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SERVICE DATA SHEET

—V1.3 | 2026.03.30

Synchrotron PXRD — General Service

Radically better XRD

5 to 5,000+ samples · ×200 better signal-to-noise ratio · reliable turnaround time · full analysis

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Measurement Parameters

Synchrotron PXRD delivers 1,000,000× the X-ray flux of laboratory XRD, enabling trace-level phase detection at high-throughput capacity.

Parameter	Specification	Why It Matters	vs. Lab XRD
X-ray energy	75.0 keV (λ = 0.165 Å)	Minimal absorption allows for penetrating thicker samples, and negligible fluorescence effects for most of the periodic table. It also enables higher structural resolution.	Standard Cu-Kα anodes (~8.04 keV) produce significant fluorescence for samples containing Co, Fe, Mn, Cr and provide less favorable structural resolution.
Geometry	Flat-plate transmission	Improved probe volume through the sample bulk and reduced effects from preferred orientation.	Reflection geometry (Bragg-Brentano) may produce signals only from the top layer for highly absorbing samples and is more prone to preferred orientation effects.
X-ray flux	~10^{14} photons/s	Great signal-to-noise in short exposure times allows for trace phase detection in seconds.	~10^{8} photons/s — 1,000,000× less flux.
Exposure time	Seconds per sample	5,000+ measurements/day. Large batches possible in weeks.	10–60 min per scan; 20–100 samples/day. Speed degrades quality.
Resolution (*ΔQ/Q*)	Approx. 0.0028(3) (as measured by the integral breadth from LaB_6).	Resolves overlapping peaks — critical for complex multi-phase systems.	Typical values on the order of 0.005–0.01 depending on configuration
***Q*-range**	0.16–9.1 $Å^{-1}$	Covers a wide *d*-spacing resolution of ~40–0.69 Å for identification of crystals with both very large and small unit cell volumes.	Maximum for Cu-Kα at 160° would be 8.03 $Å^{-1}$ (not accessible by typical instruments)
Sample thickness	1 mm	Thick sample allows beam to pass through many crystallites in the sample bulk.	Thin capillaries (e.g. 0.2–0.5 mm ID) for Debye-Scherrer geometry are difficult to fill: can lead to lower packing efficiency.
Preferred orientation effects	Reduced through transmission geometry, sample vibration and shaking during measurement.	Mass orientation of non-isotropic particles can impact quantitative data severely.	Bragg-Brentano — the most common lab setup — is particularly sensitive to this effect. Highly anisotropic particles tend to align along flat plate or thin capillary geometries.
Microabsorption effects	Reduced with high-energy X-rays	Micro-absorption adversely affects quantitative XRD results by denser particles shadowing lighter ones.	Low-energy lab sources are particularly affected.
Temperature	23.6 °C	All samples are measured at RT.	–

Characterisation Capabilities — Crystallography

Take advantage of the best quality data by using state-of-the-art analysis tools and methodologies.

Parameter	Specification	Why It Matters	vs. Lab XRD
Detection (high density phases)	Typically ~0.1–0.01 wt% (e.g. heavy metal containing phases, rare earths, noble metals, etc.)	Find trace phases that may be targeted for value or hazard assessment.	0.5–2.0 wt% typical.
Detection (low density phases)	Typically down to ~0.1 wt% depending on phase mixture (e.g. silicates).	Quantify all crystalline phases present in multiphase mixtures.	~1–5 wt% (requiring very long measurement times).
Detection (nanoparticles)	Detect phases present with < 20 nm crystallite sizes (depending on phases)	With measured background subtraction applied, identify nanocrystalline phases, e.g., small precipitates or inclusions.	Higher baseline noise and white radiation (in non-monochromated instruments) can limit practical detection.
Quantification of amorphous content	Absolute quantification via internal standard (typically down to a few wt%)	The ratio of amorphous to crystalline material impacts physicochemical properties.	Similar behaviour as for detection of low density or disordered phases.
Lattice parameter precision	5–6 significant digits	Understand solid solutions. Refinement leads to highest accuracy structures.	Detector zero errors and sample offset can lead to both lower refinement precision and overall accuracy.
Quantification	Whole pattern fitting via Rietveld refinement (TOPAS v7)	Provides the most holistic assessment of all contents of the sample.	–
Refinement output	wt%, crystallite size, unit cell, site occupancy, etc. Refined parameters depend on relative fraction and degree of crystallinity.	We can design protocols to investigate your target information.	–

Example—Phase Quantification of Clay Bearing Minerals

As an example of quantitative analysis results typical of this setup, we provide here the analysis of a multiphase sample produced to represent an old red sandstone sample for the 12th Reynold's Cup competition. In this case, NIST Silicon SRM 640c was added as an internal calibrant at loading level of 10 wt.%

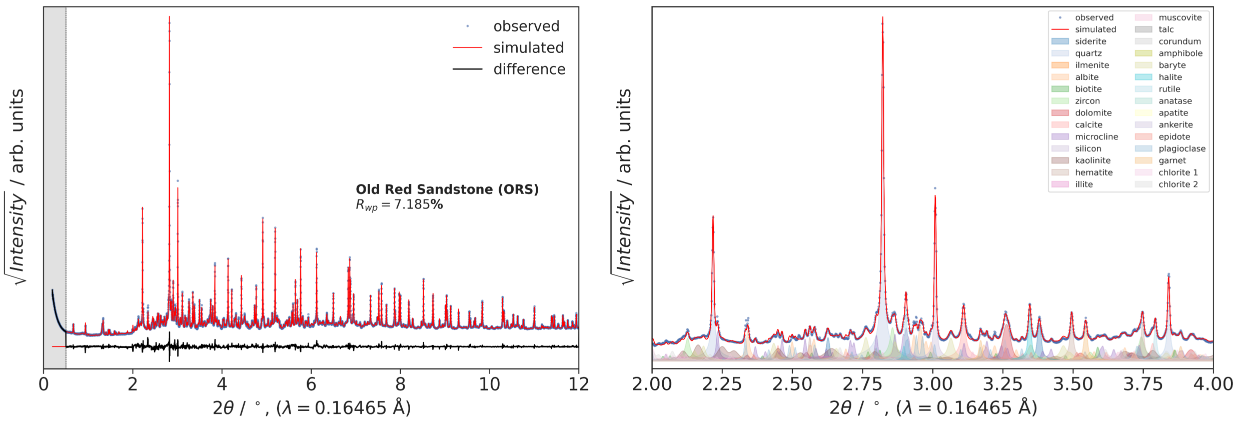

Figure 1: (left) Resulting fit from quantitative whole pattern refinement is shown and (right) individual contributions from each mineral phase accounted for are shown for reference.

Table 1: The comparison of actual values given for the reference mixture versus the determined values from the quantitative refinement, and quantification residuals..

Mineral	Actual / wt.%	Determined / wt.%	Delta / wt.%
Non-clay			
quartz	52.6	51.27	1.33
K-feldspar group	5.9	4.78	1.12
plagioclase group	8.9	7.41	1.49
garnet	2.4	1.59	0.81
epidote	0.8	0.59	0.21
zircon	1.1	1.27	-0.17
calcite	3.9	3.17	0.73
dolomite/ankerite	3.9	3.83	0.07
siderite	2.0	1.25	0.75
hematite	2.0	1.57	0.43
apatite	trace	0.10	–
rutile	2.0	1.87	0.13
anatase	0.1	–	–
halite	1.6	1.51	0.09
baryte	1.1	1.11	-0.01
amphibole	trace	–	–
corundum	0.2	0.12	0.08
ilmenite	0.1	0.01	0.09
talc	trace	0.09	–
amorphous	0	0	0
Clay			
kaolinite	3.6	3.17	0.43
mica (dioctahedral)	0.1	0.70	-0.6
illite/smectite	2.8	2.64	0.16
mica (triocahedral)	1.1	0.62	0.48
chlorite	3.8	2.18	1.62

Characterisation Capabilities — Amorphous & Local Structure

Synchrotron total scattering data and pair distribution function (PDF) analysis deliver insights for amorphous and nano-crystalline materials.

Parameter	Specification	Why It Matters	vs. Lab XRD
PDF data generation	PDFs are generated from the total scattering data using PDFgetX3 software.	The software minimises the need for tuning every individual dataset. Parameter choices can be rapidly tested, changed, and re-run as needed.	–
***Q*-range**	0.32–31 $Å^{-1}$	Covers a wide *d*-spacing range of ~20–0.2 Å with an exceptional real space resolution.	Suitable measurements typically only achieved with Mo-Kα1 or Ag-Kα1 devices and 10–30 h measurement times.
PDF Q_{max}	Typically 20–30 $Å^{-1}$ depending on sample composition	Provides maximal real space resolution, improves accuracy of data normalisation corrections, and reduces processing artefacts.	Typical Q_{max} values achieved in the lab ~15 $Å^{-1}$ (Mo-Kα1) and ~20 $Å^{-1}$ (Ag-Kα1)
Real space resolution *Δd*	Approx. ≥ 0.16–0.11 Å (determined as π/Q_{max})	Enables you to resolve partially overlapping atom pair distances in the local structure and gain high precision on bond distance estimation.	Typically approx. ≥ 0.42–0.31 Å
Maximum distances accessible in the PDF	See structural correlations up to approx. 250–300 Å.	Allows you to confidently analyse medium- and long-range correlations.	Can be similar depending on the configuration. Asymmetrical line profiles can make long-distance correlations unreliable if not corrected for.
Structure in amorphous phases	PDF patterns are automatically determined, which provide information about the bond distances and coordination numbers.	The PDF signal provides a unique local structure fingerprint for different amorphous materials, enabling more reliable identification and tracking of changes.	Lower real space resolution leads to broader peaks in the PDF. This lowers the ability to differentiate similar samples.
Differential PDF analysis	Customised data-to-data comparisons allow for unique insights into structural changes.	Extract local structure environments of supported clusters or sites in host-guest systems.	Generally no suitable statistics with laboratory measurements (e.g. see https://doi.org/10.1016/j.mtchem.2025.102776)
Local structure refinement	Precise refinement of local structures carried out using e.g., PDFgui, TOPAS, etc.	You can be confident of the structure type in ultra-small nanoparticles down to 1–2 nm and get precise values of bond distances, lattice parameters, domain size, etc.	–

Characterisation Capabilities — Small-Angle Scattering Microstructure

Small-angle X-ray scattering (SAXS) probes the material over very low spatial frequencies. This allows observations of inhomogeneity or periodicity in the density, which can be particularly useful for identifying microphase segregation or mesoporosity.

ParameterKPI	Specification	Why It Matters	vs. Lab XRD
***Q*-range**	~0.01–0.78 $Å^{-1}$	Covers a *d*-spacing range of ~630–8 Å for analysis of micropore formation and phase segregation.	Can typically provide a similar analysis range.
High sample penetration	Probe through dense solid samples.	Can analyze microstructure in highly absorbing materials not suitable for low energy X-rays.	Lab SAXS machines typically work with low energy X-rays to improve access to and resolution of small-angle features.
Micro-/mesopore analysis	Refine models including Guinier-Porod, fractal scattering, broad peaks, etc.	Assess density fluctuations from pore structures; e.g. porous carbons: help to identify interparticle correlations.	–
Microphase segregation	Fit broad peak and or structure factor models to assess segregated domain size and spacing lengthscale.	Assess density fluctuations from segregated components that are not thermodynamically compatible, e.g. in paracrystalline polymers.	–
SAXS analysis	Performed using SASview or similar for model refinement.	Standard models used, when feasible, as benchmarked against known use cases. Supporting information from the user is required to help guide appropriate model selection.	–

Sample Requirements

Requirement	Specification	Notes
Sample mass Standard measurement: For quantitative phase analysis:	 30–50 mg 0.5–10 g	Standard powder preparations work well. More powder is needed for internal standard mixing and homogenisation.
Particle size Ideal size range: Acceptable:	 < 1–5 µm < 40 µm	Large crystallites can lead to preferred orientation and higher errors on intensities. Finer particle sizes are better. Grind or mill samples when possible if degradation or unwanted sample changes can be avoided.
Accepted forms	Powders, gels, foams, slurries, suspensions, solutions. Solid forms such as pellets, discs, or films also work (assuming grain sizes as above).	Powders are preferred. Non-standard forms may be accepted. Contact us to discuss.
Sample hazards	All hazards should be stated when submitting a request. We don't accept samples requiring procedures beyond standard PPE and laboratory safety controls (e.g., fume hood, glove box, lab coat, safety goggles, gloves, mask/respirator).-	This may include samples classified as highly toxic/poisonous, radioactive, explosive, carcinogenic/mutagenic/reprotoxic (CMR), highly reactive, or biological (e.g., animal tissues, genetic materials). Please contact us first.
Air sensitive samples	Air sensitive materials can be handled and sealed into holders in a glove box to avoid degradation from moisture or oxygen.	Please indicate air sensitive samples when making a request, and provide notes on sensitivity and handling requirements. Current protocols may not be suitable for every sample.
Temperature sensitive samples	Cold storage is possible prior to sample preparation and measurements.	All sample measurements are performed at room temperature.
Shipping	Use a certified international courier only (DHL, FedEx, UPS, etc.) ensuring proper labeling and documentation. Unique package labels are provided for shipment identification upon reception.	Please note that national postal services are not acceptable and may lead to delays or rejected shipments.
Sample storage	Retained for 12 months and then destroyed. Contact us if you need samples returned.	Samples are retained for purposes of complementary analyses or reassessment if needed.

Capacity & Turnaround Time

Sample Volume	Turnaround (from reception)
Up to 1,500 samples	2–4 weeks
Up to 5,000 samples	2–6 weeks
Up to 10,000 samples	6–8 weeks
> 10,000 samples	By arrangement
Rush / recurring	Faster turnaround time with appropriate lead times

Sample Preparation

Step	What We Do
Receiving & logging	Each shipment is assigned an internal tracking number for storage and preparation activities. Chain-of-custody is documented.
Subsampling	A representative portion, typically a few mg, is extracted.
Sample labeling	Every subsample receives a unique QR code identified that connects the sample ID to the associated measurements.
Loading	Powders are packed into flat-plate transmission holders.
Standard powders	No further preparation needed.
Coarse / non-standard material	Light hand grinding by mortar and pestle up to specialised milling procedures may be needed (surcharge may apply). Contact us to discuss.
Air-sensitive samples	Loaded under an inert atmosphere: argon glove-box (O_2 and H_2O levels below 0.1 ppm). Please indicate sensitivity when submitting a request.

Analysis Methods

Method	What You Get	Best For
Measurement only	Raw diffraction data files. Your team performs the analysis.	In-house teams, AI/ML training datasets, academic research groups.
Semi-quantitative (Rietveld)	Full phase ID + Rietveld wt% with errors. Most common tier.	Product QC, formulation checks, pharmaceutical polymorph screening and solid-form studies, battery cathode development.
Full quantitative (Rietveld + internal calibrant)	Internal standard for absolute quantification incl. amorphous content.	High detail mineralogical phase quantification, analysis of cements and waste materials.
Statistical & cluster analysis	Analysis plus multivariate clustering, PCA, compositional mapping.	High-throughput screening campaigns, combinatorial materials discovery and process optimisation.
PDF / local structure analysis	Pair distribution function analysis for amorphous and nanocrystalline phases.	Amorphous APIs, battery materials incl. solid electrolytes and hard carbons, nanocatalysts, glasses, etc.
SAXS	Nanostructure analysis at the 1–100 nm scale. Particle size distributions, porosity, and mesoscale organization.	Nanoparticles, porous catalysts, framework materials (MOFs, zeolites), nanoformulations, core-shell systems, electrode architectures, colloidal dispersions.

QAQC — Applied Across All Tiers

Measures	Detail
Standards	NIST reference materials are measured every beamtime to calibrate the experiment and standardise data. Validation refinements, instrumental profile characterisation, and goodness-of-fit are provided for NIST LaB6 660b or similar for every beamtime and setup.
Replicates	Replicate subsampling and/or remeasurement can be arranged for any percentage of samples as required by the study. Please contact us to discuss your requirements.
Rwp	Weighted R-factor reported for every refinement.
Refinement precision	Rietveld-derived esd’s reported for every wt% value.
Error assessment	Measurement and quantification errors can be assessed when replicate observations are available.
Audit Trail	Raw data, all data processing steps incl. metadata and dependency files, corrections, reference standard and background measurements are stored for validation and re-processing purposes.

Applications

Package	Volume (example)	Use Case
Pilot study	5–50 samples	First-time evaluation. Validate method for your materials. Validate sensitivity to targets before scaling.
Pharmaceutical solid-form screening	100–1,000 samples	Polymorph identification, salt/co-crystal screening, assessment of amorphous solid dispersions.
Battery materials development	100–5,000 samples	Cathode/anode phase purity, degradation studies, solid-solution mapping, nanoparticle characterisation, hard carbon anodes, solid electrolytes.
Catalysts & advanced materials	100–5,000 samples	Active phase identification, support characterisation, structure-activity correlation.
AI/ML training datasets	1,000–50,000+ samples	High-quality, standardised diffraction patterns for training machine learning models. Combine with phase analysis and structure refinements for data enrichment by labeling with quantitative structural values.
QC & production monitoring	Recurring	Ongoing phase purity checks. Validation of in-line QC. Meta-analysis on production variations. 12-month credit-based purchasing available.
White Label Solution for Laboratories and Consultants	By arrangement	Overflow capacity. White-label available. High-throughput capacity and high sensitivity data for projects out-of-scope with local infrastructure.

Output & Deliverables

Deliverable	Format	Description
Raw data	Raw data images (.tif or .edf)	2D images generated during the measurement–contains information about powder scattering behaviour and can be reprocessed from scratch.
Experimental metadata	Detector definition and mask files (.edf or .npy), calibration file (.poni), integration parameters	All files and information needed to reprocess the 2D images if desired.
Processed data	Integrated, corrected, and background subtracted data (.xye)	1D datasets: scattering intensity as a function of 2θ or Q. Intermediate files are provided to show the effects of different corrections steps. Target datasets are directly ready for analysis and reporting. Correction steps can be re-run for validation.
Pair distribution function data	Normalised and transformed datasets (.iq, .sq, .fq, .gr).	PDF data are generated using PDFgetX3 software. Parameter values are provided in metadata headers and can be rapidly adjusted and re-run as needed.
Experimental reports	.pdf document	Provided with every measurement set. Presents the measurement calibration and validation details. Plots data with available processing parameter sets and provides analysis advice based on data quality metrics.
Refinement starter files	TOPAS input file (.inp) for Rietveld refinement and PDFgui (.ddp3) for PDF refinement of reference standards.	Files provide all instrumental parameter settings and refinement setup details—can be used as starter files for further refinements of target datasets.
Technical reports	.pdf document	Analysis results, data comparison and refinement fit plots. Statistical analysis, etc. depending on project requirements. Custom formats possible by discussion.
Custom formats	On request	Additional charges may apply for custom formats.

How It Works

Step	What Happens	Time
1. Ship	Send your samples using an international courier. No special preparation needed for standard powders.	—
2. Measure	Synchrotron PXRD on automated high-throughput beamline.	Depending on scheduled capacity. Average < 14 days for smaller batches.
3. Assess	Data and experimental reports are returned for general assessment and planning of next steps.	Available within 1–2 days of experiment.
4. Analyse (optional)	Rietveld refinement. Full phase ID & quantification. PDF refinement. Small-angle scattering analysis. QAQC.	Report in days to weeks depending on project scope.

Return on Investment

The economic case for synchrotron-quality PXRD is compelling across industries.

Pharmaceutical R&D — Solid-Form Screening

Typical cost of a failed polymorph in late-stage development	$50M–$100M+
MT Screening Campaign (500 samples)	€80,000
Identifying one critical polymorph or amorphous form early	Avoids reformulation, regulatory delay, patent risk
Value	One prevented failure pays for decades of screening

Ritonavir. Rotigotine. The cost of a missed polymorph is measured in product recalls and lost years. Reduce risk by testing polymorph formation under more conditions and screening formulation effects over a wider parameter space.

Battery Materials — Cathode / Anode Development

Typical cathode development programme (lab to pilot)	€2M–€10M
MT Development Campaign (1,000 samples)	€150,000
Identifying degradation phases, solid-solution boundaries, or impurity phases 6 months earlier	€500K–€2M in accelerated time-to-market
ROI	3–13× on analytical investment alone

NMC, LFP, hard carbon anodes, solid-state electrolytes — every generation demands atomic-level understanding of phase evolution. We deliver it at scale.

AI / ML Training Data

Enriched dataset (10,000 standardised patterns plus phase and structure property labels)	€1,000,000
Value of a curated, synchrotron-quality training dataset	Unique. Not available from any other commercial source
Competitive advantage	Synchrotron data outperforms lab data in information content and can be provided at statistically meaningful quantities for AI/ML applications.

High signal-to-noise. Consistent geometry. Minimal artefacts. The cleanest diffraction data available — exactly what your algorithms need.

Process Optimization

Enriched dataset (1,000 standardised patterns plus phase and process parameters)	€180,000
Identify changes in precursors and process outputs	Reduce process fluctuations and optimize performance.
Competitive advantage	Synchrotron data outperforms lab data in information content and can be provided at statistically meaningful scales.

High signal-to-noise. Consistent geometry. Minimal artefacts. The cleanest diffraction data available — track changes in output in high resolution and correlate them with process parameters.

Pricing — Measurement + Semi-Quantification

Standard powder samples. Full quantification, PDF analysis, and statistical analysis available as add-ons.

Samples	Approx. Cost	Approx. Cost Per Sample
5	€2,500	€500
10	€5,000	€500
30	€8,000	€267
50	€10,000	€200
100	€18,000	€180
300	€50,000	€167
500	€80,000	€160
1,000	€150,000	€150
5,000	€600,000	€120

12-month credit-based purchasing available for recurring programmes. Contact us for a custom quote.

Radically better XRD

5 to 5,000+ samples · ×200 better signal-to-noise ratio · reliable turnaround time · full analysis

Frequently Asked Questions

Can you install this at our site?

No. Synchrotron PXRD requires a particle accelerator nearly a kilometer in circumference — that's what gives it 1,000,000× the photon flux of a lab source. You ship samples; we return data. No CAPEX, no maintenance, no expert team on your side required.

Can turnaround be faster than listed?

Yes. Faster turnaround for special projects or regular recurring needs can be arranged with appropriate lead times.

Are the data sufficient for crystal structure solution using powder diffraction?

Yes, absolutely. The combination of high *Q*- and *d-spacing* resolution combined with accurate experimental background removal provide excellent data for structure solution. Correction of offset artifacts using NIST standards leads to high indexing accuracy. Low angle signals allow for capturing peaks due to very large unit cells such as for MOFs and COFs.

Can I quantify amorphous content without adding an internal standard?

There are various methods for amorphous quantification. We regularly apply the degree of crystallinity method for semi-quantitative analysis of amorphous content, and quantitative analysis can also be performed using PONKCS-style using reference measurements if the amorphous content can be isolated. Nevertheless, the internal standard method is generally the most straightforward approach for fully quantitative analysis. The Rietveld method normalises the total crystalline content described within the model to the known internal calibrant allowing the remaining fraction to be partitioned as the amorphous component.

Do you handle air-sensitive samples?

Yes. Moisture-sensitive and oxidising materials can be handled and prepared in an argon glove-box (O_2 and H_2O levels below 0.1 ppm). The sample holders are prepared with additional sealing on the windows before removal and kept under inert gas until just before the measurement. Air sensitivity should be indicated when submitting a request. Note, materials that react violently in air such as pyrophoric materials are not appropriate for our setup.

Do you report elemental composition?

If desired, we can propagate the elemental composition associated with the crystalline phases for comparison to other data. Note that this does not include the elements associated with amorphous or unidentified contents, and may not be sensitive to occupational doping in various cases. However, if you provide elemental analysis to us such as from ICP, XRF, CHN(O)S, EDX, etc., it can significantly enhance the reliability of phase identification and potentially enable us to constrain the composition of the amorphous phase.

What about confidentiality?

All data are treated under strict NDA unless designated otherwise. Sample details, materials, and results are never shared without written consent.

Do you work with hazardous samples?

All hazards should be stated when submitting a request. We don't accept samples requiring procedures beyond standard PPE and laboratory safety controls (e.g., fume hood, glove box, lab coat, safety goggles, gloves, mask/respirator). This typically precludes samples classified as highly toxic/poisonous, radioactive, explosive, carcinogenic/mutagenic/reprotoxic (CMR), highly reactive, or biological (e.g., animal tissues, genetic materials). If your sample might present a significant hazard, please contact us first to discuss.

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