

D8 Series

• User Manual

Instrument Performance Verification Booklet D8 ADVANCE / D8 DISCOVER / D8 ENDEAVOR

Original Instructions

Innovation with Integrity

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We have checked the contents of this manual for agreement with the hardware and software described. Since deviations cannot be precluded entirely, we cannot guarantee full agreement. However, the data in this manual are reviewed regularly and any necessary corrections are included in subsequent editions. Suggestions for improvement are welcome.

All configurations and specifications are subject to change without notice.

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1 Introduction

This guidance outlines procedures recommended by Bruker AXS for instrument verification. The procedures described apply to all Bruker AXS D8 ADVANCE, D8 DISCOVER, and D8 ENDEAVOR diffraction systems used for X-ray powder diffraction analysis in reflection mode and fully cover the functionality of all validation relevant components of these diffraction systems as provided in the following table.

Table 1.1: Diffraction systems and verification relevant components. Some combinations of accessories might not be available. For details refer to the detailed tables in section Appendices A to I [> 20]

	Bragg-Brentano Systems		Parallel Beam Systems
Diffractometer	D8 ADVANCE ¹⁾	D8 ENDEAVOR ²⁾	D8 ADVANCE ¹⁾
	D8 DISCOVER		D8 DISCOVER
Anode	Cu, Co	Cu, Co	Cu, Co
Goniometer	Theta / 2Theta	Theta / Theta	Theta / 2Theta
	Theta / Theta		Theta / Theta
Sample stage	Standard	Rotating	Standard
	Rotating		Rotating
	FLIP-STICK		FLIP-STICK
	AUTO CHANGER		AUTO CHANGER
	Centric Eulerian cradle		Centric Eulerian cradle
	Compact cradle		Compact cradle
	Compact cradle ^{plus}		Compact cradle ^{plus}
	UMC 150, UMC 150 HTS,		UMC 150, UMC 150 HTS,
	UMC 151, UMC 1516		UMC 151, UMC 1516
	Compact UMC		Compact UMC
Monochromati-	Focusing monochromator	Kβ-Filter	Primary Göbel mirror
sation:	Secondary monochromator	Discriminator settings	(60 mm)
	Kβ-Filter	(LYNXEYE XE-I)	Primary I WIN / I RIO
	Discriminator settings		Discriminator settings
			(LYNXEYE XE-T)
Slits:	Fixed divergence and	Fixed or variable	Fixed slits
	antiscatter slits	divergence slit ³⁾	Primary axial Soller slit
	antiscatter slits	air scatter screen ⁴⁾	Secondary equatorial Soller slit
	Variable divergence slit and air scatter screen	Variable divergence slit and air scatter screen ⁴⁾	Secondary TWIN optics of the PATHFINDER
	Fixed divergence slit and	Primary axial Soller slit	
	air scatter screen	Secondary axial Soller slit	
	Primary axial Soller slit		
	Secondary axial Soller slit		
	Receiving slit		
	TWIN / TRIO optics		

	Bragg-Brentano Systems		Parallel Beam Systems	
Diffractometer	D8 ADVANCE ¹⁾ D8 DISCOVER	D8 ENDEAVOR ²⁾	D8 ADVANCE ¹⁾ D8 DISCOVER	
Detector	Scintillation counter	LYNXEYE XE	Scintillation counter	
	Solid state detector (SOL-XE)	LYNXEYE XE-T LYNXEYE-2	Solid state detector (SOL-XE)	
	Linear detector VÅNTEC-1	SSD160-2	Linear detector VÅNTEC-1	
	Linear detector LYNXEYE / LYNXEYE-2 / LYNXEYE XE / LYNXEYE XE-T / SSD160 / SSD160-2		Linear detector LYNXEYE / LYNXEYE -2 / LYNXEYE XE / LYNXEYE XE-T / SSD160 / SSD160-2	
	EIGER2 R 500K		EIGER2 R 500K	
¹⁾ Including D8 ADVANCE ECO				

²⁾ Including D8 ENDEAVOR ECO

³⁾Adjustment knife edge required

⁴⁾ Including motorized and manual air scatter screen

1.1 Performance Verification Levels

For instrument verification three performance verification levels are defined, which cover the functionality of all relevant components of the diffraction system under investigation.

Measurement and evaluation procedures for each test level are detailed in section *Procedures* [> 9]. Protocol templates for full documentation are provided in the *Appendices A to I* [> 20].

Factory Acceptance Test

The factory acceptance test is performed at the manufacturer's site and designed to guarantee the perfect performance of the system after its initial assembling.

Customer Acceptance Test

The customer acceptance test is identical to the factory acceptance test but performed at the customer's site and guarantees the perfect condition of the system after delivery and installation. The customer acceptance test procedure should be also performed after instrument repairs or when the setup of the instrument has been modified.

Daily check

The daily check routine is a procedure to routinely check that the instrument is operating within specified limits.

1.2 Performance Verification in GxP Regulated Areas

GxP is a general term for *Good Practice* quality guidelines and regulations. These guidelines are used in many fields, including the pharmaceutical and food industries.

The titles of these good practice guidelines usually begin with "Good" and end in "Practice", with the specific practice descriptor in between. GxP represents the abbreviations of these titles, where x (a common symbol for a variable) represents the specific descriptor. Examples are GMP for *Good Manufacturing Practice* and GLP for *Good Laboratory Practice*.

Performance specification and verification are mandatory parts of the equipment qualification (EQ) process as defined by **GxP** regulations. If your laboratory is not required to comply with **GxP** regulations you may skip this section.

For instrument qualification Bruker AXS recommends the adaptation of the specifications and procedures provided in this booklet into your in-house EQ system according to the following schema:

Table 1.2: Instrument performance verification as part of equipment qualification

Performance Verification	Equipment Qualification		
Specifications (reference values, section 3)	Design Qualification	Defines the functional and operational specifications	
	Installation Qualification	Establishes that the instrument is received as designed and specified and that it is properly installed	
Customer Acceptance Test	Operational Qualification	Demonstrates that the instrument will function according to the operational specifications	
Daily Check	Performance Qualification	Demonstrates that the instrument will function according to a specification appropriate to its routine use	

Introduction

2 **Procedures**

For instrument verification the following three parameters are to be evaluated:

- 1. line position
- 2. relative line intensity, and
- 3. line shape.

In the following sections a standard operating procedure (SOP) is described which is valid for all performance verification levels as described in section *Performance Verification Levels* [> 6]. This procedure comprises the following steps, details of which are described in the following four sections:

Process	Section
Insertion of the standard reference sample	Certified Reference Material [9]
Setting of given instrument parameters	Instrument Parameters [> 9]
Measurement of the standard reference sample using given measurement parameters	Measurement Parameters [▶ 11]
Data evaluation and comparison of the results with specifications	Evaluation Procedures and Data Interpretation [▶ 12]

The instrument and measurement parameters to be used for the different instrument performance tests have been carefully selected to allow accurate, meaningful and holistic instrument verification within finite time. Therefore the instrument and measurement parameters provided here can be regarded as a recommendation for routine use of the instrument.

An instrument passing all tests with respect to line position, intensity and shape is automatically fit for all kinds of X-ray analysis.

For GxP regulated laboratories Bruker AXS recommends to use the procedures provided in this chapter as a base for the creation of in-house SOPs.

2.1 Certified Reference Material

The certified reference material to be used is based on the NIST standard reference material SRM1976c [1] and is delivered with each diffraction system.

This reference material is also recommended for instruments operated in transmission mode, although only suited for reflection measurements: Instruments must be switched to reflection mode for verification purposes.

2.2 Instrument Parameters

For Bragg-Brentano systems the instrumental parameters listed in the first table below are used.

For parallel beam systems equipped with a Göbel Mirror the instrument parameters to be selected depend on the length of the mirror. For 40 mm Göbel mirrors (e.g. in the TWIN optics) the required instrument parameters are provided in the second table, for 60 mm Göbel mirrors in the third table.

Instrument Parameter	Value	Value
Generator settings	Cu: 40 kV / 40 mA ^{3) 5)}	Cu: 40 kV / 40 mA ^{3) 5)}
	Co: 35 kV / 40 mA ⁽³⁾⁽³⁾	Co: 35 kV / 40 mA ^{3/3/}
	0.3° (approx. 0.6 mm)	0.3° (approx. 0.6 mm)
Axial Soller slits Primary	2.5°	2.5°
Secondary	2.5°	2.5°
Antiscatter slit ¹⁾ (only 0D detectors)	0.3° (approx. 0.6 mm)	-
Air scatter screen		Automatic mode for motorized air scatter screen
		Approx. 4 mm above the sample for manual scatter screen
Kβ filter ²⁾	12.5 μm (20 μm ⁴⁾)	12.5 µm (20 µm ⁴⁾)
Receiving slit for 0D detectors	0.1 mm	0.1 mm
Linear detector VÅNTEC-1	3° detector opening	3° detector opening
	no Debye slit	no Debye slit
	(see corresponding User Manual)	(see corresponding User Manual)
Linear detector LYNXEYE / LYNXEYE-2 / LYNXEYE XE /	3° detector opening in all available directions,	3° detector opening in all available directions
LYNXEYE XE-T ^{6) 7)} / SSD160 /	antiscatter slit max. opening	
Linear detector EICEP2 P E00(⁸⁾	(see corresponding User Manual)	
	exact value might be chosen slightly smaller in case of instrumental restrictions	

Table 2.1: Instrument parameters for Bragg-Brentano systems (incl. TWIN / TRIO Bragg-Brentano setting)

¹⁾ Variable slits must be operated in fixed mode.

²⁾ If no secondary monochromator is used, a suited K β -filter must be fitted (Ni-Filter for Cu-radiation, Fe-Filter for Co-radiation). No filter is used for focusing monochromator settings.

³⁾ Valid for long fine focus X-ray tubes.

⁴⁾ For LYNXEYE, SSD160, LYNXEYE-2, SSD160-2, VÅNTEC-1, and EIGER2 R 500K

⁵⁾ In case of D8 ADVANCE ECO or D8 ENDEAVOR ECO Cu: 40 kV / 25 mA ; Co: 35 kV / 28 mA

⁶⁾Use Discriminator Detector Settings and Veto Values for High Resolution mode

⁷⁾ A Temperature Stability of \pm 1 K for the detector environment is required.

⁸⁾EIGER2 R 500K in 1D mode; Energy threshold mode setting is set to automatic mode.

Table 2.2: Instrument parameters for parallel beam systems with 40 mm Göbel mirrors in primary TWIN / TRIO optics

Instrument Parameter	Value	
Generator settings	Cu: 40 mA / 40 kV ^{1), 2)}	
	Co: 35 mA / 40 kV ^{1),2)}	
Radiation safety slit holder	1 mm	
Göbel mirror with axial Soller slit	2.5°	
Equatorial Soller slit 0.2°		
¹⁾ Valid for long fine focus X-ray tubes, ²⁾ In case of D8 ADVANCE ECO or D8 ENDEAVOR ECO Cu: 40 kV / 25 mA ; Co: 35 kV / 28 mA		

Table 2.3: Instrument parameters for parallel beam systems with 60 mm Göbel mirrors

Instrument Parameter	Value	
Generator settings	Cu: 40 mA / 40 kV ^{1) 2)}	
	Co: 35 mA / 40 kV ^{1), 2)}	
Radiation safety slit holder	1.2 mm	
Göbel mirror with axial Soller slit	2.5°	
Equatorial Soller slit	0.2°	
¹⁾ Valid for long fine focus X-ray tubes, ²⁾ In case of D8 ADVANCE ECO or D8 ENDEAVOR ECO Cu: 40 kV / 25 mA ; Co: 35 kV / 28 mA		

2.3 Measurement Parameters

Measurement parameters to be used are listed in the first table for Cu radiation and in the second table for Co-radiation, respectively. Depending on specific measurement setups, individual reflections may not be measurable. Continuous sample rotation speed of 15 rpm is recommended. For statistical reasons each peak requires a minimum of 1000 counts at the peak maximum, step times must be adjusted accordingly.

Reflection hkl	Scan angles 20 [°] ¹⁾	Step width 20 [°] ¹⁾	Step time [s] ¹⁾
012	24.7 - 26.2	0.005	5
104	34.0 - 36.2	0.005	3
0 2 10	88.1 - 89.7	0.01	40
1 3 10	126.4 - 129.0	0.02	40
¹⁾ For linear detectors measure all reflections in one uninterrupted range (from 20° to 130° in 2Theta) with smallest possible step width and step time 0.5 s. For LYNXEYE /			

Table 2.4: Measurement parameters for Cu radiation

¹⁾ For linear detectors measure all reflections in one uninterrupted range (from 20° to 130 in 2Theta) with smallest possible step width and step time 0.5 s. For LYNXEYE / LYNXEYE XE / LYNXEYE XE-T / SSD160 / LYNXEYE-2 / SSD160-2 and EIGER2 R 500K use step size of 0.005 and step time 0.5 s. For evaluation limits use values given as scan angles for point detector.

Reflection hkl	Scan angles 20 [°]	Step width 20 [°] ¹⁾	Step time [s] ¹⁾
012	29.2 - 30.4	0.005	20
104	40.3 - 41.8	0.005	8
300	80.8 - 81.9	0.01	50
226	117.2 - 119.4	0.02	100

Table 2.5: Measurement parameters for Co radiation

¹⁾ For linear detectors measure all reflections in one uninterrupted range (from 28° to 120° in 2Theta) with smallest possible step width and step time 1 s. For LYNXEYE / LYNXEYE XE / LYNXEYE XE-T / SSD160 / LYNXEYE-2 / SSD160-2 and EIGER2 R 500K use step size of 0.005 and step time 0.5 s. For evaluation limits use values given as scan angles for point detector.

2.4 Evaluation Procedures and Data Interpretation

Line positions, intensities and shapes are determined using the **Area** feature of the program DIFFRAC.EVA, which is part of each DIFFRAC.SUITE package supplied with the diffraction system. To learn how to use EVA and its **Area** function please refer to the DIFFRAC.EVA User Manual.

Please note, that the evaluation procedure is slightly different for instruments with and without primary beam monochromator.

2.4.1 Instruments with Primary Beam Monochromator

For instruments with primary beam monochromator ($K_{\alpha 1}$) the following evaluation steps have to be performed:

- 1. Start EVA and load the .brml / .raw data to be evaluated.
- Select the Area page and create a new area using the <u>complete</u> measured range. For linear detectors use exactly the ranges defined by table 2.4 and table 2.5 in section <u>Measurement Parameters [▶ 11]</u>.
 - Note the following data as displayed in the toolbox: Line position : Obs. Max Line intensity : Net Area Line shape : FWHM

2.4.2 Instruments Without Focusing Monochromator

For instruments without primary beam monochromator the impact of the $K_{\alpha 2}$ component of the radiation emitted by the X-ray source has to be taken into account. In order to achieve line intensities as accurate as possible, the complete $K_{\alpha 1, 2}$ doublet must be used. The determination of line position and shape has to be performed on $K_{\alpha 1}$ only; therefore $K_{\alpha 2}$ has to be stripped off before calculating both parameters.

Accordingly, the following routine has to be performed:

- 1. Start EVA and load the .brml / .raw data to be evaluated.
- Select the Area page and create a new area using the <u>complete</u> measured range. For PSD use exactly ranges as defined by table 2.4 and table 2.5 in section *Measurement Parameters* [▶ 11].
 - Note the following data as displayed in the toolbox: Line intensity: Net Area
- 3. Perform a $K_{\alpha 2}$ stripping. Ensure a properly adjusted $K_{\alpha 1}/K_{\alpha 2}$ -ratio to minimize artifacts.
- 4. Create a new area using the <u>complete</u> measured range. For PSD use exactly ranges as defined by table 2.4 and table 2.5.
 - Note the following data as displayed in the toolbox: Line position: Obs. Max Line shape: FWHM

3 Reference Values

3.1 Angular Accuracy and Instrument Response

The following tables 3.1 and 3.2 list the reference values of peak positions and relative intensities including error bars for four reflections of the Corundum calibration sample to be measured. The Corundum plate is Bruker AXS's selected calibration sample, produced from a NIST SRM1976c origin to fit to a large variety of sample stages, as it is very stable, robust, long lasting, and does not require any preparation. The certificate is dedicated to Cu-radiation. However, Bruker AXS uses the d-spacing of this standard also for verifying angular accuracy (line-position and FWHM) for Co-radiation.

Line positions for Parallel Beam Geometry differ from Bragg-Brentano because of following reasons:

NIST SRM1976c includes certified lattice parameters derived from Bragg-Brentano measurements. Line positions can be calculated according Bragg's law taking into account geometrical aberrations defined by the instrumental setup (cf. reference [2] in References). These geometrical aberrations are namely:

- Width of X-ray source
- Flat specimen error
- · Width of receiving slit / spacing of equatorial Soller slit
- · Specimen transparency
- Axial divergence

For Bragg-Brentano Geometry, incl. TWIN / TRIO Bragg-Brentano Geometry, instrumental parameters (slits, axial Sollers: refer to section *Glossary* [> 20]) have been selected to realize a high resolution setup, reducing influences on Bragg's-Law below 0.005°.

For Parallel Beam Geometry geometrical aberrations are reduced to

- · Spacing of horizontal Soller slit
- Axial divergence

Instrumental parameters for Parallel Beam Geometry, incl. TWIN / TRIO Parallel Beam Geometry, have been optimized regarding X-ray flux by allowing especially for larger axial divergence. Therefore, the parallel beam geometry and obtained asymmetric peak shapes result in shifted values for the line position **Obs. Max**, when compared to Bragg-Brentano measurements.

Reference values for line positions and relative intensities are listed in table 3.1 for Cu-radiation and table 3.2 lists the line positions for Co-radiation.

In the case of Bragg-Brentano, influences from geometrical aberrations on line positions can be neglected. Reference values for Parallel Beam Geometry require, among others, correction for axial divergence. The listed reference values take this into account.

Depending on specific measurement setups, individual reflections may not be measurable. In those cases measurements must be restricted to accessible reflections.

Reflection hkl	Line position 20 [°] Bragg-Brentano	Line position 20 [°] Parallel Beam	Relative intensity (Net area rounded to 2 decimal place)
012	25.575	25.561	23.88
104	35.148	35.137	100.00
0 2 10	88.989	88.996	12.29
1 3 10	127.670	127.692	14.85

Table 3.1: Reference values for line positions and relative intensities for Cu-radiation (CuK_{a1}: $\lambda = 0.154059 \text{ nm}$)

Table 3.2: Reference values for line positions (without absorption correction) for Co-radiation (CoK_{α_1}: $\lambda = 0.178897$ nm)

Reflection hkl	Line position 2θ [°] Bragg-Brentano	Line position 2θ [°] Parallel Beam
0 1 2	29.786	29.773
104	41.049	41.041
300	81.247	81.250
226	118.142	118.165

3.1.1 Basic Setup (Bragg-Brentano, dedicated and TWIN / TRIO Optics)

The basic reference position of the D8 system is set in Bragg-Brentano geometry at factory. This must finally be done/checked in the **Configuration** plugin of the MEASUREMENT SUITE:

- 1. Theta-Theta: MotorizedDrives/Inner_Circle_Motor | Reference Position according Acceptance Test Protocol
- 2. Theta-2Theta: MotorizedDrives/Outer_Circle_Motor | Reference Position according Acceptance Test Protocol
- 3. This **Reference Position** must be saved to data base of the MEASUREMENT SUITE by the **Save configuration to data base** of the **Configuration** plugin.
 - The software will ask for a name for this configuration. The name is Instrument Verification Factory.
- 4. Save and activate this setting.

3.1.2 Additional Setups (Göbel Mirror, Parallel Beam TWIN / TRIO Optics)

Additional setups like different parallel beam setups with Göbel mirrors or the parallel beam path of the TWIN / TRIO optics have beam directions different from the basic Bragg-Brentano setup. Accordingly, this information must be added to the data base. The system takes this into account by the deflection angles of the optics. The value of the deflection angle is identical for theta-theta and theta-2theta systems. This must finally be done/checked in the **Configuration** plugin of the MEASUREMENT SUITE:

- 1. Göbel mirror: Goniometer/PrimaryTrack/GoebelMirror | Deflection angle according Acceptance Test Protocol
- 2. TWIN optics: Goniometer/PrimaryTrack/TWIN OPTICS/GoebelMirror | Deflection angle according Acceptance Test Protocol TRIO optics: Goniometer/PrimaryTrack/TRIO OPTICS/GoebelMirror | Deflection angle according Acceptance Test Protocol

- 3. The deflection angle must be saved to data base of the MEASUREMENT SUITE by the **Save configuration to data base** of the **Configuration** plugin.
 - The software will ask for a name for this configuration. The name is Instrument Verification Factory. Saving will update the older factory configuration defined with basic setup.
- 4. Save and activate this setting.

3.1.3 Factory and Customer Acceptance Test Protocol

The deviation is given by the angular difference between measured peak position and reference value given in Table 3.1 and Table 3.2.

The shift is defined as the difference between minimum and maximum deviation. If the shift is within the allowed range but the deviation is out the specified value, offset is corrected. This ensures that the deviations are in the specified accuracy specifications.

The accuracy of the tested equipment is the maximum measured deviation after offset correction.

The configuration must be saved to the database:

- 1. Insert **Instrument Verification Factory / Customer**, when asked for a configuration name by the software.
- 2. Save and activate this setting.

3.2 Instrument Resolution

Maximum values for line shape in terms of **FWHM** (Full Width at Half Maximum) are listed in the following two tables. Please note, that these values are dependent on the instrument geometry, on the detector type, and on the anode material employed.

Table 3.3: Maximum allowed values for the line shape in terms of FWHM (Cu-radiation). SC: scintillation counter, SOL-XE: energy dispersive solid state detector, position sensitive detector VÅNTEC-1, SSD160, LYNXEYE / LYNXEYE XE / LYNXEYE XE-T, LYNXEYE-2, SSD160-2 and EIGER2 R 500K

Reflection hkl		Parallel Beam (Göbel Mirror)					
	SC / SOL-XE [°]	VÅNTEC-1 [°]	LYNXEYE / LYNXEYE XE / LYNXEYE XE-T / SSD160 / LYNXEYE-2 / SSD160-2 EIGER2 R 500K [°]	SC / SOL-XE / LYNXEYE / LYNXEYE XE / LYNXEYE XE-T / SSD160 / LYNXEYE-2 / SSD160-2 ¹⁾ EIGER2 R 500K ²⁾ [°]			
012	0.055	0.07	0.06	0.22			
104	0.055	0.07	0.06	0.22			
0 2 10	0.10	0.10	0.10	0.22			
1 3 10	0.18	0.18	0.18	0.27			
¹⁾ LYNXEYE / mode	¹⁾ LYNXEYE / LYNXEYE XE / LYNXEYE XE-T / SSD160 / LYNXEYE-2 / SSD160-2 in 0D mode						

²⁾ EIGER2 R 500K in **0D** mode with 14 mm * 16 mm opening

Table 3.4: Maximum allowed values for the line shape in terms of FWHM (Co-radiation). SC: scintillation counter, SOL-XE: energy dispersive solid state detector, position sensitive detector VÅNTEC-1, SSD160, LYNXEYE / LYNXEYE XE / LYNXEYE XE-T, LYNXEYE-2, SSD160-2 and EIGER2 R 500K

Reflection hkl		Bragg-Brent	ano	Parallel Beam (Göbel Mirror)		
	SC / SOL-XE [°]	VÅNTEC-1 [°]	LYNXEYE / LYNXEYE XE / LYNXEYE XE-T / SSD160 / LYNXEYE-2 / SSD160-2 EIGER2 R 500K [°]	SC / SOL-XE / LYNXEYE / LYNXEYE XE / LYNXEYE XE-T / SSD160 / LYNXEYE-2 / SSD160-2 ¹⁾ EIGER2 R 500K ²⁾ [°]		
012	0.06	0.10	0.06	0.22		
104	0.06	0.10	0.06	0.22		
300	0.10	0.11	0.10	0.22		
226	0.18	0.18	0.18	0.27		
¹⁾ LYNXEYE / LYNXEYE XE / LYNXEYE XE-T / SSD160 / LYNXEYE-2 / SSD160-2 in 0D mode						

²⁾ EIGER2 R 500K in **0D** mode with 14 mm * 16 mm opening

For Parallel Beam Geometry the 0.2° equatorial Soller is used as standard and optimum set up. If different equatorial Sollers are used, **FWHM** values will increase accordingly.

4 References – Glossary – Appendices A to I

4.1 References

[1] NIST, National Institute of Standards and Technology, Standard Reference Materials Program, Gaithersburg, MD 20899-001, USA, *http://www.nist.gov*

[2] R. W. Cheary, A. A. Coelho, J. P. Cline, Journal of Research of the National Institute of Standards and Technology **109**, 1-25 (2004): "Fundamental Parameters Line Profile Fitting in Laboratory Diffractometers"

Table 4.1: Referenced documents

Document Title	Document Number
D8 ADVANCE Pre-Installation Guide (for installations in North America)	DOC-M88-EXX046
D8 ADVANCE Introductory User Manual (for installations outside North America)	DOC-M88-ZXX146
D8 Series D8 ADVANCE / D8 DISCOVER User Manual Vol. 1	DOC-M88-EXX153
D8 ADVANCE Supplement Folder	DOC-M88-ZXX152
D8 DISCOVER Pre-Installation Guide (for installations in North America)	DOC-M88-EXX008
D8 DISCOVER Introductory User Manual (for installations outside North America)	DOC-M88-ZXX151
D8 DISCOVER User Manual Vol. 2	DOC-M88-EXX162
D8 DISCOVER Supplement Folder	DOC-M88-EXX163
D8 Series IQ OQ PQ for D8 ADVANCE / D8 DISCOVER	DOC-M88-EXX160
D8 ENDEAVOR IQ OQ PQ	DOC-M88-EXX265
LYNXEYE and SSD160 User Manual	DOC-M88-EXX095
LYNXEYE XE User Manual	DOC-M88-EXX240
LYNXEYE-2 User Manual	DOC-M88-EXX305
SSD160-2 User Manual	DOC-M88-EXX306
LYNXEYE XE-T User Manual	DOC-M88-EXX239
EIGER2 R 500K User Manual	DOC-M88-EXX293
VÅNTEC-1	DOC-M88-EXX072
Solid state detector (SOL-XE)	DOC-M88-EXX113
MEASUREMENT.CENTER DIFFRAC.SUITE User Manual	DOC-M88-EXX191
MEASUREMENT.CENTER DIFFRAC.SUITE Installation Guide	DOC-M88-EXX190
DIFFRAC.SUITE Evaluation Package User Manual	DOC-M88-EXX200
DIFFRAC.SUITE EVA Tutorial	DOC-M88-EXX201

4.2 Glossary

Certified reference material	A reference material, accompanied by a certificate, one or more of whose property values are certified by a procedure, which establishes its traceability to an accurate realization of the unit in which the property values are expressed, and for which each certified value is accompanied by an uncertainty at a stated level of confidence.
Testing	A technical operation that consists of the determination of one or more characteristics of performance of a given product, material equipment, organism, physical phenomena, process or service according to a specified procedure.
Validation	Establishing documented evidence that provides a high degree of assurance that a specific process will consistently produce a product meeting its predetermined specifications and quality attributes.
Verification	Confirmation by examination and provision of evidence that specified requirements have been met.
	Performance verification of analytical instrumentation is the process of comparing test results with specifications / acceptance criteria and ends with the sign-off of a "Declaration of Conformity" of the instrument to specifications / acceptance criteria.

4.3 Appendices A to I

A. Factory Acceptance Test Protocol templates for Cu radiation, Bragg-Brentano

B. Factory Acceptance Test Protocol templates for Co radiation, Bragg-Brentano

C. Factory Acceptance Test Protocol templates for Cu radiation, Parallel Beam

D. Factory Acceptance Test Protocol templates for Co radiation, Parallel Beam

E. Customer Acceptance Test Protocol templates for Cu radiation, Bragg-Brentano

F. Customer Acceptance Test Protocol templates for Co radiation, Bragg-Brentano

- G. Customer Acceptance Test Protocol templates for Cu radiation, Parallel Beam
- H. Customer Acceptance Test Protocol templates for Co radiation, Parallel Beam

I. Daily check protocol template

A. Factory Acceptance Test **Protocol**

Declaration of Conformity

Bragg-Brentano Geometry with Copper Anode

NIST SRM1976c Sample: Cu

Anode:

Customer Name:	
Customer PO Number:	
Serial Number:	SAP Number (Sales Order Number):

This protocol details the results of the factory acceptance test procedure for Bruker AXS diffraction systems in Bragg-Brentano reflection geometry. The factory acceptance test procedure consists in full-profile measurements of the certified NIST standard reference material SRM1976c. Details of this procedure are outlined in the Instrument Verification Booklet, which is part of the instrument documentation.

The present verification routine covers the functionality of all relevant components of the diffraction system under investigation.

System w	YES NO					
Tested by	/:					
Name, first name:						
Testing approval: I, an authorized Bruker Employee, acknowledge that the aboreferenced system has been tested and demonstrates functionality that meets customer order specifications in accordance with mutually agreed terms.				ge that the above ality that meets eed terms.		
Date:		Signature:				
Test Supe	Test Supervisor:					
Name, first name:						
Date:		Signature:				

Part I: Instrument Details (D8 Series)

	Instrument Details			Set Values for Validation		
Diffractome- ter	D8 ADVANCE ¹⁾			Tube Power: 4 Tube Power: 4	40 kV / 40 mA (fe 40 kV / 30 mA (fe	or FL tubes) ²⁾ or FF tubes) ²⁾
Vertical goniometer	Theta/Theta Theta/2Theta					
	Height: 150					
	Radius: Primary radius Secondary radius	[mm]				
Sample stage	Standard					
	Rotating					
	FLIP-STICK			Sample position	on 5	
	AUTO CHANGER			Sample position	on A1	
	Compact Cradle / Co Cradle ^{Plus}	mpact				
	Compact UMC					
Monochro-	Kβ-Filter					
matisation	Secondary monochro	hromator				
	Focusing monochrom	nator				
				Copy values from High Resolution mode:		ition mode:
	LYNXEYE XE-T)			Low Thr. [V]	High Thr. [V]	Veto Thr. [V]
Slits	Fixed divergence slit			Divergence slit: 0.3° (approx. 0.6 mm)		0.6 mm)
	Fixed antiscatter slit			Antiscatter slit: 0.3° (approx. 0.6 mm)		
	Variable divergence	slit		Divergence slit: 0.3° (approx. 0.6 mm)		
	Variable antiscatter s	slit		Antiscatter slit: 0.3° (approx. 0.6 mm)		
	Motorized air scatter	screen		Automatic mode		
	Primary axial Soller slit			Primary axial	Soller slit: 2.5°	
	Secondary axial Soller slit			Secondary axial Soller slit: 2.5°		0
	Receiving slit			Receiving slit	0.1 mm	

Instrument Configuration D8 ADVANCE

	Instrument Details			Set Values for Validation
Detector	Scintillation counter			
(See User	LYNXEYE, SSD160		LYN	XEYE User Manual DOC-M88-EXX095
ivianuais)	LYNXEYE XE		LYN	XEYE XE User Manual DOC-M88-EXX240
	LYNXEYE XE-T		LYN	XEYE XE-T User ManualDOC-M88-EXX239
	LYNXEYE-2	🔲 LYNXEYE-2 U		XEYE-2 User Manual DOC-M88-EXX305
	SSD160-2		SSE	0160-2 User Manual DOC-M88-EXX306
	Solid state detector (SOL-XE)		SOI	XE User Manual DOC-M88-EXX113
	VÅNTEC-1		VÅN	NTEC-1 User Manual DOC-M88-EXX072
	EIGER2 R 500K		EIG	ER2 R 500K User Manual DOC-M88-EXX293
¹⁾ including D8 ²⁾ 40 kV / 25 m/	ADVANCE ECO A in case of D8 ADVANCE ECO			

Instrument Configuration D8 DISCOVER

	Instrument Details	;		Set Values for Validation		
Diffractometer	D8 DISCOVER			Tube Power: 40 Tube Power: 40 TXS Power: 50 filament, line an TXS Power: 50 filament, spot fo	kV / 40 mA (fo kV / 30 mA (fc kV / 100 mA (fc d spot focus) kV / 22 mA (for cus)	r FL tubes) or FF tubes) or 0.3x3 mm ² 0.1x1 mm ²
Vertical goniometer	Theta/Theta Theta/2Theta					
	Height: 150 214 258					
	Radius: Primary radius Secondary radius	[m [m	m] m]			
Horizontal	Theta/2Theta					
goniometer	Height: 214 258					
	Radius: Primary radius Secondary radius	[m [m	m] m]			
Sample stage	Standard					
	Rotating					
	FLIP-STICK			Sample position 5		
	AUTO CHANGER			Sample position	A1	
	Compact Cradle/ Co Cradle ^{Plus}	ompact				
	Centric Eulerian Cra	adle				
	UMC 150/151/1516	/150 HTC				
	Compact UMC					
Monochroma-	Kβ-Filter					
tisation	Secondary monochromator					
	Focusing monochromator					
	Discriminator Settin	gs		Copy values fro	m High Resolut	ion mode:
	(LYNXEYE XE / LY	NXEYE XE-T)		Low Thr. [V]	High Thr. [V]	Veto Thr. [V]

	Instrument Details			Set Values for Validation		
Slits	Fixed divergence slit			Divergence slit: 0.3° (approx. 0.6 mm)		
	Fixed antiscatter slit			Antiscatter slit: 0.3° (approx. 0.6 mm)		
	Variable divergence slit			Divergence slit: 0.3° (approx. 0.6 mm)		
	Variable antiscatter slit			Antiscatter slit: 0.3° (approx. 0.6 mm)		
	Motorized air scatter screen			Automatic mode		
	Primary axial Soller slit			Primary axial Soller slit: 2.5°		
	Secondary axial Soller slit			Secondary axial Soller slit: 2.5°		
	Receiving slit			Receiving slit 0.1 mm		
Detector	Scintillation counter					
(See User Manuals)	LYNXEYE, SSD160		LYNXEYE User Manual DOC-M88-EXX095			
Mariuais)	LYNXEYE XE		LYN	XEYE XE User Manual DOC-M88-EXX240		
	LYNXEYE XE-T		LYNXEYE XE-T User ManualDOC-M88-EXX239			
	LYNXEYE-2		LYNXEYE-2 User Manual DOC-M88-EXX305			
	SSD160-2		SSI	SSD160-2 User Manual DOC-M88-EXX306		
	Solid state detector (SOL-XE)		SOL-XE User Manual DOC-M88-EXX113			
	VÅNTEC-1		VÅI	NTEC-1 User Manual DOC-M88-EXX072		
	EIGER2 R 500K		EIG	ER2 R 500K User Manual DOC-M88-EXX293		

	Instrument Detai	ls			Set Values for	or Validation	
Diffractometer	D8 ENDEAVOR ¹⁾				Tube Power: Tube Power:	40 kV / 40 mA (f 40 kV / 30 mA (f	or FL tubes) ²⁾ or FF tubes) ²⁾
Vertical	Theta/Theta						
goniometer	Height:						
	150						
	Radius:						
	200,5						
	Rotating				Sample positi	on A1	
Monochromati-	Kβ-Filter						
sation	Discriminator Settings (LYNXEYE XE / LYNXEYE XE-T)				Copy values f	rom High Resolu	ution mode:
					Low Thr. [V]	High Thr. [V]	Veto Thr. [V]
Slits	Fixed divergence				Divergence slit: 0.3° (approx. 0.6 mm)		
	Variable divergen	се			Divergence slit: 0.3° (approx. 0.6 mm)		
	Primary / secondary axial Soller slit				Primary and secondary axial Soller slit: 2.5°		
	Air Scatter Screen				Set mode to Automatic for motorized air scatter screen. Position the air scatter scree approx. 4 mm above the sample surface for manual air scatter screen or use adjustmen tool		
	LYNXEYE XE			LYI	LYNXEYE XE User Manual DOC-M88-EXX240		
	LYNXEYE XE-T			LYNXEYE XE-T User ManualDOC-M88-EXX239			
LYNXEYE-2		LYNXEYE-2 User Manual DOC-M88-EXX305			88-EXX305		
	SSD160-2			SSI	D160-2 User M	anual DOC-M88	3-EXX306
¹⁾ including D8 ENDEAVOR ECO ²⁾ 40 kV / 25 mA in case of D8 ENDEAVOR ECO							

Instrument Configuration D8 ENDEAVOR

Part II: Angular Accuracy, Instrument Response and Resolution (D8 Series)

Anode: Cu				Bragg-Brentano Geometry									
Angular Accuracy: Difference Reference Position corr				Instrument Response: I _{rel} Instr Res						Instru Reso	ument lution		
Maximum al	lowed 2θ de	viation depend	s on height		Maximum	allowed i	ntens	sity deviatio	n for point o	detectors	± 10%	$FWHM_{obs} <$	FWHM _{max}
2θ _{obs} [°]	Differ- ence	2θ _{obs} Reference Position corr	Difference Reference Position corr	2θ _{exp} ¹⁾ [°]	I _{obs}	I _{obs} I _{exp}		$I_{rel} = \frac{I_{obs}}{N}$	I _{min}	I _{exp} ¹⁾	I _{max}	FWHM _{obs} [°]	FWHM _{max} ²⁾ [°]
				25.575					21.49	23.88	26.27		
				35.148					90.00	100.00	110.00		
				88.989					11.06	12.29	13.52		
				127.670					13.37	14.85	16.34		
Reference F ½(Difference	Position corr e _{max} +Differer	nce _{min})									$Sum = \sum$	$\frac{l_{obs}}{l_{exp}}$, $i=1\ldots 4$	
Detector ³⁾	Current Re	ference Positic	n		Shift						N =	$=\frac{Sum}{4}$	
2-Theta ³⁾	Corrected (Current Re Position co	Reference Pos eference Positi rr)	tion on - Reference			Heig	ht	Maximum	allowed sh	ift 20 for	specified a	accuracy of:	
N: scaling fa	actor; For de ∕ <i>alues [</i> ▶ 15]	tails cf. chapter			Vertical	150			0,02°		± 0,0)1°	
obs: observe	ed					214			0,03°		± 0,0	15°	
exp: expecte	ed					258			0.04°		± 0,0)2°	
corr: correct	ed				Horizontal	214			0,02°		± 0,0)1°	
rel: relative						258			0,02°		± 0,0)1°	

¹⁾ see table 3.1. For linear detector configurations intensities might be outside allowed deviations for point detectors due to reasons explained in chapter Reference Values [▶ 15]; ²⁾ see table 3.3;

³⁾ mark applicable: detector in case of Theta/Theta and 2-Theta in case of Theta/2Theta; Depending on specific measurement setups, individual reflections may not be measurable. Then measurements must be restricted to accessible reflections.

comments		

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B. Factory Acceptance Test Protocol

Declaration of Conformity

Bragg-Brentano Geometry with Cobalt Anode

NIST SRM1976c Sample: Co

Anode:

Customer Name:	
Customer PO Number:	
Serial Number:	SAP Number (Sales Order Number):

This protocol details the results of the factory acceptance test procedure for Bruker AXS diffraction systems in Bragg-Brentano reflection geometry. The factory acceptance test procedure consists in full-profile measurements of the certified NIST standard reference material SRM1976c. Details of this procedure are outlined in the Instrument Verification Booklet, which is part of the instrument documentation.

The present verification routine covers the functionality of all relevant components of the diffraction system under investigation.

System w	YES NO					
Tested by	/:					
Name, firs	et name:					
Testing ap referenced customer	oproval: I, an au d system has be order specifica	thorized Bruker een tested and de tions in accorda	Employee, acknowled emonstrates functiona nce with mutually agre	ge that the above ality that meets eed terms.		
Date:		Signature:				
Test Supe	Test Supervisor:					
Name, first name:						
Date:		Signature:				

Part I: Instrument Details (D8 Series)

	Instrument Details			Set Values for Validation		
Diffractometer	D8 ADVANCE ¹⁾			Tube Power: 3 Tube Power: 3	85 kV / 40 mA (1 85 kV / 30 mA (1	for FL tubes) ²⁾ for FF tubes) ²⁾
Vertical goniometer	Theta/Theta Theta/2Theta	Theta/Theta 📃 Theta/2Theta 🦳				
	Height: 150					
	Radius: Primary radius Secondary radius		[mm] [mm]			
Sample stage	Standard					
	Rotating					
	FLIP-STICK			Sample position	on 5	
	AUTO CHANGER			Sample position A1		
	Compact Cradle/ Compact Cradle ^{Plus}					
	Compact UMC					
Monochroma-	Kβ-Filter					
lisation	Secondary monoch					
	Focusing monochro					
	Discriminator Settings (LYNXEYE XE / LYNXEYE XE-T)			Copy values from High Resolution mode:		
				Low Thr. [V]	High Thr. [V]	Veto Thr. [V]
Slits	Fixed divergence			Antiscatter slit: 0.3° (approx. 0.6 mm)		
	Fixed antiscatter sli	t		Antiscatter slit: 0.3° (approx. 0.6 mm)		
	Variable divergence		Divergence slit: 0.3° (approx. 0.6 mm)			
	Variable antiscatter	⁻ slit		Antiscatter slit: 0.3° (approx. 0.6 mm)		
	Motorized air scatte	r screen		Automatic mode		
	Primary axial Soller	slit		Primary axial Soller slit: 2.5°		
	Secondary axial Sol		Secondary axial Soller slit: 2.5°			
	Receiving slit			Receiving slit (0.1 mm	

Instrument Configuration D8 ADVANCE

	Instrument Details			Set Values for Validation		
Detector	Scintillation counter					
(See User	LYNXEYE, SSD160		LYNX	EYE User Manual DOC-M88-EXX095		
Manuais)	LYNXEYE XE		LYNXEYE XE User Manual DOC-M88-EXX24			
	LYNXEYE XE-T		LYNXEYE XE-T User ManualDOC-M88-EX>			
	LYNXEYE-2		LYNX	EYE-2 User Manual DOC-M88-EXX305		
	SSD160-2		SSD160-2 User Manual DOC-M88-EXX306			
	Solid state detector (SOL-XE)		SOL-	XE User Manual DOC-M88-EXX113		
	VÅNTEC-1		VÅN	FEC-1 User Manual DOC-M88-EXX072		
	EIGER2 R 500K		EIGE	R2 R 500K User Manual DOC-M88-EXX293		
¹⁾ including D8 ADVANCE ECO ²⁾ 35 kV / 28 mA in case of D8 ADVANCE ECO						

	Instrument Details			Set Values for Validation		
Diffractometer	D8 DISCOVER			Tube Power: 35 kV / 40 mA (for FL tubes) Tube Power: 35 kV / 30 mA (for FF tubes)		
Vertical goniometer	Theta/Theta Theta/2Theta					
	Height: 150 214 258					
	Radius: Primary radius Secondary radius	[r	nm] nm]			
Horizontal	Theta/2Theta					
gemeneter	Height: 214 258					
	Radius: Primary radius Secondary radius	[r	nm] nm]			
Sample stage	Standard					
	Rotating FLIP-STICK AUTO CHANGER					
				Sample positio	n 5	
				Sample position A1		
	Compact Cradle/ Compact Cradle ^{Plus}					
	Centric Eulerian Cradle					
	UMC 150/151/1516/150 HTC Compact UMC					
Monochroma-	i- Kβ-Filter					
tisation	Secondary monochromator					
	Focusing monochromator					
	Discriminator Settings (LYNXEYE XE / LYNXEYE XE-T)			Copy values fro Low Thr. [V]	om High Resolu High Thr. [V]	tion mode: Veto Thr. [V]

Instrument Configuration D8 DISCOVER

	Instrument Details			Set Values for Validation	
Slits	Fixed divergence Fixed antiscatter slit			Divergence slit: 0.3° (approx. 0.6 mm)	
				Antiscatter slit: 0.3° (approx. 0.6 mm)	
	Variable divergence slit			Divergence slit: 0.3° (approx. 0.6 mm)	
	Variable antiscatter slit			Antiscatter slit: 0.3° (approx. 0.6 mm)	
	Motorized air scatter screen Primary axial Soller slit Secondary axial Soller slit Receiving slit			Automatic mode	
				Primary axial Soller slit: 2.5°	
				Secondary axial Soller slit: 2.5°	
				Receiving slit 0.1 mm	
Detector	Scintillation counter				
(See User	LYNXEYE, SSD160		LYNXEYE User Manual DOC-M88-EXX095		
	LYNXEYE XE		LYN)	KEYE XE User Manual DOC-M88-EXX240	
	LYNXEYE XE-T		LYNXEYE XE-T User ManualDOC-M88-EXX239		
	LYNXEYE-2		LYNXEYE-2 User Manual DOC-M88-EXX305		
	SSD160-2			SSD160-2 User Manual DOC-M88-EXX306	
	Solid state detector (SOL-XE)		SOL-XE User Manual DOC-M88-EXX113		
	VÅNTEC-1		VÅNTEC-1 User Manual DOC-M88-EXX072		
	EIGER2 R 500K		EIGER2 R 500K User Manual DOC-M88-EXX293		

	Instrument Details			Set Values for Validation			
--	------------------------------------	----------------	-----	---	---------------	---------------	--
Diffractometer	D8 ENDEAVOR ¹⁾			Tube Power: 35 kV / 40 mA (for FL tubes) ²⁾			
				Tube Power: 35 kV / $30 \text{ mA} (\text{for FF tubes})^2)$			
Vertical	Theta/Theta						
goniometer	Height:						
	150						
	Radius:						
	200,5						
	Rotating			Sample position	ר A1		
Monochroma-	Kβ-Filter	•					
tisation	Discriminator Settin	gs		Copy values from High Resolution mode:			
	(LYNXEYE XE /			Low Thr. [V]	High Thr. [V]	Veto Thr. [V]	
Slits	Fixed divergence			Divergence slit: 0.3° (approx. 0.6 mm)			
	Variable divergence	е		Divergence slit: 0.3° (approx. 0.6 mm)			
	Primary / secondary slit	/ axial Soller		Primary and secondary axial Soller slit: 2.5°			
	Air Scatter Screen			Set mode to Automatic for motorized air scatte screen. Position the air scatter screen approx. 4 mm above the sample surface for manual ai scatter screen or use adjustment tool			
	LYNXEYE XE		LYN	XEYE XE User N	Manual DOC-M8	8-EXX240	
	LYNXEYE XE-T		LYN	XEYE XE-T Use	r ManualDOC-M	88-EXX239	
			LYN	LYNXEYE-2 User Manual DOC-M88-EXX305			
	SSD160-2 SSD			3D160-2 User Manual DOC-M88-EXX306			
¹⁾ including D8 El ²⁾ 35 kV / 28 mA	NDEAVOR ECO in case of D8 ADVAN	NCE ECO					

Instrument Configuration D8 ENDEAVOR

Part II: Angular Accuracy, Instrument Response and Resolution (D8 Series)

Anode: Co			Bragg-Brentano Geometry								
An	gular Accuracy: I	Difference Ref	erence Positio	n corr	Instrument Resolution						
Maximum allowed 20 deviation depends on height			FWHM _{obs} < FWHM _{max}								
2θ _{obs} [°]	Difference	2θ _{obs} Reference Position corr	Difference Reference Position corr	20 _{exp} ¹⁾ [°]	FWHM _{obs} [°]			FWHM _{max} ²⁾ [°]			
				29.786							
				41.049							
				81.247							
				118.142							
Reference Position corr ¹ / ₂ (Difference _{max} +Difference _{min})						obs: observed exp: expected					
Detector ³⁾	Current Reference	e Position			corr: corrected						
									For details cf. cl [> 15]	hapter <i>Re</i>	eference Values
2-Theta ³⁾	Corrected Refere	ence Position			Shift						
	(Current Referen Position corr)	ce Position - R	eference			Height		Maximum a	Maximum allowed shift 20		ified accuracy of:
	1				Vertical	150		C).02°		± 0.01°
						214		C	0.03°		± 0.015°
						258		C).04°		± 0.02°
					Horizontal	214		C).02°		± 0.01°
						258		C).02°		± 0.01°
¹⁾ see table ²⁾ see table ³⁾ mark app	⁾ see table 3.2 ²⁾ see table 3.4 ³⁾ mark applicable: detector in case of Theta/Theta and 2-Theta in case of Theta/2Theta										

Depending on specific measurement setups, individual reflections may not be measurable. Then measurements must be restricted to accessible reflections.

Comments		

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C. Factory Acceptance Test **Protocol**

Declaration of Conformity

Parallel Beam Geometry with Copper Anode

NIST SRM1976c Sample: Cu

Anode:

Customer Name:		
Customer PO Number:		
Serial Number:		SAP Number (Sales Order Number):

This protocol details the results of the factory acceptance test procedure for Bruker AXS diffraction systems in parallel beam reflection geometry (Göbel mirror systems). The factory acceptance test procedure consists in full-profile measurements of the certified NIST standard reference material NIST SRM1976c . Details of this procedure are outlined in the Instrument Verification Booklet, which is part of the instrument documentation.

The present verification routine covers the functionality of all relevant components of the diffraction system under investigation.

System w	ithin required s	YES NO				
Tested by:						
Name, firs	st name:					
Testing approval: I, an authorized Bruker Employee, acknowledge that the above referenced system has been tested and demonstrates functionality that meets customer order specifications in accordance with mutually agreed terms.						
Date:		Signature:				
Test Supe	ervisor:					
Name, first name:						
Date:		Signature:				

Part I: Instrument Details

Instrument Configuration D8 ADVANCE

	Instrument Detail	S		Set Values for Validation			
Diffractometer	D8 ADVANCE ¹⁾			Tube Power: 40 k Tube Power: 40 k	V / 40 mA (foi V / 30 mA (foi	r FL tubes) ²⁾ r FF tubes) ²⁾	
Vertical goniometer	Theta/Theta Theta/2Theta						
	Height: 150			-			
	Radius: Primary radius Secondary radius		[mm] [mm]				
Sample stage	Standard	I					
	Rotating						
	FLIP-STICK			Sample position 5			
	AUTO CHANGER			Sample position A	.1		
	Compact Cradle/ C Cradle ^{Plus}	compact					
	Compact UMC						
Monochroma-	Primary Göbel mirr	or 60 mm		Exit slit 1.2 mm			
tisation	Primary TWIN / TR beam	IO parallel		Exit slit 1 mm			
	Discriminator Settings			Copy values from	ion mode:		
	XE-T)	NAEYE		Low Thr. [V]	High Thr. [V]	Veto Thr. [V]	
			_				
Slits	Primary axial Solle	r slit		2.5°			
	Secondary equator slit	ial Soller		0.2°			
Detector	Scintillation counte	r 🔵					
	LYNXEYE, SSD16	0	LYNXEY	EYE User Manual DOC-M88-EXX095			
	LYNXEYE XE		LYNXEY	E XE User Manual	DOC-M88-EX	XX240	
	LYNXEYE XE-T		LYNXEY	E XE-T User Manu	alDOC-M88-I	EXX239	
	LYNXEYE-2		EYE-2 User Manual DOC-M88-EXX305				
	55D160-2		SSD160-	-2 User Manual DO	C-10188-EXX3	006	
	Solid state detector (SOL-XE)	r 📃	SOL-XE	User Manual DOC-	-M88-EXX113	3	

	Instrument Details			Set Values for Validation
	VÅNTEC-1		VÅNTEC	-1 User Manual DOC-M88-EXX072
	EIGER2 R 500K		EIGER2	R 500K User Manual DOC-M88-EXX293
¹⁾ including D8 ADVANCE ECO ²⁾ 40 kV / 25 mA in case of D8 ADVANCE ECO				

Instrument Configuration D8 DISCOVER

	Instrument Details			Set Values for Validation			
Diffractome- ter	D8 DISCOVER			Tube Power: 4 Tube Power: 4 TXS Power: 50 filament, line a TXS Power: 50 filament, spot f	0 kV / 40 mA (fc 0 kV / 30 mA (f 0 kV / 100 mA (fo nd spot focus) 0 kV / 22 mA (for ocus)	or FL tubes) or FF tubes) or 0.3x3 mm ² r 0.1x1 mm ²	
Vertical goniometer	Theta/Theta Theta/2Theta						
	Height: 150 214 258						
	Radius: Primary radius Secondary radius	[mi	m] m]				
Horizontal goniometer	Theta/2Theta Height: 214 258						
	Radius: Primary radius Secondary radius	[mi	m] m]				
Sample stage	Standard						
	Rotating						
	FLIP-STICK			Sample position 5			
	AUTO CHANGER			Sample positio	n A1		
	Compact Cradle/ Cor	npact Cradle ^{Plus}					
	Centric Eulerian Crac	lle					
	UMC 150/151/1516/1	50 HTC					
	Compact UMC						
Monochro-	Primary Göbel mirror	60 mm		Exit slit 1.2 mm	ı		
matisation Primary TWIN / TRIO parallel beam			Exit slit 1 mm				
	Discriminator Settings (LYNXEYE XE / LYN	s XEYE XE-T)		Copy values fro Low Thr. [V]	om High Resolu High Thr. [V]	tion mode: Veto Thr. [V]	

	Instrument Details			Set Values for Validation		
Slits	Primary axial Soller slit			2.5°		
	Secondary equatorial Soller slit			0.2°		
Detector	Scintillation counter					
(See User	LYNXEYE, SSD160		LYN	XEYE User Manual DOC-M88-EXX095		
manuais)	LYNXEYE XE		LYNXEYE XE User Manual DOC-M88-EXX240			
	LYNXEYE XE-T		LYN	XEYE XE-T User ManualDOC-M88-EXX239		
	LYNXEYE-2		LYN	XEYE-2 User Manual DOC-M88-EXX305		
	SSD160-2			0160-2 User Manual DOC-M88-EXX306		
	Solid state detector (SOL-XE)		SO	XE User Manual DOC-M88-EXX113		
	VÅNTEC-1		VÅV	NTEC-1 User Manual DOC-M88-EXX072		
	EIGER2 R 500K		EIG	ER2 R 500K User Manual DOC-M88-EXX293		

Part II: Angular Accuracy, Instrument Response and Resolution

Anode: Cu			Parallel Beam Geometry										
Angı	ular Accui	acy: Difference	Deflection ar	ngle corr	Instrument Response: I _{rel}) Instrument Resolution							Resolution	
Maximum allowed 2θ deviation depends on height			Maximum allo	Maximum allowed intensity deviation for point detectors ± 10% FWHM _{obs} < FWHM _{max}							-WHM _{max}		
2θ _{obs} [°]	Differ- ence	2θ _{obs} Deflection angle corr	Difference Deflection angle corr	20 _{exp} ¹⁾ [°]	I _{obs}	I _{obs} I _{exp}	I _{rel} =	I _{obs} N	I _{min}	I _{exp} ¹⁾	I _{max}	FWHM _{obs} [°]	FWHM _{max} ²⁾ [°]
				25.561					21.49	23.88	26.27		
				35.137					90.00	100.00	110.00		
				88.996					11.06	12.29	13.52		
				127.692					13.37	14.85	16.34		
Deflection	angle corr ce _{max} +Diffe	rence _{min})									$Sum = \sum_{n=1}^{\infty}$	$\sum \frac{I_{obs}}{I_{exp}}, i = 1 \dots 4$	
Detector ³⁾	Curre	nt Deflection and	gle		Shift						N	$=\frac{Sum}{4}$	
2-Theta ³⁾	Corre (Curre Deflee	cted Deflection a ent Deflection ar ction angle corr)	angle ngle –			Hei	ght	Maxir	num allow	ed shift 26) [°] fo	or specified a	ccuracy of:
N: scaling	factor; For	details cf. chapt	er Reference \	/alues [▶ 15]	Vertical 150			0.02	2		± 0.0	1°	
obs: observed						214			0.0	3		± 0.07	15°
exp: expected						258			0.04	4		± 0.0	2°
corr: corrected					Horizontal	214			0.02	2		± 0.0	1°
rel: relative	•					258			0.02	2		± 0.0	1°
¹⁾ see table ²⁾ see table ³⁾ mark app	e 3.1 3.3 plicable: de	tector in case of	f Theta/Theta a	and 2-Theta in c	case of Theta/2	2Theta	Thon m	0001150	monto mu	the restri			floctions
Depending	i on specifi	c measurement	setups, individ	ual reflections i	may not be me	easurable.	i nen m	easure	ments mus	st be restri	cted to a	accessible re	TIECTIONS.

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Comments		

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D. Factory Acceptance Test Protocol

Declaration of Conformity

Parallel Beam Geometry with Cobalt Anode

Sample: NIST SRM1976c

Anode:

Co	
Customer Name:	
Customer PO Number:	
Serial Number:	SAP Number (Sales Order Number):

This protocol details the results of the factory acceptance test procedure for Bruker AXS diffraction systems in parallel beam reflection geometry (Göbel mirror systems). The factory acceptance test procedure consists in full-profile measurements of the certified NIST standard reference material NIST SRM1976c. Details of this procedure are outlined in the Instrument Verification Booklet, which is part of the instrument documentation.

The present verification routine covers the functionality of all relevant components of the diffraction system under investigation.

System w	VES NO							
Tested by	Tested by:							
Name, firs	et name:							
Testing approval: I, an authorized Bruker Employee, acknowledge that the above referenced system has been tested and demonstrates functionality that meets customer order specifications in accordance with mutually agreed terms.								
Date:		Signature:						
Test Supe	Test Supervisor:							
Name, firs	et name:							
Date:		Signature:						

Part I: Instrument Details

Instrument Configuration D8 ADVANCE

	Instrument Details				Set Values	s for Validatio	n
Diffractometer	D8 ADVANCE ¹⁾				Tube Powe tubes) ²⁾ Tube Powe tubes) ²⁾	er: 35 kV / 40 m er: 35 kV / 30 m	nA (for FL nA (for FF
Vertical goniometer	Theta/Theta Theta/2Theta						
	Height: 150						
	Radius: Primary radius Secondary radius			[mm] [mm]			
Sample stage	Standard	I					
	Rotating						
	FLIP-STICK				Sample po	sition 5	
	AUTO CHANGER				Sample po	sition A1	
	Compact Cradle/ Compact Cradle						
	Compact UMC						
Monochroma-	Primary Göbel mirror 6	60 mm			Exit slit 1.2	mm	
lisation	Discriminator Settings (LYNXEYE XE / LYNXEYE XE-T)				Copy value mode:	es from High Re	esolution
					Low Thr. [V]	High Thr. [V]	Veto Thr. [V]
				_			
Slits	Primary axial Soller slit	t 			2.5°		
Detector	Secondary equatorial S	Soller slit			0.2		
See User							
Manuals)	LYNXEYE, SSD160				E User Man F XF User N	ual DOC-1088-1 Janual DOC-M	=XXU95 88-FXX240
	LYNXEYE XE-T			LYNXEY	E XE-T Use	r ManualDOC-I	M88-EXX239
	LYNXEYE-2			LYNXEY	E-2 User Ma	anual DOC-M88	3-EXX305
	SSD160-2			SSD160-	2 User Man	ual DOC-M88-I	EXX306
	Solid state detector (SOL-XE)			SOL-XE	User Manua	I DOC-M88-EX	X113

	Instrument Details			Set Values for Validation	
	VÅNTEC-1		VÅNTEC-	-1 User Manual DOC-M88-EXX072	
	EIGER2 R 500K		EIGER2 F	R 500K User Manual DOC-M88-EXX293	
1) including D8 ADVANCE ECO 2) 35 kV / 28 mA in case of D8 ADVANCE ECO					

	Instrument Details			Set Values for Validation		
Diffractome- ter	D8 DISCOVER			Tube Power: 3 Tube Power: 3	5 kV / 40 mA 5 kV / 30 mA	(for FL tubes) (for FF tubes)
Vertical goniometer	Theta/Theta Theta/2Theta					
	Height: 150 214 258					
	Radius: Primary radius Secondary radius	[mm] 		•		
Horizontal	Theta/2Theta					
goniometer	Height: 214 258					
	Radius: Primary radius Secondary radius	[mm] 				
Sample	Standard					
stage	Rotating	Rotating				
	FLIP-STICK			Sample positio	on 5	
	AUTO CHANGER			Sample positio	on A1	
	Compact Cradle/ Compact Cradle ^{Plus}					
	Centric Eulerian Cradle					
	UMC 150/151/1516/150 H	ТС				
	Compact UMC					
Monochro- matisation	Primary Göbel mirror 60 m	ım		Exit slit 1.2 mm	1	
	Discriminator Settings (LYNXEYE XE / LYNXEYE XE-T)			Copy values fr Low Thr. [V]	om High Resc High Thr. [V]	olution mode: Veto Thr. [V]
Slits	Primary axial Soller slit					
	Secondary equatorial Soll	er slit				

Instrument Configuration D8 DISCOVER

	Instrument Details		Set Values for Validation
Detector	Scintillation counter		
	LYNXEYE, SSD160	LYN	XEYE User Manual DOC-M88-EXX095
	LYNXEYE XE	LYN	XEYE XE User Manual DOC-M88-EXX240
	LYNXEYE XE-T	LYN	XEYE XE-T User ManualDOC-M88-EXX239
	LYNXEYE-2	LYN	XEYE-2 User Manual DOC-M88-EXX305
	SSD160-2	SSI	D160-2 User Manual DOC-M88-EXX306
	Solid state detector (SOL-XE)	SO	L-XE User Manual DOC-M88-EXX113
	VÅNTEC-1	1ÅV	NTEC-1 User Manual DOC-M88-EXX072
	EIGER2 R 500K	EIG EXX	ER2 R 500K User Manual DOC-M88- K293

L	

Part II: Angular Accuracy, Instrument Response and Resolution

Anode: Co					Parallel Beam Geometry					
An	gular Accuracy:	Difference Defle	ction angle corr		Instrument Resolution					
Maximum allowed 2θ deviation depends on height					FWHM _{obs} < FWHM _{max}					
2θ _{obs} [°]	Difference	2θ _{obs} Deflection angle corr	Difference Deflection angle corr	2θ _{exp} ¹⁾ [°]	FWHM _{obs} [°]				FWHM _{max} ²⁾ [°]	
				29.773						
				41.041						
				81.250						
				118.165						
Deflection angle corr ½(Difference _{max} +Difference _{min})										
Detector ³⁾	Current Defl	ection angle		Shift						
2-Theta ³⁾	heta ³⁾ Corrected Deflection angle (Current Deflection angle - Deflection angle corr)				Hei	ght	Maximum allowe	ed shift 2θ [°]	for specified accuracy of:	
	·			Vertical	150		0.02		± 0.01°	
For details cf. c	hapter <i>Reference</i>	Values [▶ 15]		_	214		0.03	•	± 0.015°	
obs: observed				_	258		0.04		± 0.02°	
exp: expected				Horizontal	214		0.02		± 0.01°	
corr: corrected					258		0.02		± 0.01°	
¹⁾ see table 3.2 ²⁾ see table 3.4 ³⁾ mark applicat	ble: detector in ca	se of Theta/Theta	and 2-Theta in c	ase of Theta/2T	heta					
Depending on s	specific measuren	nent setups, indivi	dual reflections r	may not be mea	surable. The	en measi	urements must be	restricted to	accessible reflections.	

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Comments		

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E. Customer Acceptance Test **Protocol**

Declaration of Conformity

Bragg-Brentano Geometry with Copper Anode

NIST SRM1976c Sample: Cu

Anode:

Customer Name:	
Customer PO Number:	
Serial Number:	SAP Number (Sales Order Number):

This protocol details the results of the factory acceptance test procedure for Bruker AXS diffraction systems in Bragg-Brentano reflection geometry. The factory acceptance test procedure consists in full-profile measurements of the certified NIST standard reference material SRM1976c. Details of this procedure are outlined in the Instrument Verification Booklet, which is part of the instrument documentation.

The present verification routine covers the functionality of all relevant components of the diffraction system under investigation.

System w				
Customer	Name:			
Date:		Signature:		
Technician Name:				
Date:		Signature:		

Part I: Instrument Details (D8 Series)

	Instrument Details			Set Values for Validation		
Diffractome- ter	D8 ADVANCE ¹⁾			Tube Power: 4 Tube Power: 4	40 kV / 40 mA (fe 40 kV / 30 mA (fe	or FL tubes) ²⁾ or FF tubes) ²⁾
Vertical goniometer	Theta/Theta Theta/2Theta					
	Height: 150					
	Radius: Primary radius Secondary radius	[mm]				
Sample stage	Standard					
	Rotating		\bigcirc			
	FLIP-STICK			Sample position 5		
	AUTO CHANGER			Sample positi	on A1	
	Compact Cradle / Compact Cradle ^{Plus}					
	Compact UMC					
Monochro-	Kβ-Filter					
matisation	Secondary monochromator					
	Focusing monochromator					
	Discriminator Settings			Copy values from High Resolution mode:		
	LYNXEYE XE-T)			Low Thr. [V]	High Thr. [V]	Veto Thr. [V]
Slits	Fixed divergence slit			Divergence slit: 0.3° (approx. 0.6 mm)		
	Fixed antiscatter slit			Antiscatter slit: 0.3° (approx. 0.6 mm)		
	Variable divergence	slit	\bigcirc	Divergence slit: 0.3° (approx. 0.6 mm)		
	Variable antiscatter s	slit		Antiscatter slit: 0.3° (approx. 0.6 mm)		
	Motorized air scatter	screen		Automatic mode		
	Primary axial Soller s	lit		Primary axial Soller slit: 2.5°		
	Secondary axial Solle	er slit		Secondary axial Soller slit: 2.5°		
	Receiving slit			Receiving slit	0.1 mm	

Instrument Configuration D8 ADVANCE

	Instrument Details			Set Values for Validation		
Detector	Scintillation counter					
(See User	LYNXEYE, SSD160		LYN	XEYE User Manual DOC-M88-EXX095		
Manuais)	LYNXEYE XE		LYN	XEYE XE User Manual DOC-M88-EXX240		
	LYNXEYE XE-T			YNXEYE XE-T User ManualDOC-M88-EXX239		
	LYNXEYE-2			YNXEYE-2 User Manual DOC-M88-EXX305		
	SSD160-2		SSE	0160-2 User Manual DOC-M88-EXX306		
	Solid state detector (SOL-XE)		SOI	XE User Manual DOC-M88-EXX113		
	VÅNTEC-1		VÅN	NTEC-1 User Manual DOC-M88-EXX072		
	EIGER2 R 500K		EIG	ER2 R 500K User Manual DOC-M88-EXX293		
¹⁾ including D8 ²⁾ 40 kV / 25 m/	ADVANCE ECO A in case of D8 ADVANCE ECO					

Instrument Configuration D8 DISCOVER

	Instrument Details	;		Set Values for Validation			
Diffractometer	D8 DISCOVER			Tube Power: 40 Tube Power: 40 TXS Power: 50 filament, line an TXS Power: 50 filament, spot fo	kV / 40 mA (fo kV / 30 mA (fo kV / 100 mA (fo d spot focus) kV / 22 mA (for ocus)	r FL tubes) or FF tubes) or 0.3x3 mm ² 0.1x1 mm ²	
Vertical	Theta/Theta						
goniometer	Theta/2Theta						
	Height:						
	150						
	214						
	258						
	Radius:						
	Primary radius	[m	m]				
	Secondary radius	[m	m]				
Horizontal	al Theta/2Theta 📃						
goniometer	Height:						
	214						
	258						
	Radius:						
	Primary radius	[m	m]				
	Secondary radius	[m	m]				
Sample stage	Standard						
	Rotating						
	FLIP-STICK		\bigcirc	Sample position	n 5		
	AUTO CHANGER			Sample position	n A1		
	Compact Cradle/ Co Cradle ^{Plus}	ompact					
	Centric Eulerian Cra	adle					
	UMC 150/151/1516	/150 HTC	\bigcirc				
	Compact UMC						
Monochroma-	Kβ-Filter						
tisation	Secondary monoch	romator					
	Focusing monochro	mator					
	Discriminator Settin	gs		Copy values fro	m High Resolut	ion mode:	
	(LYNXEYE XE / LY	ŇXEYE XE-T)		Low Thr. IV1	High Thr. IV1	Veto Thr. IVI	

	Instrument Details			Set Values for Validation		
Slits	Fixed divergence slit			Divergence slit: 0.3° (approx. 0.6 mm)		
	Fixed antiscatter slit			Antiscatter slit: 0.3° (approx. 0.6 mm)		
	Variable divergence slit			Divergence slit: 0.3° (approx. 0.6 mm)		
	Variable antiscatter slit			Antiscatter slit: 0.3° (approx. 0.6 mm)		
	Motorized air scatter screen			Automatic mode		
	Primary axial Soller slit			Primary axial Soller slit: 2.5°		
	Secondary axial Soller slit			Secondary axial Soller slit: 2.5°		
	Receiving slit			Receiving slit 0.1 mm		
Detector	Scintillation counter					
(See User Manuals)	LYNXEYE, SSD160		LYNXEYE User Manual DOC-M88-EXX095			
Mariuais)	LYNXEYE XE		LYNXEYE XE User Manual DOC-M88-EXX240			
	LYNXEYE XE-T		LYNXEYE XE-T User ManualDOC-M88-EXX239			
	LYNXEYE-2		LYNXEYE-2 User Manual DOC-M88-EXX305			
	SSD160-2		SSI	SSD160-2 User Manual DOC-M88-EXX306		
	Solid state detector (SOL-XE)		SOL-XE User Manual DOC-M88-EXX113			
	VÅNTEC-1		VÅI	NTEC-1 User Manual DOC-M88-EXX072		
	EIGER2 R 500K		EIGER2 R 500K User Manual DOC-M88-EXX293			

	Instrument Detai	ls			Set Values for Validation			
Diffractometer	D8 ENDEAVOR ¹⁾			Tube Power: 40 kV / 40 mA (for FL tubes) $^{2)}$ Tube Power: 40 kV / 30 mA (for FF tubes) $^{2)}$				
Vertical	Theta/Theta							
goniometer	Height:							
	150							
	Radius:							
	200,5							
	Rotating				Sample positi	on A1		
Monochromati-	Kβ-Filter							
sation	Discriminator Settings (LYNXEYE XE / LYNXEYE XE-T)				Copy values f	rom High Resolu	ution mode:	
					Low Thr. [V]	High Thr. [V]	Veto Thr. [V]	
Slits	Fixed divergence				Divergence slit: 0.3° (approx. 0.6 mm)			
	Variable divergence				Divergence slit: 0.3° (approx. 0.6 mm)			
	Primary / secondary axial Soller slit				Primary and secondary axial Soller slit: 2.5°			
	Air Scatter Screen				Set mode to Automatic for motorized air scatter screen. Position the air scatter screen approx. 4 mm above the sample surface for manual air scatter screen or use adjustment tool			
	LYNXEYE XE			LYN	LYNXEYE XE User Manual DOC-M88-EXX240			
	LYNXEYE XE-T			LYNXEYE XE-T User ManualDOC-M88-EXX239				
	LYNXEYE-2			LYNXEYE-2 User Manual DOC-M88-EXX305				
	SSD160-2			SSD160-2 User Manual DOC-M88-EXX306				
¹⁾ including D8 EN ²⁾ 40 kV / 25 mA in	DEAVOR ECO case of D8 ENDE	AVOR ECO						

Instrument Configuration D8 ENDEAVOR

Part II: Angular Accuracy, Instrument Response and Resolution (D8 Series)

Anode: Cu				Bragg-Brentano Geometry									
Angular Accuracy: Difference Reference Position corr					Instrument Response: I _{rel} Instr Res						Instru Reso	ument lution	
Maximum allowed 2θ deviation depends on height			Maximum	Maximum allowed intensity deviation for point detectors ± 10% FWHM _{obs} < FV						FWHM _{max}			
2θ _{obs} [°]	Differ- ence	2θ _{obs} Reference Position corr	Difference Reference Position corr	2θ _{exp} ¹⁾ [°]	I _{obs}	I _{obs} I _{exp}		$I_{rel} = \frac{I_{obs}}{N}$	I _{min}	I _{exp} ¹⁾	I _{max}	FWHM _{obs} [°]	FWHM _{max} ²⁾ [°]
				25.575					21.49	23.88	26.27		
				35.148					90.00	100.00	110.00		
				88.989					11.06	12.29	13.52		
				127.670					13.37	14.85	16.34		
Reference F ½(Difference	Position corr e _{max} +Differer	nce _{min})									$Sum = \sum$	$\frac{l_{obs}}{l_{exp}}$, $i=1\ldots 4$	
Detector ³⁾	Current Re	ference Positic	n		Shift						N =	$=\frac{Sum}{4}$	
2-Theta ³⁾	Corrected (Current Re Position co	Reference Pos eference Positi rr)	tion on - Reference			Heig	ht	Maximum	allowed sh	ift 20 for	specified a	accuracy of:	
N: scaling factor; For details cf. chapter Reference Values [▶ 15]				Vertical	150		0,02° ±		± 0,0)1°			
obs: observed					214		0,03° ±		± 0,0	15°			
exp: expected					258		0.04° ±		± 0,0)2°			
corr: correct	ed				Horizontal	214			0,02°		± 0,0)1°	
rel: relative						258			0,02°		± 0,0)1°	

¹⁾ see table 3.1. For linear detector configurations intensities might be outside allowed deviations for point detectors due to reasons explained in chapter Reference Values [▶ 15]; ²⁾ see table 3.3;

³⁾ mark applicable: detector in case of Theta/Theta and 2-Theta in case of Theta/2Theta; Depending on specific measurement setups, individual reflections may not be measurable. Then measurements must be restricted to accessible reflections.

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Comments		

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F. Customer Acceptance Test **Protocol**

Declaration of Conformity

Bragg-Brentano Geometry with Cobalt Anode

NIST SRM1976c Sample: Со

Anode:

Customer Name:	
Customer PO Number:	
Serial Number:	SAP Number (Sales Order Number):

This protocol details the results of the factory acceptance test procedure for Bruker AXS diffraction systems in Bragg-Brentano reflection geometry. The factory acceptance test procedure consists in full-profile measurements of the certified NIST standard reference material SRM1976c. Details of this procedure are outlined in the Instrument Verification Booklet, which is part of the instrument documentation.

The present verification routine covers the functionality of all relevant components of the diffraction system under investigation.

System within required specifications			YES NO	
Customer Name:				
Date:		Signature:		
Technician Name:				
Date:		Signature:		

Part I: Instrument Details (D8 Series)

	Instrument Details	;		Set Values for Validation			
Diffractometer	D8 ADVANCE ¹⁾			Tube Power: 3 Tube Power: 3	5 kV / 40 mA (f 5 kV / 30 mA (f	or FL tubes) ²⁾ or FF tubes) ²⁾	
Vertical goniometer	Theta/Theta Theta/2Theta						
	Height: 150						
	Radius: Primary radius Secondary radius		.[mm] .[mm]				
Sample stage	Standard						
	Rotating						
	FLIP-STICK			Sample position 5			
	AUTO CHANGER			Sample position	on A1		
	Compact Cradle/ Compact Cradle ^{Plus}						
	Compact UMC						
Monochroma-	Kβ-Filter						
tisation	Secondary monoch						
	Focusing monochro						
	Discriminator Setting		Copy values from High Resolution mode:				
	LYNXEYE XE-T)			Low Thr. [V]	High Thr. [V]	Veto Thr. [V]	
Slits	Fixed divergence			Antiscatter slit: 0.3° (approx. 0.6 mm)			
	Fixed antiscatter sli	t		Antiscatter slit: 0.3° (approx. 0.6 mm)			
	Variable divergence slit			Divergence slit: 0.3° (approx. 0.6 mm)			
	Variable antiscatter slit			Antiscatter slit: 0.3° (approx. 0.6 mm)			
	Motorized air scatte	r screen		Automatic mode			
	Primary axial Soller	slit		Primary axial Soller slit: 2.5°			
	Secondary axial Sol	ller slit		Secondary axi	Secondary axial Soller slit: 2.5°		
	Receiving slit		Receiving slit ().1 mm			

Instrument Configuration D8 ADVANCE

	Instrument Details			Set Values for Validation		
Detector	Scintillation counter					
(See User Manuals)	LYNXEYE, SSD160		LYNX	EYE User Manual DOC-M88-EXX095		
	LYNXEYE XE		LYNXEYE XE User Manual DOC-M88-EXX2			
	LYNXEYE XE-T		LYNXEYE XE-T User ManualDOC-M88-EXX239			
	LYNXEYE-2		LYNXEYE-2 User Manual DOC-M88-EXX305			
	SSD160-2		SSD1	60-2 User Manual DOC-M88-EXX306		
	Solid state detector (SOL-XE)		SOL-	XE User Manual DOC-M88-EXX113		
	VÅNTEC-1		VÅN	EC-1 User Manual DOC-M88-EXX072		
	EIGER2 R 500K		EIGE	R2 R 500K User Manual DOC-M88-EXX293		
¹⁾ including D8 ADVANCE ECO ²⁾ 35 kV / 28 mA in case of D8 ADVANCE ECO						

	Instrument Details			Set Values for Validation			
Diffractometer	D8 DISCOVER			Tube Power: 3 Tube Power: 3	35 kV / 40 mA (fo 35 kV / 30 mA (f	or FL tubes) or FF tubes)	
Vertical goniometer	Theta/Theta Theta/2Theta						
	Height: 150 214 258						
	Radius: Primary radius Secondary radius	[r	nm] nm]				
Horizontal	Theta/2Theta						
gomometer	Height: 214 258						
	Radius: Primary radius Secondary radius	[r [r	nm] nm]				
Sample stage	Standard						
	Rotating						
	FLIP-STICK			Sample position	on 5		
	AUTO CHANGER			Sample position A1			
	Compact Cradle/ Co Cradle ^{Plus}	ompact					
	Centric Eulerian Cradle						
	UMC 150/151/1516/150 HTC						
	Compact UMC						
Monochroma- tisation	Kβ-Filter						
	Secondary monoch	romator					
	Focusing monochro	mator					
	Discriminator Settings			Copy values f	rom High Resolu	tion mode:	
		,		Low Thr. [V]	High Thr. [V]	Veto Thr. [V]	

Instrument Configuration D8 DISCOVER

	Instrument Details			Set Values for Validation		
Slits	Fixed divergence			Divergence slit: 0.3° (approx. 0.6 mm)		
	Fixed antiscatter slit			Antiscatter slit: 0.3° (approx. 0.6 mm)		
	Variable divergence slit			Divergence slit: 0.3° (approx. 0.6 mm)		
	Variable antiscatter slit			Antiscatter slit: 0.3° (approx. 0.6 mm)		
	Motorized air scatter screen			Automatic mode		
	Primary axial Soller slit			Primary axial Soller slit: 2.5°		
	Secondary axial Soller slit			Secondary axial Soller slit: 2.5°		
	Receiving slit			Receiving slit 0.1 mm		
Detector	Scintillation counter					
(See User Manuals)	LYNXEYE, SSD160		LYNXEYE User Manual DOC-M88-EXX095			
	LYNXEYE XE		LYNXEYE XE User Manual DOC-M88-EXX240			
	LYNXEYE XE-T		LYN)	NXEYE XE-T User ManualDOC-M88-EXX239		
	LYNXEYE-2		LYNXEYE-2 User Manual DOC-M88-EXX305			
	SSD160-2		SSD)160-2 User Manual DOC-M88-EXX306		
	Solid state detector (SOL-XE)		SOL-XE User Manual DOC-M88-EXX113			
	VÅNTEC-1		VÅN	NTEC-1 User Manual DOC-M88-EXX072		
	EIGER2 R 500K		EIGER2 R 500K User Manual DOC-M88-EXX293			
	Instrument Details	;		Set Values for	Validation	
--	------------------------------------	----------------	--	---	-------------------	---------------------------
Diffractometer	D8 ENDEAVOR ¹⁾			Tube Power: 35	5 kV / 40 mA (for	FL tubes) ²⁾
				Tube Power: 35	5 kV / 30 mA (fo	r FF tubes) ²⁾
Vertical	Theta/Theta					
goniometer	Height:					
	150					
	Radius:					
	200,5					
	Rotating			Sample positior	ו A1	
Monochroma-	Kβ-Filter					
tisation	Discriminator Settings			Copy values fro	m High Resoluti	on mode:
	(LYNXEYE XE / LYNXEYE XE-T)			Low Thr. [V]	High Thr. [V]	Veto Thr. [V]
Slits	Fixed divergence			Divergence slit: 0.3° (approx. 0.6 mm)		
	Variable divergence	е		Divergence slit: 0.3° (approx. 0.6 mm)		
	Primary / secondary slit	/ axial Soller		Primary and secondary axial Soller slit: 2.5°		
	Air Scatter Screen			Set mode to Automatic for motorized air scatte screen. Position the air scatter screen approx. 4 mm above the sample surface for manual ai scatter screen or use adjustment tool		
	LYNXEYE XE		LYNXEYE XE User Manual DOC-M88-EXX240			
	LYNXEYE XE-T		LYNXEYE XE-T User ManualDOC-M88-EXX239			
			LYNXEYE-2 User Manual DOC-M88-EXX305			
	SSD160-2 SSE			160-2 User Man	ual DOC-M88-E	XX306
¹⁾ including D8 El ²⁾ 35 kV / 28 mA	NDEAVOR ECO in case of D8 ADVAN					

Instrument Configuration D8 ENDEAVOR

Part II: Angular Accuracy, Instrument Response and Resolution (D8 Series)

Anode: Co			Bragg-Brentano Geometry								
An	gular Accuracy: I	Difference Ref	erence Positio	n corr	Instrument Resolution						
Maximum allowed 2θ deviation depends on height				FWHM _{obs} < FWHM _{max}							
2θ _{obs} [°]	Difference	2θ _{obs} Reference Position corr	Difference Reference Position corr	20 _{exp} ¹⁾ [°]	FWHM _{obs} [°]				FWHM _{ma} , [°]	2)	
				29.786							
				41.049							
				81.247							
				118.142							
Reference Position corr ¹ / ₂ (Difference _{max} +Difference _{min})						obs: observed exp: expected					
Detector ³⁾	Current Reference	e Position			corr: corrected						
									For details cf. cl [> 15]	hapter <i>Re</i>	eference Values
2-Theta ³⁾	Corrected Refere	ence Position			Shift						
	(Current Referen Position corr)	ce Position - R	eference			He	ight	Maximum a	allowed shift 20	for spec	ified accuracy of:
	1				Vertical	150		C).02°		± 0.01°
						214		C	0.03°		± 0.015°
						258		C).04°		± 0.02°
					Horizontal	214		C).02°		± 0.01°
						258		C).02°		± 0.01°
¹⁾ see table ²⁾ see table ³⁾ mark app	¹⁾ see table 3.2 ²⁾ see table 3.4 ³⁾ mark applicable: detector in case of Theta/Theta and 2-Theta in case of Theta/2Theta										

Depending on specific measurement setups, individual reflections may not be measurable. Then measurements must be restricted to accessible reflections.

comments		

G. Customer Acceptance Test **Protocol**

Declaration of Conformity

Parallel Beam Geometry with Copper Anode

NIST SRM1976c Sample: Cu

Anode:

Customer Name:	
Customer PO Number:	
Serial Number:	SAP Number (Sales Order Number):

This protocol details the results of the factory acceptance test procedure for Bruker AXS diffraction systems in parallel beam reflection geometry (Göbel mirror systems). The factory acceptance test procedure consists in full-profile measurements of the certified NIST standard reference material NIST SRM1976c . Details of this procedure are outlined in the Instrument Verification Booklet, which is part of the instrument documentation.

The present verification routine covers the functionality of all relevant components of the diffraction system under investigation.

System within required specifications			
Customer	Name:		
Date:		Signature:	
Technicia	n Name:		
Date:		Signature:	

Part I: Instrument Details

Instrument Configuration D8 ADVANCE

	Instrument Detail	S		Set Values for Validation			
Diffractometer	D8 ADVANCE ¹⁾			Tube Power: 40 kV / 40 mA (for FL tubes) ²⁾			
				Tube Power: 40 k	V / 30 mA (for	r FF tubes) ²⁾	
Vertical	Theta/Theta						
goniometer	Theta/2Theta						
	Height:						
	150						
	Radius:						
	Primary radius		[mm]				
	Secondary radius		[mm]				
Sample stage	Standard						
	Rotating						
	FLIP-STICK			Sample position 5			
	AUTO CHANGER			Sample position A	.1		
	Compact Cradle/ C Cradle ^{Plus}	Compact Cradle/ Compact Cradle ^{Plus}					
	Compact UMC						
Monochroma-	Primary Göbel mirr	or 60 mm		Exit slit 1.2 mm			
tisation	Primary TWIN / TR beam	IO parallel		Exit slit 1 mm Copy values from High Resolution mode:			
	Discriminator Settir	ngs					
	(LYNXEYE XE / LY XE-T)	'NXEYE		Low Thr. [V]	High Thr. [V]	Veto Thr. [V]	
Slits	Primary axial Solle	r slit		2.5°			
	Secondary equator slit	ial Soller		0.2°			
Detector	Scintillation counte	r 🔵					
	LYNXEYE, SSD16	0	LYNXEY	E User Manual DO	C-M88-EXX0	95	
	LYNXEYE XE		LYNXEY	E XE User Manual	DOC-M88-EX	XX240	
	LYNXEYE XE-T		LYNXEY	E XE-T User Manu	alDOC-M88-I	EXX239	
	LYNXEYE-2	LYNXEY	E-2 User Manual D	OC-M88-EX	<305		
	SSD160-2 SSI			2 User Manual DO	C-M88-EXX3	06	
	Solid state detector (SOL-XE)	r 🔵	SOL-XE	SOL-XE User Manual DOC-M88-EXX113			
	VÅNTEC-1		VÅNTEC	-1 User Manual DC	C-M88-EXX	072	

	Instrument Details			Set Values for Validation		
	EIGER2 R 500K		EIGER2	R 500K User Manual DOC-M88-EXX293		
¹⁾ including D8 ADVANCE ECO ²⁾ 40 kV / 25 mA in case of D8 ADVANCE ECO						

Instrument Configuration D8 DISCOVER

	Instrument Details			Set Values for Validation		
Diffractome- ter	D8 DISCOVER			Tube Power: 4 Tube Power: 4 TXS Power: 50 filament, line al TXS Power: 50 filament, spot f	0 kV / 40 mA (fc 0 kV / 30 mA (fc 0 kV / 100 mA (fc nd spot focus) 0 kV / 22 mA (for ocus)	or FL tubes) or FF tubes) or 0.3x3 mm ²
Vertical goniometer	Theta/Theta Theta/2Theta					
	Height: 150 214 258					
	Radius: Primary radius Secondary radius	[m	m] m]			
Horizontal	Theta/2Theta					
goniometer	Height: 214 258					
	Radius: Primary radius Secondary radius	[m	m] m]			
Sample stage	Standard		\bigcirc			
	Rotating					
	FLIP-STICK			Sample positio	n 5	
	AUTO CHANGER		\bigcirc	Sample positio	n A1	
	Compact Cradle/ Cor	npact Cradle ^{Plus}				
	Centric Eulerian Crac	lle				
	UMC 150/151/1516/1	50 HTC				
	Compact UMC					
Monochro-	Primary Göbel mirror 60 mm		\bigcirc	Exit slit 1.2 mm	ı	
matisation	Primary TWIN / TRIC	parallel beam		Exit slit 1 mm		
	Discriminator Setting (LYNXEYE XE / LYN	s XEYE XE-T)		Copy values fro Low Thr. [V]	om High Resolu High Thr. [V]	tion mode: Veto Thr. [V]
Slits	Primary axial Soller s	lit		2.5°		
	Secondary equatorial Soller slit			0.2°		

	Instrument Details		Set Values for Validation
Detector	Scintillation counter		
(See User	LYNXEYE, SSD160	LYN	XEYE User Manual DOC-M88-EXX095
Manuals)	LYNXEYE XE	LYN	XEYE XE User Manual DOC-M88-EXX240
	LYNXEYE XE-T	LYN	XEYE XE-T User ManualDOC-M88-EXX239
	LYNXEYE-2	LYN	IXEYE-2 User Manual DOC-M88-EXX305
	SSD160-2	SSE	0160-2 User Manual DOC-M88-EXX306
	Solid state detector (SOL-XE)	SOI	XE User Manual DOC-M88-EXX113
	VÅNTEC-1	VÅN	NTEC-1 User Manual DOC-M88-EXX072
	EIGER2 R 500K	EIG	ER2 R 500K User Manual DOC-M88-EXX293

Part II: Angular Accuracy, Instrument Response and Resolution

	Anode: Cu			Parallel Beam Geometry									
Angı	Ilar Accura	acy: Difference	Deflection ar	igle corr	Instrument Response: I _{rel}) Instrument Resolution								Resolution
Maximum allowed 2θ deviation depends on height		Maximum allo	Maximum allowed intensity deviation for point detectors ± 10% FWHM _{obs} < FWHM _{max}							-WHM _{max}			
2θ _{obs} [°]	Differ- ence	2θ _{obs} Deflection angle corr	Difference Deflection angle corr	2θ _{exp} ¹⁾ [°]	I _{obs}	I _{obs} I _{exp}	I _{rel} =	Iobs N	I _{min}	I _{exp} ¹⁾	I _{max}	FWHM _{obs} [°]	FWHM _{max} ²⁾ [°]
				25.561					21.49	23.88	26.27		
				35.137					90.00	100.00	110.00		
				88.996					11.06	12.29	13.52		
				127.692					13.37	14.85	16.34		
Deflection	angle corr ce _{max} +Differ	rence _{min})									$Sum = \sum$	$\sum \frac{I_{obs}}{I_{exp}}, i = 1 \dots 4$	
Detector ³⁾	Curren	t Deflection ano	gle		Shift						N	$=\frac{Sum}{4}$	
2-Theta ³⁾	Corrected Deflection angle (Current Deflection angle – Deflection angle corr)				Hei	ght	Maxir	num allow	ed shift 26) [°] fo	or specified a	ccuracy of:	
N: scaling f	factor; For o	details cf. chapt	er Reference \	/alues [▶ 15]	Vertical	150			0.02	2		± 0.0	1°
obs: observed					_	214			0.0	3		± 0.01	15°
exp: expected						258			0.04	4		± 0.0	2°
corr: corrected					Horizontal	214			0.02	2		± 0.0	1°
rel: relative						258			0.02	2		± 0.0	1°
¹⁾ see table ²⁾ see table ³⁾ mark app	3.1 3.3 licable: det	ector in case of	Theta/Theta a	nd 2-Theta in c	case of Theta/2	2Theta	Thon ~	0000	monto mu	at he rest-			flactions
Depending	on specific	measurement	setups, individ	uai reflections l	may not be me	easurable.	i nen m	easure	ments mus	si de restri	clea to a	accessible re	nections.

Comments		

H. Customer Acceptance Test **Protocol**

Declaration of Conformity

Parallel Beam Geometry with Cobalt Anode

NIST SRM1976c Sample: Co

Anode:

Customer Name:		
Customer PO Number:		
Serial Number:	S	AP Number (Sales Order Number):

This protocol details the results of the factory acceptance test procedure for Bruker AXS diffraction systems in parallel beam reflection geometry (Göbel mirror systems). The factory acceptance test procedure consists in full-profile measurements of the certified NIST standard reference material NIST SRM1976c . Details of this procedure are outlined in the Instrument Verification Booklet, which is part of the instrument documentation.

The present verification routine covers the functionality of all relevant components of the diffraction system under investigation.

System within required specifications			YES NO	
Customer	Name:			
Date:		Signature:		
Technicia	n Name:			
Date:		Signature:		

Part I: Instrument Details

Instrument Configuration D8 ADVANCE

	Instrument Details			Set Values for Validation			
Diffractometer	D8 ADVANCE ¹⁾			Tube Powe tubes) ²⁾ Tube Powe tubes) ²⁾	er: 35 kV / 40 m er: 35 kV / 30 m	nA (for FL nA (for FF	
Vertical goniometer	Theta/Theta Theta/2Theta Height: 150 Radius:			-			
	Primary radius Secondary radius		[mm] .[mm]				
Sample stage	Standard						
	Rotating						
	FLIP-STICK			Sample po	sition 5		
	AUTO CHANGER			Sample po	sition A1		
	Compact Cradle/ Com	pact Cradle					
	Compact UMC						
Monochroma-	Primary Göbel mirror 6	60 mm		Exit slit 1.2	mm		
tisation	Discriminator Settings (LYNXEYE XE / LYNX		Copy value mode:	es from High Re	esolution		
				Low Thr. [V]	High Thr. [V]	Veto Thr. [V]	
Slits	Primary axial Soller slit	t		2.5°			
	Secondary equatorial S	Soller slit		0.2°			
Detector	Scintillation counter						
(See Oser Manuals)	LYNXEYE, SSD160 LYNXEYE XE LYNXEYE XE-T LYNXEYE-2 SSD160-2 Solid state detector (SOL-XE)		LYNXEY LYNXEY LYNXEY SSD160- SOL-XE	E User Man E XE User N E XE-T Use E-2 User Man 2 User Manua	ual DOC-M88-I /anual DOC-M r ManualDOC-I anual DOC-M88-I ual DOC-M88-I I DOC-M88-EX	EXX095 88-EXX240 M88-EXX239 8-EXX305 EXX306 XX113	

	Instrument Details			Set Values for Validation	
	VÅNTEC-1		VÅNTEC-	-1 User Manual DOC-M88-EXX072	
	EIGER2 R 500K		EIGER2 F	R 500K User Manual DOC-M88-EXX293	
1) including D8 ADVANCE ECO 2) 35 kV / 28 mA in case of D8 ADVANCE ECO					

	Instrument Details			Set Values fo	r Validation	
Diffractome- ter	D8 DISCOVER			Tube Power: 3 Tube Power: 3	5 kV / 40 mA 5 kV / 30 mA	(for FL tubes) (for FF tubes)
Vertical goniometer	Theta/Theta Theta/2Theta					
	Height: 150 214 258					
	Radius: Primary radius Secondary radius	[mm] [mm]				
Horizontal goniometer	Theta/2Theta Height: 214					
	258					
	Radius: Primary radius Secondary radius	 [mm] 				
Sample	Standard					
stage	Rotating					
	FLIP-STICK			Sample position	on 5	
	AUTO CHANGER			Sample positio	on A1	
	Compact Cradle/ Compac Cradle ^{Plus}	t				
	Centric Eulerian Cradle					
	UMC 150/151/1516/150 H	ITC				
	Compact UMC					
Monochro-	Primary Göbel mirror 60 m	nm		Exit slit 1.2 mn	n	
matisation	Discriminator Settings (LYNXEYE XE / LYNXEYI	E XE-T)		Copy values fr	om High Reso	olution mode:
		,		Low Inr. [V]	Fign Thr. [V]	veto inr. [V]
Slits	Primary axial Soller slit					
	Secondary equatorial Soll	er slit				

Instrument Configuration D8 DISCOVER

	Instrument Details		Set Values for Validation
Detector	Scintillation counter		
	LYNXEYE, SSD160	LYN	XEYE User Manual DOC-M88-EXX095
	LYNXEYE XE	LYN	XEYE XE User Manual DOC-M88-EXX240
	LYNXEYE XE-T	LYN	XEYE XE-T User ManualDOC-M88-EXX239
	LYNXEYE-2	LYN	XEYE-2 User Manual DOC-M88-EXX305
	SSD160-2	SSI	D160-2 User Manual DOC-M88-EXX306
	Solid state detector (SOL-XE)	SO	L-XE User Manual DOC-M88-EXX113
	VÅNTEC-1	VÅI	NTEC-1 User Manual DOC-M88-EXX072
	EIGER2 R 500K	EIG EX	ER2 R 500K User Manual DOC-M88- K293

L	

Part II: Angular Accuracy, Instrument Response and Resolution

Anode: Co					Parallel Beam Geometry					
Angular Accuracy: Difference Deflection angle corr					Instrument Resolution					
Maximum allowed 2θ deviation depends on height					FWHM _{obs} < FWHM _{max}					
2θ _{obs} [°]	Difference	2θ _{obs} Deflection angle corr	Difference Deflection angle corr	2θ _{exp} ¹⁾ [°]	FWHM _{obs} [°]		bs	FWHM _{max} ²⁾ [°]		
				29.773						
				41.041						
				81.250						
				118.165						
Deflection angle corr ½(Difference _{max} +Difference _{min})										
Detector ³⁾	Current Defl	ection angle		Shift						
2-Theta ³⁾	Corrected D (Current Def Deflection a	eflection angle lection angle - ngle corr)			Hei	ght	Maximum allowed shift 2θ [°] for specified ac		for specified accuracy of:	
	·			Vertical	150		0.02		± 0.01°	
For details cf. chapter <i>Reference Values</i> [▶ 15]					214		0.03		± 0.015°	
obs: observed					258		0.04		± 0.02°	
exp: expected				Horizontal	214		0.02		± 0.01°	
corr: corrected					258		0.02		± 0.01°	
¹⁾ see table 3.2 ²⁾ see table 3.4 ³⁾ mark applicat	ble: detector in cas	se of Theta/Theta	and 2-Theta in c	ase of Theta/2	Theta					
Depending on a	specific measuren	nent setups, indivi	dual reflections n	nay not be mea	surable. The	en measi	urements must be r	estricted to	accessible reflections.	

Comments		

I. Daily Check Protocol

System No.:							
Sample:							
Anode:							
Reflection (hkl):		2θ _{exp} : Maximum allowed 2θ deviation: ± 0.01°			FWHM _{exp} : Maximum allowed FWHM (< FWHM _{max})		
Date	Line Postion	Line Intensity	Line Shape	Pass / I	Fail	Operator	Signature

Date	Line Postion	Line Intensity	Line Shape	Pass / Fail	Operator	Signature

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