APPENDIX A

DESCRIPTION OF CURRENT FACILITIES AT SECTOR 17

Current Capabilities:

IMCA-CAT currently operates Sector 17 at the Advanced Photon Source (APS). Sector 17 is equipped with an insertion device beamline (17-ID) utilizing an APS standard undulator A, and a bending magnet beamline (17-BM). Both beamlines are dedicated to macromolecular crystallography.

Insertion Device Beamline:

The insertion device beamline, 17-ID, provides monochromatic X-rays through a Daresbury double-crystal constant off-set monochromator. The optical system includes a cryogenically cooled Si(111) channel-cut first crystal and a flat Si(111) second crystal in the monochromator, a P5 integral shutter assembly, an F2 filter rack operating as a monochromatic filter assembly, and an L2-20 slit assembly located in the experiment end station. The beam is currently unfocused. The undulator may be operated on its first or third harmonic. On the first harmonic, operations have been carried out between 6 keV and 13.6 keV. Due to limitations in the geometry of the monochromator, however, the highest energy achievable on the third harmonic is about 16 keV. Routine monochromatic and multiwavelength anomalous dispersion (MAD) experiment capabilities over an energy range from 6 to 13.6 keV are currently available.

The experiment end station is equipped with an ADSC Quantum 210 CCD detector, a 2 x 2 array of detector modules with a total active area of 210 mm x 210 mm and 51 micron pixels in a 4096 grid. The detector is mounted on a Crystal Logic goniostat with omega and 2 theta (0° to 45°) rotations and detector translation (85 mm to 585 mm). The optical system for viewing sample crystals includes two Thales Optem zoom 160 lenses, one mounted with a SONY monochrome video digital camera and the other mounted with a SONY color digital camera, and positioned 110° apart. A standard scintillation detector (Bicron) is used to measure fluorescence spectra of anomalously-scattering samples. The sample crystal is cooled to 100 K with an Oxford Instruments Cryojet. Automatic filling of the liquid nitrogen dewars is direct from the APS central distribution system. Recently installed and currently in commissioning is a Rigaku/MSC ACTOR robot for automatic crystal transport, orientation and retrieval.

Bending Magnet Beamline:

The IMCA-CAT bending-magnet beamline, 17-BM, operates in monochromatic beam mode. The first beamline component, a CRSII water- cooled mask, defines maximum horizontal acceptance of the beamline of 2 mrad, and vertical acceptance of 0.6 mrad. A water cooled L3-20 slits assembly is located downstream of the mask, and determines the

size of the beam which impinges a Pd-coated-Si water cooled white beam collimating mirror (InSynch, LR Design bender). The angle of deflection for the collimating mirror is set to 3 mrad. A pink beam, reflected by the collimating mirror is intercepted by a Daresbury double-crystal constant off-set monochromator with a water-cooled Si(111) first crystal. The second crystal of the monochromator, a sagittally bent Si(111), focuses the beam in the horizontal direction. Vertical focusing is implemented by a Pt/Pd-coated ULE mirror (InSynch, Daresbury bender design), located downstream of the monochromator. The angle of the deflection for the mirror is set to 3 mrad so downstream of the mirror the monochromatic beam is horizontal. All optical components used in focusing the beam are located at close to 1:1 geometry. A P6 / modified integral shutter assembly is located downstream of the focusing mirror and is the last optical component in front end station. A L3-20 modified slit assembly and a XIA monochromatic beam filter are situated in the experiment end station.

Routine monochromatic experiment capabilities over an energy range from 6 to 17 keV are currently available, with an energy resolution of ~0.02%. The size of the focused beam is ~100 μ in the vertical direction and ~270 μ in the horizontal direction. The experimental end station is equipped with a marUSA 165 mm ccd detector, a single 4k x 4k chip with simultaneous four-channel readout of 2048 x 2048 pixel images in 3.5 seconds per image. The detector is mounted on a marresearch desktop beamline (dtb) goniometer system with phi and 2 theta (0° to 30°) rotations and detector translation (20 mm to 370 mm). A standard scintillation detector (Bicron) is used to measure fluorescence spectra of anomalously-scattering samples. The sample crystal is cooled to 100 K with an Oxford Cryosystems 600 series Cryostream Cooler mounted at a fixed angle of 45° about the beam axis (5° towards the source). Automatic filling of the liquid nitrogen dewars is direct from the APS central distribution system. Data acquisition is driven by the marccd software which is integrated with the beamline control system (MX) such that the monochromator energy changes for an entire multiwavelength experiment can be controlled from a single data acquisition menu.

ADDITIONAL HARDWARE.

Significant pieces of additional hardware available for a future 17-ID upgrade and not mentioned in the previous description are

1. Daresbury vertical focusing mirror , tank and bender. 1 e.a.
2. Daresbury horizontal focusing mirror , tank and bender. 1 e.a.
3. InSynch ULE substrate Pt/Pd coated mirror 1m long 2 e.a.
4. LR Design bender for sagittal focusing 1 e.a.
5. LR Design guard slits assembly 1 e.a.
6. Oxford Instruments T2 motion stages system 1 e.a.
   for L5-20 indulator white beam slits

Equipment Pool:

IMCA-CAT maintains an additional marUSA 165 mm CCD detector and a marResearch standard base as backup units. Additionally, IMCA-CAT maintains an Oxford Cryosystems 600 series Cryostream Cooler as a spare sample cooling unit.

Computing and Networking:

The computational capabilities available to users include resources for data collection, data processing, and data archiving. Four software packages for data processing are routinely available: HKL2000, X-GEN, D*Trek, and MOSFLM. IMCA-CAT provides Linux, SGI IRIX, and Microsoft Windows 2000 computer workstations for users. Each beamline provides the ability to write data to CD-R media as well as external SCSI and FireWire (IEEE 1394) hard drives. Data can also be written to DAT and DLT tape from the Laboratory Office Module. The computer network connecting IMCA-CAT computers is capable of up to 100BaseTX Fast Ethernet. A gigabit ethernet network is in the planning stages and should be in place by summer 2004. Each beamline provides two Ethernet cables for plugging in a laptop computers. The network provides automatic DHCP configuration eliminating the need for the user to configure a laptop's network settings as long as the laptop operating system supports the DHCP protocol. Lastly, each beamline has a dedicated printer.

Office, Biochemistry and Electronics Laboratories:

Building 435A contains 1450 square feet (SF) of office space, consisting of nine offices and a conference room. The IMCA-CAT facility includes a ~625-SF biochemistry laboratory for crystal growth and sample preparation, equipped with a standard fume hood. Also available are a 4°C cold room, a -20°C freezer, a variable temperature refrigerator, three Olympus stereo microscopes of which one is configured with an Olympus DP11 digital camera. The IMCA-CAT facility includes a ~625-SF electronics laboratory for working on beamline components. A portion of this lab has been set aside as office area for general users.

Description of Facilities Available to General Users:

The insertion device beamline, 17-ID, having declared full operations on October 1, 1999, is scheduled with general users for 25% of the total available beam time. IMCA-CAT staff in general provide training and operations support to general users. The general user is expected to have sufficient expertise in macromolecular crystallography to efficiently design and perform single-wavelength and SAD/MAD experiments and to effectively produce high quality science. Scientific support is offered on a collaborative basis. The equipment on the insertion device beamline and in the biochemistry laboratory, along with the associated computing resources (described in ‘Current Capabilities’) are available to general users. The bending magnet beamline, 17-BM, is in commissioning phase and is

expected to be available to general users by January 1, 2005 at the same 25% general user level.

Beamline Staff

The current staff of the IMCA-CAT beamline consists of a director, 3 additional Ph.D. level scientists, and 3 non-Ph.D. support personnel. The CAT currently has 2 open head count. Staff CVs are available upon request upon completion of the confidentiality agreement, enclosed in Appendix C. The IMCA beamline staff represents a valuable resource for the contractor in seamlessly transitioning from current operations and the IMCA supervisory board believes that every reasonable effort should be made to retain the current staff.