

X-ray Laboratory SOPs, Troubleshooting, Maintenance and Budget

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Disclaimer: The information in this document is provided in good faith for general guidance only. Despite reasonable care, it may contain unintentional errors or become out of date, and we cannot accept responsibility for any loss, damage or injury arising from its use. It does not replace the manufacturer's manuals, your institution's approved procedures, or the advice of your radiation protection officer. Always consult your local experts and follow applicable regulations before operating any equipment.

Purpose, scope and safety

These SOPs cover safe, reproducible operation of laboratory X-ray powder and thin-film diffractometers and a benchtop XRF spectrometer, grouped by instrument class rather than by one model. Local rules, the manufacturer's manual and the radiation-protection officer's instructions always take precedence over this document.

Who may operate

- Only trained users who are signed off for the specific instrument and the configuration they use (for example Bragg–Brentano, thin film or a heating chamber).
- Optics changes, alignment, tube changes and anything that requires bypassing an interlock are done only by the instrument responsible or the service engineer.
- New users run their first sessions with a trained user present.

Radiation safety rules for every instrument

1. Never defeat, bridge or tape an interlock, and never open a housing panel.
2. Check the "X-RAY ON" and "SHUTTER CLOSED" lamps before opening the doors; if any lamp is out or contradicts the software, stop and report it.
3. Close the doors gently and fully: a door not seated in its interlock trips the safety circuit and switches off the high voltage.
4. Wear a personal dosimeter where the local radiation-protection programme requires one.
5. Pregnant users, and anyone unsure about exposure, consult the radiation-protection officer before working.
6. Report any alarm, unusual noise, smell of burning, coolant leak or damaged lead glass immediately and do not use the instrument until it is cleared.
7. Operation follows national law: for example the Swedish Radiation Safety Authority (SSM) regulations in Sweden, the Ionising Radiations Regulations 2017 in the UK, and state regulations in the USA.

General lab rules

- Book the instrument, and sign the logbook at the start and end of every session: date, user, group, instrument configuration, kV/mA, samples and any problem seen.
- No food or drink. Wear gloves when handling powders and holders, and take them off before touching keyboards and door handles.
- Toxic, radioactive, air-sensitive or beryllium-containing samples need prior approval and the correct sealed holder.
- No USB sticks on instrument PCs; move data through the network or the facility's transfer drive. Raw data on the instrument PC are deleted after a fixed period, so copy them the same day.
- Leave the instrument in standby (typically 20–30 kV, 5–10 mA) unless the local rule is to switch the generator off. Leave the control software running if the manufacturer requires it for standby.

Instrument landscape

Almost every laboratory powder diffractometer in use worldwide falls into one of five classes, and each class has its own SOP below. The table lists current and common legacy models by manufacturer. The SOP letter shows which procedure applies.

Manufacturer	Model	Status (as of Oct 2026)	Class (SOP)	Geometry and optics	Detector	Typical use
Bruker	D2 PHASER	Current	Benchtop (A)	Bragg–Brentano, low-power sealed tube, optional 6-position changer	LYNXEYE 1D strip	Teaching, phase ID, QC
Bruker	D6 PHASER	Current (2023)	Benchtop (A)	Higher-power benchtop, exchangeable optics	1D strip	Research-grade benchtop work
Bruker	D4 ENDEAVOR. D8 ENDEAVOR	Current	Floor, automated (B)	Bragg–Brentano with large sample changer	1D strip	Industrial process control (cement, mining)
Bruker	D8 ADVANCE (incl. TwinTwin, K α 1,	Current	Floor (B, C)	θ – θ , motorised slits, optional Johansson K α 1 or switchable B–B / parallel	LYNXEYE XE-T (energy-resolving), EIGER2 R	Multipurpose powder, non-ambient, PDF

Manufacturer	Model	Status (as of Oct 2026)	Class (SOP)	Geometry and optics	Detector	Typical use
	DAVINCI)			beam		
Bruker	D8 DISCOVER	Current	Thin film (D)	Göbel mirror, Eulerian cradle, monochromators	0D/1D/2D	GIXRD, XRR, HRXRD, RSM, texture, stress
Siemens / Bruker AXS	D500 , D5000 , D8 Focus	Legacy	Floor (B, D)	θ - 2θ or θ - θ , fixed slits; D5000 also with Göbel mirror	Scintillation counter, early PSD	Routine powder and thin film
Malvern Panalytical	Aeris	Current	Benchtop (A)	Compact Bragg-Brentano	1D pixel detector	QC, mining, cement, teaching
Malvern Panalytical	Empyrean	Current	Floor (B, C, D)	Multipurpose, exchangeable PreFIX optics, reflection, transmission, capillary	0D/1D/2D/3D pixel detectors	Powder, thin film, SAXS, PDF, CT
Malvern Panalytical	X'Pert³ Powder , X'Pert³ MRD	Current	Floor (B), thin film (D)	Powder: B-B; MRD: mirror, Ge(220) monochromator, triple axis, cradle	Proportional, PIXcel	Powder; HRXRD, RSM, XRR, texture, stress
Philips / PANalytical	PW1710/ PW3710, X'Pert PRO MPD , X'Pert MRD	Legacy	Floor (B, D)	θ - 2θ , fixed slits, graphite secondary monochromator	Proportional, X'Celerator	Routine powder, thin film
Rigaku	MiniFlex , MiniFlex XpC	Current	Benchtop (A)	Vertical goniometer, 600–800 W tube	D/teX Ultra 1D, optional 2D HPAD	Phase ID, Rietveld, QC
Rigaku	SmartLab	Current	Floor (B, D)	θ - θ , 3 kW	D/teX Ultra	Powder,

Manufacturer	Model	Status (as of Oct 2026)	Class (SOP)	Geometry and optics	Detector	Typical use
	SE, SmartLab			sealed tube or 9 kW rotating anode, in-plane arm	250, HyPix-3000	thin film, SAXS, in-plane, operando
Rigaku	Ultima IV, D/MAX series	Legacy	Floor (B)	θ - θ or θ -2 θ	Scintillation, D/teX	Routine powder
Thermo Fisher	ARL EQUINOX 100, 1000, 3000, 3500	Current	Benchtop or floor (A, C)	No moving detector arm; reflection or transmission, capillary	Curved PSD covering 90–120° 2 θ at once	Fast, real-time kinetics, QC
Shimadzu	XRD-6100, XRD-7000	Current	Floor (B)	6100: vertical θ -2 θ (axes can be driven independently); 7000: θ - θ	Scintillation or 1D	Routine powder, stress, thin film options
STOE	STADI P, STADI MP	Current	Transmission/capillary (C)	Debye-Scherrer and flat transmission, Ge(111) K α 1	MYTHEN strip, image plate	Air-sensitive samples, structure solution
Anton Paar	XRDynamic 500	Current (2021)	Floor (B, C)	Automated switching of beam geometries, evacuated beam path, large radius	Hybrid pixel	Automated powder, non-ambient, SAXS
Huber	Imaging-plate Guinier camera G670	Current (niche)	Transmission (C)	Guinier focusing, K α 1 monochromator	Image plate	High-resolution phase work
Evident (Olympus)	TERRA II, BTX III	Current	Portable / benchtop (A)	Transmission, very small sample	Combined XRD/XRF	Field geology,

Manufacturer	Model	Status (as of Oct 2026)	Class (SOP)	Geometry and optics	Detector	Typical use
				amounts	CCD	mining

Many instruments are configured on site, so a single model can need more than one SOP: a D8 ADVANCE TwinTwin, for example, follows SOP B in Bragg–Brentano mode and SOP D in parallel-beam mode.

SOP A – Benchtop powder diffractometers

Applies to D2/D6 PHASER, Aeris, MiniFlex, ARL EQUINOX 100 and similar compact instruments. They have low-power tubes, fixed optics and built-in interlocks, so routine users do not change hardware.

Start-up

1. Check the logbook for open problems and the room for coolant leaks; check the internal or external cooler is running if the model has one.
2. Switch on the instrument, then the PC, and start the control software. Wait for the self-test and drive initialisation to finish.
3. If the tube has been off for more than the manufacturer's limit (often a few days), run the tube-conditioning routine before any measurement.
4. Ramp to the operating power set by the instrument responsible. Never exceed the tube rating on the tube label.

Sample preparation

1. Grind to about 5–10 μm in an agate mortar, dry or under ethanol; avoid over-grinding soft or metastable phases.
2. Fill the holder flush with the rim, ideally by back-loading to reduce preferred orientation. Use a zero-background silicon holder for less than about 20 mg.
3. Wipe the holder rim so no powder falls into the instrument, and label the holder.

Measurement

1. Open the door only when the shutter-closed lamp is on, load the holder and close the door until it clicks.
2. Start from a facility template; a typical Cu K α survey is 5–80° 2 θ , 0.02° steps, about 10–30 min in total, with sample rotation on.
3. Use a smaller divergence slit or a knife edge for data below about 10° 2 θ ; record any change in the logbook.
4. Save with a file name containing date, user and sample ID.

Shut-down

1. Unload the sample, close the door and leave the generator at standby or switch off as the local rule says.

2. Clean the holder, copy the data and sign out of the logbook.

Weekly check (instrument responsible): measure a corundum or Si standard; corundum 104 should be within ± 0.01 – 0.02° of 35.15° 2θ for Cu $K\alpha_1$, and intensity should not fall more than about 10–20% from its reference value.

SOP B – Floor-standing Bragg–Brentano diffractometers

Applies to D8 ADVANCE (including TwinTwin in Bragg–Brentano mode), Empyrean, X'Pert³ Powder, SmartLab, XRD-6100/7000, XRDynamic 500 and legacy D5000, X'Pert PRO and PW1710/3710 systems. These use 1.5–3 kW sealed tubes with water cooling, so the order of start-up and shut-down matters.

Start-up

1. Check that the chiller or building water is on, at the set temperature and pressure (for example about 20–26 °C and the flow on the chiller label). Legacy systems: start the chiller 5–10 min before the generator.
2. Switch on the main power and the generator (key switch, then HV button), then start the control software (DIFFRAC.Measurement Center, Data Collector, SmartLab Studio II or legacy DIFFRACplus).
3. Initialise all drives with the doors closed.
4. Raise power in steps: **kV first, then mA**, about 5–10 units per step with 30–60 s between steps, to the facility setting (commonly 40 kV, 40 mA for Cu). Do not start a scan until the requested and actual values agree.
5. If the tube has been off for more than a few days, run the conditioning routine instead of a manual ramp.

Hardware set-up (trained users)

1. Confirm the optics against the logbook: divergence and anti-scatter slits (fixed or motorised), Soller slits, Ni filter or $K\alpha_1$ monochromator, detector mode.
2. Motorised slits: use fixed-angle mode for quantitative work, or variable mode with a stated irradiated length (for example 10–12 mm) and convert the data before Rietveld refinement.
3. Energy-resolving strip detectors (for example LYNXEYE XE-T): select the energy window for your anode to suppress $K\beta$ and Fe/Co/Mn fluorescence.
4. Never remove Soller slits or the knife edge to "gain counts" for data you will analyse quantitatively.

Measurement

1. Load samples into the changer positions noted in the logbook, or onto the stage, with spinning on unless the sample may slide.
2. Build a job list from facility templates: sample position, ID, method and file path. Check the summary before pressing start.
3. Typical Cu $K\alpha$ parameters: 5– 90° 2θ , 0.01– 0.02° steps, total time 15 min to 2 h depending on purpose; quantitative and Rietveld work needs the longer scans.

4. Watch the first scan for overloads, unexpected $K\beta$ peaks or a rising low-angle background, which point to a wrong optic.
5. Overnight or weekend runs only with the instrument responsible's approval.

Shut-down

1. Unload all samples and close the doors gently.
2. Lower power: **mA first, then kV**, back to standby (for example 20–30 kV, 5–10 mA), or switch off if the local rule says so.
3. Do not close the control software if the instrument uses it to manage standby.
4. Legacy systems switched off fully: leave the cooling water on for about 30 min after the generator.
5. Copy data, convert files if needed (raw to xy or brml), clean holders and sign the logbook.

Based on published SOPs for a [Siemens D5000](#), a [Bruker D8](#) and a [Bruker D8 ADVANCE with LYNXEYE XE-I](#).

SOP C – High-resolution $K\alpha_1$ and transmission/capillary instruments

Applies to Johansson $K\alpha_1$ set-ups (for example D8 ADVANCE with Ge(111) monochromator), STOE STADI P/MP, Emyrean in transmission or capillary mode, Huber Guinier cameras and ARL EQUINOX in transmission. Start-up and shut-down follow SOP B; only the differences are listed.

Before measuring

1. Check the monochromator alignment with a Si or LaB_6 standard weekly: no $K\alpha_2$ shoulder and peak widths at their reference values. Only the instrument responsible re-aligns the monochromator.
2. Expect roughly half the intensity of a filtered beam; plan longer scans instead of opening slits.

Capillary samples

1. Choose the capillary diameter for the sample's absorption: about 0.3–0.5 mm for strongly absorbing samples, 0.5–1.0 mm for organics with Cu or for Mo radiation.
2. Fill 2–3 cm of capillary, tapping or using a vibrator; air-sensitive samples are filled and sealed in a glovebox (flame-sealing or wax).
3. Mount in the goniometer head and centre it so the capillary does not wobble while spinning; check with the camera or by eye.
4. Always spin the capillary during measurement.

Flat transmission samples

1. Spread a thin, even layer between two X-ray-transparent foils (for example Kapton or polyester), with a little grease or oil if needed.
2. Measure an empty foil once per batch so it can be subtracted.

Measurement

1. Typical Cu $K\alpha_1$ indexing data: 2–90° 2 θ , 0.01° steps or finer, 1–4 h. Mo $K\alpha_1$ reaches higher Q for PDF or strongly absorbing samples.
2. Record capillary diameter and filling height in the logbook; absorption corrections need them.

SOP D – Parallel-beam and thin-film diffractometers

Applies to D8 DISCOVER, X'Pert³ MRD and legacy X'Pert MRD, SmartLab, Empyrean and D8 ADVANCE in parallel-beam mode, and D5000 with Göbel mirror. The direct beam can reach the detector in these set-ups, so alignment always starts with an absorber in place.

Start-up and optics

1. Start up as in SOP B and raise the tube from standby (for example 20 kV/10 mA) to operating power (for example 40 kV/40 mA).
2. Confirm the optics for the task: Göbel mirror with a 0.1–0.2 mm slit and Soller slits for GIXRD and XRR; mirror plus Ge(220) or Ge(022) monochromator and analyser for HRXRD and reciprocal space maps; lens or polycapillary for texture and stress.
3. Optics changes are done only by trained users, with the generator at standby and the shutter closed, and recorded in the logbook.
4. Do not touch detector entrance windows: many contain beryllium.

Alignment (every sample)

1. Clear previous offsets. Insert the absorber (or set it to a fixed attenuation) so the direct beam cannot saturate the detector.
2. Detector zero: 2 θ scan from –0.5 to +0.5° with $\omega = 0$; set zero only if a clear peak appears.
3. Height (z) scan, for example –1 to +2 mm in 0.01 mm steps; set z at half the direct-beam intensity.
4. Rocking (ω) scan, $\pm 1^\circ$; set the peak as $\omega = 0$ so the surface is parallel to the beam.
5. Repeat the z-scan and the rocking scan until both stop changing; for HRXRD also align χ (ψ) and then the substrate peak.
6. Return the absorber to automatic before measuring.

Measurement types

Task	Typical settings
GIXRD (phases in films down to ~20 nm)	Fixed incidence $\omega = 0.3\text{--}2^\circ$; detector scan 10–90° 2 θ ; parallel-plate collimator or equatorial Soller
XRR (thickness, density, roughness)	Coupled θ –2 θ from 0 to 3–5°, steps 0.002–0.005°, automatic absorber, knife edge close to the surface
HRXRD and rocking curves	Monochromator and analyser; ω scans around substrate and layer peaks; at least 9–10 points across the FWHM
Reciprocal space maps	Series of ω –2 θ scans at stepped ω around a

Task	Typical settings
	symmetric and an asymmetric reflection
Texture (pole figures)	Fixed 2θ ; χ 0–75°, φ 0–360° on the Eulerian cradle
Residual stress	$\sin^2\psi$ method: one high-angle peak at 5–7 ψ tilts

Shut-down: remove the sample, return all drives to their park positions, set the generator to standby and leave the control software open if required.

Alignment steps follow the [Princeton D8 DISCOVER procedure](#) and the [EPFL D8 DISCOVER alignment guide](#); MRD optics settings follow the [UNSW MRD description](#).

SOP E – Non-ambient chambers

Applies to oven and low-temperature chambers fitted to SOP B or D instruments, for example the Anton Paar [HTK 1200N](#) (25–1200 °C, vacuum to about 10^{-4} mbar, air or inert gas, at most 1 bar overpressure, samples up to 16 mm diameter), the TTK 600 low-temperature chamber and domed hot stages such as the DHS 1100. Only users trained on the chamber may run it, and every run is entered in the chamber's own logbook.

Before the run

1. Check that the sample, holder material and atmosphere are compatible at the highest temperature: no reactions with alumina, Pt or Ni holders, no melting onto the heater and no toxic decomposition products. Ask the instrument responsible if unsure.
2. Check the chamber cooling water is flowing and the windows (Kapton or Be) are intact.
3. Mount the sample, close the chamber and leak-test: pump to vacuum or purge with gas for the time set in the method before heating.
4. Align the sample height at room temperature; plan a height correction (motorised z or a Si/Al₂O₃ internal standard) because the sample and holder expand on heating.

During the run

1. Heat and cool at the rates in the method and let the temperature settle before each scan.
2. Never vent the chamber hot, and never open it above about 50 °C.
3. Low-temperature runs: keep the window heater or dry gas on to avoid ice; wear face shield and cryogenic gloves when filling liquid nitrogen, and keep the room ventilated because nitrogen gas displaces oxygen.

After the run

1. Let the chamber return to room temperature (cold chambers: let them warm under dry gas before opening, to avoid condensation).
2. Remove the sample, clean the holder, and note any deposits on windows or the heater in the logbook.
3. Calibrate the temperature scale yearly with a standard of known thermal expansion or phase transition.

SOP F – Benchtop energy-dispersive XRF

Applies to Malvern Panalytical Epsilon 1, Epsilon 3 (now succeeded by [Epsilon 4](#)) and similar EDXRF spectrometers, which are often run next to diffractometers to check composition. The X-ray tube switches on only while the interlocked lid is closed.

Start of session

1. Leave the spectrometer powered on between sessions unless the local rule says otherwise; open the software.
2. Run the energy-calibration (gain) check when the software asks. Handle the reference sample with gloves: some references contain beryllium.
3. For light elements (Na–Cl), switch on the helium flush or vacuum if fitted and let it purge before measuring.

Sample preparation

1. Loose powders and liquids: sample cup with a thin X-ray film (for example 3.6 µm Mylar or polypropylene), film stretched taut and free of wrinkles; fill at least a few millimetres deep.
2. Quantitative work: pressed pellets with a binder or fused beads give better repeatability than loose powders.
3. Never measure wet, corrosive or volatile samples without a sealed liquid cup and the instrument responsible's approval.

Measurement and results

1. Choose a facility application: standardless screening (for example Omnian) for unknowns, a calibrated application for routine analysis.
2. Enter the sample name, close the lid and start; a full standardless scan takes about 10–30 min.
3. Check the spectrum for misidentified peaks before reporting results, and record the film type and the compound or balance setting used.
4. Do not overwrite facility applications; copy them under your own name.

End of session: remove and dispose of sample cups in the labelled waste, clean any spilled powder from the measurement window area with the approved method, copy results and sign the logbook.

Based on the [UC San Diego Epsilon 1 SOP](#).

General troubleshooting

Most problems are sample or set-up issues that the user can fix; anything involving the generator, interlocks, cooling or optics alignment goes to the instrument responsible. When in doubt: close the shutter, set the generator to standby, take a screenshot, write the problem in the logbook and report it.

Symptom	Likely cause	What the user does	Escalate when
High voltage switches off when doors close or	Door not seated in its interlock; safety circuit	Close doors fully; do not	Always, if it

Symptom	Likely cause	What the user does	Escalate when
during a run	tripped	reset the circuit yourself	trips again
Alarm lamp flashing at standby	Cooling water too cold or flow low at low power (often clears at operating power)	Check chiller display; do not start a scan with a solid alarm	Alarm stays on or is solid
Generator will not ramp or keeps falling back	Tube needs conditioning, cooling fault, generator fault	Run the conditioning routine if allowed	Ramp fails twice
Drive error, "not initialised" or goniometer stuck	Collision, lost reference position, door opened mid-move	Re-initialise drives with doors closed	Drive will not initialise or makes noise
All peaks shifted the same amount	Zero error	Measure Si or corundum standard	Standard is off by more than $\pm 0.02^\circ$
Peaks shifted, most at low angle	Sample surface too high or low, transparent organic sample	Refill holder flush; thinner layer; use an internal standard	Never: sample issue
Intensity much lower than usual	Absorber or wrong slit in, monochromator mis-set, ageing tube	Check optics against the logbook and the template	Standard intensity down more than about 20%
Strong extra peaks about 10% of main peaks at lower 2θ	K β not removed: filter missing or wrong detector window	Check filter or energy window	Filter missing from the instrument
High, flat background	Fluorescence (Fe, Co, Mn under Cu) or missing filter	Energy-resolving detector window, or Co/Fe tube	-
Rising background below $\sim 15^\circ 2\theta$	Anti-scatter slit or knife edge missing, slit too wide	Refit or lower knife edge; narrower divergence slit	-
Asymmetric low-angle peaks, poor resolution	Soller slits removed or wrong	Refit correct Soller slits	Slits missing
Relative intensities vary between repeats	Coarse grains or preferred orientation	Grind finer, back-load, spin; check 2D image if available	-
Sharp peaks from Al, steel or glass	Beam spilling onto the holder; too little sample	Narrower slit at low angle; more sample; zero-	-

Symptom	Likely cause	What the user does	Escalate when
		background holder	
Flat-topped or doubled strongest peaks	Detector saturation	Use attenuator or lower mA for that scan	Persists at normal power
Sample changer fails to pick or drops a holder	Holder not seated, wrong position, wrong holder type	Stop the job, retrieve holder with the door open and X-rays off	Mechanical damage
XRR shows no fringes	Sample not aligned or not parallel; very rough film	Repeat z and rocking scans	–
Vacuum not reached in a chamber	O-ring dirty or seated wrong, window damaged	Clean and reseal O-ring	Window damaged
Ice or fog on a cold-chamber window	Window heater or dry-gas purge off	Restore purge, warm and dry before restarting	–
XRF gain check fails or results drift	Reference not seated, film contaminated, helium low	Repeat with clean reference; check helium	Fails twice
Software lost connection to the instrument	Communication fault	Do not power-cycle the generator; save work and report	Always

Maintenance

A short, regular schedule keeps tubes, detectors and cooling systems running for years; the instrument responsible owns it and records every task in the instrument logbook.

Frequency	Task	Who
Every session	Logbook entry; check lamps, chiller display and doors; leave instrument at standby; clean holders	User
Weekly	Measure the Si or corundum standard and plot position, width and intensity on a control chart; back up data; clean the sample changer and stage	Instrument responsible
Monthly	Check chiller water level, filter and flow; check tube hours; inspect Be and Kapton windows; test door interlocks and warning lamps	Instrument responsible
Every 6–12 months	Change chiller water and filter (with corrosion inhibitor); radiation leakage survey around the enclosure; full alignment check	Instrument responsible, radiation-protection

Frequency	Task	Who
		officer
Yearly	Manufacturer service visit: generator, interlocks, goniometer and optics alignment, detector calibration; temperature calibration of non-ambient chambers	Service engineer
As needed	Tube conditioning after long idle periods; tube replacement when standard intensity has fallen to about half or the tube fails	Instrument responsible, service engineer

Spares worth keeping on site: a sealed tube for each anode in use, Ni filters, Soller and divergence slits, knife-edge and beam-stop parts, Kapton foil and O-rings for chambers, sample holders, chiller filters and fuses listed in the manual.

Records: tube serial number and installation date, tube hours, standard-sample control chart, service reports, radiation survey results and training sign-offs. These records are what auditors and the radiation-protection authority ask for first.

Budgeting and financing

The largest recurring costs of an X-ray lab are staff time, service contracts and X-ray tubes. Plan them as one annual budget, recover part through user fees, and fund new instruments through infrastructure grants. Fill the template below with local quotes; prices vary by vendor, country and contract.

Annual running-cost template

Item	Basis for the estimate	Annual cost (local currency)
Staff (instrument responsible, technician share)	FTE × salary incl. overheads	[]
Service contracts	Vendor quote per instrument; preventive visit plus repairs	[]
X-ray tubes	Tube price ÷ expected life, per instrument and anode	[]
Detector and optics repairs	Reserve, or covered by the contract	[]
Chillers, water filters, inhibitor	Consumables plus chiller service	[]
Consumables	Holders, zero-background plates, capillaries,	[]

Item	Basis for the estimate	Annual cost (local currency)
	Kapton, XRF cups and film, helium, liquid N ₂	
Software licences	Control, search-match database (for example ICDD PDF), Rietveld	[]
Radiation protection	Dosimeters, leakage surveys, training	[]
Electricity and premises	Local internal rent model	[]
Replacement reserve	Purchase price ÷ planned service life	[]

Setting user fees: a full-cost hourly rate divides the costs not covered by subsidies by the hours actually billed.

$$\text{Hourly rate} = (\text{annual running costs} - \text{subsidies}) \div \text{billable hours per year}$$

Most facilities set a lower internal academic rate, a higher external academic rate and a commercial rate, plus a separate rate for staff-run service. Published examples:

Facility	Internal	External academic	Commercial or staff service
UNSW Sydney, all XRD (2023–24)	AU\$35/h	AU\$70/h	AU\$150/h user, AU\$250/h service
Caltech, Rigaku SmartLab (2023)	US\$30/h	US\$50/h (non-profit)	US\$100/h staff assistance
University of Guelph, powder XRD	\$10/h self-use	\$15/h self-use	\$40/h staff collection (industry)

Funding sources

- **Department or core-facility budget:** base funding for staff and service contracts, usually in return for open access and reporting of usage.
- **User fees:** from research projects, collaborators and industry; record usage per project in the booking system.
- **Research grants:** equipment lines in project grants, or shared purchases by several groups.
- **National infrastructure funding:** in Sweden, for example, the Swedish Research Council's [grants to research infrastructures of national interest](#) (about SEK 965 million for 2024–2028 across 21 infrastructures in the 2023 call) and the Knut and Alice Wallenberg Foundation's [infrastructure grants](#) (SEK 203 million in 2014). These are examples only: check the schemes available in your own country (in the UK, for example, UKRI).
- **Industry partnerships:** service agreements or co-funded instruments with companies that need regular analysis.

Plan instrument replacement before the manufacturer ends support for spare parts and software, and include installation, room preparation, training and the first service contract in the purchase budget.

Sources

This document is a summary in original wording and cites the published sources below; please consult the original manuals and SOPs for authoritative detail. Product and company names are trademarks of their respective owners; no affiliation with or endorsement by any manufacturer is implied.

Published SOPs and manuals

- [Siemens D5000 SOP, University of Puerto Rico Mayagüez](#)
- [Bruker D8 XRD SOP, University of Washington](#)
- [Bruker D8 ADVANCE PXRD SOP, Westlake University](#)
- [Bruker D8 DISCOVER operating procedure, Princeton University](#)
- [Bruker D8 DISCOVER SOP, University of Michigan](#)
- [Bruker D8 DISCOVER sample alignment, EPFL](#)
- [PANalytical X'Pert MRD configurations, UNSW Sydney](#)
- [Epsilon 1 XRF SOP, UC San Diego](#)

Instrument and manufacturer information

- [X-ray laboratory, Ångström Laboratory, Uppsala University](#)
- [Bruker diffractometer range](#) and [D6 PHASER announcement](#)
- [Malvern Panalytical X-ray diffractometers](#)
- [Rigaku XRD product comparison](#)
- [Thermo Fisher ARL EQUINOX 3000](#)
- [Shimadzu XRD-6100](#)
- [Powder diffractometers including STOE STADI P, University of Freiburg](#)
- [Anton Paar XRDynamic 500 launch, IUCr Newsletter](#)
- [Anton Paar HTK 1200N](#)
- [Olympus TERRA II and BTX III launch](#)

Fees and funding

- [UNSW access costs 2023](#), [Caltech XRPD fees](#), [University of Guelph XRD rates](#)
- [Swedish Research Council infrastructure grants 2023](#), [Knut and Alice Wallenberg Foundation infrastructure grants](#)