	QIKR shall be designed to accept pulses from the STS moderator designed to support a downward-directed neutron beam	S.4-R09
S.04.08.01-R8	QIKR must be able to provide and maintain the level of optical component alignment required to meet the instrument's performance goals over the lifetime of the instrument <i>Note: This may mean providing monitoring of alignment over time and ensuring it will be possible to perform realignment if needed</i>	S.4-R14
S.04.08.01-R9	QIKR equipment shall be designed following all applicable standards for personnel safety. <i>Note: Safety hazards will be evaluated within the framework of a formal hazards analysis identifying consequences, likelihood and proposed mitigation of hazardous events</i>	S.4-15
S.04.08.01-R10	QIKR shall be designed to limit radiation exposure in adjacent areas that are accessible to personnel during beam-on and beam-off conditions to less than 0.25 mrem/hr	S.4-R16
S.04.08.01-R11	QIKR must provide accommodation for additional shielding to be added to achieve low background: <2 counts/minute "dark count" (shutter closed) and <5 counts/sec with the shutter open and detector not viewing the beam <i>Note: The requirement is only to provide the <u>ability</u> to add shielding after beam-on if the detector counts require it</i>	S.4-R01

Req. No.	Description	Traceability
S.04.08.01-R12	QIKR must provide two main incident beams, one viewing the moderator from above the horizon, and one from below.	S.4-R01 S.4-R09 S.4-R13
S.04.08.01-R13	QIKR must be able to operate each beam path independently of the other	S.4-R01 S.4-R09 S.4-R13
S.04.08.01-R14	QIKR must provide multiple incident angles on both solid and liquid samples	S.4-R01 S.4-R09 S.4-R13
S.04.08.01-R15	QIKR must provide user facilities and equipment sufficient to prepare samples containing liquids for testing and to safely collect experiment data	S.4-R08
S.04.08.01-R16	Personnel must have safe access to each end station within 30sec of closing the corresponding shutter <i>Note: This will be determined by material and shielding choices</i>	S.4-R04 S.4-R08 S.4-R15
S.04.08.01-R17	There must be at least 46cm (1.5 feet) of clear space to the side of the sample for user access on each of the upper and lower beam paths	S.4-R08
S.04.08.01-R18	Deleted, Rev02	
S.04.08.01-R19	QIKR sample stage must accommodate sample equipment that fit within a 60cm x 60cm x 200cm volume (Length x Width x Height)	S.4-R01
S.04.08.01-R20	Horizontal beam footprint at sample = 5x10 mm to 25x75 mm	S.4-R01
S.04.08.01-R21	QIKR must accept 95% of the viewable neutron trajectories from the moderator at the spectrum peak ($\lambda = 2.5 \text{ \AA}$)	S.4-R01 S.4-R09
S.04.08.01-R22	QIKR must be able to operate at both 15 and 7.5 Hz	S.4-R01 S.4-R02
S.04.08.01-R23	Q-resolution $0.02 \leq \Delta Q / Q \leq 0.07$	S.4-R01
S.04.08.01-R24	Min Bandwidth (lower path) Min Bandwidth (upper path) $\Delta\lambda = 16.8 \text{ \AA}$ at 7.5 Hz $\Delta\lambda = 14 \text{ \AA}$ at 7.5 Hz $\Delta\lambda = 8.4 \text{ \AA}$ at 15 Hz $\Delta\lambda = 7.0 \text{ \AA}$ at 15 Hz	S.4-R01 S.4-R02
S.04.08.01-R25	QIKR shall be optimized for a relative angular resolution of 0.025, but shall support resolutions as large as 0.07	S.4-R01
S.04.08.01-R26	The nominal sample position must be 2m away from the end of the guide, measured along the guide centerline	S.4-R01 S.4-R09
S.04.08.01-R27	The nominal detector position must be on a 2m radius centered on the nominal sample position	S.4-R01 S.4-R09

4. OPTICS (S.04.08.02)

The neutron guide system will be designed to have the highest transmission efficiency for neutrons of wavelengths $\geq 2.5 \text{ \AA}$ and will completely reject wavelengths $\leq 0.25 \text{ \AA}$. The guide system will also provide a sufficient number of wave vector transfers at the sample to allow a variety of neutron incident angles without requiring tilting of the sample itself. Configuration and Quality Level of the Optics System is given in the S04080200-QAI10000 document.

Req. No.	Description	Value/Error	Traceability (S.04.08.01)
S.04.08.02-R1	The QIKR neutron guide system shall have a design vacuum level less than 5×10^{-3} torr.		R13, R21, R23, R24, R25
S.04.08.02-R2	Deleted, Rev02		
S.04.08.02-R3	The range of wave vector transfers (neutron incident angles) supplied at the sample position shall be:	$0.005-0.5 \text{ \AA}^{-1}$	R13, R14
S.04.08.02-R4	Neutron attenuation by the slits shall be:	$<10^{-5}$ at 1 \AA	R13, R21, R23, R24, R25
S.04.08.02-R5	Alignment of optical components must be such that each beam path transmits $2.5 \text{ \AA} - 25 \text{ \AA}$ neutrons from the moderator to the sample with an efficiency of:	$>90\%$ of the simulated neutron transport	R08, R13, R21, R23, R24, R25
S.04.08.02-R6	Deleted, Rev02		
S.04.08.02-R7	Deleted, Rev02		
S.04.08.02-R8	Variation in position between guide <u>elements</u> must be less than the following maximums (refer to figures 1-2): horizontal/vertical linear: longitudinal linear: angular about the longitudinal axis: angular about the x or y axis:	$\Delta x, \Delta y \leq 20 \text{ \mu m}$ $\Delta z \leq 100 \text{ \mu m}$ $\Delta \theta \leq 2.0 \times (10)^{-3}$ radians $\Delta \phi \leq 2.0 \times (10)^{-3}$ radians	R08, R13, R21, R23, R24, R25
S.04.08.02-R9	Variation in position between guide <u>sections</u> must be less than the following maximums (refer to figures 1-2): horizontal/vertical linear: longitudinal linear: angular about the longitudinal axis: angular about the x or y axis:	$\Delta x, \Delta y \leq 50 \text{ \mu m}$ $\Delta z \leq 2 \text{ mm}$ $\Delta \theta \leq 2.0 \times (10)^{-3}$ radians $\Delta \phi \leq 2.0 \times (10)^{-3}$ radians	R08, R13, R21, R23, R24, R25
S.04.08.02-R10	QIKR must supply a means to evacuate the guide that is separate from the central bunker vacuum supply		R2, R6

Req. No.	Description	Value/Error	Traceability (S.04.08.01)
S.04.08.02-R11	QIKR must supply a means to back-fill evacuated guides with house nitrogen <i>Note: this can be through the same connection where local vacuum is supplied</i>		R2, R6
S.04.08.02-R12	A high-pass wavelength filter must be present to reject unwanted long wavelength neutrons from prior pulses. <i>Note: The frequency cutoff is variable and is adjusted by filter angular position. The cutoff depends on instrument operation rate (7.5Hz or 15Hz) and the settings required for a particular experiment.</i>		R22, R24

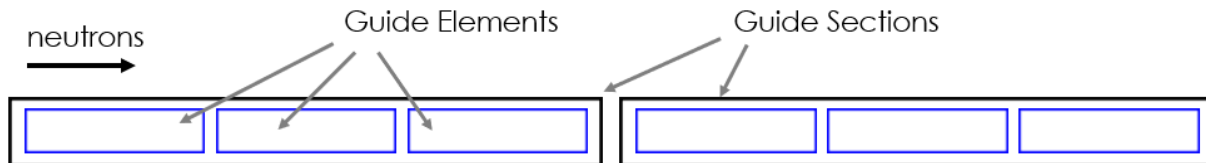


Figure 1: Description of guide elements and guide sections. Guide elements are individual pieces of guide glass. Guide sections are each a single housing that contains multiple guide elements. Alignment requirements are applied both between guide elements and between guide sections.

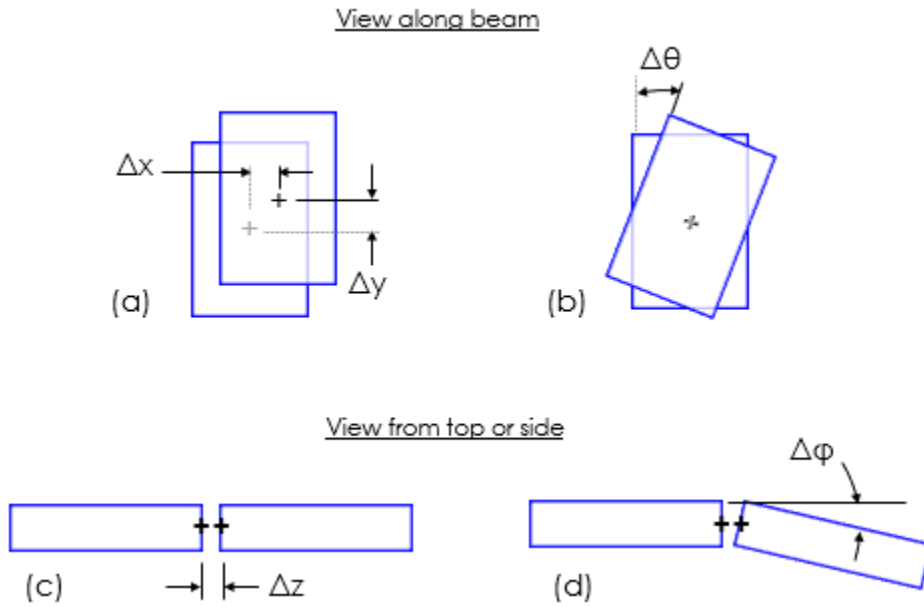


Figure 2: Description of misalignment types: (a) misalignment of centers of adjacent guide element ends or guide section ends, (b) rotational misalignment between adjacent guide elements or guide sections along the longitudinal axis of the downstream guide element or guide section, (c) variation in longitudinal distance between adjacent guide element (or guide section) end centers, and (d) rotational displacement of a guide element's (or guide section's) downstream end center from its nominal position.

5. CHOPPERS (S.04.08.03)

QIKR will have bandwidth choppers sufficient to pass the desired wavelength range for each beam path and to reject all other wavelengths to the highest degree possible. To allow frame skipping, each chopper will also be able to rotate at half the source frequency (7.5Hz).

Req. No.	Description	Value/Error	Traceability (S.04.08.01)
S.04.08.03-R1	Neutron choppers shall have an availability requirement $\geq 97\%$ to be operating within specification during beam operations		R2, R13
S.04.08.03-R2	Choppers must be removable within 24 hours of beam shutdown		R2, R4, R13
S.04.08.03-R3	Chopper rotation frequency:	15Hz, 7.5Hz	R13, R22
S.04.08.03-R4	Choppers must supply a variable angular aperture		R13, R24
S.04.08.03-R5	Attenuation of neutrons outside of the desired wavelength range of 2.5 -23.5 Å shall be:	$<10^{-5}$ at 1 Å	R13, R21, R23, R24

6. SHIELDING (S.04.08.04)

QIKR will need sufficient shielding to both ensure that background radiation at the sample and detector is minimal, that safe radiation levels are always maintained outside the cave, and that safe radiation levels are maintained within the cave when the shutter is closed. Additionally, shielding within the cave will allow either the upper or lower beam path to be in full operation while the other is being accessed by personnel. QIKR has no separate beam transport shielding section: the cave begins immediately at the outer surface of the bunker wall. Material and size requirements for the shielding will be determined by neutronic analysis.

Req. No.	Description	Traceability (S.04.08.01)
S.04.08.04-R1	The beamline shielding, cave walls, and beam stop shall limit dose rates to the maximum dose rates given in S04080400-DCD10000.	R6, R9, R10, R13
S.04.08.04-R2	There shall be sufficient shielding in the bunker to absorb line-of-sight neutrons prior to the cave	R10, R11, R13, R16
S.04.08.04-R3	All shielding within the bunker space, within the bunker wall penetration window, and within the cave must be removable	R4, R13
S.04.08.04-R4	The QIKR cave must provide shielding to allow personnel access to one beam path's sample while the other beam path is operating	R10, R13, R16
S.04.08.04-R5	QIKR must have separate beam stops in the cave areas, one each for the upper and lower beam paths	R4, R10, R13, R16

7. DETECTORS (S.04.08.05)

QIKR will need detectors with high spatial resolution and the ability to see reflections from the sample over a range of angles about both the vertical axis (diffuse reflections) and the horizontal axis transverse to the beam (specular-plane reflections).

Req. No.	Description	Value/Error	Traceability (S.04.08.01)
S.04.08.05-R1	QIKR detectors shall be capable of being grounded to a dedicated infrastructure for instrument system use		R09, R13
S.04.08.05-R2	Spatial pixel area shall be:	$\leq 0.1 \times 0.1 \text{ cm}^2$	R13, R20, R23, R24, R25
S.04.08.05-R3	Minimum detector area shall be:	$20 \times 20 \text{ cm}^2$	R13, R20, R23, R24, R25
S.04.08.05-R4	Precision of time-of-flight detection shall be:	10 μsec	R13, R20, R23, R24, R25
S.04.08.05-R5	Total instantaneous rate shall be: Time-average rate shall be: Maximum dead time at these rates must be $\leq 1\%$	$\geq 20,000/\text{sec}$ $\geq 10,000/\text{sec}$	R13, R20, R23, R24, R25
S.04.08.05-R6	Detector efficiency shall be:	$\geq 60\% @ 2.5 \text{ \AA}$	R13, R20, R23, R24, R25
S.04.08.05-R7	Diffuse angular range (rotation about the vertical axis) shall be:	$-1^\circ \leq 2\phi \leq 15^\circ$	R13, R20, R23, R24, R25
S.04.08.05-R8	Specular-plane angular range (rotation about the horizontal axis perpendicular to the beam path) shall be:	$-15^\circ \leq 2\theta \leq 15^\circ$	R13, R20, R23, R24, R25

8. MOTION (S.04.08.06)

In this section, the z-axis is defined to be along the centerline of the beam between the end of the beam guide and the sample (downstream is positive), the x-axis is horizontal, and the y-axis is perpendicular to x and z (upward is positive). The axes follow a right-handed coordinate system sign convention.

QIKR will have fixed beam path directions but will be able to change the angle of neutrons incident on the sample by selecting various beam intensities exiting from the guide at discrete angles and positioning the sample to intersect one of those beams, and/or by changing the orientation of the sample. The motion axes downstream of the guide end will select the desired incident angles and provide the desired detection coverage while controlling beam divergence and shaping the beam footprint on the sample. They will also place the sample in a y-position that intersects one of several desired beam intensity angles. Either upstream or downstream of the guide end will be located a beam attenuator that allows to user to reduce the overall beam intensity in discrete increments

The Maintenance Shield for QIKR will be a custom version of the standard design since it must accommodate two separate beam paths. The customization will be limited to the range of motion, overall size of the shield, and the total number of shield positions. The overall design and method of operation will otherwise be the same as the standard maintenance shield.

Each beam path will have its own Shutter, located downstream of that path's chopper. Each Shutter will be operated independently of the other so that the upper beamline may be operational while the lower beamline is accessible to personnel (and vice versa). A heavy shutter may be used, but since QIKR is a curved beamline, it may be possible to use a lighter style of shutter, such as a guillotine.

Additional Motion Requirement details are given in **S04080600-SRD10000**.

Req. No.	Description	Value/Error	Traceability (S.04.08.01)
S.04.08.06-R1	QIKR must provide three collimating apertures upstream of the sample that have remotely adjustable openings.		R5, R20, R23, R25
S.04.08.06-R2	The apertures upstream of the sample must be movable along the beam path direction. <i>Note: This motion may be either manual or motorized, preference for manual motion</i>		R5, R13, R19, R20, R25
S.04.08.06-R3	QIKR must be able to remotely and collectively rotate all collimating apertures about an x axis drawn through the center of the guide glass end.		R5, R13, R14
S.04.08.06-R4	QIKR must be able to remotely adjust the sample position about its nominal location in the x-z plane.		R5, R13, R19, R26, R27
S.04.08.06-R5	QIKR must be able to remotely adjust the y axis position of the sample about its nominal location. <i>Note: There are three nominal y-positions of the guide defined by the three highest intensity beams exiting the guide end</i>		R5, R13, R14, R19, R26, R27
S.04.08.06-R6	QIKR must be able to remotely adjust the angle of the sample about each of the x and z axes relative to a horizontal plane.		R5, R13, R14, R19

Req. No.	Description	Value/Error	Traceability (S.04.08.01)
S.04.08.06-R7	QIKR must be able to remotely adjust the position of the detector about an x axis through the center of the nominal sample location.		R5, R13, R14, R26, R27
S.04.08.06-R8	QIKR must be able to remotely adjust the position of the detector about a y-axis through the center of the nominal sample position.		R5, R13, R26, R27
S.04.08.06-R9	Maintenance shield must be based on the standard design and accommodate both upper and lower beam paths.		R3, R7, R10, R12, R13
S.04.08.06-R10	Each shutter must be based on the standard design and be placed such that personnel can access one cave while the other is operating.		R6, R9, R10, R12, R13, R16
S.04.08.06-R11	QIKR must provide the ability to remotely move multiple samples sequentially into and out of the sample position.		R5, R6, R13, R15
S.04.08.06-R12	Top level assemblies of motion components located within the cave must withstand additional loading beyond the loads generated by the assembly weight itself		R2, R6, R9
S.04.08.06-R13	The detector must have position adjustments independent of the sample position to allow for initial setup and alignment		R8
S.04.08.06-R14	Motion components and assemblies must be protected from accidental changes in their desired location		R8
S.04.08.06-R15	Motion components and assemblies within the cave must not permanently locate components within a given envelop about the nominal sample center position: <i>Note: This is meant to preserve clear space for sample environments. Motion components may be within this area for smaller sample environments but must be movable to accommodate larger sample environments.</i>	.35m below lowest y-pos .50m above highest y-pos .50m all other directions	R19
S.04.08.06-R16	All motion components as well as their associated cabling and control rack spaces must be located outside of the required clear space for the user next to the sample		R17
S.04.08.06-R17	A beam attenuator shall be provided that allows the user to reduce the overall beam intensity in multiple discrete increments <i>Note: A reduction in beam intensity may be to allow accurate measurements in some situations</i>		R23, R25
S.04.08.06-R18	The high-pass wavelength filter must have an adjustable linear position for initial alignment to the beam path, and an adjustable angular position to select the desired wavelength cut-off		R22, R24

9. SAMPLE ENVIRONMENT

Section deleted, R02. All Sample Environments moved out of Instruments' scope.

10. INFRASTRUCTURE & UTILITIES (S.04.08.08)

QIKR will have the following infrastructure items in common with the majority of beamlines: a control hutch with furniture and workstation equipment, standard connections to building utilities (electrical power, water, HVAC, networking), SCE, IPPS and ODH equipment, smoke detectors, fire alarms, and sprinklers. Infrastructure and utility items that are unique to QIKR are listed in the table below:

Req. No.	Description	Traceability (S.04.08.01)
S.04.08.09-R1	QIKR equipment must be able to interface to standard STS utility distribution systems	R6, R9, R13
S.04.08.09-R2	QIKR design shall make provisions for all required safety systems	R6, R9, R13
S.04.08.09-R3	QIKR must provide a sample prep area with storage for samples and sample prep materials. The prep area will also provide a water supply with a filtrations system, a sink with a drain for rinsing glassware, and a fume hood.	R13, R15
S.04.08.09-R4	QIKR must provide a means of moving guide sections, in-cave shielding, sample environments, and any other in-cave equipment weighing more than 25lbs into and out of the cave	R4, R6, R9, R13, R15
S.04.08.09-R5	QIKR must provide an in-cave location in each cave to store multiple samples	R5, R13, R15

11. INTEGRATED CONTROLS/ SOFTWARE (S.06.04.08)

Instrument Control Systems (ICS) shall meet the requirements in S06040200-SR0001, *Integrated Control Systems Instruments Control and Data Acquisition Requirements Document*.

12. SCIENTIFIC SOFTWARE (S.04.02)

Scientific software includes development of robust data reduction, visualization, and analysis for STS instruments. Requirements for scientific software will be developed prior to CD2.