

XRD CONVERSION

USER'S MANUAL

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Introduction

The *XRD Conversion* program was developed to convert raw, legacy X-Ray diffraction data into a usable format, from UDF files to UDI files. The program consists of two windows: conversion and editing. This program allows the conversion of multiple data files.

Document Layout

This document is broken into five sections. The first two describe how to start the *XRD Conversion* program and the main program features. The next three sections describe how to select files for conversion, how to actually convert the files, and how to edit converted or unconverted files.

Starting XRD Conversion

Start the *XRD Conversion* program by clicking on the XRD icon, or by opening it from the **Start Menu** (Explorer Window).

The first window to appear is the main conversion window (See Figure 1).

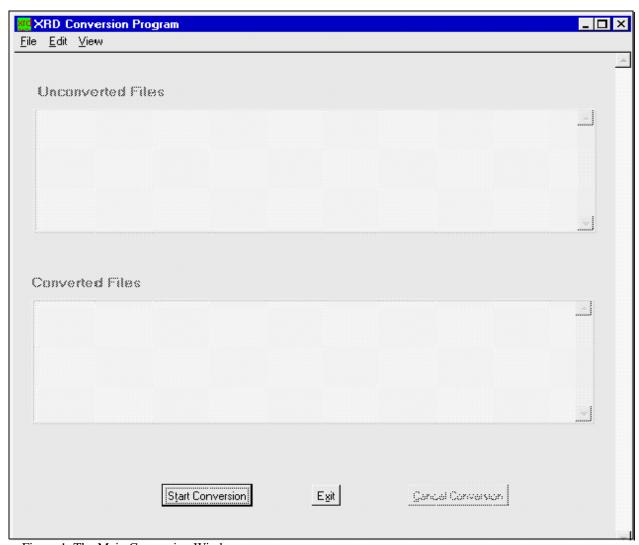


Figure 1. The Main Conversion Window.

XRD Conversion Main Window

Important Features

- There is a menu bar at the top of the window. The three menu lists provide access to all available program functions.
- The top dialog box, "Unconverted Files", will display the unconverted (raw data) files selected from a specified folder(s). This box does not become active until files have been added.
- The bottom dialog box, "Converted Files", will display the files after they are converted. This box becomes active when the converted files are displayed.
- The two buttons at the bottom of the window allow you to begin a conversion, or exit the *XRD Conversion* program completely.
- Clicking on the green **XRD** box next to the title opens a list of options. These options allow you to move, size, minimize, maximize, or close the screen.

The Menu bar

The menu bar contains three menu lists–File, Edit, and View (See Below).



Selecting a Fuction

You can **select** a function in one of three ways. (1) Select an option from one of the three lists by clicking on it with the mouse. OR (2) Next to the function on the menu list, a control key command is given. Hit the **Ctrl** key + the key of the underlined letter in the function name (e.g. to activate "Select Files" hold down **Ctrl+S**). OR (3) Hit the **Alt** key + the letter button that is underlined in a function to activate that particular function (e.g. to active "Select Files" click on **Alt+S**).

Options Under "File"

- <u>Select Files</u> this option allows you to select raw data files for conversion. Choose the files using the "Raw Data Files" dialog box that appears upon option selection. (See "Selecting Files for Conversion" p. 4).
- <u>Start Conversion</u> this option starts the conversion once the appropriate files are loaded into the "Unconverted Files" box. Performs the same function as the **Start** Conversion button located at the bottom of the window. After the conversion is

complete, the program opens an alert box displaying the number of files converted.

• Exit – this option exits the *XRD Conversion* program completely. Performs the same function as the Exit button.

Options Under "Edit"

• <u>Delete File</u> – this option performs different actions, depending on where the file is located. For <u>unconverted files</u>, it deletes the selected file from the "Unconverted File" box and the XRD program. It does **NOT** delete the raw data from the original file! For <u>converted files</u>, it deletes the selected file from the "Converted File" box and also from the folder to which it is sent after conversion. The converted file is completely deleted, but the <u>raw data</u> still exists in its original folder.

Options Under "View"

• <u>Open File</u> – this option allows you to select a file and open it for editing. This selection will open the "Edit Text File" window with either the raw data or the converted data, depending on which file you select. **From this window you can edit any of the data available** (See "Editing Files" p. 7).

Selecting Files for Conversion

Downloading Data

Before any file can be selected for conversion, the data files must be downloaded to your local machine. Be sure to place them in a location that is easily identifiable by anyone who will use the conversion program.

Selecting the Files

1. From the main Conversion window, choose **Select Files** from the **File** menu. This opens the "Raw Data Files" dialog box (See Figure 2).

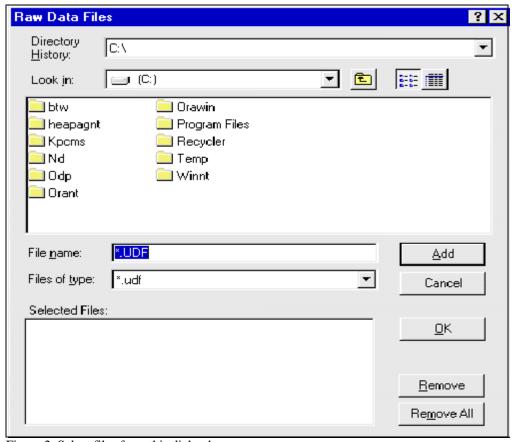


Figure 2. Select files from this dialog box.

- 2. If you know the directory address, enter it in the **Directory History** box. If not, use the **Look in:** box to navigate through the directory tree until you find the files you need.
- 3. **Add** the raw data files to the "Selected Files" box by either double clicking on a file, or by first highlighting the file, then pressing the **Add** button.
- 4. Remove a file at any time by highlighting it and clicking the **Remove** button for one file, or **Remove** All to remove all files displayed.
- 5. Once all the raw data files you want to be converted are listed, click the **OK** button. The files are exported to the XRD "Unconverted Files" box on the main window. They are now ready for conversion.

Converting Files

Your files should now be listed in the "Unconverted Files" box on the main conversion window (See Figure 3).



Figure 3. Unconverted files ready for conversion.

NOTE: Once your files are listed in the "Unconverted Files" box, do NOT leave this screen until you have converted your files. If you leave this screen to select more files from the "Raw Data Files" dialog box, the files already listed will be deleted. Make sure you always convert the files listed before trying to import more files into the "Unconverted Files" box.

- 1. Start the conversion in one of three ways: (1) select **Start Conversion** from the **File** menu, (2) click on the **Start Conversion** button at the bottom of the screen, (3) or press the **Ctrl+T** keys.
- 2. After the conversion is complete, you will receive a message indicating the number of files converted (See Figure 4).



Figure 4. Message indicating number of files converted.

- 3. Click on **OK** to see the converted file(s) listed in the "Converted Files" box.
- 4. The converted files are saved in the same directory where the raw data files are located. The converted file is listed with a UDI extension (e.g. 1105a001.udi).

Editing Files

Both the unconverted and converted files can be accessed for editing.

Opening a File

- 1. From the main conversion window, highlight the file you want to edit. It can be an unconverted or a converted file.
- 2. From the View menu, select Open File. This opens the "Edit Text File" window.
- 3. An unconverted file, once opened, should look similar to Figure 5.

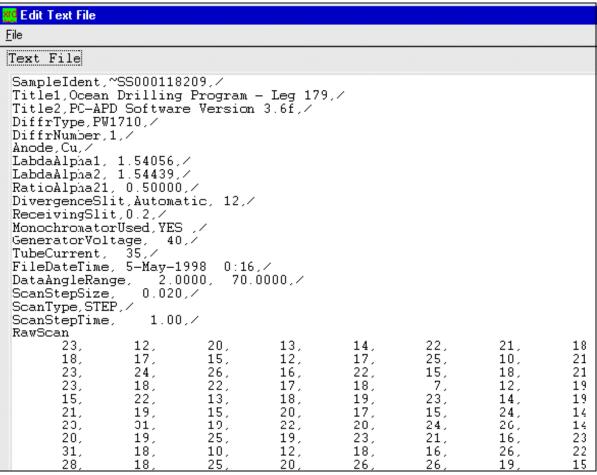


Figure 5. An unconverted file in "Edit" mode.

4. A converted file, once opened, should look similar to Figure 6. **Notice that the data is now sorted into labeled columns**.

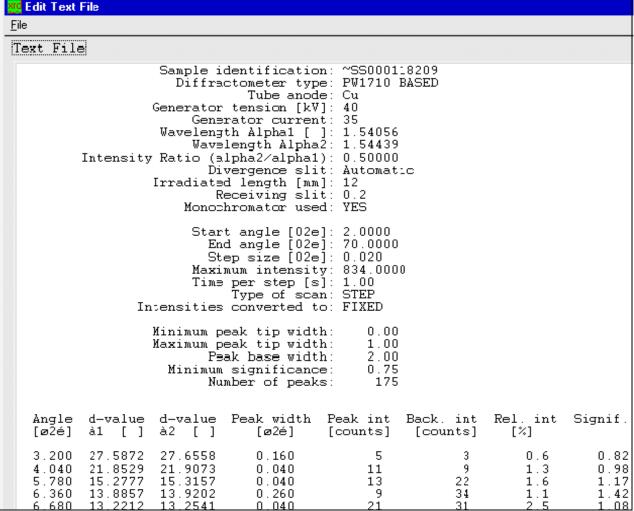


Figure 6. A converted file in "Edit" mode.

5. Edit the data as you deem necessary.

The "File" Menu

Click on **File** in the corner of the editing window to display its list of options (See Figure 7).

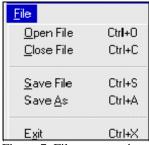


Figure 7. File menu options

Open File

This option allows you to open text files in "edit" mode. Clicking on this option opens the "Text Files" dialog box (See Figure 8). From this box you can select the file you want to open in the "Edit Text File" window.

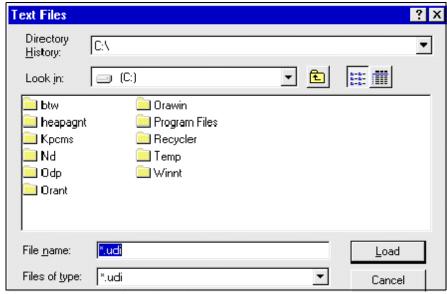


Figure 8. The "Text Files" dialog box.

Close File

This option closes the currently opened file in the editing window.

Save File

This option allows you to save the editing changes. Use the "Save File" dialog box to select the appropriate folder (See Figure 8). This does not show text files opened within the text edit window. It only displays files opened in the conversion window.

Save As

This option allows you to save your edited file as a new file, or in another location. Selecting this option brings up the "Save File" dialog box (See Figure 9).



Figure 9. The "Save File" dialog box.

Exit

This option closes the editing window and re-opens the main conversion window.

Appendix. Installation and Setup

The files required for program installation and delivery are located on the "Appsdev" server. From this server, the files are located in two places: the "Develop" and the "Deliver" directories. Use the directory to which you have access.

Deliver Directory

- 1. The three installation files in the "Deliver" directory are located at V:\Deliver\Apps\XRD\XRD_Conv.
- 2. The three files in the XRD_Conv folder required for installation are: **setup.exe**, **Xrd.001**, and **Xrd.002**.
- 3. **Copy** these three files.
- 4. Create a "Temp" folder on your local hard drive. **Paste** the three files into the "Temp" folder.
- 5. Go to the **Start** menu and click on **Run**.
- 6. Find the "Setup" executable and run the setup.
- 7. While the setup is running, a dialog box will appear. The box informs you that the files are being placed on your local hard drive at **C:\ODP\XRD**.
- 8. Click on the **Finish** button.
- 9. A window with the **XRD Convert** and **Uninstall Executable** will open. **Copy** the XRD Convert.
- 10. Go to the desktop. Right click the mouse and select **Paste** from the menu displayed. This creates an icon for the XRD program on your desktop.

Develop Directory

- 1. The three installation files in the "Develop" directory are located at V:\Develop\XRD_Conv\Exe.
- 2. All remaining steps are identical to the installation from the "Deliver" directory. Once the three installation files are located, start at step #2 from above.