Experimental Envelope for the SBC 19BM Facility

(September 2001)

The commissioning envelope described below does not define the limits of the beamline capabilities but describes conditions for crystallographic experiments conducted successfully at the beamline.

Sample Characteristics

- Crystals of macromolecules known to diffract (10 - 500 kDa/AU)
- Unit cell dimension: longest ≤ 600 Å
- Number of heavy atom sites validated
- Anomalous scatterers within the beamline energy limits (results demonstrated for Se, Co, Fe, Pt, Hg, S, Xe, I; currently maximum number of sites – 12/A.U.)
- Crystal size: 0.05 – 1.0 mm
- Cryofreezing protocol established
- Mosaicity ≤ 2˚

Sample Preparation Capabilities

- Crystallization facility at the SBC available (special arrangements on request)
- On-site sample freezing in liquid nitrogen, nitrogen cold stream, or liquid propane
- Cold room available (4˚ C)
- Wet lab and modest lab equipment available (users bring their own chemicals or arrange for shipment to ANL)

X-ray Beam Characteristics 19ID

- Energy: 6.5 - 13 keV (special arrangements request)
- Energy band width: 1.8 x 10E-4
- Collimator size: 0.2 mm x 0.15mm
- Flux: As needed, limited by sample degradation (max. 6 x 10^{12} x-ray Ph/sec/mm^2)
- Beamstop – 1 mm, designed for MAD phasing to limit fluorescence interference

Data Acquisition Conditions

- Exposure: 1 - 180 sec per frame
- Sample temperature: ≥ 94 K (Oxford)
- Detector-sample distance: ≥ 120 - ≤ 960 mm
- Detector 2 theta angle: -5˚ - +38˚
- Detector offset –100 - +400 mm
- Kappa goniostat operational (motor-driven phi rotation and z-translation, manual x- and y-translation)
- Omega angle: ± 120˚ continuous scan range
- Omega angle drive rate: ≤ 10˚/sec
- Oscillation angle: fine or wide slicing (0.1 - 4.0^o)
- Mounting pin type: Yale, Harvard, Hampton, (special arrangements on request)

- MAD experiments: presently with operator assistance

Special Instrumentation

- **Fluorescence detectors**
  - Amptek Model CR100, energy resolution ~350 eV at 12 keV, 1-2K cps for linear detection
  - BICRON, poor energy resolution, but 30-40K cps for linear detection
- **X-ray area detector (SBC-1 and SBC-2) characteristics**
  - Nine-element CCD
  - Surface area: 210 x 210 mm
  - Pixel size: 0.068 mm
  - Unbinned images: 3072 x 3072 pixels (18.5 Mb image size, 2.9 sec deadtime)
  - Binned images: 1536 x 1536 pixels (4.5 Mb image size, 1.6 sec deadtime)
  - Data acquisition rate – up to approximately 30 images/min

Data Processing and Management

- HKL2000 v0.96.511, d*TREK v.7.1/v.7.2
- Automated data management (transfer and archiving)
- Data transfer rates 3.5-4.5 Mb/sec
- Data archive rates approximately 2.8 Mb/sec
- SGI Challenge computer (2 x 200 MHz processors) with 50 Gb disk space
- One PC LINUX workstation with dual processors (450 MHz), two with dual processors (1 GHz), two with dual processors (700 MHz) and two 220 Gb RAID5 disk storage spaces
- Archive data to user-provided DLT (20/35/70 Gb capacity; compressed) or DAT (12/8/4 Gb capacity) tape

Personnel and Administration

- Independent investigator agreement between user's institution and the APS
- Completion of proposal review form and safety review form
- Identification of spokesperson designated by the principal investigator
- Completion of DOE-approved radiation safety training (available at the APS)
- Completion of ANL-approved beamline training (available at the SBC)
- Current SBC support team assigned to each user group

User support: day one: full support 9 am to 9 pm, subsequent days: full support during regular hours; weekends and off-hour support only by special arrangement