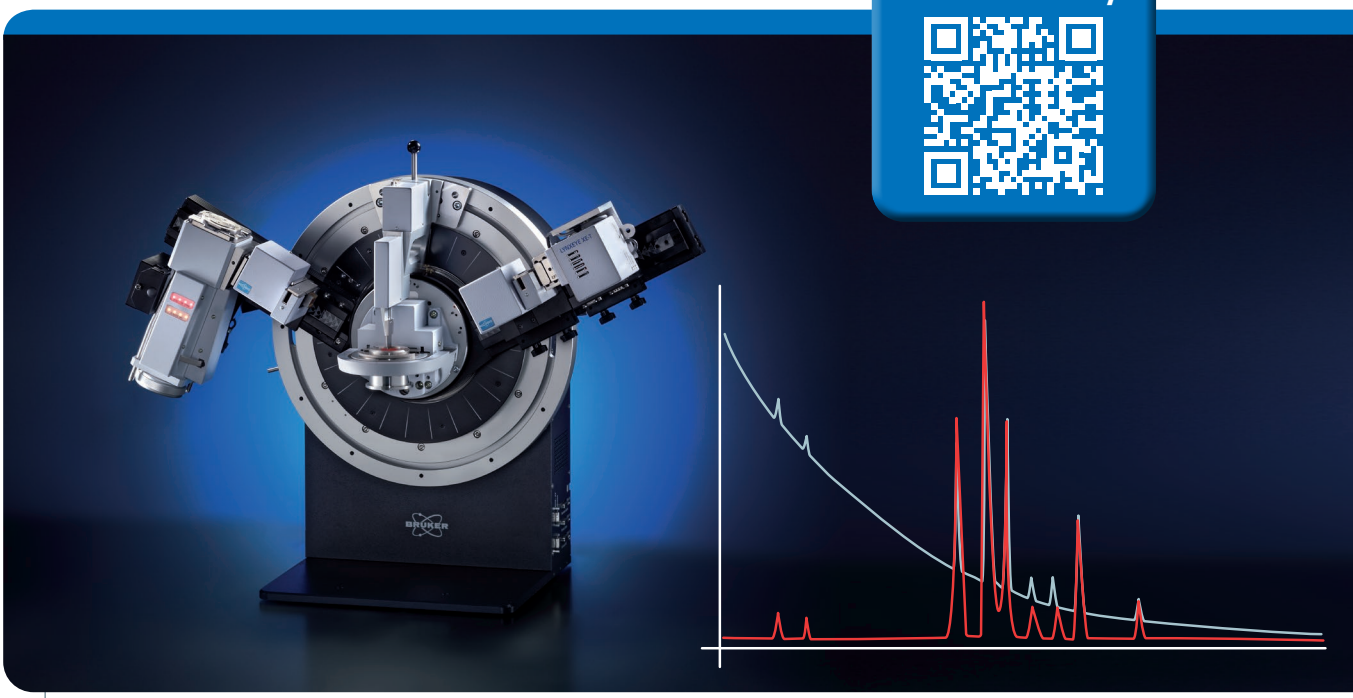
Perfect powder data, automatically



## Product Sheet XRD 52

# Dynamic Beam Optimization

- Superior Suppression of Air and Instrument Scattering

### Introduction

Bruker's unique Dynamic Beam Optimization™ feature sets a significant new benchmark in terms of data quality for X-ray diffraction and scattering applications.
The software controlled synchronization of a motorized divergence slit, motorized anti-scatter screen, and variable detector field of view provides measurement data virtually free of air, instrument, and sample holder scattering – specifically at low angles 2θ.

DBO is available for the D8 ADVANCE, D8 DISCOVER, and the D8 ENDEAVOR diffractometer families. Existing diffractometers can be easily upgraded.

### Key benefits

- Powder data virtually free of air, instrument, and sample support scattering
- Significantly enhanced lower limits of detection and quantification for minor crystalline and amorphous phases
- Superb data quality for materials with low angle peaks (large d-spacings) such as clays, pharmaceuticals, zeolites, and porous framework materials

## What is "Dynamic Beam Optimization"?

Real-world factors are commonly introduced into all XRD experiments and can adversely affect data quality. One of the most common – though largely avoidable – factors is unwanted scattering from a variety of sources:

- Air scattering along the beampath
- Instrument parts, mostly the sample holder
- Sample fluorescence

Common to all of these effects is a strongly increased backgound, most notable at low angles $2\theta$, that is often accompanied by additional peaks originating from the sample environment. The consequence is an unpleasant looking powder pattern with a significant reduction in sensitivity, both in terms of lower limits of detection and quantification, and errors in relative peak intensities.

With Dynamic Beam Optimization (DBO) three technologies merge, resulting in perfect powder data, automatically:

1. Motorized Divergence Slit
2. Motorized Anti-Scatter Screen
3. Variable Detector Field of View (FoV)

The net result is a system with performance greater than the sum of its parts, and sets a new benchmark in terms of data quality as is instantly apparent from the data. The effective elimination of all sorts of unwanted scattering directly results in superb peak-to-background ratios and low-angle background performance. Additionally, when employing the unique energy dispersive LYNXEYE XE-T detector, fluorescence radiation can be completely filtered without intensity loss.

DBO delivers not only unrivalled powder diffraction data quality, but also the experiments just got simpler: there is no beam-spill, no cropping of the beam, and no need for a beam-stop.


**Would you like to see how DBO works? Watch this video to learn how to acquire perfect powder data everytime, automatically.**


## Maximum flexibility

Dynamic Beam Optimization perfectly adapts to the requirements of your applications. Each component provides a unique benefit in terms of data quality and can be used independently. Employed together, the three technologies – the Motorized Divergence Slit, Motorized Anti-Scatter Screen and Variable Detector FoV – deliver best data quality and maximum ease-of-use. Combined with other DAVINCI optics, stages or even detectors, the DBO components complement your existing set-up.

## Do you want to

- Switch from Bragg-Brentano to parallel beam geometry?
  → Easy! Dynamic Beam Optimization supports both geometries.
- Use a non-ambient chamber or any other sample stage which would collide with the Motorized Anti-Scatter Screen
  → Easy! Take it out.
- Use a capillary stage or perform reflectometry experiments?
  → Easy! Move the Motorized Anti-Scatter Screen to the desired position and keep it fixed.
- Measure samples without low angle peaks?
  → Easy! Switch off the Variable Detector FoV with a mouse click.

### Benefits

- Superior data quality free of parasitic scattering
  → Acquisition of diffraction data with virtually no instrument background starting at angles as low as about 0.3° 2θ
  → Superior suppression of white radiation and sample fluorescence with the LYNXEYE XE-T
- Ultimate ease-of-use
  → Fully automatic, software controlled synchronization of Motorized Divergence Slits, Motorized Anti-Scatter Screen, and Variable Detector FoV
- Maximum flexibility and compatibility
  → Supports a wide range of different instrument setups
  → Fully compatible with both the Bragg-Brentano geometry (fixed as well as variable divergence slits) and parallel beam geometry

# Dynamic Beam Optimization – Key Components


**Motorized Divergence Slit**


Motorized Anti-Scatter Screen


Variable Detector FoV

## 1 Motorized Divergence Slit

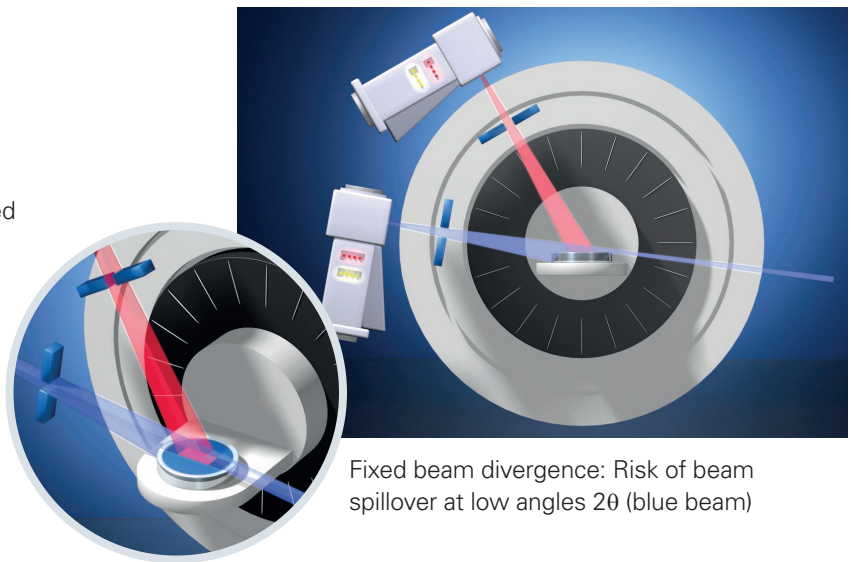
**Full prevention of sample support scattering**

The function of divergence slits is to control the vertical beam divergence in order to illuminate as much of the sample surface as possible without illuminating the sample support as well.

Where fixed slits are employed, the divergence of the X-ray beam is kept constant, but the illuminated sample length changes as a function of 2θ. As a result, at low angles 2θ, there is a risk of illuminating the sample support (beam spillover). Once the sample support is illuminated, there is increasing scattering at low angles 2θ in the form of "amorphous bumps" and additional peaks. Reducing the slit size reduces the risk of beam spillover but also results in significant intensity loss.

Motorized Divergence Slits vary the beam divergence to keep the illuminated sample length constant at all angles 2θ. They are an effective solution to the spillover problem enabling highest possible intensities at all angles 2θ. When beam spillover is not an issue, Motorized Divergence Slits can also be used in fixed slit mode.

- Can be operated in fixed and variable slits mode
- Prevents parasitic scattering from the sample support
- Enables highest possible intensities at all angles 2θ



Fixed beam divergence: Risk of beam spillover at low angles 2θ (blue beam)

Variable beam divergence: The beam is confined within the sample at all angles 2θ

# Dynamic Beam Optimization – Key Components


Motorized Divergence Slit


**Motorized Anti-Scatter Screen**

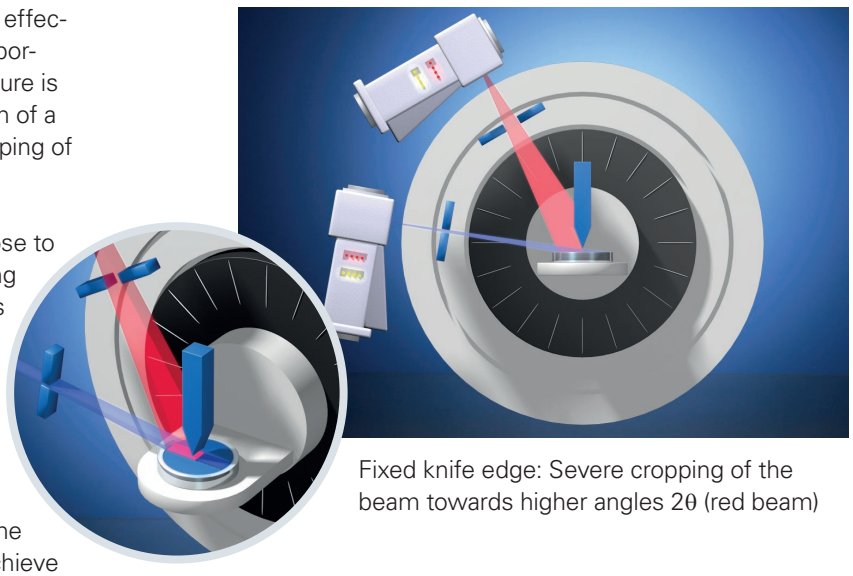

Variable Detector FoV

## 2 Motorized Anti-Scatter Screen – Superior shielding of low to high angle air scattering

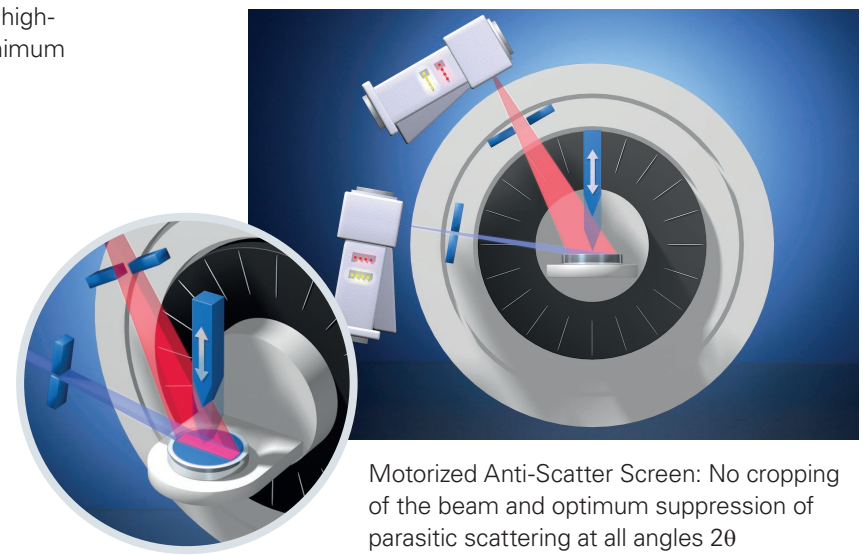
The Motorized Anti-Scatter Screen is a device for effective shielding of instrument background, most importantly air-scattering at low angles 2θ. The key feature is the fully software controlled, continuous retraction of a knife edge as a function of 2θ to prevent any cropping of the beam, especially at higher angles 2θ.

Traditional fixed knife edges have to be placed close to the sample surface to suppress parasitic scattering at low angles 2θ. Consequently, the X-ray beam is cropped at higher angles. This effect is most pronounced for the Bragg-Brentano geometry when using variable slits (constant illuminated sample length). As a result, intensities at high angles will be affected by large systematic errors.

With the unique Motorized Anti-Scatter Screen, the knife edge position is automatically adjusted to achieve maximum suppression of parasitic scattering without cropping the beam at any angles 2θ. As a result, highest-quality data with accurate intensities and minimum instrument background will be obtained.



Fixed knife edge: Severe cropping of the beam towards higher angles 2θ (red beam)



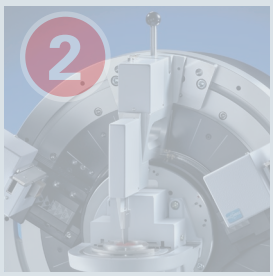
Motorized Anti-Scatter Screen: No cropping of the beam and optimum suppression of parasitic scattering at all angles 2θ

### Features

- Bragg-Brentano geometry:
  - → Fixed as well as automatic operation.
  - → Fixed as well as variable beam divergence
- Parallel and focusing capillary transmission geometry:
  - → Fixed operation

# Dynamic Beam Optimization – Key Components


Motorized Divergence Slit




Motorized Anti-Scatter Screen

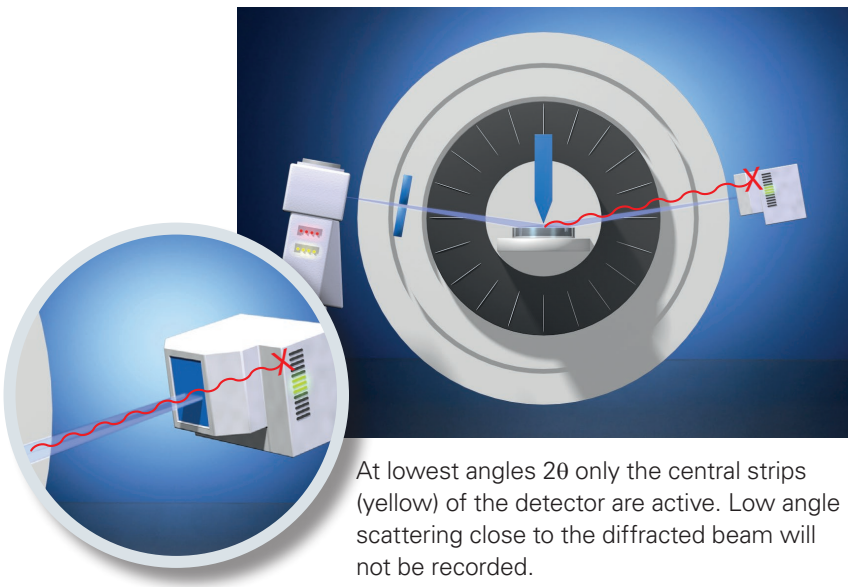

Variable Detector FoV

## 3 Variable Detector FoV – Superior reduction of very low angle air scattering

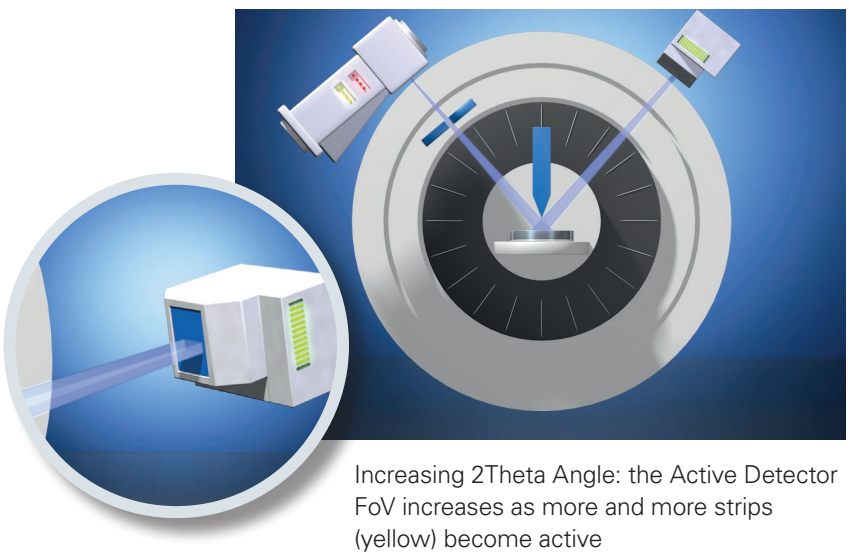
Data acquisition at low angles, smaller than ~20° 2θ requires sophisticated beam conditioning to minimize air scattering, which otherwise is the most prominent contribution to the data. This is of particular concern at very low angles smaller than ~5° 2θ, the small angle X-ray scattering (SAXS) regime, where background suppression is of highest importance.

Bruker's unique Variable Detector FoV provides for excellent reduction of very low angle background scattering. This is achieved by automatic, software-controlled change of the active detector window size as a function of 2θ: At 0° 2θ, the active detector window is closed and gradually opens as the detector moves to higher angles 2θ. As a consequence, the use of beamstops to minimize scattering becomes obsolete, and high quality data with virtually no instrument background can be collected starting at angles as low as ~0.3° 2θ.

- Electronically controlled active detector window, no mechanical slits
- Effectively shields scattering at very low angles down to ~0.3° 2θ
- Unambiguous detection of SAXS signals

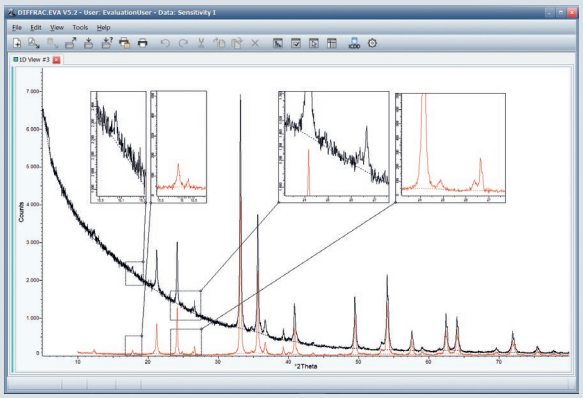


At lowest angles 2θ only the central strips (yellow) of the detector are active. Low angle scattering close to the diffracted beam will not be recorded.



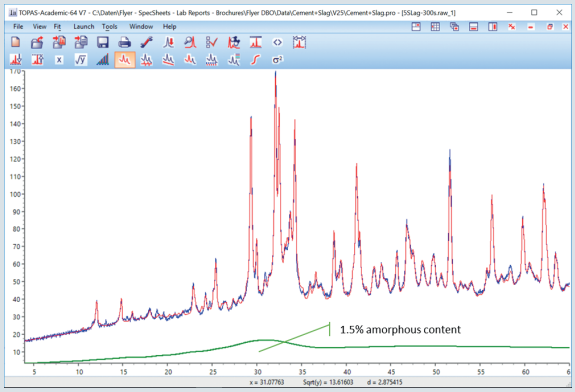
Increasing 2Theta Angle: the Active Detector FoV increases as more and more strips (yellow) become active

# Application Examples



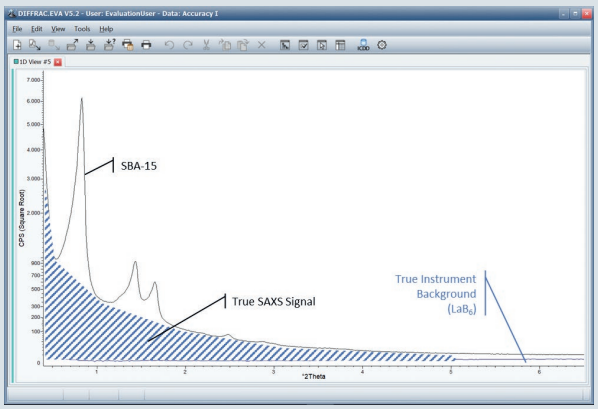
## Sensitivity (I): Crystalline materials

High instrument background may not only reduce lower limits of detection and quantification significantly, but can entirely obscure important reflections. This figure shows data taken without (black scan) and with Motorized Anti-Scatter Screen (red scan). Using the Motorized Anti-Scatter Screen, instrument background is reduced to the bare minimum, allowing reliable detection and quantification of minor phases down to levels less than 0.05wt% absolute.



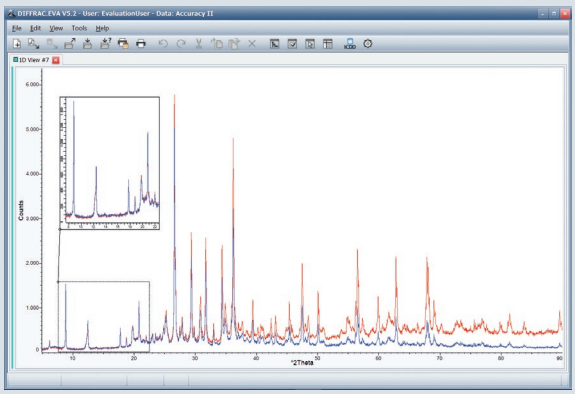

## Sensitivity (II): Amorphous materials

The analysis of amorphous materials is more challenging than for crystalline materials. The former contribute broad bumps rather than sharp peaks to the observed pattern, which are difficult to distinguish from instrument background. When using the Motorized Anti-Scatter Screen, small levels of amorphous material can be accurately quantified even in highly complex powder patterns. Lower levels of detection and quantification of down to or less than 1.5wt% absolute are achievable.




## Accuracy (I): Low angle (SAXS) data

It is at very low angles, where the combination of the Motorized Anti-Scatter Screen and the Variable Detector FoV shines. Successful reduction of air scattering close to the primary beam enables accurate measurements of SAXS data as shown in the figure for SBA-15. (black scan). The true instrument background can be determined using a standard such as LaB6 (blue scan). The result is SAXS data, virtually free of instrument background.



## Accuracy (II): High angle data

Intensities at both low and high angle are measured accurately using the Motorized Anti-Scatter Screen. Fixed knife edges cannot suppress low angle instrument background without severely cropping intensities at higher angles (black scan). With the unique Motorized Anti-Scatter Screen, the knife edge position is automatically adjusted to achieve maximum suppression of instrument background without cropping the beam at any angles (red scan).

# Technical specifications

| Motorized Divergence Slit |
|---|
| Fully software controlled |
| Can be used in fixed and variable beam divergence mode |

| Motorized Anti-Scatter Screen |
|---|
| Fully software controlled |
| Tool-free and alignment-free mounting and unmounting |
| Compatibility with sample stages:<br>■ Automatic operation with Rotating Sample Stage, Flip-Stick, and Auto-Changer<br>■ Manual mode allows fixed distance setting for compatibility with capillary stage, XYZ stages, and Eulerian cradles<br>■ Operation of Standard Sample Stage and any non-ambient chambers requires unmounting of the Motorized Anti-Scatter Screen<br>■ Other stages on request |
| Max. 2θ range up to 140° 2θ, dependent on accessories, instrument geometry and instrument radius |
| For θ/θ goniometers only |

| Variable Detector FoV |
|---|
| Fully software controlled |
| Available with all members of the LYNXEYE detector family (SSD160-2, LYNXEYE-2, LYNXEYE XE-T) and EIGER2 detectors |
| Automatic normalization of intensity according to effective exposure time |
| No beamstop required to minimize air-scattering |

## Upgrade

**DBO is available for the D8 ADVANCE, D8 DISCOVER, and the D8 ENDEAVOR diffractometer families. Existing diffractometers can be easily upgraded.**



**Bruker AXS GmbH**

info.baxs@bruker.com

**www.bruker.com**

**Worldwide offices**

bruker.com/baxs-offices

**Online information**

bruker.com/xrd