D8 Series

- User Manual

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

Original Instructions

Innovation with Integrity

XRD

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Contents

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

	Bragg-Brentano Systems		Parallel Beam Systems
Diffractometer	**D8 ADVANCE[1)]** **D8 DISCOVER**	**D8 ENDEAVOR[2)]**	**D8 ADVANCE[1)]** **D8 DISCOVER**
Detector	Scintillation counter Solid state detector (SOL-XE) Linear detector VÅNTEC-1 Linear detector LYNXEYE / LYNXEYE-2 / LYNXEYE XE / LYNXEYE XE-T / SSD160 / SSD160-2 EIGER2 R 500K	LYNXEYE XE LYNXEYE XE-T LYNXEYE-2 SSD160-2	Scintillation counter Solid state detector (SOL-XE) Linear detector VÅNTEC-1 Linear detector LYNXEYE / LYNXEYE -2 / LYNXEYE XE / LYNXEYE XE-T / SSD160 / SSD160-2 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 "**G**ood" and end in "**P**ractice", 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

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.

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

Instrument Parameter	**Value**	**Value (with air scatter screen)**
Generator settings	Cu: 40 kV / 40 mA [3) 5)] Co: 35 kV / 40 mA [3) 5)]	Cu: 40 kV / 40 mA [3) 5)] Co: 35 kV / 40 mA [3) 5)]
Divergence slit [1)]	0.3° (approx. 0.6 mm)	0.3° (approx. 0.6 mm)
Axial Soller slits Primary Secondary	2.5° 2.5°	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 no Debye slit (see corresponding User Manual)	3° detector opening no Debye slit (see corresponding User Manual)
Linear detector LYNXEYE / LYNXEYE-2 / LYNXEYE XE / LYNXEYE XE-T [6) 7)] / SSD160 / SSD160-2 Linear detector EIGER2 R 500K[8)]	3° detector opening in all available directions, antiscatter slit max. opening (see corresponding User Manual) exact value might be chosen slightly smaller in case of instrumental restrictions	3° detector opening in all available directions

[1)] Variable slits must be operated in fixed mode.
[2)] If no secondary monochromator is used, a suited Kβ-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 ± 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.

Table 2.4: Measurement parameters for Cu radiation

Reflection hkl	Scan angles 2θ [°] [1)]	Step width 2θ [°] [1)]	Step time [s] [1)]
0 1 2	24.7 - 26.2	0.005	5
1 0 4	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 / 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.			

Table 2.5: Measurement parameters for Co radiation

Reflection hkl	Scan angles 2θ [°] [1)]	Step width 2θ [°] [1)]	Step time [s] [1)]
0 1 2	29.2 - 30.4	0.005	20
1 0 4	40.3 - 41.8	0.005	8
3 0 0	80.8 - 81.9	0.01	50
2 2 6	117.2 - 119.4	0.02	100

[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.
2. Select the **Area** page and create a new area using the complete measured range. For linear detectors use exactly the ranges defined by table 2.4 and table 2.5 in section *Measurement Parameters [▶ 11]*.
   - 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.
2. Select the **Area** page and create a new area using the complete 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 complete 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.

Table 3.1: Reference values for line positions and relative intensities for Cu-radiation ($CuK_{\alpha 1}$: λ = 0.154059 nm)

Reflection hkl	Line position 2θ [°] Bragg-Brentano	Line position 2θ [°] Parallel Beam	Relative intensity (Net area rounded to 2 decimal place)
0 1 2	25.575	25.561	23.88
1 0 4	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 3.2: Reference values for line positions (without absorption correction) for Co-radiation ($CoK_{\alpha 1}$: λ = 0.178897 nm)

Reflection hkl	Line position 2θ [°] Bragg-Brentano	Line position 2θ [°] Parallel Beam
0 1 2	29.786	29.773
1 0 4	41.049	41.041
3 0 0	81.247	81.250
2 2 6	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	**Bragg-Brentano**			**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)] [°]**
0 1 2	0.055	0.07	0.06	0.22
1 0 4	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 / 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-Brentano**			**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] [°]**
0 1 2	0.06	0.10	0.06	0.22
1 0 4	0.06	0.10	0.06	0.22
3 0 0	0.10	0.11	0.10	0.22
2 2 6	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

Sample: **NIST SRM1976c**

Anode: **Cu**

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**
Tested by:			
Name, first 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 Supervisor:			
Name, first name:			
Date:		**Signature:**	

Comments

Part I: Instrument Details (D8 Series)

Instrument Configuration D8 ADVANCE

	Instrument Details		Set Values for Validation
Diffractometer	**D8 ADVANCE** [1]		Tube Power: 40 kV / 40 mA (for FL tubes) [2] Tube Power: 40 kV / 30 mA (for 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 A1
	Compact Cradle / Compact Cradle^{Plus}	☐	
	Compact UMC	☐	
Monochromatisation	Kβ-Filter	☐	
	Secondary monochromator	☐	
	Focusing monochromator	☐	
	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 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

	Instrument Details		Set Values for Validation
Detector (See User Manuals)	Scintillation counter	☐	
	LYNXEYE, SSD160	☐	LYNXEYE User Manual DOC-M88-EXX095
	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	☐	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

[1] including D8 ADVANCE ECO
[2] 40 kV / 25 mA in case of D8 ADVANCE ECO

Comments

Instrument Configuration D8 DISCOVER

	Instrument Details		Set Values for Validation
Diffractometer	**D8 DISCOVER**		Tube Power: 40 kV / 40 mA (for FL tubes) Tube Power: 40 kV / 30 mA (for FF tubes) TXS Power: 50 kV / 100 mA (for 0.3x3 mm^2 filament, line and spot focus) TXS Power: 50 kV / 22 mA (for 0.1x1 mm^2 filament, spot focus)
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] .....[mm]	
Sample stage	Standard	☐	
	Rotating	☐	
	FLIP-STICK	☐	Sample position 5
	AUTO CHANGER	☐	Sample position A1
	Compact Cradle/ Compact Cradle^{Plus}	☐	
	Centric Eulerian Cradle	☐	
	UMC 150/151/1516/150 HTC	☐	
	Compact UMC	☐	
Monochroma-tisation	Kβ-Filter	☐	
	Secondary monochromator	☐	
	Focusing monochromator	☐	
	Discriminator Settings (LYNXEYE XE / LYNXEYE XE-T)	☐	Copy values from High Resolution mode: 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 (See User Manuals)	Scintillation counter	☐	
	LYNXEYE, SSD160 LYNXEYE XE LYNXEYE XE-T LYNXEYE-2 SSD160-2	☐ ☐ ☐ ☐ ☐	LYNXEYE User Manual DOC-M88-EXX095 LYNXEYE XE User Manual DOC-M88-EXX240 LYNXEYE XE-T User ManualDOC-M88-EXX239 LYNXEYE-2 User Manual DOC-M88-EXX305 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

Comments

Instrument Configuration D8 ENDEAVOR

	Instrument Details		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 goniometer	Theta/Theta	☐	
	Height: 150	☐	
	Radius: 200,5	☐	
	Rotating	☐	Sample position A1
Monochromati-sation	**Kβ-Filter**	☐	
	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	☐	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 LYNXEYE XE-T LYNXEYE-2 SSD160-2	☐ ☐ ☐ ☐	LYNXEYE XE User Manual DOC-M88-EXX240 LYNXEYE XE-T User ManualDOC-M88-EXX239 LYNXEYE-2 User Manual DOC-M88-EXX305 SSD160-2 User Manual DOC-M88-EXX306

[1] including D8 ENDEAVOR ECO
[2] 40 kV / 25 mA in case of D8 ENDEAVOR ECO

Comments

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}**	**Instrument Resolution**
Maximum allowed 2θ deviation depends on height	Maximum allowed intensity deviation for point detectors ± 10%	$FWHM_{obs} < FWHM_{max}$

$2\theta_{obs}$ [°]	Differ-ence	$2\theta_{obs}$ Reference Position corr	Difference Reference Position corr	$2\theta_{exp}$ [1] [°]	I_{obs}	$\frac{I_{obs}}{I_{exp}}$	$I_{rel} = \frac{I_{obs}}{N}$	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 Position corr ½($Difference_{max}$+$Difference_{min}$)										$Sum = \sum \frac{I_{obs}}{I_{exp}}, i = 1 \dots 4$		
Detector[3]	Current Reference Position			**Shift**						$N = \frac{Sum}{4}$		
2-Theta[3]	Corrected Reference Position (Current Reference Position - Reference Position corr)				Height		Maximum allowed shift 2θ		for specified accuracy of:			
N: scaling factor; For details cf. chapter *Reference Values [▶ 15]*				Vertical	150	☐	0,02°		± 0,01°			
obs: observed					214	☐	0,03°		± 0,015°			
exp: expected					258	☐	0.04°		± 0,02°			
corr: corrected				Horizontal	214	☐	0,02°		± 0,01°			
rel: relative					258	☐	0,02°		± 0,01°			

[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

B. Factory Acceptance Test Protocol

Declaration of Conformity

Bragg-Brentano 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 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**
Tested by:			
Name, first 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 Supervisor:			
Name, first name:			
Date:		**Signature:**	

Comments

Part I: Instrument Details (D8 Series)

Instrument Configuration D8 ADVANCE

	Instrument Details		Set Values for Validation
Diffractometer	**D8 ADVANCE** [1]		Tube Power: 35 kV / 40 mA (for FL tubes) [2] Tube Power: 35 kV / 30 mA (for 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 A1
	Compact Cradle/ Compact Cradle^{Plus}	☐	
	Compact UMC	☐	
Monochroma-tisation	Kβ-Filter	☐	
	Secondary monochromator	☐	
	Focusing monochromator	☐	
	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 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

	Instrument Details		Set Values for Validation
Detector (See User Manuals)	Scintillation counter	☐	
	LYNXEYE, SSD160	☐	LYNXEYE User Manual DOC-M88-EXX095
	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	☐	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
[1] including D8 ADVANCE ECO [2] 35 kV / 28 mA in case of D8 ADVANCE ECO			

Comments

Instrument Configuration D8 DISCOVER

	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	 .....[mm] .....[mm]	
Horizontal goniometer	Theta/2Theta	☐	
	Height: 214 258	 ☐ ☐	
	Radius: Primary radius Secondary radius	 .....[mm] .....[mm]	
Sample stage	Standard	☐	
	Rotating	☐	
	FLIP-STICK	☐	Sample position 5
	AUTO CHANGER	☐	Sample position A1
	Compact Cradle/ Compact Cradle^{Plus}	☐	
	Centric Eulerian Cradle	☐	
	UMC 150/151/1516/150 HTC	☐	
	Compact UMC	☐	
Monochroma-tisation	Kβ-Filter	☐	
	Secondary monochromator	☐	
	Focusing monochromator	☐	
	Discriminator Settings (LYNXEYE XE / LYNXEYE XE-T)	☐	Copy values from High Resolution mode: Low Thr. [V] / High Thr. [V] / Veto Thr. [V]

	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 (See User Manuals)	Scintillation counter	☐	
	LYNXEYE, SSD160 LYNXEYE XE LYNXEYE XE-T LYNXEYE-2 SSD160-2	☐ ☐ ☐ ☐ ☐	LYNXEYE User Manual DOC-M88-EXX095 LYNXEYE XE User Manual DOC-M88-EXX240 LYNXEYE XE-T User ManualDOC-M88-EXX239 LYNXEYE-2 User Manual DOC-M88-EXX305 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

Comments

Instrument Configuration D8 ENDEAVOR

	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 mA (for FF tubes)[2]
Vertical goniometer	Theta/Theta	☐	
	Height: 150	☐	
	Radius: 200,5	☐	
	Rotating	☐	Sample position A1
Monochroma-tisation	**Kβ-Filter**	☐	
	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	☐	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 LYNXEYE XE-T LYNXEYE-2 SSD160-2	☐ ☐ ☐ ☐	LYNXEYE XE User Manual DOC-M88-EXX240 LYNXEYE XE-T User ManualDOC-M88-EXX239 LYNXEYE-2 User Manual DOC-M88-EXX305 SSD160-2 User Manual DOC-M88-EXX306

[1] including D8 ENDEAVOR ECO
[2] 35 kV / 28 mA in case of D8 ADVANCE ECO

Comments

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

Anode: Co	Bragg-Brentano Geometry
Angular Accuracy: Difference Reference Position corr	**Instrument Resolution**
Maximum allowed 2θ deviation depends on height	$FWHM_{obs} < FWHM_{max}$

$2\theta_{obs}$ [°]	Difference	$2\theta_{obs}$ Reference Position corr	Difference Reference Position corr	$2\theta_{exp}$ [1] [°]	$FWHM_{obs}$ [°]	$FWHM_{max}$ [2] [°]
				29.786		
				41.049		
				81.247		
				118.142		

Reference Position corr ½(Difference$_{max}$+Difference$_{min}$)			obs: observed	
			exp: expected	
Detector[3]	Current Reference Position		corr: corrected	
			For details cf. chapter *Reference Values [▷ 15]*	
2-Theta[3]	Corrected Reference Position (Current Reference Position - Reference Position corr)		**Shift**	

	Height		Maximum allowed shift 2θ	for specified accuracy of:
Vertical	150	☐	0.02°	± 0.01°
	214	☐	0.03°	± 0.015°
	258	☐	0.04°	± 0.02°
Horizontal	214	☐	0.02°	± 0.01°
	258	☐	0.02°	± 0.01°

[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

C. Factory Acceptance Test Protocol

Declaration of Conformity

Parallel Beam Geometry with Copper Anode

Sample: **NIST SRM1976c**

Anode: **Cu**

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			☐ **YES** ☐ **NO**
Tested by:			
Name, first 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 Supervisor:			
Name, first name:			
Date:		**Signature:**	

Comments

Part I: Instrument Details

Instrument Configuration D8 ADVANCE

	Instrument Details		Set Values for Validation
Diffractometer	**D8 ADVANCE** [1)]		Tube Power: 40 kV / 40 mA (for FL tubes)[2)] Tube Power: 40 kV / 30 mA (for 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 A1
	Compact Cradle/ Compact Cradle[Plus]	☐	
	Compact UMC	☐	
Monochroma-tisation	Primary Göbel mirror 60 mm	☐	Exit slit 1.2 mm
	Primary TWIN / TRIO parallel beam	☐	Exit slit 1 mm
	Discriminator Settings (LYNXEYE XE / LYNXEYE XE-T)	☐	Copy values from High Resolution mode: Low Thr. [V] / High Thr. [V] / Veto Thr. [V] (/ /)
Slits	Primary axial Soller slit	☐	2.5°
	Secondary equatorial Soller slit	☐	0.2°
Detector	Scintillation counter	☐	
	LYNXEYE, SSD160 LYNXEYE XE LYNXEYE XE-T LYNXEYE-2 SSD160-2	☐ ☐ ☐ ☐ ☐	LYNXEYE User Manual DOC-M88-EXX095 LYNXEYE XE User Manual DOC-M88-EXX240 LYNXEYE XE-T User ManualDOC-M88-EXX239 LYNXEYE-2 User Manual DOC-M88-EXX305 SSD160-2 User Manual DOC-M88-EXX306
	Solid state detector (SOL-XE)	☐	SOL-XE User Manual DOC-M88-EXX113

	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			

Comments

Instrument Configuration D8 DISCOVER

	Instrument Details		Set Values for Validation
Diffractometer	**D8 DISCOVER**		Tube Power: 40 kV / 40 mA (for FL tubes) Tube Power: 40 kV / 30 mA (for FF tubes) TXS Power: 50 kV / 100 mA (for 0.3x3 mm^2 filament, line and spot focus) TXS Power: 50 kV / 22 mA (for 0.1x1 mm^2 filament, spot focus)
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] .....[mm]	
Sample stage	Standard	☐	
	Rotating	☐	
	FLIP-STICK	☐	Sample position 5
	AUTO CHANGER	☐	Sample position A1
	Compact Cradle/ Compact Cradle^{Plus}	☐	
	Centric Eulerian Cradle	☐	
	UMC 150/151/1516/150 HTC	☐	
	Compact UMC	☐	
Monochromatisation	Primary Göbel mirror 60 mm	☐	Exit slit 1.2 mm
	Primary TWIN / TRIO parallel beam	☐	Exit slit 1 mm
	Discriminator Settings (LYNXEYE XE / LYNXEYE XE-T)	☐	Copy values from High Resolution mode:

Low Thr. [V]	High Thr. [V]	Veto Thr. [V]

	Instrument Details		Set Values for Validation
Slits	Primary axial Soller slit	☐	2.5°
	Secondary equatorial Soller slit	☐	0.2°
Detector (See User Manuals)	Scintillation counter	☐	
	LYNXEYE, SSD160	☐	LYNXEYE User Manual DOC-M88-EXX095
	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	☐	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

Comments

Part II: Angular Accuracy, Instrument Response and Resolution

Anode: Cu	Parallel Beam Geometry	
Angular Accuracy: Difference Deflection angle corr	**Instrument Response: I_{rel})**	**Instrument Resolution**
Maximum allowed 2θ deviation depends on height	Maximum allowed intensity deviation for point detectors ± 10%	$FWHM_{obs} < FWHM_{max}$

$2\theta_{obs}$ [°]	Differ-ence	$2\theta_{obs}$ Deflection angle corr	Difference Deflection angle corr	$2\theta_{exp}$ [1)] [°]	I_{obs}	$\frac{I_{obs}}{I_{exp}}$	$I_{rel} = \frac{I_{obs}}{N}$	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 ½(Difference$_{max}$+Difference$_{min}$)										$Sum = \sum \frac{I_{obs}}{I_{exp}}, i = 1 \dots 4$		
Detector[3)]	Current Deflection angle				**Shift**					$N = \frac{Sum}{4}$		

2-Theta[3)]	Corrected Deflection angle (Current Deflection angle – Deflection angle corr)			Height		Maximum allowed shift 2θ [°]	for specified accuracy of:
N: scaling factor; For details cf. chapter *Reference Values [▷ 15]*			Vertical	150		0.02	± 0.01°
obs: observed				214		0.03	± 0.015°
exp: expected				258		0.04	± 0.02°
corr: corrected			Horizontal	214		0.02	± 0.01°
rel: relative				258		0.02	± 0.01°

[1)] see table 3.1
[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

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 within required specifications			☐ **YES** ☐ **NO**
Tested by:			
Name, first 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 Supervisor:			
Name, first name:			
Date:		**Signature:**	

Comments

Part I: Instrument Details

Instrument Configuration D8 ADVANCE

	Instrument Details		Set Values for Validation
Diffractometer	**D8 ADVANCE** [1]		Tube Power: 35 kV / 40 mA (for FL tubes)[2] Tube Power: 35 kV / 30 mA (for 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 A1
	Compact Cradle/ Compact Cradle Plus	☐	
	Compact UMC	☐	
Monochroma-tisation	Primary Göbel mirror 60 mm	☐	Exit slit 1.2 mm
	Discriminator Settings (LYNXEYE XE / LYNXEYE XE-T)	☐	Copy values from High Resolution mode: Low Thr. [V] / High Thr. [V] / Veto Thr. [V] [ ] / [ ] / [ ]
Slits	Primary axial Soller slit	☐	2.5°
	Secondary equatorial Soller slit	☐	0.2°
Detector (See User Manuals)	Scintillation counter	☐	
	LYNXEYE, SSD160 LYNXEYE XE LYNXEYE XE-T LYNXEYE-2 SSD160-2	☐ ☐ ☐ ☐ ☐	LYNXEYE User Manual DOC-M88-EXX095 LYNXEYE XE User Manual DOC-M88-EXX240 LYNXEYE XE-T User ManualDOC-M88-EXX239 LYNXEYE-2 User Manual DOC-M88-EXX305 SSD160-2 User Manual DOC-M88-EXX306
	Solid state detector (SOL-XE)	☐	SOL-XE User Manual DOC-M88-EXX113

	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) 35 kV / 28 mA in case of D8 ADVANCE ECO			

Comments

Instrument Configuration D8 DISCOVER

	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	 ..... [mm] ..... [mm]	
Horizontal goniometer	Theta/2Theta	☐	
	Height: 214 258	 ☐ ☐	
	Radius: Primary radius Secondary radius	 ..... [mm] ..... [mm]	
Sample stage	Standard	☐	
	Rotating	☐	
	FLIP-STICK	☐	Sample position 5
	AUTO CHANGER	☐	Sample position A1
	Compact Cradle/ Compact Cradle^{Plus}	☐	
	Centric Eulerian Cradle	☐	
	UMC 150/151/1516/150 HTC	☐	
	Compact UMC	☐	
Monochromatisation	Primary Göbel mirror 60 mm	☐	Exit slit 1.2 mm
	Discriminator Settings (LYNXEYE XE / LYNXEYE XE-T)	☐	Copy values from High Resolution mode: Low Thr. [V] / High Thr. [V] / Veto Thr. [V] ( ) / ( ) / ( )
Slits	Primary axial Soller slit	☐	
	Secondary equatorial Soller slit	☐	

	Instrument Details		Set Values for Validation
Detector	Scintillation counter	☐	
	LYNXEYE, SSD160	☐	LYNXEYE User Manual DOC-M88-EXX095
	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	☐	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

Comments

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	$FWHM_{obs} < FWHM_{max}$

$2\theta_{obs}$ [°]	Difference	$2\theta_{obs}$ Deflection angle corr	Difference Deflection angle corr	$2\theta_{exp}$ [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 Deflection angle		**Shift**				
2-Theta[3]	Corrected Deflection angle (Current Deflection angle - Deflection angle corr)			Height		Maximum allowed shift 2θ [°]	for specified accuracy of:
			Vertical	150	☐	0.02	± 0.01°
For details cf. chapter *Reference 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 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

E. Customer Acceptance Test Protocol

Declaration of Conformity

Bragg-Brentano Geometry with Copper Anode

Sample: **NIST SRM1976c**

Anode: **Cu**

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:**	

Comments

Part I: Instrument Details (D8 Series)

Instrument Configuration D8 ADVANCE

	Instrument Details		Set Values for Validation
Diffractometer	**D8 ADVANCE** [1]		Tube Power: 40 kV / 40 mA (for FL tubes) [2] Tube Power: 40 kV / 30 mA (for 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 A1
	Compact Cradle / Compact Cradle^{Plus}	☐	
	Compact UMC	☐	
Monochromatisation	Kβ-Filter	☐	
	Secondary monochromator	☐	
	Focusing monochromator	☐	
	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 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

	Instrument Details		Set Values for Validation
Detector (See User Manuals)	Scintillation counter	☐	
	LYNXEYE, SSD160	☐	LYNXEYE User Manual DOC-M88-EXX095
	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	☐	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

[1] including D8 ADVANCE ECO
[2] 40 kV / 25 mA in case of D8 ADVANCE ECO

Comments

Instrument Configuration D8 DISCOVER

	Instrument Details		Set Values for Validation
Diffractometer	**D8 DISCOVER**		Tube Power: 40 kV / 40 mA (for FL tubes) Tube Power: 40 kV / 30 mA (for FF tubes) TXS Power: 50 kV / 100 mA (for 0.3x3 mm^2 filament, line and spot focus) TXS Power: 50 kV / 22 mA (for 0.1x1 mm^2 filament, spot focus)
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] .....[mm]	
Sample stage	Standard	☐	
	Rotating	☐	
	FLIP-STICK	☐	Sample position 5
	AUTO CHANGER	☐	Sample position A1
	Compact Cradle/ Compact Cradle^{Plus}	☐	
	Centric Eulerian Cradle	☐	
	UMC 150/151/1516/150 HTC	☐	
	Compact UMC	☐	
Monochroma-tisation	Kβ-Filter	☐	
	Secondary monochromator	☐	
	Focusing monochromator	☐	
	Discriminator Settings (LYNXEYE XE / LYNXEYE XE-T)	☐	Copy values from High Resolution mode: 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 (See User Manuals)	Scintillation counter	☐	
	LYNXEYE, SSD160 LYNXEYE XE LYNXEYE XE-T LYNXEYE-2 SSD160-2	☐ ☐ ☐ ☐ ☐	LYNXEYE User Manual DOC-M88-EXX095 LYNXEYE XE User Manual DOC-M88-EXX240 LYNXEYE XE-T User ManualDOC-M88-EXX239 LYNXEYE-2 User Manual DOC-M88-EXX305 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

Comments

Instrument Configuration D8 ENDEAVOR

	Instrument Details		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 goniometer	Theta/Theta	☐	
	Height: 150	☐	
	Radius: 200,5	☐	
	Rotating	☐	Sample position A1
Monochromati-sation	**Kβ-Filter**	☐	
	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	☐	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 LYNXEYE XE-T LYNXEYE-2 SSD160-2	☐ ☐ ☐ ☐	LYNXEYE XE User Manual DOC-M88-EXX240 LYNXEYE XE-T User ManualDOC-M88-EXX239 LYNXEYE-2 User Manual DOC-M88-EXX305 SSD160-2 User Manual DOC-M88-EXX306

[1] including D8 ENDEAVOR ECO
[2] 40 kV / 25 mA in case of D8 ENDEAVOR ECO

Comments

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}**	**Instrument Resolution**
Maximum allowed 2θ deviation depends on height	Maximum allowed intensity deviation for point detectors ± 10%	$FWHM_{obs} < FWHM_{max}$

$2\theta_{obs}$ [°]	Differ-ence	$2\theta_{obs}$ Reference Position corr	Difference Reference Position corr	$2\theta_{exp}$ [1] [°]	I_{obs}	$\frac{I_{obs}}{I_{exp}}$	$I_{rel} = \frac{I_{obs}}{N}$	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 Position corr ½($Difference_{max}$+$Difference_{min}$)											$Sum = \sum \frac{I_{obs}}{I_{exp}}, i = 1 \dots 4$		
Detector[3]	Current Reference Position				**Shift**						$N = \frac{Sum}{4}$		
2-Theta[3]	Corrected Reference Position (Current Reference Position - Reference Position corr)					Height		Maximum allowed shift 2θ		for specified accuracy of:			
N: scaling factor; For details cf. chapter *Reference Values [▶ 15]*					Vertical	150	☐	0,02°		± 0,01°			
obs: observed						214	☐	0,03°		± 0,015°			
exp: expected						258	☐	0.04°		± 0,02°			
corr: corrected					Horizontal	214	☐	0,02°		± 0,01°			
rel: relative						258	☐	0,02°		± 0,01°			

[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

F. Customer Acceptance Test Protocol

Declaration of Conformity

Bragg-Brentano 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 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:**	

Comments

Part I: Instrument Details (D8 Series)

Instrument Configuration D8 ADVANCE

	Instrument Details		Set Values for Validation
Diffractometer	**D8 ADVANCE** [1]		Tube Power: 35 kV / 40 mA (for FL tubes) [2] Tube Power: 35 kV / 30 mA (for 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 A1
	Compact Cradle/ Compact Cradle^{Plus}	☐	
	Compact UMC	☐	
Monochroma-tisation	Kβ-Filter	☐	
	Secondary monochromator	☐	
	Focusing monochromator	☐	
	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 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

	Instrument Details		Set Values for Validation
Detector (See User Manuals)	Scintillation counter	☐	
	LYNXEYE, SSD160	☐	LYNXEYE User Manual DOC-M88-EXX095
	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	☐	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
[1] including D8 ADVANCE ECO [2] 35 kV / 28 mA in case of D8 ADVANCE ECO			

Comments

Instrument Configuration D8 DISCOVER

	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	 .....[mm] .....[mm]	
Horizontal goniometer	Theta/2Theta	☐	
	Height: 214 258	 ☐ ☐	
	Radius: Primary radius Secondary radius	 .....[mm] .....[mm]	
Sample stage	Standard	☐	
	Rotating	☐	
	FLIP-STICK	☐	Sample position 5
	AUTO CHANGER	☐	Sample position A1
	Compact Cradle/ Compact Cradle^{Plus}	☐	
	Centric Eulerian Cradle	☐	
	UMC 150/151/1516/150 HTC	☐	
	Compact UMC	☐	
Monochroma-tisation	Kβ-Filter	☐	
	Secondary monochromator	☐	
	Focusing monochromator	☐	
	Discriminator Settings (LYNXEYE XE / LYNXEYE XE-T)	☐	Copy values from High Resolution mode: Low Thr. [V] / High Thr. [V] / Veto Thr. [V]

	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 (See User Manuals)	Scintillation counter	☐	
	LYNXEYE, SSD160 LYNXEYE XE LYNXEYE XE-T LYNXEYE-2 SSD160-2	☐ ☐ ☐ ☐ ☐	LYNXEYE User Manual DOC-M88-EXX095 LYNXEYE XE User Manual DOC-M88-EXX240 LYNXEYE XE-T User ManualDOC-M88-EXX239 LYNXEYE-2 User Manual DOC-M88-EXX305 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

Comments

Instrument Configuration D8 ENDEAVOR

	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 mA (for FF tubes)[2]
Vertical goniometer	Theta/Theta	☐	
	Height: 150	☐	
	Radius: 200,5	☐	
	Rotating	☐	Sample position A1
Monochroma-tisation	**Kβ-Filter**	☐	
	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	☐	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 LYNXEYE XE-T LYNXEYE-2 SSD160-2	☐ ☐ ☐ ☐	LYNXEYE XE User Manual DOC-M88-EXX240 LYNXEYE XE-T User ManualDOC-M88-EXX239 LYNXEYE-2 User Manual DOC-M88-EXX305 SSD160-2 User Manual DOC-M88-EXX306

[1] including D8 ENDEAVOR ECO
[2] 35 kV / 28 mA in case of D8 ADVANCE ECO

Comments

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

Anode: Co	Bragg-Brentano Geometry
Angular Accuracy: Difference Reference Position corr	**Instrument Resolution**
Maximum allowed 2θ deviation depends on height	$FWHM_{obs} < FWHM_{max}$

$2\theta_{obs}$ [°]	Difference	$2\theta_{obs}$ Reference Position corr	Difference Reference Position corr	$2\theta_{exp}$ [1] [°]	$FWHM_{obs}$ [°]	$FWHM_{max}$ [2] [°]
				29.786		
				41.049		
				81.247		
				118.142		

Reference Position corr ½($Difference_{max}$+$Difference_{min}$)				obs: observed	
				exp: expected	
Detector[3]	Current Reference Position			corr: corrected	
				For details cf. chapter *Reference Values [▷ 15]*	

2-Theta[3]	Corrected Reference Position (Current Reference Position - Reference Position corr)		**Shift**		
				Height	Maximum allowed shift 2θ / for specified accuracy of:
			Vertical	150	0.02° / ± 0.01°
				214	0.03° / ± 0.015°
				258	0.04° / ± 0.02°
			Horizontal	214	0.02° / ± 0.01°
				258	0.02° / ± 0.01°

[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

Sample: **NIST SRM1976c**

Anode: **Cu**

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			☐ **YES** ☐ **NO**
Customer Name:			
Date:		**Signature:**	
Technician Name:			
Date:		**Signature:**	

Comments

Part I: Instrument Details

Instrument Configuration D8 ADVANCE

	Instrument Details		Set Values for Validation
Diffractometer	**D8 ADVANCE** [1)]		Tube Power: 40 kV / 40 mA (for FL tubes)[2)] Tube Power: 40 kV / 30 mA (for 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 A1
	Compact Cradle/ Compact Cradle[Plus]	☐	
	Compact UMC	☐	
Monochroma-tisation	Primary Göbel mirror 60 mm	☐	Exit slit 1.2 mm
	Primary TWIN / TRIO parallel beam	☐	Exit slit 1 mm
	Discriminator Settings (LYNXEYE XE / LYNXEYE XE-T)	☐	Copy values from High Resolution mode: Low Thr. [V] / High Thr. [V] / Veto Thr. [V] (/ /)
Slits	Primary axial Soller slit	☐	2.5°
	Secondary equatorial Soller slit	☐	0.2°
Detector	Scintillation counter	☐	
	LYNXEYE, SSD160 LYNXEYE XE LYNXEYE XE-T LYNXEYE-2 SSD160-2	☐ ☐ ☐ ☐ ☐	LYNXEYE User Manual DOC-M88-EXX095 LYNXEYE XE User Manual DOC-M88-EXX240 LYNXEYE XE-T User ManualDOC-M88-EXX239 LYNXEYE-2 User Manual DOC-M88-EXX305 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

	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

Comments

Instrument Configuration D8 DISCOVER

	Instrument Details		Set Values for Validation
Diffractometer	**D8 DISCOVER**		Tube Power: 40 kV / 40 mA (for FL tubes) Tube Power: 40 kV / 30 mA (for FF tubes) TXS Power: 50 kV / 100 mA (for 0.3x3 mm^2 filament, line and spot focus) TXS Power: 50 kV / 22 mA (for 0.1x1 mm^2 filament, spot focus)
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] .....[mm]	
Sample stage	Standard	☐	
	Rotating	☐	
	FLIP-STICK	☐	Sample position 5
	AUTO CHANGER	☐	Sample position A1
	Compact Cradle/ Compact Cradle^{Plus}	☐	
	Centric Eulerian Cradle	☐	
	UMC 150/151/1516/150 HTC	☐	
	Compact UMC	☐	
Monochromatisation	Primary Göbel mirror 60 mm	☐	Exit slit 1.2 mm
	Primary TWIN / TRIO parallel beam	☐	Exit slit 1 mm
	Discriminator Settings (LYNXEYE XE / LYNXEYE XE-T)	☐	Copy values from High Resolution mode: Low Thr. [V] | High Thr. [V] | Veto Thr. [V] | |
Slits	Primary axial Soller slit	☐	2.5°
	Secondary equatorial Soller slit	☐	0.2°

	Instrument Details		Set Values for Validation
Detector (See User Manuals)	Scintillation counter	☐	
	LYNXEYE, SSD160	☐	LYNXEYE User Manual DOC-M88-EXX095
	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	☐	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

Comments

Part II: Angular Accuracy, Instrument Response and Resolution

Anode: Cu	Parallel Beam Geometry	
Angular Accuracy: Difference Deflection angle corr	**Instrument Response: I_{rel})**	**Instrument Resolution**
Maximum allowed 2θ deviation depends on height	Maximum allowed intensity deviation for point detectors ± 10%	$FWHM_{obs} < FWHM_{max}$

$2\theta_{obs}$ [°]	Differ-ence	$2\theta_{obs}$ Deflection angle corr	Difference Deflection angle corr	$2\theta_{exp}$ [1)] [°]	I_{obs}	$\frac{I_{obs}}{I_{exp}}$	$I_{rel} = \frac{I_{obs}}{N}$	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 ½(Difference$_{max}$+Difference$_{min}$)										$Sum = \sum \frac{I_{obs}}{I_{exp}}, i = 1 \dots 4$		
Detector[3)]	Current Deflection angle				**Shift**					$N = \frac{Sum}{4}$		

2-Theta[3)]	Corrected Deflection angle (Current Deflection angle – Deflection angle corr)			Height		Maximum allowed shift 2θ [°]	for specified accuracy of:
N: scaling factor; For details cf. chapter *Reference Values [▷ 15]*			Vertical	150		0.02	± 0.01°
obs: observed				214		0.03	± 0.015°
exp: expected				258		0.04	± 0.02°
corr: corrected			Horizontal	214		0.02	± 0.01°
rel: relative				258		0.02	± 0.01°

[1)] see table 3.1
[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

H. Customer 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 within required specifications			☐ **YES** ☐ **NO**
Customer Name:			
Date:		**Signature:**	
Technician Name:			
Date:		**Signature:**	

Comments

Part I: Instrument Details

Instrument Configuration D8 ADVANCE

	Instrument Details		Set Values for Validation
Diffractometer	**D8 ADVANCE** [1]		Tube Power: 35 kV / 40 mA (for FL tubes)[2] Tube Power: 35 kV / 30 mA (for 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 A1
	Compact Cradle/ Compact Cradle Plus	☐	
	Compact UMC	☐	
Monochroma-tisation	Primary Göbel mirror 60 mm	☐	Exit slit 1.2 mm
	Discriminator Settings (LYNXEYE XE / LYNXEYE XE-T)	☐	Copy values from High Resolution mode: Low Thr. [V] / High Thr. [V] / Veto Thr. [V] [ ] / [ ] / [ ]
Slits	Primary axial Soller slit	☐	2.5°
	Secondary equatorial Soller slit	☐	0.2°
Detector (See User Manuals)	Scintillation counter	☐	
	LYNXEYE, SSD160 LYNXEYE XE LYNXEYE XE-T LYNXEYE-2 SSD160-2	☐ ☐ ☐ ☐ ☐	LYNXEYE User Manual DOC-M88-EXX095 LYNXEYE XE User Manual DOC-M88-EXX240 LYNXEYE XE-T User ManualDOC-M88-EXX239 LYNXEYE-2 User Manual DOC-M88-EXX305 SSD160-2 User Manual DOC-M88-EXX306
	Solid state detector (SOL-XE)	☐	SOL-XE User Manual DOC-M88-EXX113

	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) 35 kV / 28 mA in case of D8 ADVANCE ECO			

Comments

Instrument Configuration D8 DISCOVER

	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	 ..... [mm] ..... [mm]	
Horizontal goniometer	Theta/2Theta	☐	
	Height: 214 258	 ☐ ☐	
	Radius: Primary radius Secondary radius	 ..... [mm] ..... [mm]	
Sample stage	Standard	☐	
	Rotating	☐	
	FLIP-STICK	☐	Sample position 5
	AUTO CHANGER	☐	Sample position A1
	Compact Cradle/ Compact Cradle^{Plus}	☐	
	Centric Eulerian Cradle	☐	
	UMC 150/151/1516/150 HTC	☐	
	Compact UMC	☐	
Monochromatisation	Primary Göbel mirror 60 mm	☐	Exit slit 1.2 mm
	Discriminator Settings (LYNXEYE XE / LYNXEYE XE-T)	☐	Copy values from High Resolution mode: Low Thr. [V] / High Thr. [V] / Veto Thr. [V] ( ) / ( ) / ( )
Slits	Primary axial Soller slit	☐	
	Secondary equatorial Soller slit	☐	

	Instrument Details		Set Values for Validation
Detector	Scintillation counter	☐	
	LYNXEYE, SSD160 LYNXEYE XE LYNXEYE XE-T LYNXEYE-2 SSD160-2	☐ ☐ ☐ ☐ ☐	LYNXEYE User Manual DOC-M88-EXX095 LYNXEYE XE User Manual DOC-M88-EXX240 LYNXEYE XE-T User ManualDOC-M88-EXX239 LYNXEYE-2 User Manual DOC-M88-EXX305 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

Comments

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	$FWHM_{obs} < FWHM_{max}$

$2\theta_{obs}$ [°]	Difference	$2\theta_{obs}$ Deflection angle corr	Difference Deflection angle corr	$2\theta_{exp}$ [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 Deflection angle		**Shift**				
2-Theta[3]	Corrected Deflection angle (Current Deflection angle - Deflection angle corr)			Height		Maximum allowed shift 2θ [°]	for specified accuracy of:
			Vertical	150	☐	0.02	± 0.01°
For details cf. chapter *Reference 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 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

I. Daily Check Protocol

System No.:	
Sample:	
Anode:	

Reflection (hkl):	**$2\theta_{exp}$: Maximum allowed 2θ deviation: ± 0.01°**	**$FWHM_{exp}$: Maximum allowed FWHM (< $FWHM_{max}$)**

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

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

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