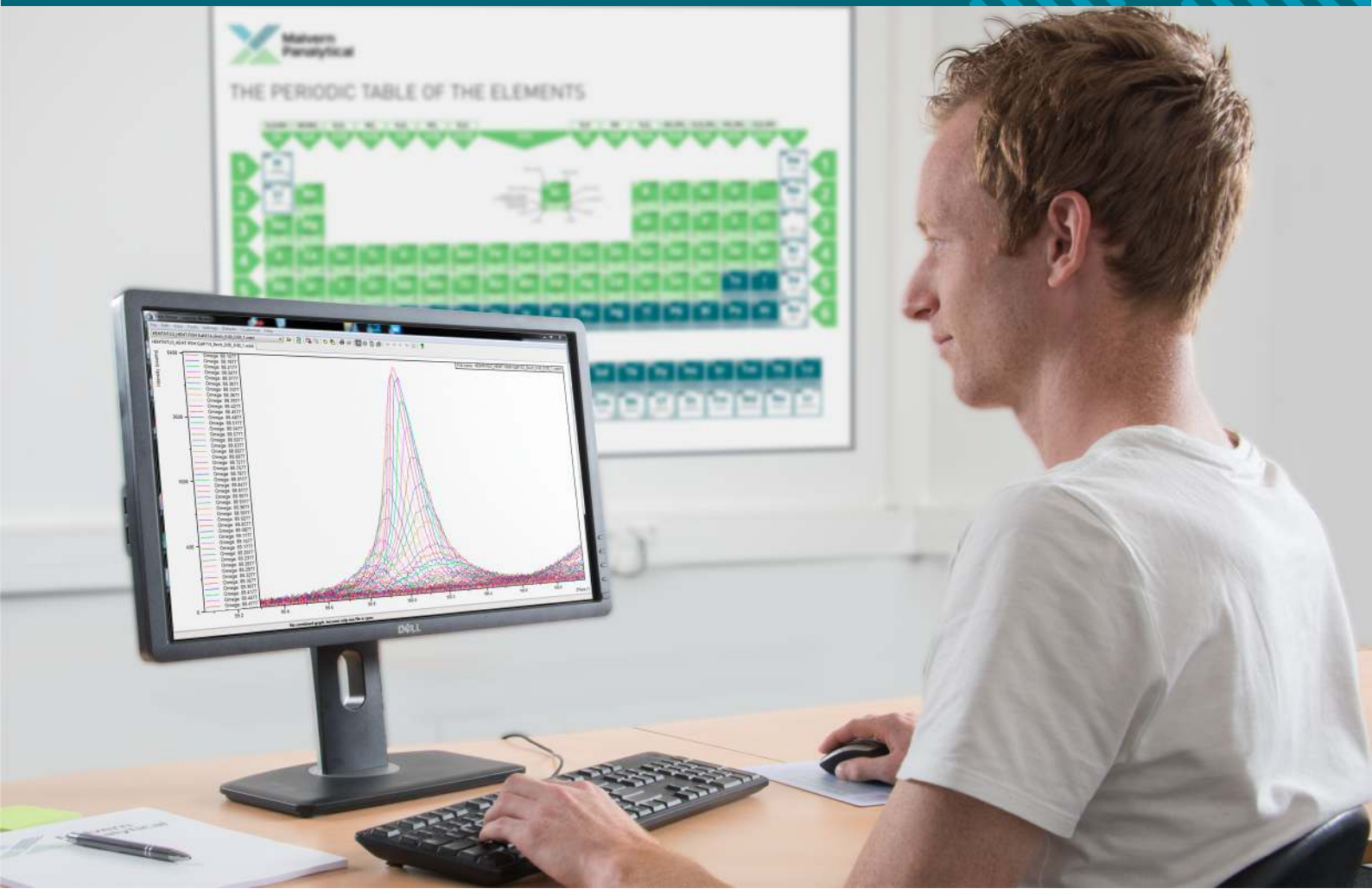
Malvern Panalytical
a spectris company

DATA VIEWER
QUICK START GUIDE



DATA VIEWER
QUICK START GUIDE

EDITION NOTICE: 4023 004 04170, May 2021
This is the original publication of Edition 10 of this document, to be used with Data Viewer version 2.1 or higher.

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CHAPTER 1 INTRODUCTION

This Quick Start Guide helps you to get started with Data Viewer quickly.

The examples in this Quick Start Guide show you how to use the software to do simple tasks.

The files used in these examples are supplied together with Data Viewer. With a standard installation, you can find them in **C:\PANalytical\Data Viewer\Tutorial**.

For all the tasks in the examples, there can be other possible ways to complete them, but then you must experiment with Data Viewer and learn the other possibilities yourself.

There can be differences between the example screens in this Quick Start Guide and what you see on your screen. If that occurs, follow the instructions on your screen.

After Data Viewer is installed, the items **View** and **Convert** are added to the right-click pop-up menu of an XRDML file.

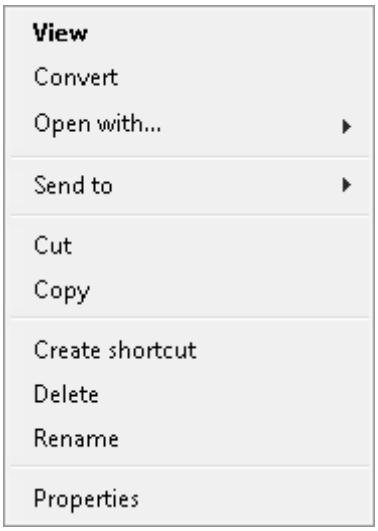


Figure 1.1 Pop-up menu of an XRDML file

Table 1.1 Description of View and Convert

Item	Description
View	Opens the file.
Convert	Converts the file to a different file type with the defaults specified in **Defaults > Conversion**. **NOTE:** If there is a file with the same name, Data Viewer always makes a backup of the file automatically.

1.1 Regulated environment

If you are in a regulated environment, there can be small differences between your situations and these given here. If that occurs, follow the instructions on your screen.

Refer to Data Viewer Help for more detailed instructions about the regulated environment.

1.2 Start Data Viewer

To start Data Viewer, use one of these procedures:

- On the desktop, double-click the icon 

.
- Click the Windows Start button and then on the list of apps or programs, go to **PANalytical Data Viewer > Data Viewer**.
- On the Windows Start menu, go to **Start > All Programs > PANalytical Data Viewer > Data Viewer**.
- Double-click an XRD data file to open it.
- Right-click an XRD data file to open the pop-up menu, and then select **View**.

1.3 Log in to Data Viewer

It is possible that Data Viewer users must log in to Data Viewer with the Windows user name and password. This is related to the configuration. When it occurs, do as follows:

1. In the **User Authentication** window, enter your Windows user name and password.

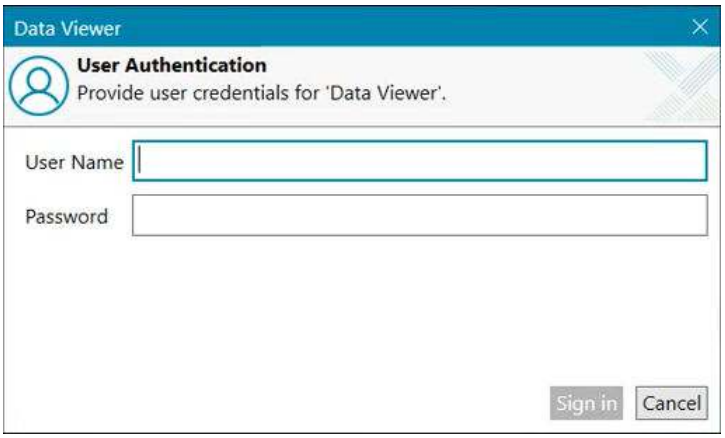


Figure 1.2 User authentication window

2. If Data Viewer is in the restricted mode, make sure that your user account is authorized to use Data Viewer. For more information, refer to OmniAccess Help.
3. Click **Sign in**. After you log in to Data Viewer. Your user name is shown on the title bar of Data Viewer.

CHAPTER 2 EXAMINE MEASUREMENTS

2.1 Introduction

With Data Viewer, you can examine most of Malvern Panalytical's XRD measurements.

You can use these measurement views and tools:

- Measurement views
  - Graphs
  - Pole figures
  - HTML reports
  - ASCII text (only for XRDML and other ASCII file types)
- Tools
  - Spectral lines
  - Peak parameters

2.2 Measurement types

Data Viewer can show most of Malvern Panalytical's XRD measurements. Here are some examples:

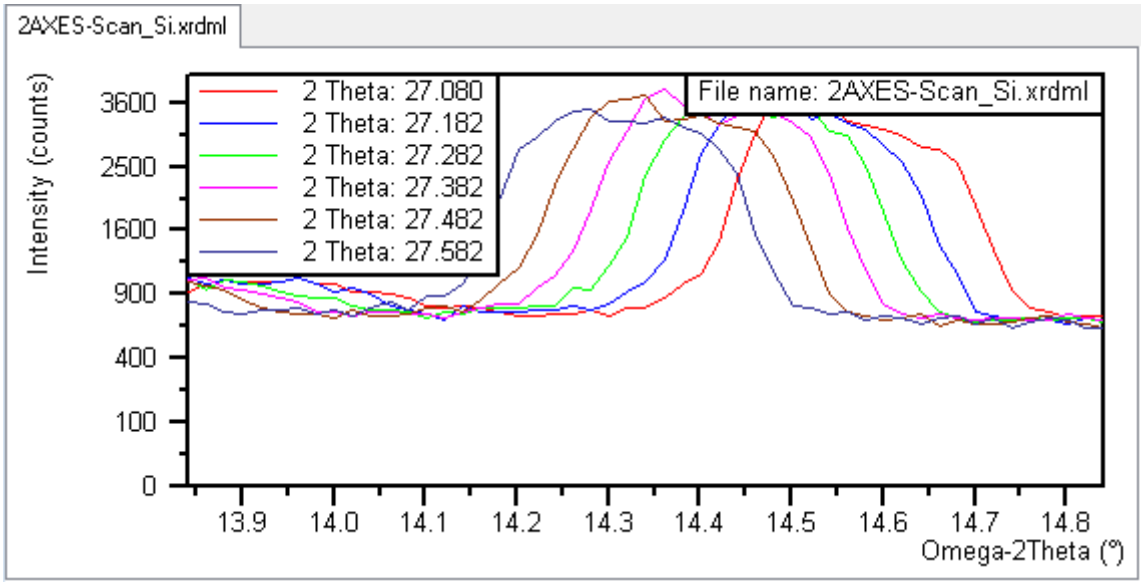


Figure 2.1 Multiple scan measurement

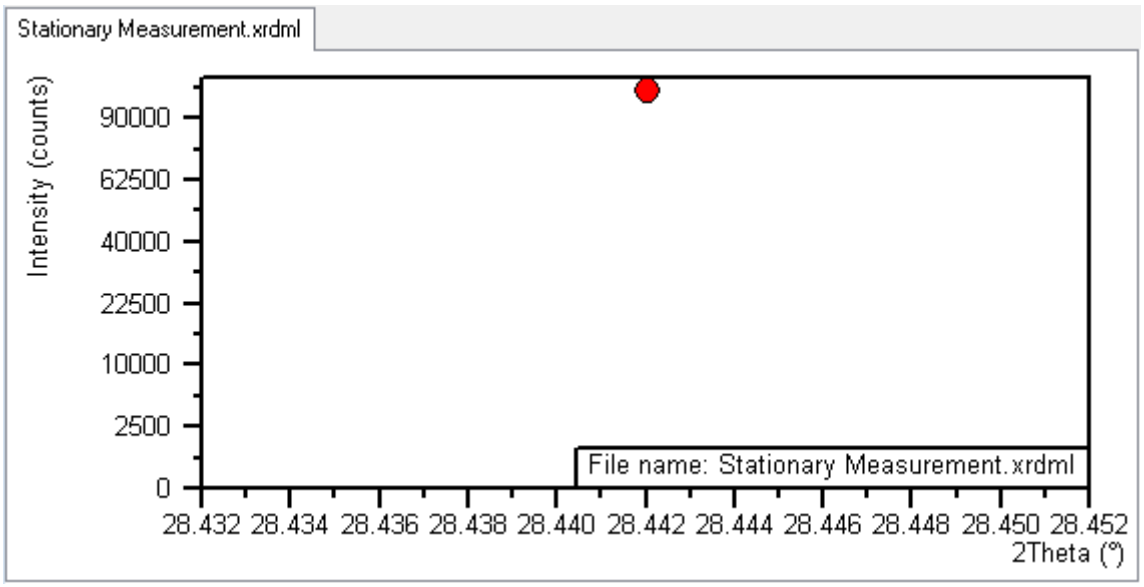


Figure 2.2 Stationary measurement

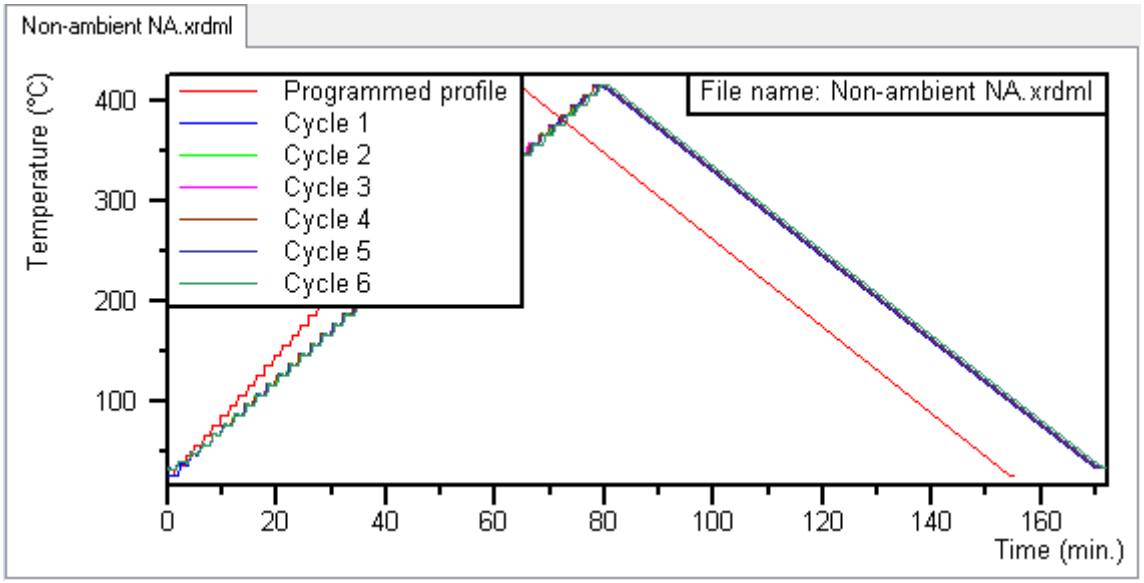


Figure 2.3 Non-ambient measurement (resulting temperatures)

2.3 Measurement views

Data Viewer has these measurement views:

- Graph: To show the measurement as a graph, go to **View > Graph**, or click the button. If you open 2 or more files with the same scan axis, they will be automatically combined into a combined graph on the **Combined Graph** tab. Refer to Section 2.3.1.

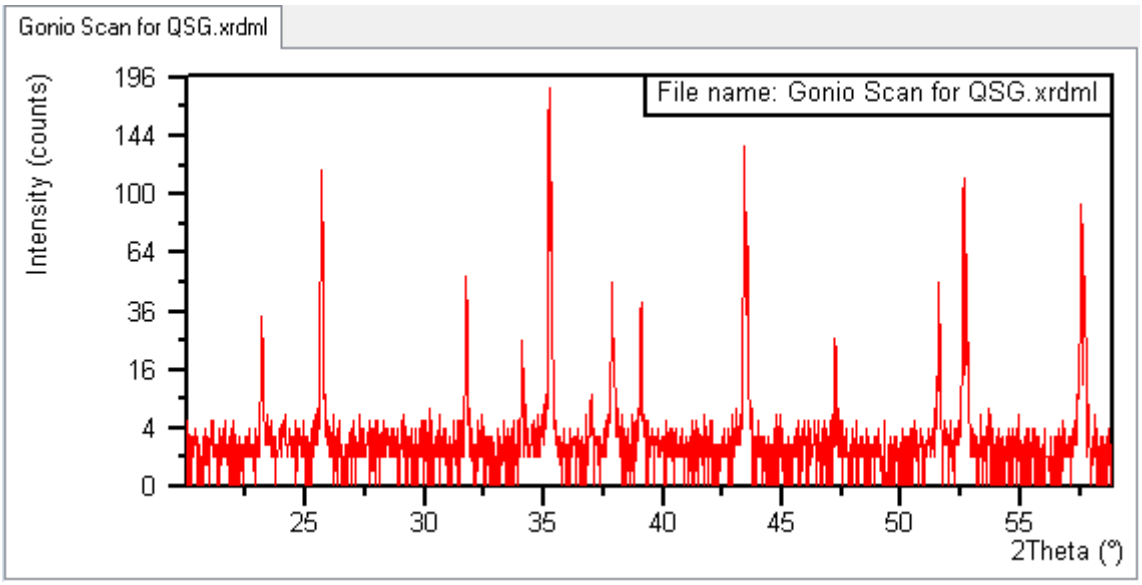


Figure 2.4 Graph

- Pole figure: To show the measurement as a pole figure, go to **View > Graph**, or click the button. This measurement view is only available for texture pole figure measurements.

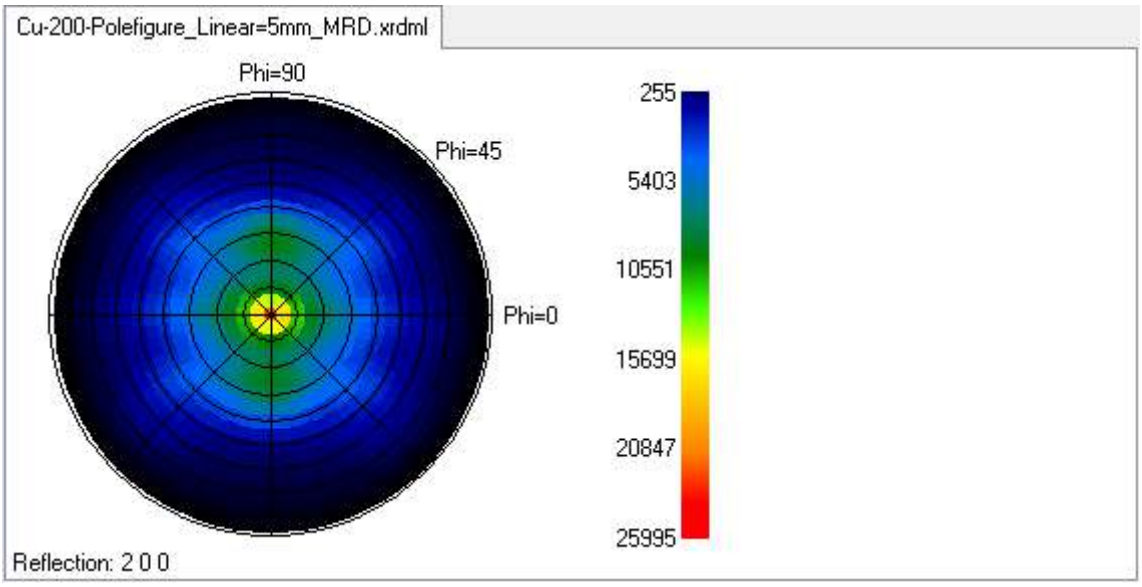


Figure 2.5 Pole figure

- Report: To show the measurement as a report, go to **View > Report**, or click the button.

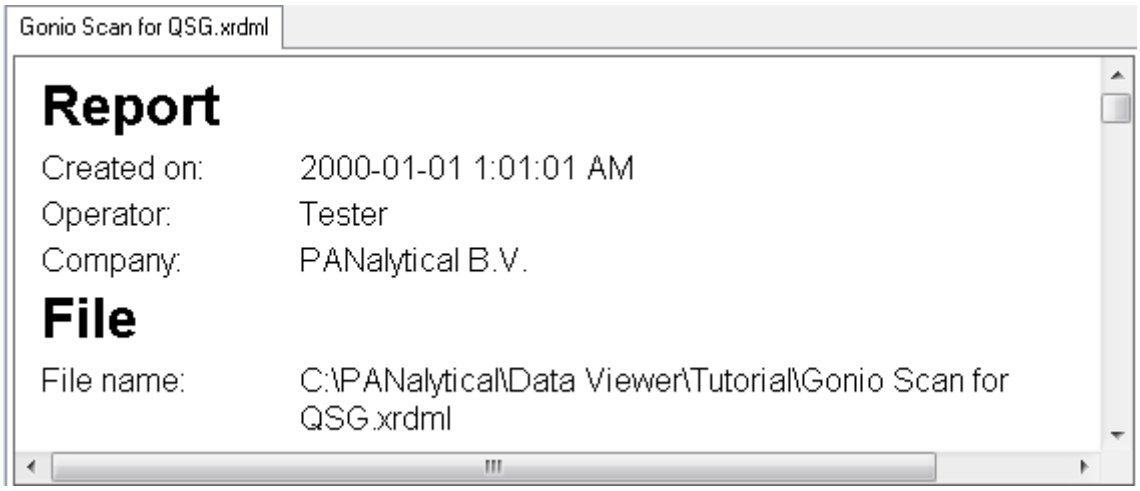


Figure 2.6 Report

- Data file: To show the measurement as a data file, go to **View > Data File**, or click the button. This measurement view is available for all ASCII file types, such as XRDML, UDF, XNN.

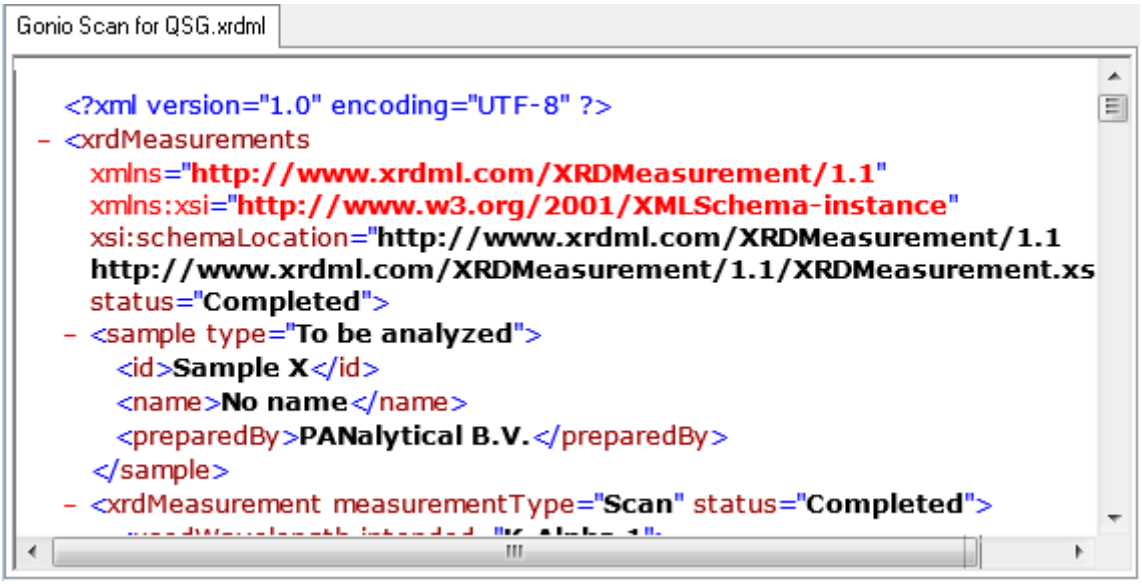


Figure 2.7 Data file

2.3.1 Combined graph

If you open 2 or more files with the same scan axis, they will be automatically combined into a combined graph on the **Combined Graph** tab.

To see a combined graph, in this example, do as follows:

1. Open the file "Gonio Scan for QSG.xrdml".

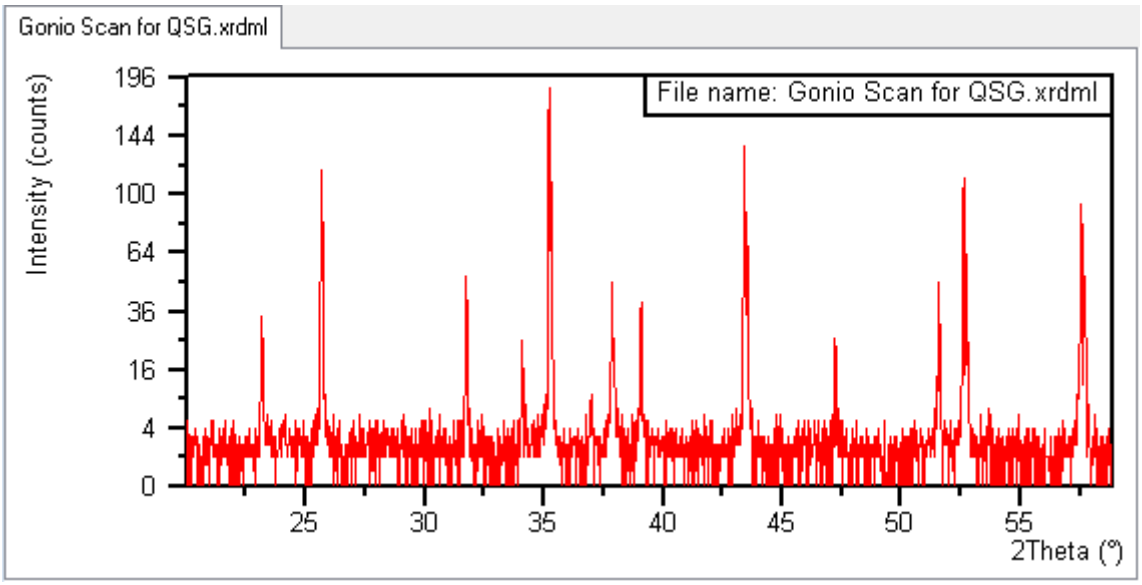


Figure 2.8 First file opened

2. Open the file "Gonio Scan 2 for QSG.xrdml".

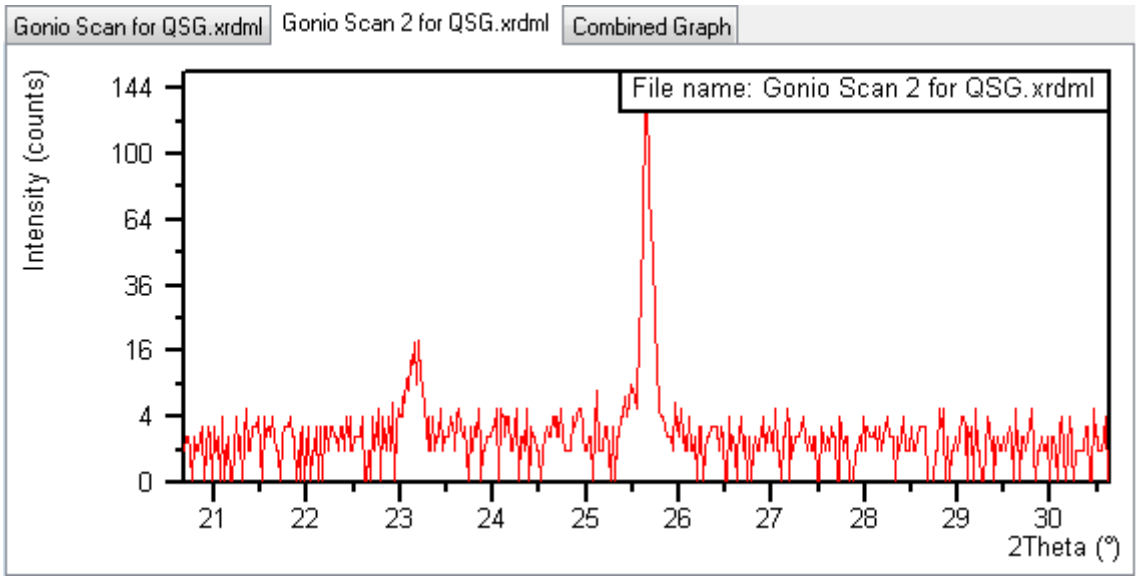


Figure 2.9 Second file opened

The 2 graphs will be automatically combined into a combined graph on the **Combined Graph** tab.

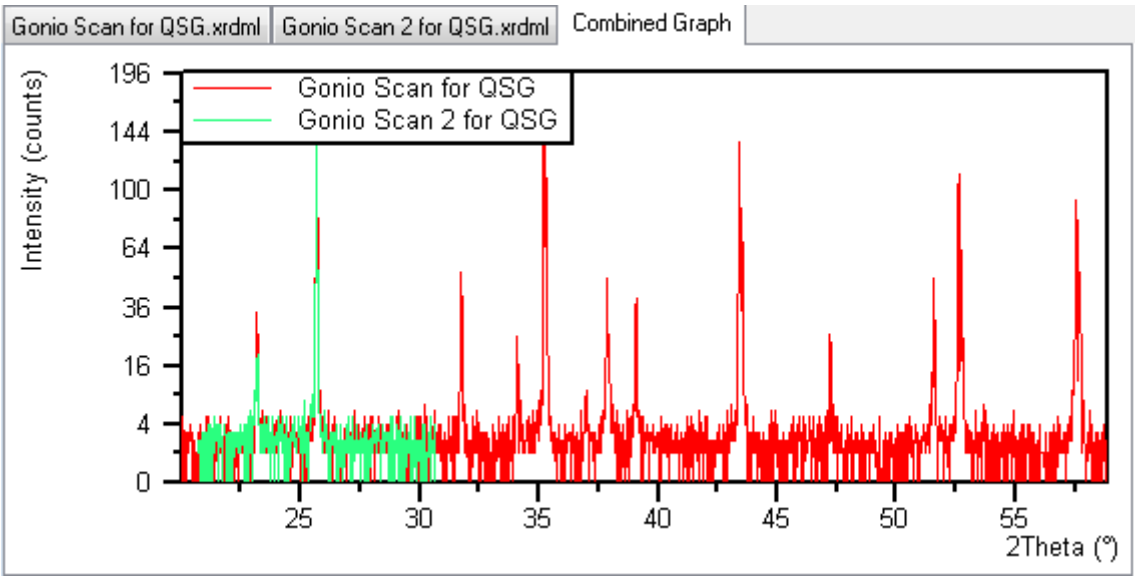


Figure 2.10 Combined graph

2.3.2 Graph properties settings

In the graph view, you can change these properties:

- Title
- Background & grid
- Horizontal axis
- Vertical axis
- Legend
- Information box
- Annotations
- Data sets

The examples in the next sections show you how to change the settings for the title, the annotations, the information box, and the legend.

2.3.2.1 Title

In this example, you will add a title to a measurement.

1. Open the file "Gonio Scan 2 for QSG.xrdml".
2. Go to **Settings > Graph Properties**.
3. Click **Title**.

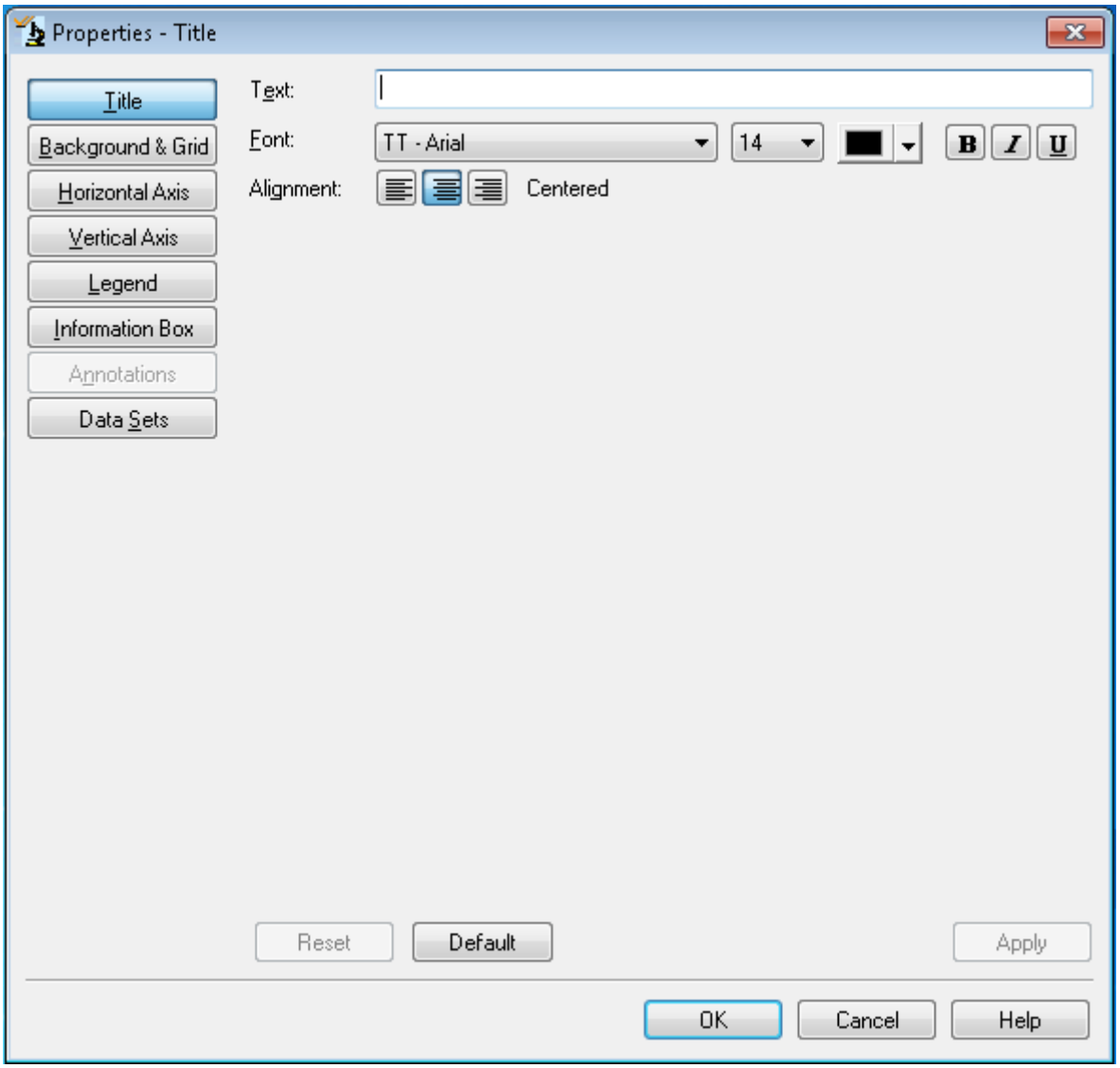


Figure 2.11 Properties for title

4. In the **Text** field, enter "Gonio Scan 2".
5. Click **OK**. The new title **Gonio Scan 2** is shown above the graph.

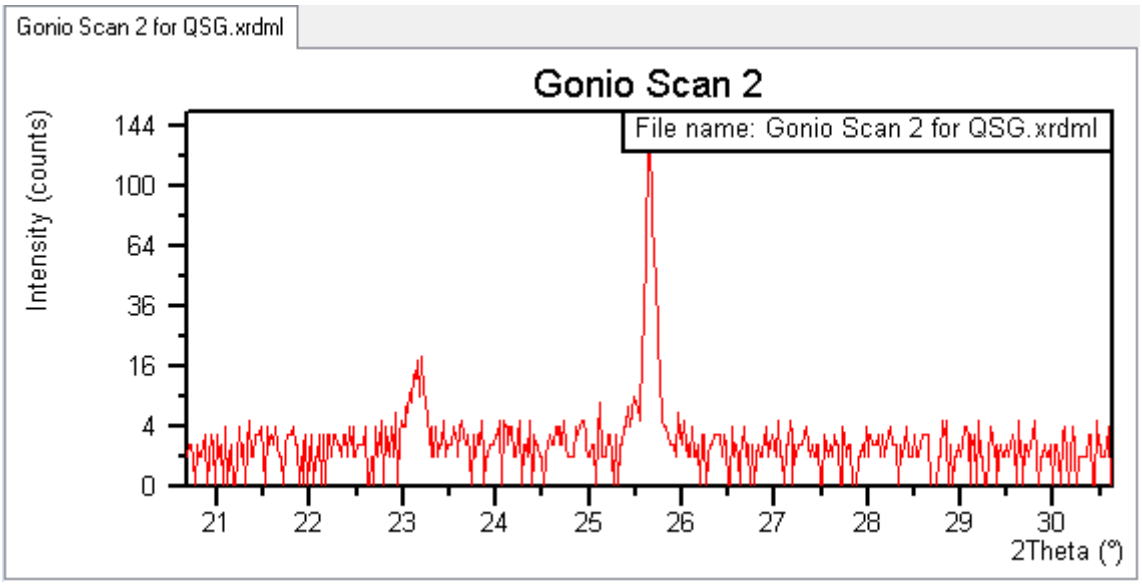


Figure 2.12 New title shown

6. If necessary, right-click the title to open the pop-up menu. Then you can align the title to the left, center, or right.

2.3.2.2 Annotations

In this example, you will make new annotations, move, rotate, and then remove them.

1. Open the file "Gonio Scan 2 for QSG.xrdml".
2. Go to **Tools > New Annotation**.
3. If this window opens, click **OK**.

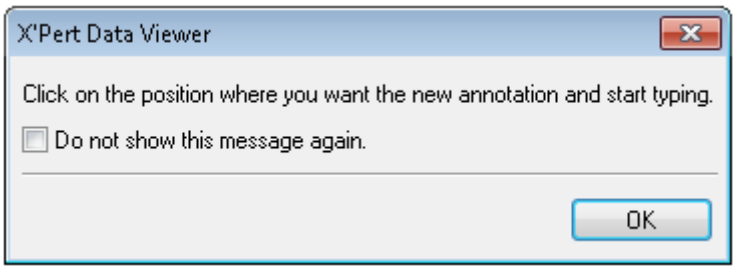


Figure 2.13 Window that tells how to add a new annotation

4. After cursor changes into , click near the peak.
5. As an alternative for steps 2 to 4, you can do as follows:
   a. Right-click near the peak.
   b. On the pop-up menu, select **New Annotation**.
6. Enter the annotation text "Peak".
7. Press **Enter**, or click outside the annotation.
8. Make the second annotation "Noise" above the noise on the left of the peak.

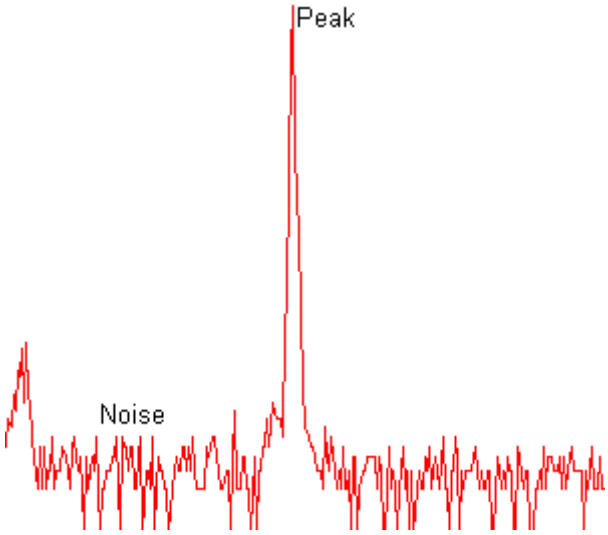


Figure 2.14 *Annotations added*

9. Drag and move the annotation "Noise" to the right of the peak.

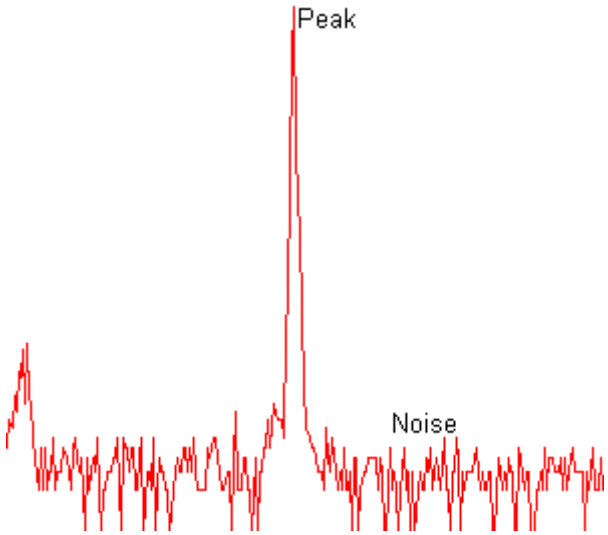


Figure 2.15 *Annotation position changed*

10. Press **Alt**, and drag the annotation "Peak" to an angle to rotate it.

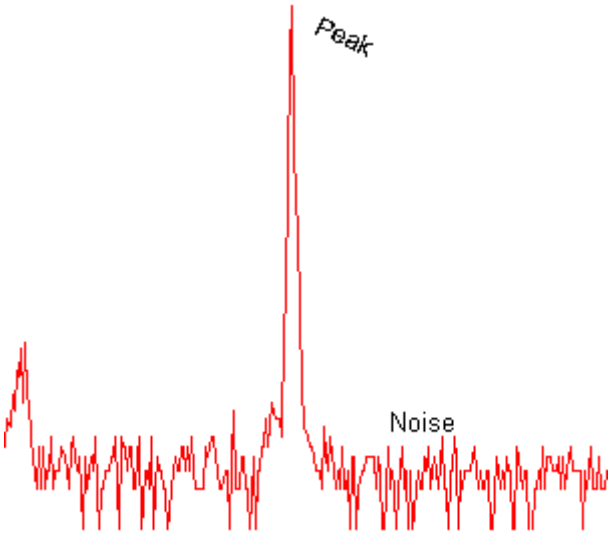


Figure 2.16 Annotation rotated

11. To remove the annotations, do as follows:
    a. Right-click an annotation.
    b. On the pop-up menu, select **Remove**.
    c. Do steps 11a and 11b again to remove the second annotation.

2.3.2.3 Information box

NOTE: The information box cannot be added in a combined graph.

To change the settings for the information box, do as follows:

1. Open the file "Gonio Scan 2 for QSG.xrdml".
2. Go to **Settings > Graph Properties**.
3. Click **Information Box**.

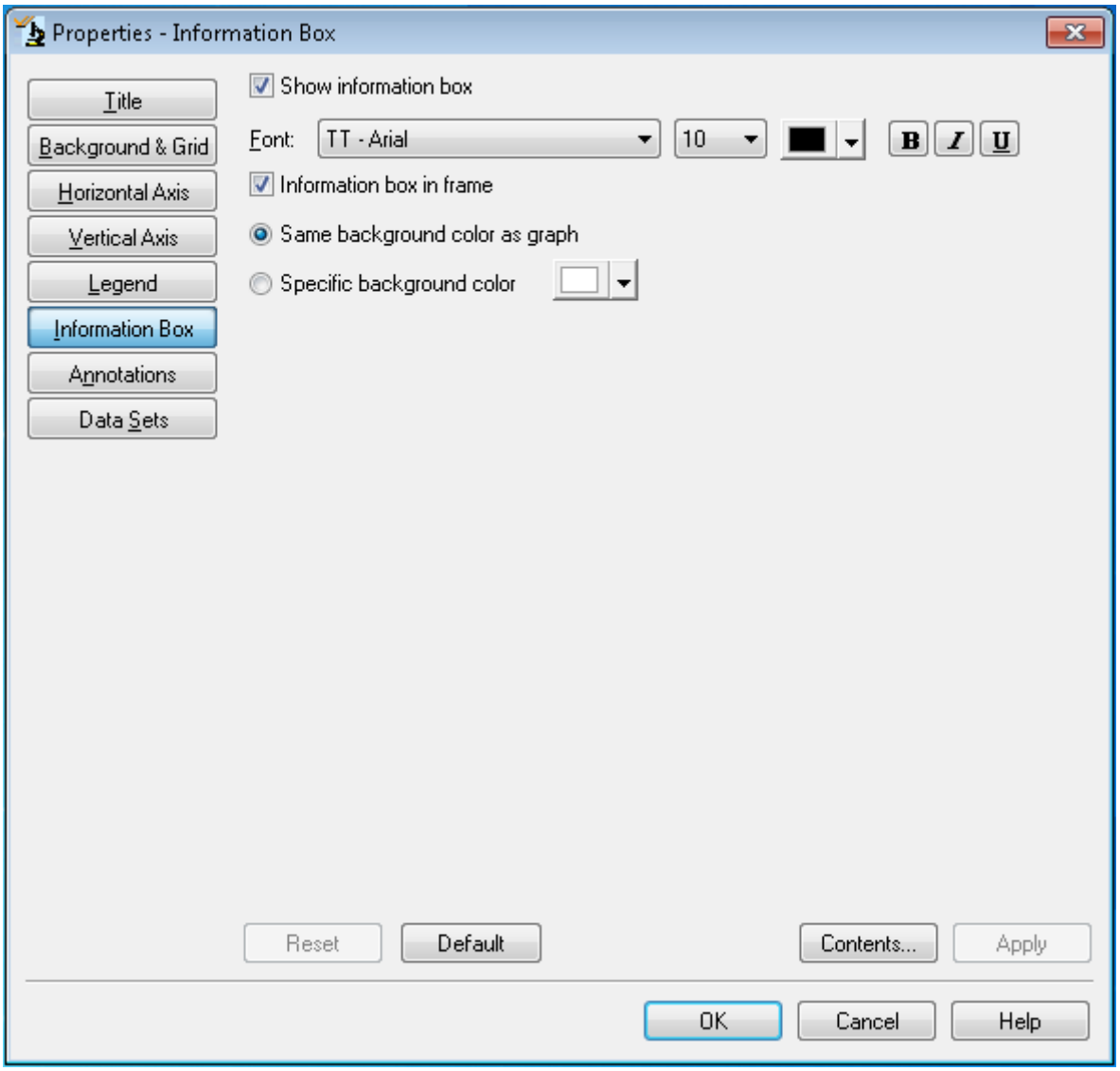


Figure 2.17 Properties for information box

4. Select the **Show Information Box** check box to show the information box.
5. Select the **Information box in frame** check box to add a frame to the information box.
6. If necessary, change the background color.
7. Click **OK**.

2.3.2.4 Legend

To change the settings for the legend, do as follows:

1. Open the file "Gonio Scan 2 for QSG.xrdml".
2. Go to **Settings > Graph Properties**.
3. Click **Legend**.

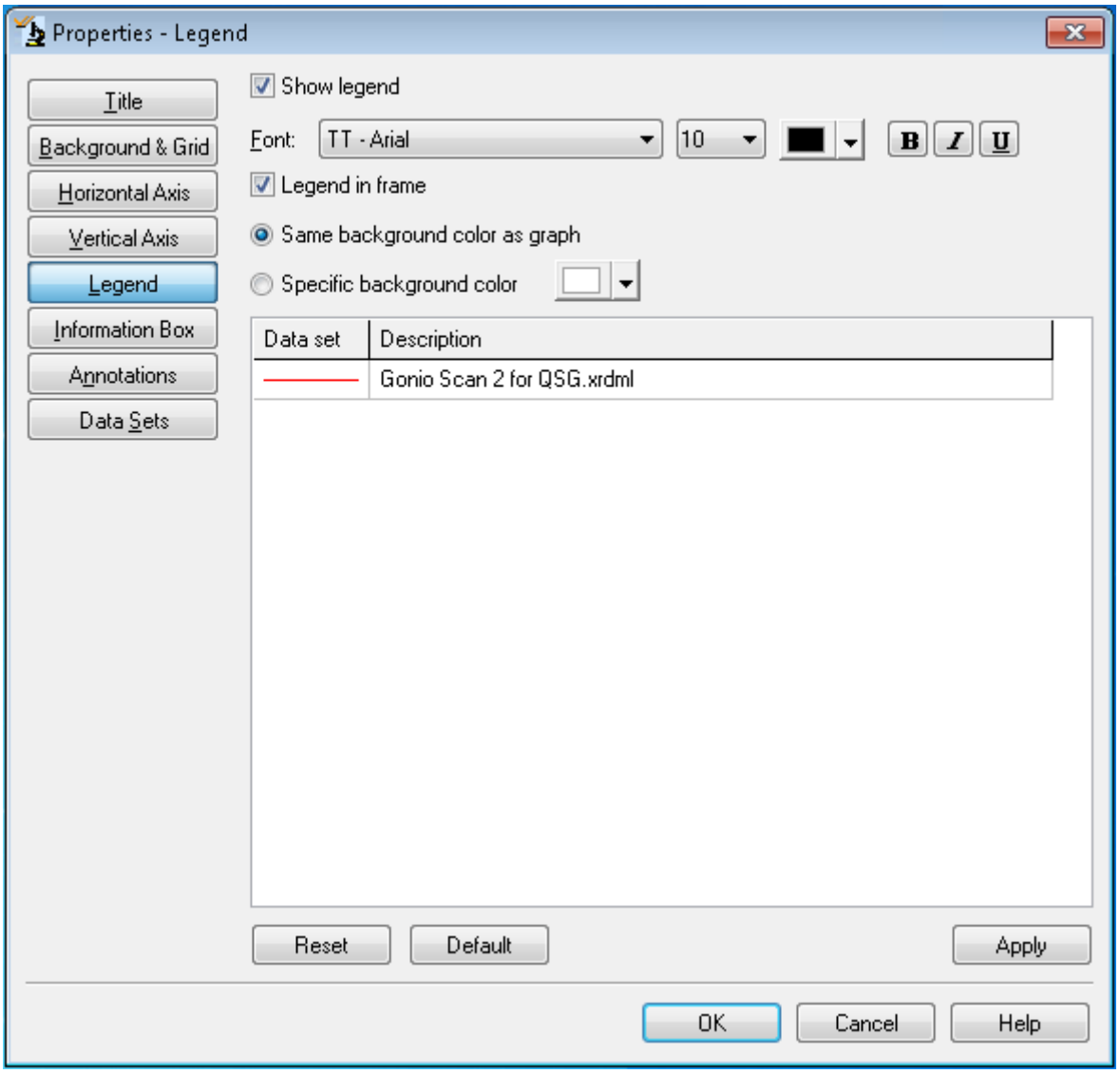


Figure 2.18 Properties for legend

4. Select the **Show legend** check box to show the legend.
5. Select the **Legend in frame** check box to add a frame to the legend.
6. If necessary, change the background color.
7. Click **OK**.

2.3.3 Report properties settings

In this example, you will change the settings for report.

1. Open the file "Gonio Scan 2 for QSG.xrdml".
2. Go to **Settings > Report**. The **Report settings window** opens.

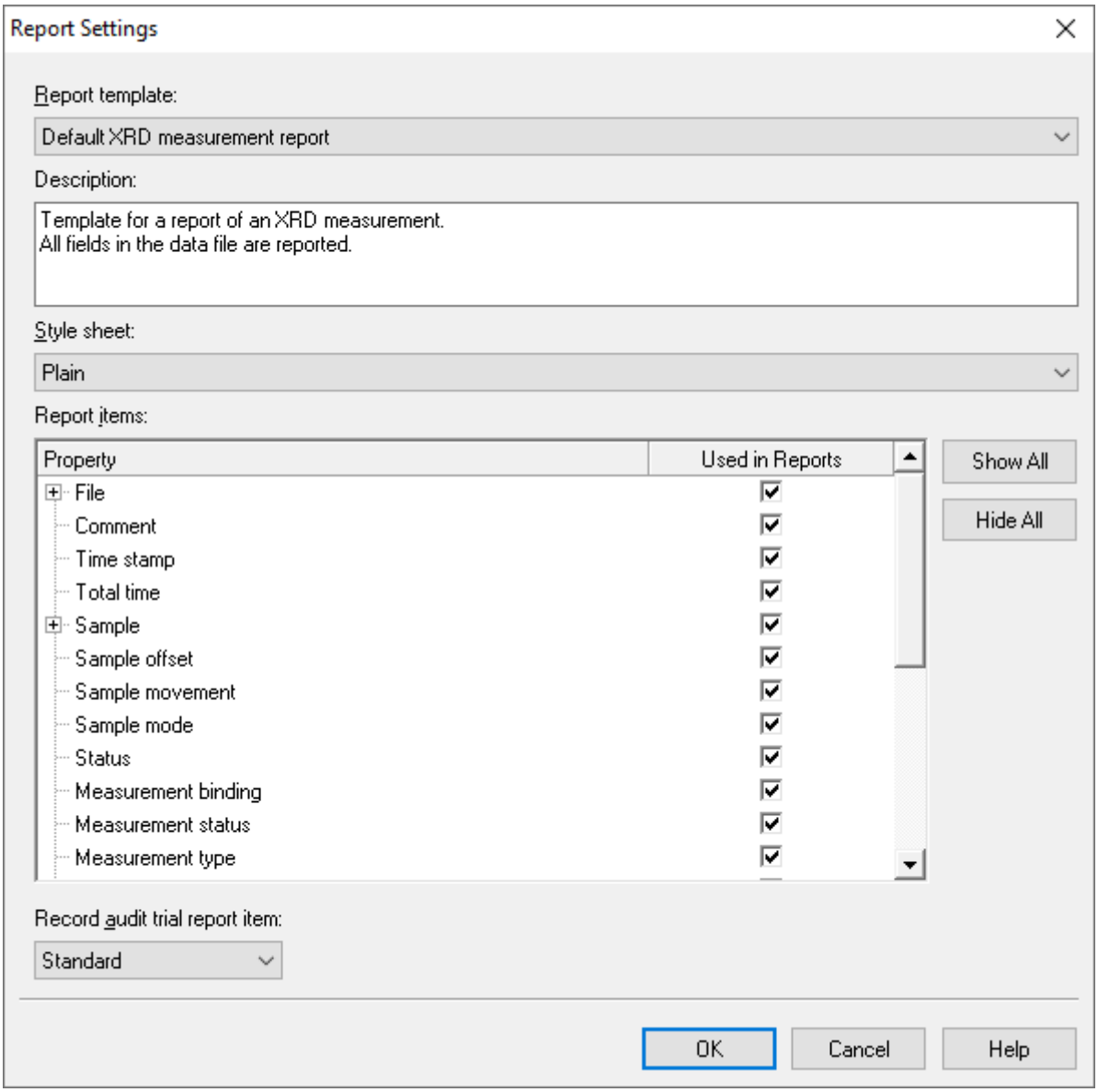


Figure 2.19 Report settings window

3. From the **Report template** drop-down list, select a report template. In a report template, the report items and their style are specified. In this example, select **Default XRD measurement report**.
4. From the **Style sheet** drop-down list, select a style sheet. In a style sheet, the style of the report is specified. In this example, select **Plain**.

   NOTE: For some report templates, you cannot use a style sheet.
5. In the **Report items** frame, select the report items that will be included in the report. In this example, click **Show All** to include all report items in the report.

   NOTE: If a report item is not found in the file, it will not be shown in the report.

   For some report templates, you cannot use select or clear report items.
6. Click **OK**.
7. Go to **View > Report**. Data Viewer makes a report with the settings you specified.

2.4 Tools

2.4.1 Spectral lines

With spectral lines, you can examine spectral relationships.

In this example, you will switch on spectral lines, change the settings, and switch off spectral lines.

1. Open the file "Gonio Scan 2 for QSG.xrdml".
2. Go to **Tools > Spectral Lines**.

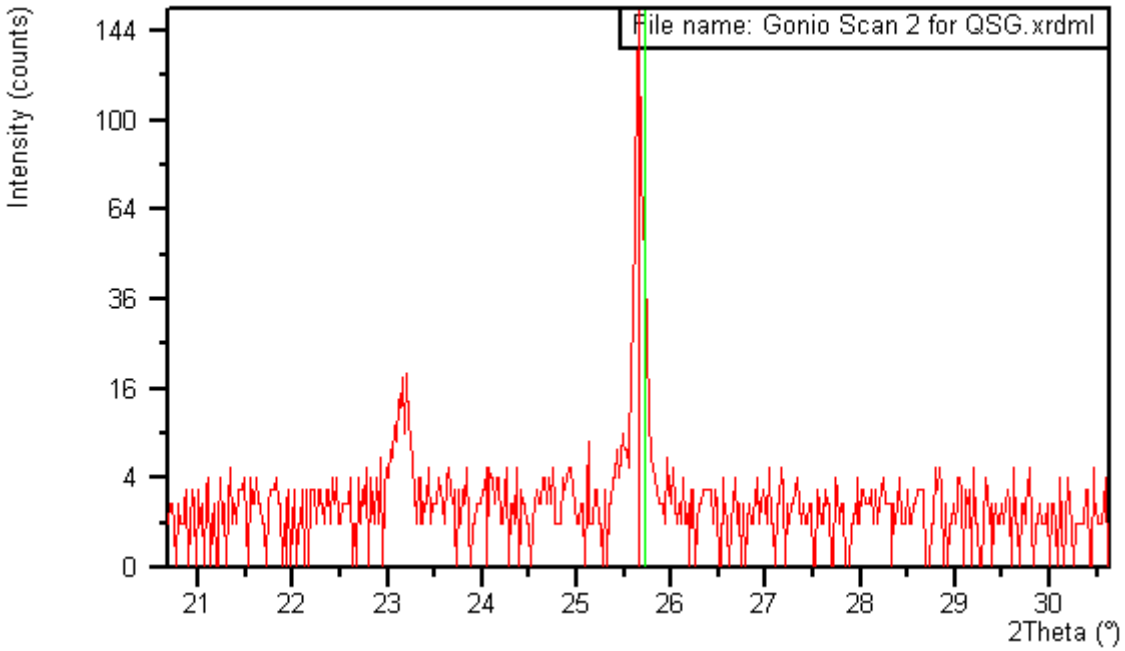


Figure 2.20 Spectral lines shown

The status bar below the graph gives information about the spectral lines.



Figure 2.21 Status bar

3. Go to **Settings > Spectral Lines**.
4. Change the settings. In this example, use these settings:
   - **K-Alpha1 line** with color red and 1 pixel width
   - **K-Alpha2 line** with color green and 1 pixel width
   - **K-Beta line** with color magenta and 1 pixel width
   - **Tungsten (W) L-Alpha1 line** with color cyan and 1 pixel width

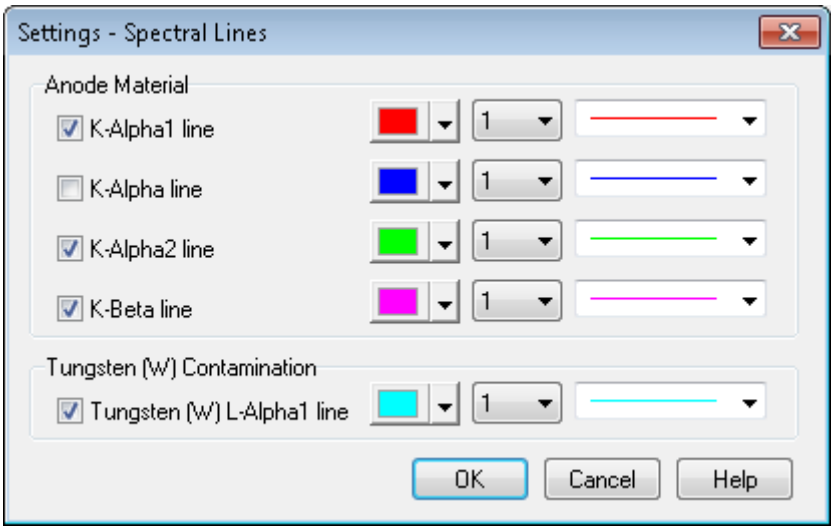


Figure 2.22 Settings changed

5. Click **OK**.

   In the graph, there is a Kβ-peak (the magenta line), but there is no tungsten contamination (the cyan line).

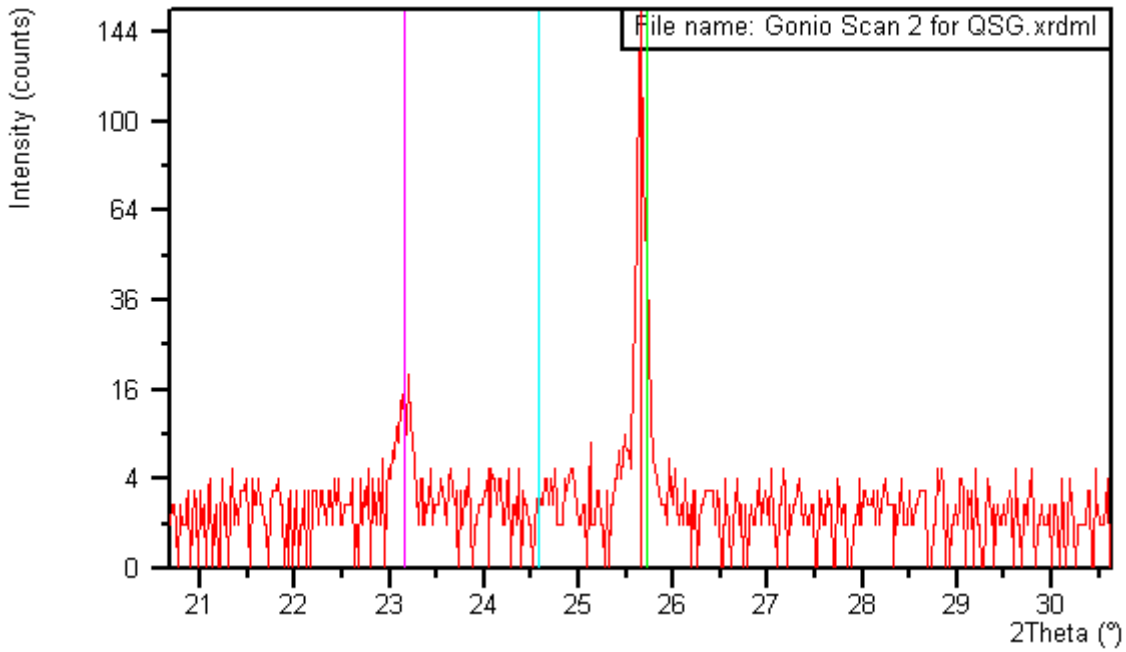


Figure 2.23 Spectral lines with new settings

6. Go to **Tools > Spectral Lines** again to switch off spectral lines.

2.4.2 Peak parameters

With peak parameters tool, you can examine the shape, position, height, and width of a peak for analysis purposes.

In this example, you will zoom in a peak, use the peak parameters tool to examine peak parameters, and then switch off the peak parameters tool.

1. Open the file "Gonio Scan 2 for QSG.xrdml".
2. Zoom in on the peak at 25.65°:
   a. Put your cursor at the bottom of the graph at approximately 25°.
   b. Click and then drag the cursor to the top of the graph at about 27°.
   c. Release the mouse.

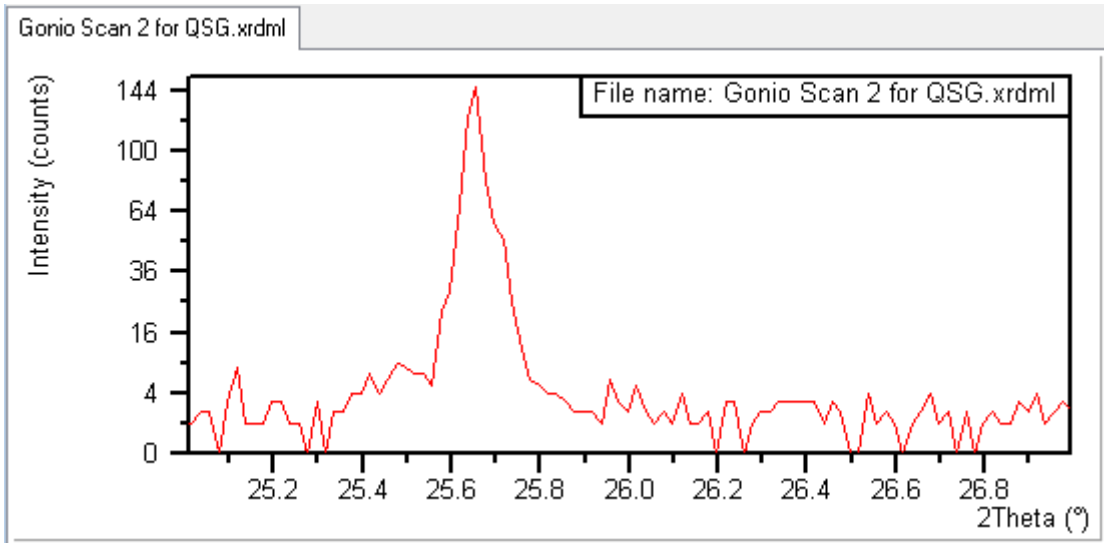


Figure 2.24 Peak after you zoom in

3. Switch on the peak parameters tool:
   a. Go to **Tools > Peak Parameters**.
   b. If this window opens, click **OK**.

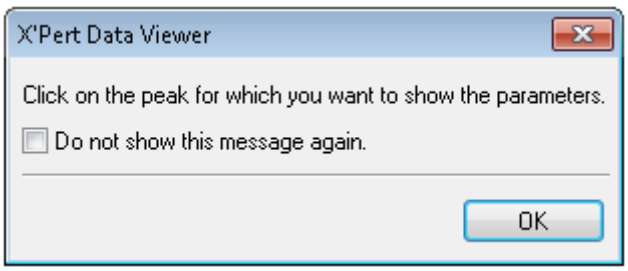


Figure 2.25 Window that tells how to show the parameters

After you switch on the peak parameters tool, the cursor changes to .

4. As an alternative for step 3, you can do as follows:
   a. Right-click a peak.
   b. From the pop-up menu, select **Peak Parameters**.

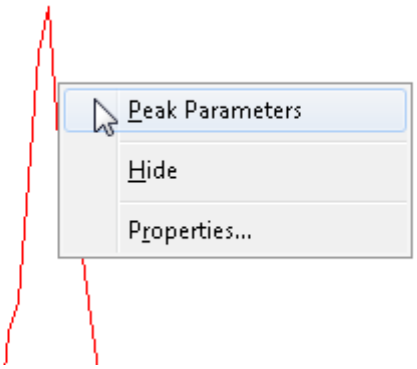


Figure 2.26 Pop-up menu

5. Click a peak to show these items:
   - Vertical line that shows the position and height of the peak
   - Annotation that gives the position and height values
   - Horizontal line across the peak that shows the Full Width at Half Maximum (FWHM)
   - Annotation that shows the FWHM value
   - Background line that shows the background level
   - **Peak Parameters** window that shows numerical values

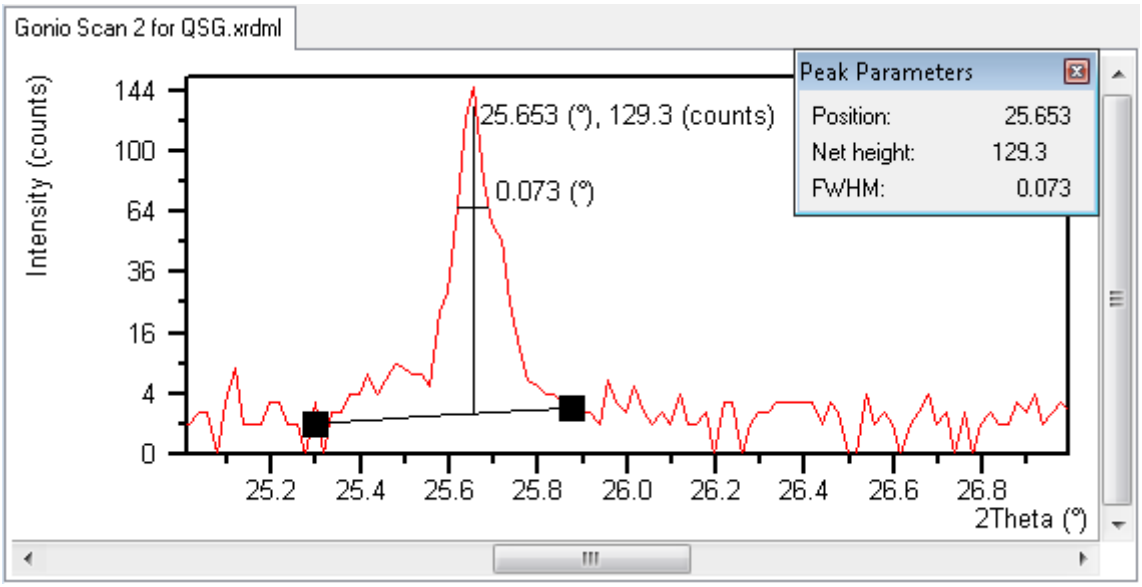


Figure 2.27 Peak parameters shown

6. If necessary, go to **Customize > Peak Parameters** to select which values are shown in the **Peak Parameters** window. Refer to Section 2.4.2.1.
7. To change the background level, drag the solid black boxes at the ends of the background line at the bottom of the peak.
8. To see the peak parameters of a different peak, click the peak.
9. Close the **Peak Parameters** window to switch off the peak parameters tool.

2.4.2.1 Peak Parameters window

In this example, you will select which parameters must be shown in the **Peak Parameters** window, and see the full name of a parameter in the **Peak Parameters** window.

1. If the **Peak Parameters** window is not open, open it. Refer to Section 2.4.2.
2. Go to **Customize > Peak Parameters**. The **Customize Peak Parameters** window opens.
3. Select **Position**, **Net height** and **FWHM**, and clear the remaining check boxes.

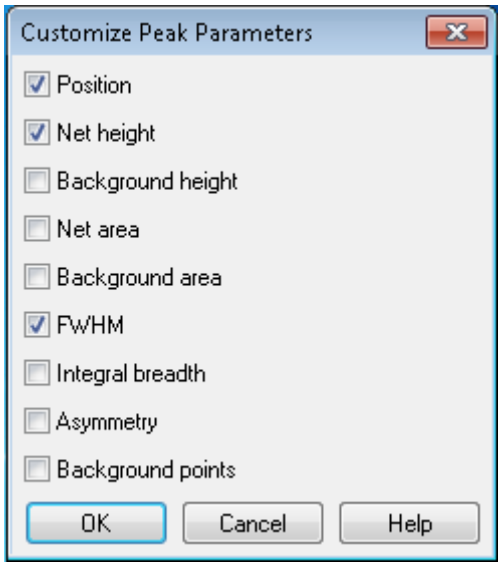


Figure 2.28 Peak parameters selected

4. Click **OK**. The **Peak Parameters** window shows the peak parameters that you selected.
5. Hover over a peak parameter in the **Peak Parameters** window, a pop-up menu shows the full name of the peak parameter. For example, the pop-up shows **Net height** is short for **Net height (counts)**.

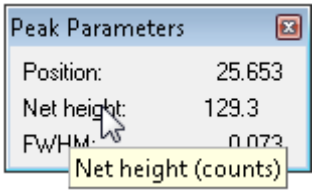


Figure 2.29 Peak Parameters window

CHAPTER 3 CONVERT FILES

3.1 Introduction

Some XRD programs cannot use XRDML files. To use these programs, you must first convert the XRDML files into other file types.

Which file type you convert to relates to the measurement and scan type you convert and the program that you will use.

Table 3.1 Conversion table

Measurement type	Scan type	File type that can be converted to
Single scan - 2θ based	gonio	RD, UDF, XNN, JCP, CSV, XY
	2θ	RD, XNN, JCP, CSV, XY
	2θ - ω	RD, XNN, JCP, CSV, XY
Single scan - ω based	ω	OD, XNN, JCP, CSV, XY
	ω - 2θ	RD, XNN, JCP, CSV, XY
Single scans - other axes	φ	XNN, JCP, CSV, XY
	ψ	XNN, JCP, CSV, XY
	Q	CSV
	X	XNN, JCP, CSV, XY
	Y	XNN, JCP, CSV, XY
	Z	XNN, JCP, CSV, XY
2-axes measurement		YNN, CSV
Stress measurement	Stress	RSC, CSV
	Single scans	RD, XNN, JCP
Texture measurement	Pole figure	RW1, CSV, RAW, DFB
	Correction file	COR, CSV
	Background	COR, CSV
X-Y (wafer) map	Refer to single scans	
Non-ambient measurements	Refer to single scans	

Refer to "Supported file types" in Data Viewer Help for more information about file types.

NOTE: When you convert an XRDML file to one of the older file formats, some details in the XRDML file will be lost.

3.2 Convert an XRDML file to an RD file

In this example, you will convert the file "Gonio Scan 2 for QSG.xrdml" to an RD file.

1. Open the file "Gonio Scan 2 for QSG.xrdml".
2. Go to **File > Convert**. The **Convert Scan Measurement** window opens.

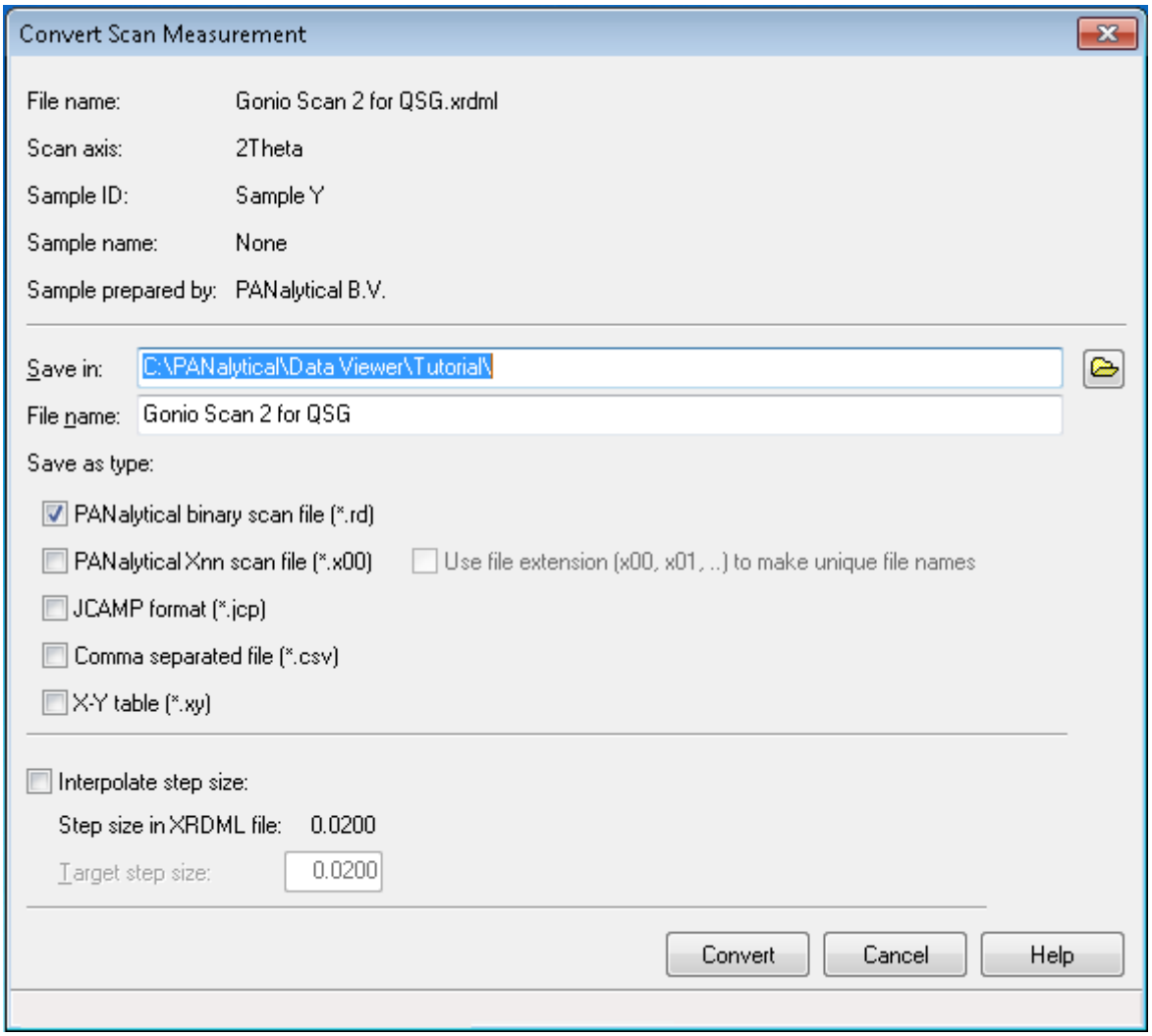


Figure 3.1 Convert Scan Measurement window

3. Enter the destination folder, or click the button to select it.
4. Enter the file name of the RD file. In this example “Gonio Scan 2 for QSG”.
5. Make sure that the **PANalytical binary scan file (*.rd)** check box is selected.
6. Make sure that the **Interpolate step size** check box is cleared.
7. Click **Convert**. The file is converted and saved in the destination folder you specified.

3.3 Convert an RD file to an XRDML file

In this example, you will convert the file "Gonio Scan 2 for QSG.rd" to an XRDML file.

1. Open the file “Gonio Scan 2 for QSG.rd”. This is the file that you made. Refer to Section 3.2.

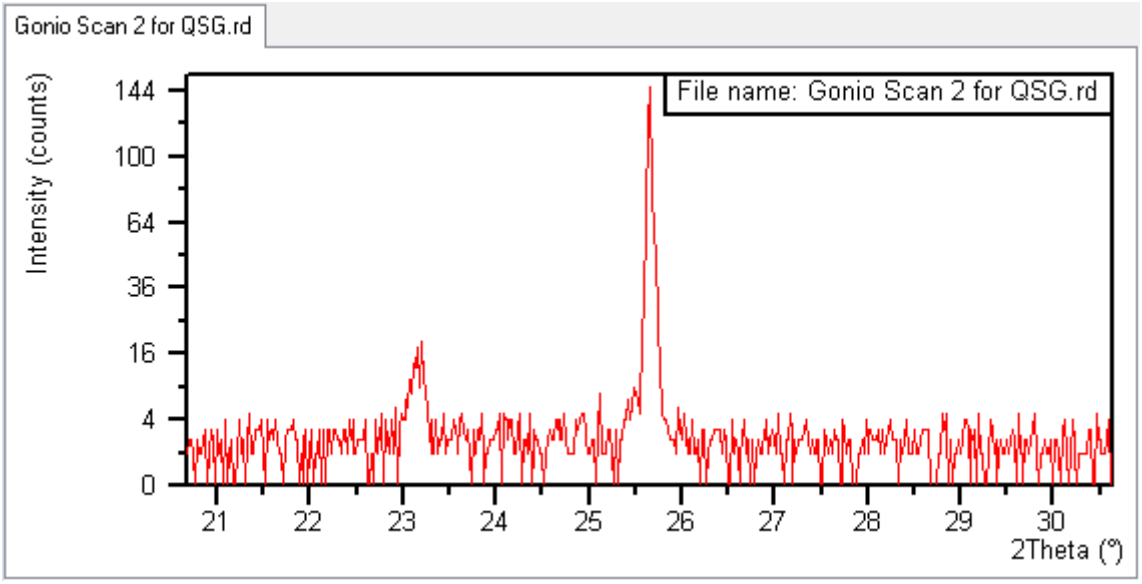


Figure 3.2 File opened

2. Go to **File > Save As XRDML File**. The **Save As** window opens.

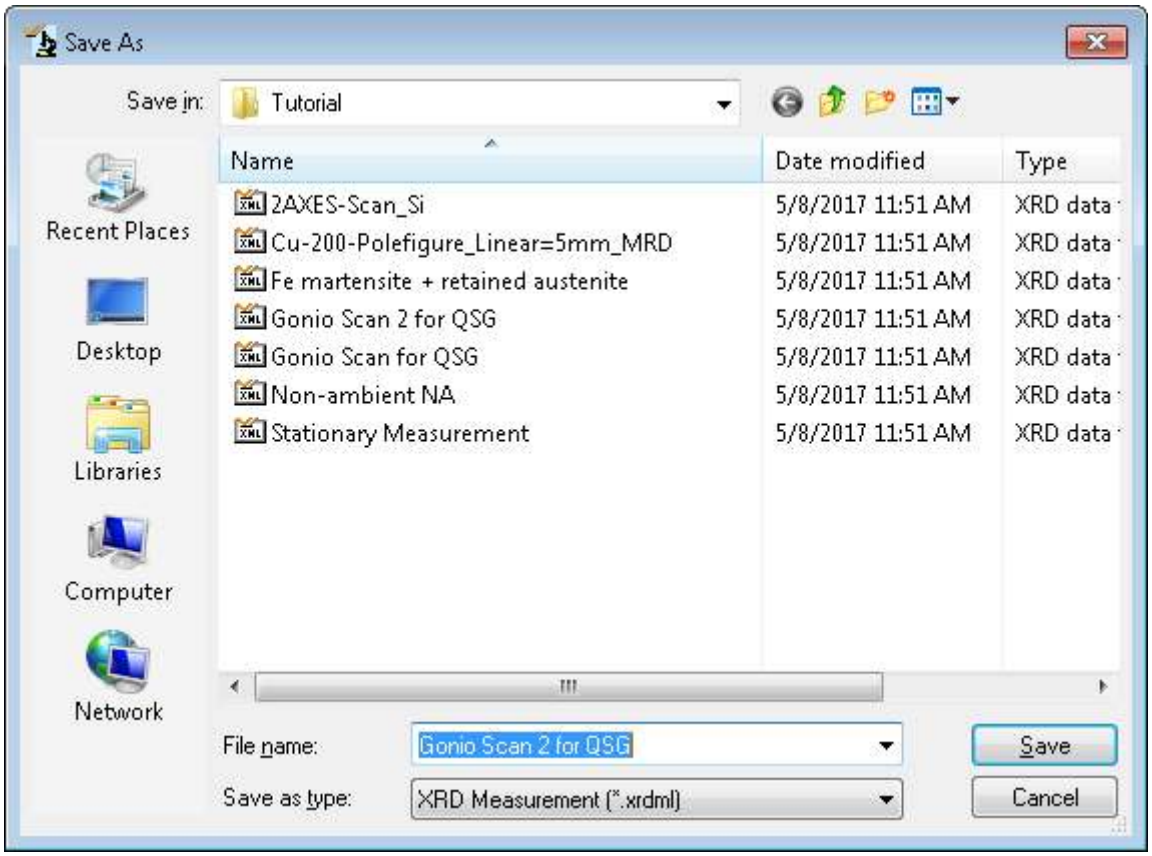


Figure 3.3 Save as window

3. Click **Save**. The **Confirm Save As** window opens.

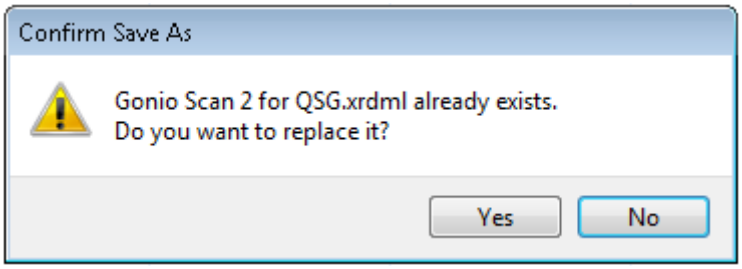


Figure 3.4 Confirm Save As window

4. Click **No**.
5. Change the file name to "Gonio Scan 2 for QSG from RD.xrdml".
6. Click **Save**. Data Viewer saves the file as an XRDML file.