Final Beamline Design Report

Insertion Device Beamline

Biophysics Collaborative Access Team

BioCAT

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3Section
Page

1.0 OVERVIEW

This document represents the Final Design Report for the Biophysics Collaborative Access Team (BioCAT), sector 18 at the Advanced Photon Source. This document can be considered as a revision and update of the BioCAT PDR and so is free-standing. All of the material in the BioCAT PDR is also addressed here. Every attempt has been made to address each of the criteria for the Preliminary and Final Design Beamline Design Review outlined in APS document TB-14. Whenever a particular criterion has been specifically addressed, it is identified by number and reproduced in this document to aid the reviewer.

The research focus of BioCAT is on structural studies of partially ordered biological materials using X-ray scattering and X-ray absorption fine structure (XAFS) spectroscopy, with particular emphasis on:

• time resolved experiments
• polarized XAFS
• resonant (anomalous) and nonresonant diffraction with emphasis on time-resolved studies
• polarized XAFS,
• hybrid diffraction/spectroscopic techniques
• novel techniques that exploit the unique properties of the APS

The primary systems of interest for XAFS are metalloprotein solutions, oriented films, and oriented single crystals. X-ray scattering studies address a wide range of systems, including solutions, fibers, membranes, Langmuir Blodgett films and monolayers, liquid crystals, and colloids.

While the successes of X-ray protein crystallography in structural biology have been impressive in recent years, it must be realized that most biological systems are not crystalline *in vivo*, and that a broad range of relevant biological structures and dynamics is not amenable to direct study by crystallographic methods. It is the partially ordered (i.e. non-crystalline) biological structures and particularly the *dynamics* of those structures that BioCAT specifically attempts to address. Several other CATs (SBC, IMCA, Bio-CARS) at the APS address well the needs of the crystallographic community. The specific intent of BioCAT is to provide a national user facility to a large research community comprising a wide variety of subspecialties and investigators having diverse interests in structural and molecular biology, and which complements the proposed beamlines of other CATs and offers significantly enhanced capabilities over beamlines at existing synchrotron radiation sources.

BioCAT operates as an NIH Research Resource under a cooperative agreement with NIH. BioCAT will perform the core and collaborative research, service, training & dissemination functions required of NIH Research Resources. Grant Bunker, Associate Professor of Physics at Illinois Institute of Technology, is the Director of BioCAT and as such, is the Principal Investigator on the BioCAT NIH Research Resource Grant. An Advisory Committee composed of recognized experts in biological synchrotron radiation research advises the CAT management on policy, strategic, management, and technical issues relevant to the CAT.

The permanent operations and maintenance staff is anticipated to be about seven full time equivalents beginning in 1998. During the first five year period only the insertion device (ID) line will be constructed.

1.1 TECHNICAL SCOPE:

(PDR Criterion 5.2.1.2 - The overall beamline layout and components are compatible with the intended science.)

The BioCAT beamline will be used both for biological small-angle diffraction and scattering and X-ray spectroscopy. Many of the proposed experimental projects make use of a combination of proven techniques such as small angle X-ray scattering and time averaged fluorescence XAFS, but applied to particularly demanding systems; other experiments will push the state of the art, such as those implementing advanced flow systems for time resolved XAFS and diffraction. Some experiments will require time resolutions in the millisecond range or faster; others require resolution of spatial periodicities on the order of several thousand Å; others require high fluxes ($\sim 10^{13}$ - 10^{14} photons/sec 3 eV bandwidth) into spot sizes on the order of 100 μm or less; yet others require a high degree of linear polarization of the X-ray beam, and onto relatively small (<100 μm) crystalline samples. In some cases a relatively large amount of angular divergence can be tolerated, so that a small spot size can be obtained by focusing optics. In other cases the intrinsic high collimation of the undulator source will be required. Thus the optics must be designed to be rather flexible.

Both the XAFS and some scattering experiments require a high energy resolution ($\Delta E/E \sim 10^{-4}$) scanning monochromator. The principal energies needed for BioCAT XAFS experiments span the K-edges of the first series transition metals (particularly Mn-Zn ~6.5-10.5 KeV); this energy range is also appropriate for most scattering experiments. Anomalous scattering experiments require tunability to selected edges which are sample dependent. The L_{III} edges (which can provide high contrast because of their intense absorption peaks due to d-final states) of the rare earth elements are about the same energy as the K-edges of primary interest for XAFS studies. Other interesting L_{III} edges (e.g. gold and mercury) are also within the accessible energy range. The K-edges of the biologically relevant Mo, Cd, and I edges extend above 33 KeV, but the rapid increase with respect to atomic number of the core-hole lifetime broadening make higher energy XAFS experiments of diminishing utility.

The scientific program of BioCAT specifically takes advantage of the unique properties of planar undulator radiation: simultaneously a high flux ($\sim 10^{13}$ - 10^{14} photons/sec) into a small angular divergence (~50 μrad) with a small source size (~100 μm vertical). The high q resolution ($q=2\pi \sin\theta / \lambda$) scattering experiments require minimum angular divergence/convergence and small spot sizes in at least one direction, so a high degree of demagnification cannot be tolerated in those cases. In other cases a smaller spot size (~40-100 μm) is desired which can be achieved by focusing when greater convergence angle can be tolerated. For highly anisotropic systems such as oriented fibers the criteria may differ in vertical and horizontal directions. The use of separate horizontal and vertical focusing elements affords independent control to permit optimal matching to the experiment. The predicted performance of the BioCAT beamline is shown in Table I.

Table I Insertion Device Beam Line Design Parameters	
Insertion Device	APS undulator A
Monochromator Type	Cryogenically Cooled Si111 Crystal
Energy Range(Undulator Fundamental)	3.5 - 13 keV
Energy range (Undulator Third Harmonic)	10.5-39 keV
Energy Resolution ($\Delta E/E$)	2×10^{-4}
Spot size	< 40 µm (FWHM vertical)
(focused at sample)	< 120 µm (FWHM horizontal)
Angular Resolution	.16 mrad (FWHM vertical
(focused at sample)	.19 mrad (FWHM horizontal)
Spot size	<50 µm (FWHM vertical)
(focused at detector 2 m from sample)	< 150 µm (FWHM horizontal)
Spot size	<100 µm (FWHM vertical)
(focused at detector 8 m from sample)	< 240 µm (FWHM horizontal)
Spot Size	1500 µm (FWHM vertical)
(at sample, no focusing)	3500 µm (FWHM horizontal)
Angular Resolution	.025 mrad (FWHM vertical)
(no focusing)	.056 mrad (FWHM horizontal)

The XAFS experiments, which primarily are in fluorescence mode, do not normally place any special demands on the angular convergence of the beam. However, high flux into a small spot size is required for many practical time resolved XAFS experiments, particularly those which employ flow systems. To reduce sample consumption, the irradiated sample volume must be minimized. Also, in time resolved XAFS experiments, when the sample is perturbed by pressure jump, temperature jump, pulsed fields, photoexcitation by laser, rapid mixing etc, both the sample volume and X-ray window area must be minimized, requiring beams of small cross-sectional area. The small beam sizes afforded by focusing optics, which ideally demagnify the source approximately 10:1 in the proposed design, should realistically provide beam sizes much less than 100 µm by 300 µm. Furthermore, experience has shown the utility of mirrors for harmonic rejection even if they are not required for focusing. For DAFS experiments and other hybrid scattering/XAFS experiments on layered materials the independent control over convergence angle in two directions will be very beneficial. Finally, for polarized XAFS and anomalous scattering experiments the high degree of linear polarization at the first and third harmonic of the undulator is a significant benefit.

XAFS places stringent demands on the scanning stability of the monochromator. At the NSLS we have found servo controlled DC motor step scanning to be practical and desirable, as a DC motor drive reduces the vibrations caused by the pulsing of stepping motors, and the motors have higher torque with less heat generation. Further, we expect that slew scanning will be very desirable to minimize the point to point settling time overhead, particularly if the scan time is relatively short, on the scale of seconds.

Thus, in addition to the focusing capability, one major requirement is that the monochromatic beam energy must be continuously scannable over the range of biological interest. Undulator “A” has been chosen as a source of very intense monochromatic radiation in the 3.2 - 14 keV range (1st harmonic, 9.6-42 keV 3rd harmonic) with very low angular divergence and the ability to dynamically scan the fundamental energy by scanning the undulator gap. For fast scans, energy ranges on the order of 1 KeV can be achieved by tapering the undulator gap.

One important aspect of the layout is the relatively long white-beam-transport lines and enclosures. The long white-beam-path is a result of the requirement for high demagnification of the beam by the optics in order to achieve the small focal spot size required to match specimen size and/or detector pixel size. Many of the target experimental systems (eg. single muscle fibers) have very small (~50 μm) cross-sections to the beam. The proposed optical arrangement allows for great flexibility in determining the beam dimensions at the sample and detector. Thus camera lengths from a few cm up to 10 m (maximum) can be employed in order to match the varied beam size and divergence requirements of a very broad range of SAX experiments. This flexibility also allows one to deliver the maximum flux to small samples in spectroscopy experiments. The NIH Special Study Section that reviewed the BioCAT NIH Proposal and the BioCAT Advisory Committee (which contain specialists in XAFS and scattering) have examined the design and confirm that the layout of the components is appropriate for the proposed scientific program.

Although the scientific mission remains unchanged, because of advances in available technology (e.g. thin crystal cryogenic optics), the final design for the ID line outlined in this document has evolved considerably from that described in the BioCAT Conceptual Design Report submitted several years ago. In consultation with G. Rosenbaum (beam line designer for the Structural Biology Center CAT and a consultant on the BioCAT project) it became evident that substantial savings in design costs and time could be realized by taking over virtually intact the design of the SBC-CAT ID beam line, without compromising (indeed, enhancing) the scientific mission in any way. The major differences between the BioCAT and SBC-CAT design lie in the layout and equipment of the end-station, and control software. As of this writing, as-built assembly and detail drawings exist for all major components of the beamline . In addition, the design of the SBC-CAT undulator beam line has received APS final design approval and is now in early operations stage. The decision to adopt this design which was reviewed and approved by the BioCAT Advisory Committee Meeting Aug. 4, 1995.

During the initial phase of operation, BioCAT will not construct a bending magnet beamline because of insufficient funding. Additional funding will be sought in the second 5 year cycle of NIH funding to construct the bending magnet beamline, at which time a new preliminary design report will be submitted. Alternative sources of funding are also being considered.

Additional background on the scientific and technical scope of the BioCAT project can be found in several prior documents. These are:

1. BioCAT: Biophysics Collaborative Access Team (proposal to NIH, February, 1994)
2. BioCAT Conceptual Design Report (January, 1994)
3. APS Project Management Plan for the Construction of the BioCAT facility (December, 1995)

The design for the BioCAT ID line (the primary subject of this report) is based substantially on the design for the SBC-CAT sector which has been documented and approved in several reports. The relevant documents are:

1. Structural Biology Center: A Proposed National User Facility at the Advanced Photon Source, February 1992 (SBC-CAT 00-0164-01)
2. SBC-CAT Conceptual Design Report, May, 1993 (SBC-CAT 00-0174-01)
3. APS Project Management Plan for the Construction of the Structural Biology Center, March, 1994 (SBC-CAT 01-0002-01)
4. Title I Design Summary Report for the Technical Facilities of the Structural Biology Center Construction Project, May 1994 (SBC-CAT 01-0151-01)
5 SBC-CAT Control System Requirements, February 1995, (SBC-CAT 01-0007-01)
6. SBC-CAT Preliminary Beamline Design Report (SBC-CAT 01-0150-01)
7. SBC-CAT Final Design Report (SBC-CAT 01-0268-01)

1.2 RATIONALE FOR THE CHOICE OF INSERTION DEVICE

The Insertion Device beamline configuration is based on APS Undulator A as described in ANL/APS/TB-17, "Undulator A Characteristics and Specifications: Enhanced Capabilities". Since the ID line will be used both for experiments requiring high q-space resolution and high r-space resolution over a continuous energy range, with a tunable, high-brilliance source, the undulator represents the best choice for scattering experiments. Since dynamic scanning and/or tapering of the undulator gap will be possible, the same insertion device will also be appropriate for the planned spectroscopy experiments.

The BESSRC- CAT and SRI-CAT teams have had excellent success with the implementation of cryogenic cooling of thin Si crystals for an ID monochromator suitable for an undulator beam line ("The Cryogenic Cooling Program at the Advanced Photon Source", C.S. Rogers, et al., ANL/APS/TB-18). Their design has been tested and has been proven to be a solution of the undulator A high heat-load problem in a manner that is compatible with the overall optical configuration required for BioCAT. The proposed design has been incorporated into the monochromator now being commissioned by SBC-CAT. Alternative designs are also being tested by SBC-CAT, MR-CAT and IMCA-CAT.

1.3 SECTOR LAYOUT

(PDR Criterion 5.2.1.1 - An overall beamline/sector layout has been provided showing beamline components, personnel safety system components, support equipment (racks, etc.), and furniture.)

(FDR Criterion 1.1)

A plan and elevation of the beamline layout has been provided with clearly identified beamline components (e.g., slits, shutters, mirrors, monochromators, shutters, stops, etc.), beamline support facilities (e.g., beamline controls and data acquisition electronics, compressed gas storage areas, etc.), and aisle ways. CAD files of the layout have been provided to the Design Exchange.

Figure 1 overall plan view of the BioCAT sector. Figure 9 shows the plan view of the BIOCAT Insertion Device beamline showing locations of major components. The layout of the beamline is very similar to that of Figure 1b of the BIOCAT Preliminary Beamline Design Report. The only changes in the layout of beamline that are different from that of the PDR are:

- The Heat Filter Assembly, F2-30, has been moved from a location in the ID-A enclosure at about 27m from the source to a location in the ID-C enclosure at about 51.5m from the source. This was done to reduce the heat load on the filter since the primary aperture located at 51m from the source will absorb a significant fraction of the radiation not intended to strike the monochromator crystal.

- With the removal of the F2-30, the positions of the pumping station and beam position monitor located at 27 m were reversed in order to simplify the support stand. This has no significant effect on the beam line design.

- The monochromatic beam photon shutter and horizontal collimation slits located at about 57-58m from the source have had their positions switched. This was done so that the photon shutter would better shield the opening in the lead tube around the beam pipe which penetrates through the common wall of the ID-C and ID-D. This is an improvement in the shielding as it increases the number of “bounces” a photon must go through in order to pass through the beam pipe into ID-D.

Apart from these changes, the layout is identical to that in the PDR.

FDR Criterion 1.2
Changes from the PDR layout have been clearly identified, and the impact on the beamline functionality is described.

The changes identified above have no impact on beamline functionality.

Figures 1 shows the overall footprint of the BioCAT sector, #18, at the APS experimental hall with the shielding enclosures and internal equipment indicated. The sector layout indicates electronic racks, and work stations. The sector area for the bending magnet beamline has been left clear of ID beamline equipment to facilitate future construction. Figure 2 (Drawing #1.1.1.1.2-002-DD-0B) shows the details of the shielding layout including the thicknesses of the wall and roof panels. Figure 8 (Drawing #B01-0001B) shows the layout of the PSS components, associated utility conduit and cable trays.

(PDR Criterion 5.2.1.3 - Life Safety Code compliant egress aisles are indicated on the sector layout.)

The location of the egress route for the sector labeled in accordance with the Life Safety Code [ANL/APS/TB-9] is indicated in Figure 1. In particular, note the egress route which permits one to pass from the walkway between Sectors 18 and 19, under the ID beamline into Sector 18 (duck-under), and out through the walkway between Sectors 17 and 18. This is necessary because the walkway between Sectors 18 and 19 could represent a dead-end pocket.

(PDR Criterion 5.2.1.4 - Some indication of the survey and alignment plan is provided.)

The survey and alignment of all beamline components and in particular the bremsstrahlung shielding will be accomplished as described in the APS Technical Update No. 6, "Experimental Hall Surveying Reference", contained in ANL/APS/TB-14, "APS Beamline Design and Construction Requirements: A reference manual for Designers and Builders". BioCAT will request that the APS survey group assist with component alignment. All Bremsstrahlung collimators and stops are in atmosphere and outside of vacuum tanks. Their size and location can be verified by direct survey. The locations of masks, slits and stops intercepting white beam are precisely referenced to externally accessible features such as vacuum flanges or tank walls. Their location can be verified by survey of the external references.

APS Survey personnel will be provided with a list coordinates of bolt-hole locations for beamline components. We will request that they locate and mark them on the floor.
Once stands have been installed, we will request the assistance of survey personnel to locate critical components such as bremsstrahlung collimators, white beam stops, white beam mask, monochromator and mirror.

2.0 INSERTION DEVICE BEAMLINE

2.0.1 ID BEAMLINE LAYOUT

The ID beamline (Fig. 9) has been designed for monochromatic operation between 3.5 keV to 15.0 keV, with an energy resolution ($\Delta E/E$) of approximately 2 x 10^{-4}. The unfocussed beam size at the sample position will be about 1.6 x 3.8 mm (FWHM). The initial monochromator optics will be liquid nitrogen-cooled silicon (111) crystals. The required experimental energy range will necessitate the use of the fundamental and the third harmonic of the Undulator A as described in ANL/APS/TB-17) As the undulator gap is expected to be scannable under beamline control (albeit indirectly via requests sent by beamline computers to APS computers), undulator gap scan rates of 1mm/sec would permit XAFS scans of 0.6 KeV on the scale of seconds. This will permit rapid scan XAFS ("QXAFS") experiments, for which the monochromator must scan in synchrony with the undulator. The monochromator and control system will accommodate such experiments.

The ID beamline consists of four radiation shielded regions:

1)	White Beam First Optical Enclosure (FOE)	(18-ID-A)
2)	White Beam Transport (WBT)	(18-ID-WBT)
3)	White Beam Second optical enclosure(SOE)	(18-ID-C)
4)	Monochromatic Experimental Station(ES)	(18-ID-D)

The radiation shielding considerations for each of these regions are discussed in the Safety Specifications in Section 3.

A vertically focusing, cylindrically-bent grazing incidence mirror and a double crystal monochromator with a sagittally focusing second crystal will allow independent focusing in both horizontal or vertical planes. By applying an asymmetric couple, a smaller radius of curvature can be applied to the downstream end of the mirror, better approximating the ideal elliptical figure. Both of these optics can be operated in unbent or variably bent modes. In particular, the angle of the mirror relative to the X-ray beam can be adjusted, so that the mirror can serve as a low pass filter in order to reject harmonics energies passed by the monochromator. Furthermore, the mirror can be completely withdrawn from the beam under computer control if desired. The placement of the two focusing optics (as shown in Figure 9) would yield maximum theoretical geometric demagnification factors of about 7:1 in the horizontal and 11:1 in the vertical resulting in a theoretical minimum spot size of 20 μm (vertical, FWHM) by 110 μm (horizontal, FWHM) at the nominal sample position and about 50 μm (vertical, FWHM) and 250 μm (horizontal, FWHM) at the detector position for a (maximum) 10 m SAX camera (assuming the numbers given in ANL/APS TB-3, Undulator A Characteristics and Specifications). The maximum convergence angles (focused at the sample) would be 0.16 mrad vertically and 0.19 mrad horizontally. Of course, real optics have aberrations, but calculations and ray tracing simulations indicate that a 40 μm vertical focus at the sample position should be readily achievable. The focusing mirror will result in a maximum deflection (4 keV, uncoated ULE glass ceramic mirror) of the beam trajectory of approximately 8 cm below the orbital plane in the vertical at the sample position and 24 cm at the maximum detector position of 9 m past the sample position.

To minimize downtime during operations, the design specifies two monochromator assemblies in series; the downstream unit will employ Si(111) crystals for scattering and most XAFS experiments, and the upstream device will employ Si(220) or higher order crystals to obtain a narrower band pass for better energy resolution, and to cover the energies above the range covered by the Si(111) monochromator.

In the following discussion, beamline components and subsystems are specified with reference to their Work Breakdown Structure numbers given in section 4.

WBS# 2.1 RADIATION ENCLOSURES

The BioCAT ID beamline consists of four radiation enclosed regions (Fig. 2):

1)	White Beam First Optical Enclosure (FOE)	(18-ID-A)
2)	White Beam Transport (WBT)	(18-ID-WBT)
3)	White Beam Second Optical Enclosure	(18-ID-C)
4)	Monochromatic Experimental Station	(18-ID-D)

18-ID-A: The FOE will be 11 meters in length with variable width to accommodate the features of the ratchet wall. The radiation shielding for the first optical enclosure will be designed as an APS-standard ID FOE similar to the SRICAT 2-ID-A radiation enclosure**.** The rear wall of the enclosure will be a steel-lead-steel sandwich with a lead thickness of 62 mm. The thickness of the lead shielding for all of the enclosures is detailed in Appendix A.

18-ID-WBT: The white beam transport (Figure 3) is based on the SBC-CAT design where 6” OD beam pipe is encased inside an interlocking base and cover. The components are constructed from a steel-lead-steel sandwich with 1/2” thick lead. The BioCAT design has an extra sealing strip to reduce the potential of radiation scattering outside of the white beam transport. Figure 4 shows the Hutch Entry Shield Weldment which penetrate through the exit and entrance shield walls of ID-A and ID-C, respectively, and extend approximately 11” into the white beam transport. Both the plate and the tube are lined with 1/2” thick lead.

18-ID-C The Second Optical Enclosure (SOE) will contain most of the optics including the monochromator(s) and mirror assemblies. The SOE will be similar to the second optical enclosure described in SBC Document #SBC01-0149-01 except that the downstream wall thickness has been increased to 37.5 mm. Two additional labyrinths have been added since the PDR (Figure 2). A standard lower labyrinth has been added on the wall common to ID-C and ID-D. A non-standard labyrinth, which has been approved by the APS, has been added on the entrance wall of ID-C (Figures 6 and 7). This labyrinth allows the liquid nitrogen transfers lines from the cryopumping system located outside the enclosure to pass through the wall and into the enclosure. The details of the SBC-CAT designed guillotine between ID-C and ID-D are provided in Figures 5a and 5b.

18-ID-D: The experimental station will be 12 meters long and 5 meters wide. The radiation shielding for the experimental station will be as specified for an APS-standard monochromatic station.

The design for these shielded enclosures are a **modified version of the APS design** represented by the shielding panels in drawings #P41050903-210000 and #P41050903-230000. The radiation enclosures’ specifications are as discussed in the Bio-CAT Shielding Enclosure Design document “Title II summary of the shielding enclosures” which is attached as Appendix A.

Design Basis: modified version of the APS design
Design Status: Title III complete
Ref. Drawing: #P41050903-210000 and P41050903-230000 and Figures 2, 3, 4, 5a, 5b, 6 and 7.

WBS#2.2. UTILITIES

General layout of the utilities is given in Figure 1. Consider effort was expended to make sure that the capacities for electricity and water matched actual expected needs with a comfortable margin of extra capacity. The water system was designed to have a cooling capacity of 24 kW. A water conditioning and circulating system was installed in the mezzanine which can deliver 1-2 Megohm water which allowed use of copper piping throughout with considerable cost savings. The clean and utility electrical requirements were adequately met by the two 30 KVA transformers provided for the ID Beamline Power by the APS. The transformers for the BM Beamline Power have not been tapped.

WBS#2.3. SAFETY

WBS#2.3.1 PERSONNEL SAFETY SYSTEM (PSS)

The truth table describing the operation of the PSS will be **specified by BioCAT to the APS**. The PSS equipment **will subsequently be built and installed by the APS.** Section 3.5 contains a discussion of the proposed logic and operation information for this system. Position of PSS components is shown in Fig. 8.

Design Basis: PSS will be BioCAT-defined, built by APS
Design Status: Title II complete
Ref. Drawing: Fig. 8

WBS# 2.3.2 EQUIPMENT PROTECTION SYSTEM

The EPS equipment will be assembled and installed by BioCAT personnel**.** It will incorporate VME modules designed by J. Haumann of the ANL ECT Division which were built for SBC-CAT. Vacuum valve controllers designed and built by ANL ECT Division are also considered part of the EPS. Section 3.6 contains a discussion of logic and operation information for this system.

Design Basis: EPS will be BioCAT-defined built by ECT
Design Status: Title III complete
Ref. Drawing: N/A.

WBS# 2.5 ID BEAMLINE COMPONENTS

(Criterion 5.2.2.1 - Each component is identified as being in one of the following categories: APS standard components adopted without modification, APS standard components that have been modified, or non-standard components.)

The components of the beamline are based on either APS Standard Components used as-is, APS Standard Components with some modification, SBC-CAT designs, or BioCAT designs. Each component in the following discussion is identified as belonging to one of these categories with additional details for non-standard components.

Each component is identified by its WBS code from the WBS prepared for the BioCAT Management Plan which is reproduced in Table 4.1 of section 4 of this document.

Although every effort has been made to make this document self-contained, the reviewer may find additional discussion and clarification of the design bases for the major beamline components in the document entitled "Title I Design Summary Report for the Technical Facilities of the Structural Biology Center Construction Project", SBC-CAT Document # SBC01-00151-01, which is available from the SBC-CAT or BioCAT for FDR reviewers if necessary.

For convenience, we will use the designations "Title I (preliminary design), Title II (final engineering design), Title III (fabrication/procurement) to refer to the status of the design for each component, these designations corresponding roughly to DOE definitions.

(**Criterion 5.2.2.2 - Adequately detailed drawings are provided for all non-standard components.**

and

Criterion 5.2.2.3 - Appropriate specifications are provided for non-standard components.)

In the discussion which follows all non- standard components have been identified and have drawings and detailed design specifications included in this report.

<u>WBS# 2.5.1 COMMISSIONING WINDOW ASSEMBLY AND MASK</u>

During initial operation the APS installed commissioning windows W1-91, W1-93 and W1-94, and the fixed mask L5-83 (4.5 mm by 4.5 mm aperture) will be used without modification as shown in Figure 9. In the near future, we plan to operate windowless in order to reduce the significant attenuation of the commissioning windows at low photon energies.

The white beam window will be the APS commissioning window which is shown in APS drawing #P4102010109-900000-01 and will be provided by the APS.

Design Basis:	APS Commissioning Window and mask
Design Status:	Design Exchange
Ref. Drawing:	#P4102010109-900000-01 and #P4105091505-200000-00

<u>WBS# 2.5.2 PRIMARY APERTURE</u>

For this device we will use a **modified version of P4105091505-200000-00.** We are using an SBC-CAT design which calls for an aperture of about 2.1 mm by 4.2 mm (Figure 10).

The aperture limits the beam size and power intercepted by the cryogenically-cooled monochromator crystal.

Design Basis: modified APS standard component, SBC-CAT design
Design Status: Title III complete
Ref. Drawing: #D1.2.3.3.1.1-050-DD-OE

WBS# 2.5.2.1. PRIMARY APERTURE POSITIONER

The aperture will be mounted on a stage that permits translation in the two directions perpendicular to the beam direction for alignment purposes (Figure 11).

Design Basis: SBC DESIGN
Design Status: Title III complete
Ref. Drawing: #D1.1.2.3.3.3-052-DE-OC

WBS# 2.5.3 HEAT FILTER ASSEMBLY

An APS-designed F2-30 twin filter stack assembly which was designed to handle the raw undulator beam will be located without modification 51.5 meters from the source. For this device we will use the **APS component shown in drawing P4105091302-300000-01, so-called F2-30, without modification.**

Design Basis APS standard component
Design Status: Title III complete
Ref. Drawing: #P4105091302-300000-01

WBS # 2.5.4 VACUUM SYSTEMS

(Criterion 5.2.2.4 - The Preliminary Design is in compliance with the APS vacuum policy at the component level.)

All components have been designed in accordance with the APS vacuum policy, contained in ANL/APS/TB-14 dated October, 1994 ("APS Beamline Design and Construction Requirements. A Reference Manual for Designers and Builders", version 1.0, May 1994).

BioCAT would like to keep open the option of windowless operation on the ID beamline. Therefore, the ID beamline has been designed to be UHV compatible. Each of the major beamline components can be vacuum isolated from the rest of the beamline by the use of gate valves located upstream and downstream of the components. The beamline vacuum pumps will be 220 l/sec ion pumps. Roughing/vacuum gauging stations are located along the beamline to allow an isolated vacuum region to be roughed down by a mobile turbomolecular pump system. The vacuum in each of the isolated vacuum regions will be monitored and be part of the beamline Equipment Protection System. The vacuum in each of the subsections will be at least 10^{-7} torr. During initial operation, the ID beamline will be vacuum isolated from the storage ring by the APS-provided commissioning window. If the ID beamline has a future windowless operation phase, we will implement whatever measures are required by the APS to ensure the vacuum integrity of the storage ring. The vacuum components themselves will be assembled from **off-the-shelf components** available from standard suppliers e.g. MDC, Varian. They will be UHV components and will include pumps, gauges, pipe, valves, flanges, etc.

Design Basis: SBC design
Design Status: Title III complete
Ref. Drawing: See Figure 9 for component locations

WBS# 2.5.5 WHITE BEAM TRANSPORT

We will employ a modification of the white beam transport shielding as implemented on the SBC-CAT ID line as described by T. Fornek at the December, 1995 TWG meeting. The Design is discussed in more detail in section 3.11 below.

Design Basis: SBC design
Design Status: Title III complete
Ref. Drawing: Fig. 3 & 4

WBS# 2.5.6 SUPPORT STRUCTURES

These structures support the vacuum components and bremsstrahlung collimators of the beamline. They will be **BioCAT**, **CSRRI** and **SBC-designed components.** The generic stands which support pumping station on the beamline are shown in Fig. 9. The stand which supports the vacuum components downstream of the mirror ("Downstream Support Assembly") is shown in Fig. 17. Stands for the individual components such as the monochromator and mirror are considered to be part of those components and are considered along with those designs.

Design Basis:	SBC design
Design Status:	Title III complete
Ref. Drawing:	Fig. 9 and 17

WBS# 2.5.7 DOUBLE CRYSTAL MONOCHROMATOR

This device will be **an SBCCAT-designed component, based on the APS cryogenically-cooled monochromator crystal design and the design used at NSLS Beamline X9.**

An assembly drawing for this device is shown in Fig. 13. The intention is to build two identical devices that will be in the beamline simultaneously, but only one set of crystals will intercept the beam at a time. One device will have Si(111) crystals and the other Si(220) or higher cut crystal**.** Thus the desired energy range and resolution can be selected using one or the other device without opening a vacuum tank and changing crystals. The broad scientific program (especially spectroscopy applications) will require changing the photon energy and resolution often and over a large range**.** The reduction in downtime required to change monochromator crystal configurations justifies deployment of resources for a second monochromator assembly.

The non-dispersive double crystal monochromator is designed to provide a constant exit height beam whose direction is parallel to the incident beam but is offset by 35 mm over its entire energy range. The second crystal will be dynamically bent in order to focus the beam in the horizontal plane (sagittal focusing). The design is based on the first and second versions of the monochromator used at NSLS beamline X9. It combines the ruggedness of the pseudomonolithic first X9 monochromator design (both crystals are supported by a common base that is rotated around a horizontal axis) with the focusing, and constant-exit-height capability, of the second X9 monochromator design. This monochromator has been installed in the SBC-CAT ID-line and is presently in use.

An external, high-precision rotary table is used to control the Bragg-angle of the crystals for precise energy selection. A ferrofluidic rotary seal is used for friction-free feedthrough of the rotating shaft into the vacuum tank. A bellows between the rotary seal and vacuum tank helps reduce vibrations. The first crystal is mounted on this shaft, with its surface tangent to the axis of rotation. This design has been used for both monochromators at X9 and has given years of reliable operation. The lower and upper limit of the Bragg-angle is set to 7.5° and 35°, respectively corresponding to a possible energy range of 3.5-15 keV for Si(111) crystals.

The second crystal is mounted on a translation stage, to keep the beam reflected from the first crystal centered on the second crystal. The track of the translation stage is attached to the rotating shaft. Its direction of motion is parallel to the lattice planes of the first crystal, and in the direction of the beam. With a vertical offset between the output and input beams of about 35 mm, the total travel of the translation stage is about 130 mm. To maintain a constant exit height of the beam, the second crystal must also be translated perpendicular to the crystal surface. The total travel of this perpendicular translation is about 6 mm. This includes compensation for bending of the second crystal.

The desired focal point of the beam is in the experimental enclosure and is between 60 and 70 m from the source. The horizontal demagnification ranges from 0.14 (7.5 m/52.5 m) to 0.33 (17.5 m/52.5 m) for the upstream (high resolution) monochromator and from 0.12 (6.5 m/52.5 m) to 0.31 (16.5 m/52.5 m) for the downstream (Si(111)) monochromator**.** The design of the bending stage is based on the device that has been used at NSLS beamline X9 for more than four years. This sagittally-focusing monochromator accepts 4 mrad of horizontal divergence and produces a focus of 0.35 mm FWHM (full width at half maximum) at 0.28 magnification. The measured width is ~15% larger than the pinhole image of the source. The ratio of measured vs. calculated flux is ~0.8. The focusing stage has been used at magnifications between 0.25 to 0.46. It has proven to be highly reproducible, with less than 5% variation of the focal width when returning to the same motor settings.

The rotary table is supported by a vibration isolation table. For vibrations transmitted from the floor, the vibration isolation table used at X9 has been shown to reduce by a factor ~30 vibrations in the range of 1 to 100 Hz.

The high resolution monochromator assembly will be identical to this device except for the crystals.

Design Basis: SBCCAT design based on X9
Design Status: Title III complete
Ref. Drawing: Fig. 13

WBS# 2.5.7 CRYOGENIC FIRST MONOCHROMATOR CRYSTAL

The first monochromotor crystal will be a cryogenic crystal based on the Knapp/Rogers design.(Fig. 14) The cryogenic closed loop system will be manufactured by Messer Griesheim, liquid nitrogen will be circulated using a Barber/Nichols BNCP30 pump (Fig. 15)

Design Basis: BioCAT design
Design Status: Title III complete
Ref. Drawing: Fig. 14 & 15

WBS# 2.5.8 VERTICAL FOCUSSING MIRROR ASSEMBLY

This device will be the SBC Rosenbaum-designed component, the design of which is based on extensive experience on NSLS Beamline X9 and beamlines at DESY. This device has completed Title III design as of this writing and an assembly drawing is shown as Fig. 16. An assembled device is now operating on the SBC-CAT beamline.

The vertically-focusing mirror provides two functions: focusing the beam in the vertical plane and reducing the intensity of harmonics passed by the monochromator. Effective rejection of harmonics is essential for XAFS experiments, particularly at sources like APS that produce copious high energy radiation.

The mirror is centered at about 56 m from the source. The focal position in the experimental enclosure can vary from 61 to 70 m from the source. Thus the vertical demagnification will range from 0.089 (5 m/56 m) to 0.25 (14 m/56 m). At commissioning, the mirror will be 1000 mm long and 100 mm wide. The vacuum tank and the base will be designed to permit possible future (after the construction project is completed and depending on the properties of the synchrotron source) extension of the mirror to 1.5 m total length, in 500-mm segments, in order to intercept a larger fraction of the vertical divergence of the beam. The specifications for the mirror to be installed at commissioning are given in Table 2.1

In order to provide the required harmonic rejection capability with sharp energy cutoff, high reflectivity of the fundamental energy, and a narrow range of angular beam deflections, the mirror coating will consist of parallel stripes of the following materials: ULE glass ceramic (uncoated substrate), rhodium, and platinum. Experience on beamline X9A at the NSLS with a Nickel coated mirror has shown that if the detection system is sufficiently linear, variations in the reflectivity vs. energy due to absorption edges in the substrate can be compensated for. The ULE glass ceramic surface will be most suitable for photon energies below 8 keV. The Rhodium surface will be used for 8-15 keV, and the Pt surface for energies above 15 keV.

Focusing is achieved by dynamically bending the flat mirror substrate around a horizontal axis by the application of bending couples at both ends. With a demagnification ratio of 11, it is expected that this mirror will produce a vertical focus width considerably better than 0.05 mm. The calculated image of the positron beam source at the focal point should be about 0.02 mm. In this design, gravitational sag of the mirror is partially compensated for over the length of the mirror.

Design Basis: SBC design based on X9
Design Status: Title III complete
Ref. Drawing: Fig. 16

TABLE 2.1 VERTICAL MIRROR SPECIFICATIONS

Length	1.0 m
Width	0.1m
Substrate	ULE glass ceramic
Thickness	38 mm
Coating	Three stripes Pt, Rhodium and uncoated
RMS Roughness	2Å
RMS Form Error	1 μrad

WBS# 2.5.9 & 2.5.10 MONOCHROMATIC COLLIMATION SLITS

This device will be **an SBC-designed component.** Collimation slits are used to limit the spatial extent of the monochromatic radiation scattered in the forward direction by the optical components. The optimum position of the collimation slits is about halfway between the scatterer and the focus. The **horizontal (Fig.18) and vertical (Fig. 19)** slits will be located at 57.5 m and 59 m respectively from the source. The collimaotr slits can also be used to limit the spatial extend of the monochromatic beam.

Design Basis: SBC design

Design Status: Title III complete
Ref. Drawing: Fig.18 & 19

WBS# 2.5.11 PHOTON SHUTTER

This device a **modified version of APS drawing** #P4105090908-200000-01 (P8). The photon shutter enables access to the hutch for specimen change or adjustment while the main safety shutters are open, thus keeping the optics at steady heat load.

Design Basis: Modified APS standard component
Design Status: Title III complete
Ref. Drawing: Fig. 20, SBC #1.1.2.2.1-050-DE-OA

WBS# 2.5.12 BEAM POSITION MONITORS

This device monitors the monochromatic beam position and direction. Will not be needed for initial commissioning and running.

Design Basis: SBC design based on X8 beamline component
Design Status: Title I in progress
Ref. Drawing: No drawing at this time

WBS# 2.5.13 BREMSSTRAHLUNG COLLIMATORS.

These are an SBC-CAT designed component and are described more fully in Section 3 below.

Design Basis: SBC design
Design Status: Title III complete
Ref. Drawing: Figure 24 and 25

WBS# 3.0 EXPERIMENTAL STATION

WBS# 3.1- 3.5 IN-HUTCH EQUIPMENT

Upstream of the sample, this equipment will include an evacuated vacuum flight path for reducing air scatter which will incorporate the attenuator foils, fast shutter, guard slits and exit window described below. The sample will be either mounted on a remotely controllable optical table (primarily for spectroscopy experiments) or on a 22 m long vibration isolation table (for scattering experiments). Fixtures on the optical table will be designed to mount various types of sample holders, a variable length 30 cm diameter evacuated flight path, motorized beamstop positioner and detector mountings.

Design Basis: BioCAT design
Design Status: Title I in progress
Ref. Drawing: no drawing at this time

WBS# 3.4 GUARD SLITS

This device will be **an SBC or BioCAT-designed component.**
Guard slits are used to limit the spatial extent of the radiation scattered by the collimation slits. Guard slits will be located just upstream of the exit window in the experimental enclosure. They require a different design than the collimation slits so that they may be placed as close as possible to the sample without interfering with experimental apparatus.

Design Basis: SBC or BioCAT design
Design Status: Title I in progress
Ref. Drawing: no drawing at this time

WBS# 3.5 MONOCHROMATIC EXIT WINDOW

The **monochromatic exit window (Fig. 21) is based on a modified SBC-CAT design**. The window material is a 200 micron thick beryllium disk of type IF-1 from Brush Wellman.

Design Basis: Modified SBC-CAT design
Design Status: Title III complete
Ref. Drawing: Fig. 21, Drawing 1.1.2.3.1-050-DC-OC

WBS# 3.7 ATTENUATOR SYSTEM

This device will be a commercial unit acquired from X-ray Instrumentation Associates. This device incorporates both attenuator foils and a shutter (~100 ms minimum exposure). The shutter will be under computer control to reduce radiation damage to the sample during detector readout or during periods of experimental protocols where data is not being collected for whatever reason. This cannot be done with shutters involved in the PSS system. Two of these in series will be located in the experimental enclosure.

Design Basis: Commercial Unit
Design Status: N/A
Ref. Drawing: N/A

WBS# 4.0 CONTROL SYSTEMS

This refers to the computer software and hardware that controls the beamline itself, the mirror, monochromator, diagnostic equipment, experimental equipment, and data acquisition including time sliced energy dispersive and two dimensional area detectors. The BCS will be based on the EPICS control system. BioCAT is working with the ECT division of Argonne, which has been instrumental in developing the SBC control system, to port enough of their code to ensure basic functionality in time for commissioning. Data acquisition and control will be an ongoing development project by BioCAT staff.

Design Basis: BioCat design
Design Status: Title II in progress
Ref. Drawing: N/A

3.0 SAFETY SPECIFICATIONS

3.1 SHIELDING

3.1.1 RADIATION ENCLOSURES.

(PDR Criterion 5.2.6.1 - The shielding design is in compliance with APS shielding standards.)

Specification of the lead thickness in the panels has been done using guidelines in the APS document ANL/APS/TB-7 combined with the more recent EGS4 calculations of ANL/APS/TB-20, the ANL document "The Effect of Incident Angle on the Shielding Thickness for Secondary Bremsstrahlung", and the extensive calculations done by Gerd Rosenbaum of the SBC-CAT. The overall layout of the enclosures in described in section 2.1 above, detailed radiation enclosure specifications are as described in Appendix A.

3.1.2 BREMSSTRAHLUNG SHIELDING

(PDR Criterion 5.2.2.5 - Optical apertures and shielding apertures are shown to be adequate.)

In addition to the radiation enclosures, there are bremsstrahlung collimators along the beamline and a beam dump at the end of the experiment enclosure. The ID beamline is designed for monochromatic operation with a 35 mm offset between the incident white beam and the diffracted beam in each case. Figs 22-27 show the anamorphic drawings for the apertures relevant to determining the positions and dimensions of the shielding components along the beamline. These have been fully specified with reference to ANL/APS/TB-7 and ANL/APS/TB-20. Ray tracings (Figs. 22-27) shows the bremsstrahlung, secondary bremsstrahlung, and synchrotron radiation apertures to be adequate.

3.1.3 PHOTON SHUTTERS

The ID beamline has three X-ray shutters:

1) Front end dual safety shutter
2) First monochromatic shutter in the P8/mod Integral Beam Stop/Shutter Assembly
3) Second monochromatic shutter in the P8/mod Integral Beam Stop/Shutter Assembly

Shutter 1 is the APS supplied safety shutter in the beamline front end which prevents any beam from entering the beamline while closed.

Shutters 1 and 2 are incorporated in the device based on a **modified version of APS drawing** #P4105090908-200000-01 (P8). The photon shutter enables access to the hutch for specimen change or adjustment while the main safety shutters are open, thus keeping the optics at steady heat load. The device incorporates two identical shutters installed in series for redundancy as required by the APS for all personnel safety systems.

3.2 OZONE MITIGATION

(PDR Criterion 5.2.5.2 - If white beam is to be propagated in an experimental station, a preliminary analysis of ozone production and the general plan for mitigation is provided.)

The ID beamline does not have a white beam open air path but will have a monochromatic open air path in the experimental hutch (18-ID-D). The problem of Ozone production will be handled following the recommendations in the "Guidelines for Ozone Mitigation at the APS" (May 1994). The radiation enclosures will be equipped with appropriate ventilation/exhaust systems vented directly onto the experimental floor.

3.3 PROGRAM SPECIFIC HAZARDS

(PDR Criterion 5.2.6.4 - A preliminary safety analysis is provided for program-specific hazards.)

We have not identified any program specific hazards at this time.

3.4 PERSONNEL SAFETY SYSTEM

(PDR Criterion 5.2.6.2 - A preliminary safety analysis is provided for the beamline Personnel Safety System.)

3.4.1 OVERVIEW

The purpose of the Personnel Safety System (PSS) is to protect the beamline user from accidental X-ray exposure either by the direct photon beam or scattered radiation. The PSS system will be designed and implemented by the APS in conjunction with the individual CAT beamline configuration. The PSS described in this section is meant as a guideline as to the type of system we would like implemented on the BioCAT ID beamline. This section is based on the document “Title I Design Description for the SBC PSS”, SBC Document #SBC01-0183-02.

3.4.2 DESIGN REQUIREMENTS

The complete design requirements for the PSS are addressed by the APS. The following are some key requirements:

- The PSS shall be designed to be fail safe to common failures, redundant, and reliable.
- The PSS shall provide access controls to protect personnel from ionizing radiation.
- The PSS shall provide emergency beam shut-off devices, emergency exit mechanisms not inhibited by the PSS, and audio visual warnings.

3.4.3 DESIGN DESCRIPTION

Key components of the PSS include emergency beam shut-off devices, emergency exit mechanisms not inhibited by the PSS, audio/visual warning devices, search buttons, and inputs to beam shutter interlocks .

The arrangement of the insertion device beamline enclosures, search buttons and doors is shown on Drawing B01-0001B(Fig. 8). The shielding consists of the following enclosures and areas:

18-ID-A First Optical Enclosure (FOE) (This enclosure is a modified version of the APS SRI-CAT hutch number 2-ID-A.)

18-ID-WBT White beam transport shielding area

18-ID-C White Beam Optical Enclosure (SOE)

18-ID-D Experimental Enclosure

None of the enclosures is allowed to be occupied when the beam is allowed to that particular enclosure or an enclosure further downstream. Only the area surrounding the white beam transport (18-ID-WBT) can be occupied when the beam is on. The white beam transport line is adequately shielded to allow personnel up to the shield covers.

3.4.3.1 Beamline components requiring interlocks

3.4.3.1.1 Shutters - The following shutters require interlocks

Photon shutter (WBS #2.5.11) located in enclosure 18-ID-C

3.4.3.1.2 Doors - The following is a listing of all doors requiring interlocks.

Enclosure 18-ID-A	Door 18-ID-A1A	Pneumatically-operated
Enclosure 18-ID-C	Door 18-ID-C1A	Pneumatically-operated
Enclosure 18-ID-C	Door 18-ID-C1B	Manual
Enclosure 18-ID-D	Door 18-ID-D1A	Pneumatically-operated
Enclosure 18-ID-D	Door 18-ID-D1B	Manual
Enclosure 18-ID-D	Door 18-ID-D2A	Manual
Enclosure 18-ID-D	Door 18-ID-D2B	Pneumatically-operated

3.4.3.2 Components requiring administrative control

The white beam transport shielding shall be under administrative control. The covers must be installed and secured before beam can be allowed into this section.

3.4.4 BEAMLINE ACTION LOGIC

The BioCAT sector 18 insertion device beamline operates in only one mode. The beamline action logic for this mode is given in Table 3.1**. (The entry in bold has been corrected from the PDR. It was changed from False to Does Not Matter).**

TABLE 3.1 BEAMLINE ACTION LOGIC FOR THE SECTOR 18 INSERTION DEVICE BEAMLINE

(REFER TO DRAWING NUMBER B01-0001B, Figure 8)

Component or Subsystem Status	18-ID-A & 18-ID-C Secure	18-ID-D Secure	APS Front End Shutter Closed	Photon Shutter Closed
Beamline Actions Desired				
Beam to 18-ID-A & 18-ID-C allowed, but not simultaneously to 18-ID-D	T	X	F	T
Access to 18-ID-A & 18-ID-C allowed	F	X	T	X
Beam to 18-ID-A, 18-ID-C & 18-ID-D allowed	T	T	F	F
Access to 18-ID-D allowed	**X**	F	T	X
Access to 18-ID-D allowed	X	F	X	T

T - True, F - False, X - Status Does Not Matter

3.4.5. SEARCH PROCEDURE FOR THE SECTOR 18 INSERTION DEVICE BEAMLINE

The description of the search procedure has been changed from that described in the PDR only to properly identify the doors by the names used in drawing number B01-0001B, Figure 8.

HUTCH 18-ID-A

Enter enclosure through door 18-ID-A1A. Search the enclosure toward the ratchet wall and push search button A1. Move toward the other end of the enclosure and verify that the bremsstrahlung collimators are in place and secure. Push search button A2. Exit enclosure. Close and interlock door 18-ID-A1A.

AREA 18-ID-WBT

Visually inspect the white beam transport shielding to verify that the covers under administrative control are secured in place.

HUTCH 18-ID-C

Close and secure 18-ID-C1B. Enter enclosure through door 18-ID-C1A. Search the enclosure toward the ratchet wall and push search button C1. Move toward the other end of the enclosure and verify that the bremsstrahlung collimators upstream and downstream of the monochromator are in place and secure. Push search button C2. Exit enclosure. Close and interlock door 18-ID-C1A.

HUTCH 18-ID-D

Close and secure all doors except one of either 18-ID-D1A or 18-ID-D2B. Enter the enclosure through either 18-ID-D1A or 18-ID-D2B. Search enclosure toward search button D1. Press search button D1. Search enclosure toward search button D2. Press search button D2. Search enclosure toward search button D3. Press search button D3. Exit enclosure. Close and interlock the door used to enter the enclosure.

The PSS should be designed such that the interlocks on any hutch can remain on for an indefinite time without needing resetting. An example would be that if the interlock on hutch 18-ID-A is removed for access to the hutch and the interlock for 18-ID-C is not removed, only hutch 18-ID-A needs to be searched prior to beam activation.

3.5 EQUIPMENT PROTECTION SYSTEM

(PDR Criterion 5.2.6.3 - A preliminary safety analysis is provided for the beamline Equipment Protection System.)

The primary purpose of the Equipment Protection System (EPS) is to ensure the safe use of the individual beamline components. BioCAT has identified equipment that needs to be monitored in order to provide protection against loss of vacuum, loss of water flow, or elevated temperature. The sensors monitored by the EPS are shown in Table 3.2. If any of these signals are not true, the EPS will trip causing a relay contact to open, preventing operation of the beamline. Interrogation of input status and resetting of the EPS monitoring circuit can be effected manually or through software via the VME IOC. The EPS circuit functionality is otherwise independent of the VME crate.

TABLE 3.2 BioCAT ID BEAMLINE EPS SENSOR CHART

(This table has been corrected since the PDR t o prorperly identify the components.)

Component	**Signal**
Primary aperture - (fixed mask)	water flow present (1 signal)
F2-30 Filter	water flow present (1 signal)
Monochromator beam dump	water flow present (1 signal)
Monochromator crystal	Liquid nitrogen flow present (1 signal)
Gate valves	gate valve fully open (1/valve)

Note that the vacuum controlling circuitry will be such that unacceptable vacuum in any section of the beam-line will automatically (in hardware) close the relevant gate valves which will then trip the EPS logic circuit. Beam will only be permitted when all gate valves are fully open. Valve closed and intermediate positions and fault conditions will be indicated by panel lights. The temperature and analog output of the flow meters will be monitored and logged for all water cooled components listed in Table 3.2; however, they will not form part of EPS circuit.

4.0 WORK BREAKDOWN STRUCTURE

(Criterion 5.2.3.1 - A work breakdown structure, consistent with the design and broken down to the component level, is provided.)

The attached WBS, Table 4.1, is that included in the APS management plan for the BioCAT sector. Figure 5.1 shows a timeline for the project through 10/97, and Figure 5.2 shows a high level schedule of tasks in section 5 below.

TABLE 4.1
WORK
BREAKDOWN
STRUCTURE

1 0	Project Management
2 0	Insertion Device (ID) Beamline Installation
2 1	Radiation Enclosures
2 2	Utilities
2 3	Safety
2 4	Materials and Services, System Integration
2 5	ID beamline components
2 5 1	Front end white beam mask assembly
2 5 2	Primary Aperture assembly
2 5 3	Heat Filter Assembly
2 5 4	Vacuum components
2 5 5	Beam transport components
2 5 6	Support stands
2 5 7	Monochromator assembly
2 5 8	Vertical Mirror Assembly
2 5 9	Horizontal collimator slit Assembly
2 5 10	Vertical collimator slit Assembly
2 5 11	P8 integral beam stop and shutter
2 5 12	Beam Position Monitors
2 5 13	Lead Bremsstrahlung Collimators
3 0	Experimental Station
4 0	Data Acquisition and Control
4 1	Networking
4 2	Workstations
4 3	VME based electronics
4 6	Motor Controllers
4 7	Diagnostic Electronics
4 8	Data Acquisition and control software
5 0	X-ray Fluorescence Analyzer/Detector
6 0	Scientific Computation
7 0	Lab Office Module

5.0 COST ESTIMATES AND SCHEDULING TIME LINES

5.1 CONSTRUCTION COST ESTIMATES

All of the following three Criteria will be discussed together below. Cost estimates for the WBS in section 4 are summarized at a high level in Table 5.1 below.

(Criterion 5.2.4.1 - Cost estimates and schedules are provided and are consistent with the WBS.)

In August of 1995 cost and schedules estimates for the project were presented to the BioCAT Advisory Committee and were the basis of the Cooperative Agreement between IIT and NIH. The proposed Total Estimated Cost and completion date remain as agreed with NIH.

(Criterion 5.2.4.2 - The engineering design effort costs have been included.)

See the above discussion on the WBS. Engineering design effort costs are minimal since the sector 18-ID line major components will be essentially identical to the sector 19 SBC-CAT beam line. Dr. G. Rosenbaum, the designer of sector 19-ID, is a paid consultant on the project and his fees are included. Costs are included for staff time to complete specifications, review the designs, and modify drawings as necessary.

(Criterion 5.2.4.3 - The cost estimates for procurements and fabrications are reasonable.)

Cost estimates are based on vendor quotations and current APS contract options. The costs for the major WBS elements are shown in Table 5.1 below. All major and most minor components have now been procurred. The overall equipment costs are within budget

Table 5.1 Major costs of the BioCAT project (Year 1-2)

		EQUIPMENT CAPITAL COST (K$)	SUPPLIES EXPEND COST (K$)
	DESCRIPTION	2,516.07	125.50
10	Project Management	60.00	40.00
20	Insertion Device (ID) Beamline Installation	**99.56**	
21	Radiation Enclosures	**634.00**	
22	Utilities	**148.21**	
23	Safety Systems (EPS & PSS)	**23.00**	
24	Materials and Services, System Integration		30.00
25	ID beamline components	997.08	
30	Experimental Station	80.57	4.00
40	Data Acquisition and Control	265.15	11.50
50	X-Ray Fluorescence Analyzer/Detector	149.52	8.00
60	Scientific Computation	20.00	5.00
70	Lab Office Module	39.00	27.00

5.2 SCHEDULING TIMELINES

(Criterion 5.2.4.4 - The schedule is reasonable.)

The high-level timeline at the supertask level for completion of tasks are shown in Figures 5.1. This represents an effort to plan in detail the design, construction, and commissioning activities for the ID beamline and to integrate and coordinate tasks relevant to interactions with the APS. The timeline relies heavily on the fact that the SBC beamline design is complete, and the SBC beamline is currently operational. Commissioning of the BioCAT undulator beamline will begin in June of 1997. Table 5.2 shows significant dates for the BioCAT project and interactions with the APS.

FIGURE 5.1 BioCAT INSERTION DEVICE BEAMLINE INSTALLATION TIMELINE

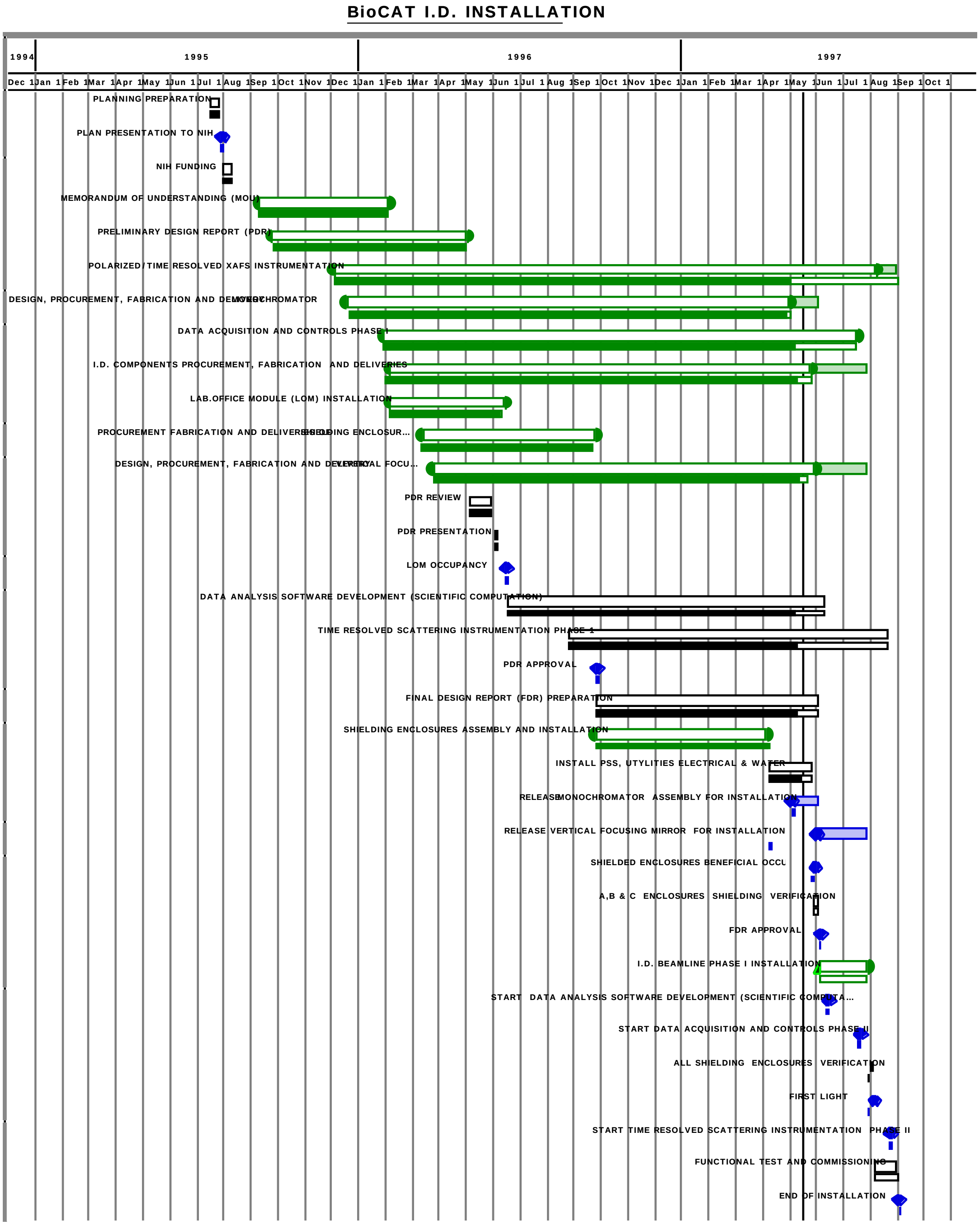

TABLE 5.2

DATES OF SIGNIFICANT MILESTONES REQUIRING APS INTERACTION

LOM BENEFICIAL OCCUPANCY	5/96
BioCAT STAFF MOVE TO LOM	6/96
PDR SUBMITTED TO APS	3/96
FDR SUBMITTED TO APS	5/97
ENCLOSURE PROCUREMENT/ CONSTRUCTION BEGINS	4/96
ID SHIELDING READY FOR TESTING	5/97
SHIELDED ENCLOSURES BENEFICIAL OCCUPANCY	5/97
WHITE BEAM COMMISSIONING A-C ENCLOSURES	6/97
INSTALLATION ID COMPONENTS	6/97
FIRST MONOCHROMATIC LIGHT	7/97

(PDR Criterion 5.2.5.3 - Cost and schedule information is provided for LOM build-out.)

The LOM buildout has been completed within budget. Figure 1 shows the floor plan for the LOM.

6.0 QA/QC

Quality assurance in all aspects of the design, fabrication, and assembly of the BioCAT ID beamline is recognized to be of great importance to the timely construction and reliable operation of the beamline. Consequently, we will follow quality assurance procedures and guidelines to assure achieving the technical goals of the lines. We will, in some instances, rely on APS quality assurance procedures by using APS standard components. For the following non-standard components, we will take the following steps to assure suitable performance of components to be fabricated or procured.

Preparation of technical specifications: Since it is the intent of BioCAT to purchase most of the components of the beam lines from commercial vendors, it is most important to develop appropriate, rigorous technical specifications that can be realistically achieved by suppliers.

Since we are using SBC-CAT designs for all non APS-standard components, we will rely on their specifications for procurement. In the case of anticipated (minor) changes from the SBC-CAT design, we will determine specifications by one or more of the following procedures: by modeling optical performance using ray tracing techniques, by evaluating thermal and mechanical performance by finite element analysis, by fabricating and testing prototypes developed in our laboratories, or by field-testing prototype components provided by potential suppliers. All the major beam line components will have been field tested by SBC-CAT in their insertion device line during the upcoming few months. We will employ their final as-built and tested drawings and specifications for procurement. BioCAT will also use the technical specifications developed by the APS for their standard beamline components

Conveyance of technical specification to potential vendors: Once the technical specifications have been developed and, when appropriate, reviewed by external experts, these specifications will be communicated to potential vendors in written form with tolerances, required delivery times, and clear statements of acceptance criteria.

Qualification of vendors: In order to assure that vendors can deliver a product of appropriate quality in a timely manner, it will be necessary to visit potential vendors to effectively inspect and evaluate their capabilities. A part of the evaluation must include a consideration of the vendors' QA/QC capabilities and policies. These evaluations will be performed by the BioCAT Directorate and those members of the BioCAT staff whose qualifications would make their input to the evaluation appropriate; when necessary, BioCAT will use third-party experts and consultants in evaluating the capabilities of potential vendors or suppliers. Particular attention will be paid to sound, safe engineering practices as well as production capabilities.

Acceptance inspection and testing: Whenever possible, performance criteria will be used for acceptance criteria. This may not always be practical, since the actual performance of many critical components (e.g. monochromators, mirrors, etc.) cannot be properly evaluated until the X-ray beams are available, and it is doubtful that vendors will permit installation prior to payment. In these cases, BioCAT staff will develop acceptance criteria based on bench testing - i.e. testing of achievable, measurable aspects of the components that will give accurate information on the probable performance in the synchrotron beam. BioCAT is planning on using the QC facility which the APS has established for the acceptance testing of the front end and SRICAT components when applicable.

Establish procedures for fabrication, assembly, testing, and installation phases: BioCAT technical staff will necessarily work closely with vendors of components to assure that specifications are met in each phase of the procurement of components. As an example, it will be necessary to maintain communications with vendors of mirrors to evaluate performance at intermediate steps of the fabrication of a mirror assembly - after substrate forming and polishing, after coating and roughness evaluations, after mounting and testing for form errors that could arise from the mounting system, after mounting in a vacuum chamber, and so on. Each component will require its own set of procedures, which will be documented and transmitted to both the vendor and the BioCAT Directorate.

Documenting and controlling design and specification changes: It is critical to document any changes made in design or specifications in order to avoid time loss due to confusion within the group. All specifications will be maintained on file, as will documentation of all communications, written or oral, with vendors or suppliers. In addition, all specification or design changes will be discussed and presented in weekly BioCAT staff technical meetings, and all suggested modifications will be communicated, in writing, to the BioCAT director in the form of CSRRI Technical Memoranda. (The CSRRI staff have been writing Technical Memoranda on all aspects of the beam line development since 1992, and these Memoranda, which are kept on file in the CSRRI Administrative Office are circulated to all staff. Further, they are cross-referenced by author, date, and keywords. Thus, they are the natural medium for documentation of design or specification changes.)

7.0 RESEARCH AND DEVELOPMENT

(Criterion 5.2.7.1 - R&D schedules are consistent with construction schedules.)

7.1 OVERVIEW

It has been the strategy of BioCAT to make use of either APS or SBC-CAT designed beamline components wherever feasible. The design for the ID beamline presented in this Preliminary Design Report has implemented APS or SBC-CAT designs for all major components, so minimal R&D will be required for implementing the ID line in its initial commissioning configuration, up to and excluding the experimental hutch equipment.

Only modest experimental hutch equipment will be available at first light (summer, 1997), but it will suffice for a broad range of the initially proposed experiments. Further development of the hutch equipment is planned for years 3-5 of the initial funding period, and is outside the scope of this document. We anticipate this to be an on going process with incremental improvements continuing in subsequent funding periods.

7.2 MULTILAYER ANALYZER XAFS DETECTOR

It is expected that the photon flux will increase by a factor of 100 to 1000 at the ID line of BioCAT over the spectroscopic beamlines at the NSLS. This development provides real opportunities for biological XAFS applications in determining the structure and time course of a time-resolved reaction, and on even more dilute systems. However, these dramatic photon flux increases will have little effect on XAFS data collection speed of dilute systems using traditional detector systems. Without significant improvements in detector throughput, the most-commonly used energy-resolving fluorescence detector, the Multi-element Ge detector, will have to operate very inefficiently to avoid detector saturation. The same is true, to a greater or lesser extent, for any detector that carries out energy discrimination through processing of detector signals. Only a detector system that removes the unwanted background *before* it reaches the detector electronics can, in our opinion, solve the dilemma of detectors always lagging behind increasing available fluxes.

To address this problem, BioCAT is developing an energy-resolving detector system using synthetic multilayers. The lack of adequate detectors have been a significant impediment to efficient XAFS data collection at existing synchrotron sources and would become very much so at the APS. The proposed multilayer-based analyzer/detector system will essentially remove that bottleneck by combining high data collection efficiency with very high count rate capability, and a reasonable solid angle of acceptance. Simulation and comparison of the multilayer array detector with the conventional detectors, such as the ionization chamber and 13-element Ge detectors, shows that the detector will be superior to them, in particular with its ability to handle the increased photon fluxes available from insertion devices, and to allow decreased sample concentration. The design specifications for this detector are shown in Table 7.1. This type of detector will provide tremendous opportunities for XAFS measurements on dilute systems, such as biological systems, at third generation synchrotron sources. Note that the tunable energy range can be altered through use of multilayers of different d-spacing.

Table 7.1 Design Specifications for Energy Resolving Fluorescence Detector with 40 Multilayer Array.

Energy Range	5 to 9.5 keV (Mn - Zn Kα)
Solid Angle Acceptance	0.5 to 0.6 Sterradian
Energy Resolution	200-300 eV @ 7 KeV
Background Rejection Factor	> 80-100
Count Rate Limitation	None
Time Resolution	20 ns in Photon Counting Mode
Sample Vertical Dimension	< 0.4 mm

The detector development R&D program is consistent with the commission and operation schedule of the facility. A prototype multilayer detector will be designed and fabricated at the beginning of 1997. A full scale array detector will be constructed at the end of 1997. Test and operation of the detector will take place in 1998 when the ID line is operational.

7.3 ADDITIONAL R&D

The bulk of the experimental program requires R&D of an evolutionary nature; there are no critical design issues which, if unsolved, would seriously compromise the bulk of the scientific program. However, as BioCAT is attempting to accommodate novel experiments, some R&D is required. Careful attention will be necessary to ensure that the control/data acquisition system is sufficiently precise, reproducible, and flexible to carry out the diverse experimental modalities anticipated for the BioCAT beamlines. For example, for QXAFS experiments, we intend to rapidly scan the undulator gap and monochromator in synchrony, following stimulation of the sample by laser flash or rapid mixing. The control system must be designed to accommodate this mode. For stimulation of the sample a novel stopped flow system will be constructed.

In addition, careful attention must be paid to positioning and alignment systems for small (~20μm) samples of low contrast, and through use of appropriate and perhaps novel materials, to minimizing scatter from windows at low angles. Good alignment hardware and software improves the quality of experimental data and promotes efficient use of beam time.

8.0 INFRASTRUCTURE

Illinois Institute of Technology (IIT), located about three miles south of downtown Chicago, is a private university which offers undergraduate and graduate degrees principally in technical fields. IIT employs all BioCAT staff, including the Director and Associate Director, and provides procurement, project accounting, and regulatory services.

IIT is participating in BioCAT through its Center for Synchrotron Radiation Research and Instrumentation (CSRRI). The Center was established in 1992 to promote synergy between the various activities in synchrotron radiation research at IIT, which includes participation of three APS CATs, as well as external contracts, and educational and outreach functions. Six IIT physics and biophysics faculty are directly involved in CAT development, and several other faculty participate collaboratively. In late 1995 Dean Chapman became Director of the CSRRI.

The CSRRI facilities include:

- Crystal optics fabrication laboratory
- X-ray test and alignment laboratory (single axis Bond orienter, monochromator alignment testbed, rocking curve measurements)
- Computer facilities: source calculations, finite element analysis, raytracing, project management
- Staff shop
- Machine shop
- Conference, seminar, and meeting facilities

APPENDIX A

BIOPHYSICS COLLABORATIVE ACCESS TEAM

ILLINOIS INSTITUTE OF TECHNOLOGY

3301 South Dearborn Street

Chicago, Illinois 60616

DOCUMENT NO. Bio01-0187-01

OUTLINE SPECIFICATION FOR BioCAT

INSERTION DEVICE BEAMLINE ENCLOSURES

IN SECTOR 18

Note:

This document was derived from the SBC document No. SBC01-0187-01 for which the Disclaimer and Government License here appended is with the BioCAT agreement.

1.0 SCOPE

This Outline Specification establishes the BioCAT-specific requirements for the fabrication, inspection, delivery, erection, and testing of the BioCAT 18 ID Beamline White Beam Optical Enclosures (18-ID-C WBOE), and the 18 ID Monochromatic Beam Experimental Enclosure (18-ID-D MBEE). These items are lead-lined enclosures for white and monochromatic beam experiment instrumentation hardware, and are located on the APS experimental floor. These enclosures generally conform to the APS enclosure design. Unless definitely stated in this specification, the requirements of the APS Document No. 41050101-00002, - Technical Specifications for APS Beamline First Optics and White Beam Experimental Enclosures in Sectors 1,2 and 3 - apply.

1.1 **Construction**: The BioCAT Beamline White Beam Optics Enclosures, and Monochromatic Beam Experimental Enclosures shall be structures fixed to and supported by the floor of the experimental hall. These enclosures shall be modular in construction and the module is a panel, 1 meter wide and 3.3 meters hide for side panels, or approximately 1.75 to 5 meters long for ceiling panels. These panels shall be manufactured as a steel/lead/steel sandwich with a steel frame welded to the inside. Where practical, the lead shall be comprised of two sheets to reduce the probability of pinholes through the entire lead sheet. The assembled panels must create a structural system capable of supporting the enclosure and attached equipment.

1.2 **Access Doors**: The Monochromatic Beam Experimental Enclosure (18-ID-D) shall have two pneumatically actuated doors. All other enclosure doors are manually actuated. The pneumatically-operated doors and manually-operated doors shall be physically identical except for the operator and safety provisions.

The 18-ID-C White Beam Optical Enclosure shall have a 3 meter doorway located on the side wall adjacent to Sector 17 (near side wall) which is comprised of a 2 meter panel and 1 meter panel. All door panels shall be manually-operated.

The 18-ID-D Monochromatic Beam Experimental Enclosure shall have two doors each of which is comprised of two 1 meter panels on the near side wall. The 1 meter panel nearest the front wall (the wall through which the X-ray beam enters the enclosure) and the 1 meter panel nearest the back wall (the wall which constitutes the end of the beamline) shall be pneumatically actuated doors.

1.3 **Utility Access**: The cable and utility access for the BioCAT Beamline Enclosures shall be through labyrinth ceiling or walls panels as shown on the drawings, and the beam transport pipe shall be through various "entry" panels as shown on the drawings.

1.4 **Shielding Integrity**: The BioCAT Beamline Enclosure shall be X-radiation tight. All panel joints and corners, access penetrations, doors and removable panels shall be suitably overlapped and fitted to prevent and X-radiation leakage. Field conditions may necessitate custom fitting of panels to ensure a radiation-tight enclosure.

1.5 **Cranes**: The BioCAT Beamline White Beam Optical Enclosure (18-ID-C) shall be equipped with 1000 Kg (1 Ton) bridged crane with a manual hoist for equipment handling as shown on the applicable drawing. The BioCAT Beamline Monochromatic Beam Experimental Enclosure (18-ID-D) may be equipped with a crane with hosts near the front and back of the enclosure.

2.0 APPLICABLE DRAWINGS

The following drawing specifies the BioCAT Beamline Enclosures which are to be fabricated by the contractor. These drawings, and their associated sub-tier drawings, are attached to this Technical Specification.

Drawings Number	Description
BIO-1.1.1.1.2-002-DD-00	Sector Layout Shielding Floor Plan & Elevations (Fig. 2)

3.0 TECHNICAL REQUIREMENTS

3.1 Design Requirements: The designs of the BioCAT Beamline First Optics Enclosure, White Beam Optical Enclosure and Monochromatic Beam Experimental Enclosure are defined in the drawings, and their associated sub-tier drawings, which are listed in Section 2.0 of this Technical Specification. Since the Enclosures are fabricated from standardized panels, the construction details of the Standard APS Shielding enclosures can be used for the BioCAT enclosures where applicable. The size of the panels, the lead thickness’, the number and placement of the door panels and other items must be adjusted to conform to the specific requirements of each enclosure, as defined on the applicable drawing as listed in Section 2.0.

3.1.1 Mechanical.

3.1.1.1 Enclosure Dimensions: The outside dimensions for each enclosure are defined on the applicable assembly drawing as listed in section 2.0.

3.1.1.2 Shielding Requirements: The shielding requirements and lead thickness’ are given on Drawing BIO-1.1.1.1.2-002-DD-00, Sector Layout Shielding Floor Plan & Elevations. "Back wall" refers to the wall through which the X-ray beam exits the enclosure. "Front wall" refers to the wall opposite from the "back wall". "Side walls" are all other walls. "Entry Panels" are the specific panels through which the X-ray beam pipe passes.

3.1.1.3 Piping: Only piping required for the pneumatic door operation shall be provided.

3.1.1.4 Pneumatic Access Door: Push buttons to open and close each door shall be located on the outside of the enclosures. Door release buttons shall be located on the inside of the enclosures to vent the cylinders and permit egress from the enclosures. The leading edge of each door shall be equipped with a safety trip switch which, when contacting an obstacle while closing, will cause the door to open and prevent personnel injury.

3.1.2 Electrical: No electrical equipment shall be provided.

3.1.3 Welding: Complete dye penetrant testing of all welds in NOT required as long as pre-qualified weld joints are used as provided in the Structural Welding Code, ANSI/AWS D1.1-90.

3.2 Fabrication Requirements: Fabrication of the BioCAT 18 ID Beamline White Beam Optical Enclosure (18-ID-C WBOE) and the 18 ID Monochromatic Beam Experimental Enclosure (18-ID-D MBEE) shall be in accordance with the drawings which are listed in Section 2.0 of this Technical Specification, and with all the provisions of this Specification.

3.3 Painting: The BioCAT Optics Enclosures and Experimental Enclosure shall be painted according to APS document no. 4105-00024, Technical Specification for Painting Requirements of Beamline Structures.

3.4 Drawings: The drawings and documents listed in Section 2.0 define the basic fabrication requirements of the BioCAT Beamline White Beam Optical Enclosure and Monochromatic Beam Experimental Enclosure. The contractor is responsible for the preparation of detail and shop drawings. The new drawings by the contractor shall be submitted to ANL for approval.