Central Facility for X-Ray Materials Characterization

X-Ray data file access and format conversion

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X-Ray Diffraction data file access

X-Ray diffraction data files are stored on the computers that control the instruments. These files can be accessed in 2 ways:

- **Direct file access** - Data files can be retrieved directly from the instrument computers using floppy disk, USB flash drives, CD-R/CD-RW media, and sent to another location via the Internet (e.g. e-mail account).

- **Network file sharing** - Data files can also be retrieved by accessing the Instrument computers through the UNL Network using File sharing for Microsoft Networks.

Rigaku D/Max-B data files

Network Computer Name	🖥 Rigaku-xrd
Microsoft Networks workgroup	**PHYSICS & ASTRO**
Data file location	**c:\data**

Direct File Access:

1. On the Rigaku D/Max-B Instrument computer, using windows explorer, navigate to the data file directory **c:\data**.
2. If the names of the data files are unknown, access the detailed file list given in the file manager in the Rigaku software.

> **How?** - In the c:\data directory, locate the file fildir.dat open it with a text editor such at Notepad or Wordpad. If this file has been associated with a word processor, it can be opened by double-clicking. This file contains detailed information for each XRD data file such as the Sample ID and Date and time of the scan. Note: This information can also be viewed with the File Directory Display Utility in the Rigaku software.

3. Copy the data files to the desired destination. Be sure you leave the original file intact (i.e. do not "cut").

Network file sharing from compatible computer:

1. A "compatible computer" is one that:
   a. Has **Client for Microsoft Networks** over the **TCP/IP Protocol** enabled.
   b. Is a member of the **Physics & Astro** workgroup.
   ** Note all computers in the X-Ray lab are compatible computers.
2. Go to **START | Search | Computers or People | A Computer on the Network**. If a shortcut is already on the desktop, double-click it and go to step 4.
3. For computer name type **Rigaku-xrd** and click Search
4. When it finds the computer it will be listed in the search results pane. Double-click on the **Rigaku-xrd** entry
5. If there are no networking problems, you should see a list of available shares on Rigaku-xrd. Double click on **Data**.
6. Eventually it will list the files in the c:\data directory of the Rigaku D/Max-B Instrument comptuer.
7. If the names of the data files are unknown, locate the file **fildir.dat** in the directory you just opened and load it with a text editor such at Notepad or Wordpad. This file contains detailed information for each XRD data file such as the Sample ID, Date and time of the scan.
8. Copy the data file(s) to the desired destination.

Bruker-AXS D8 Discover data files

Network Computer Name	Bruker-xrd
Microsoft Networks workgroup	PHYSICS & ASTRO
Data file location	c:\frames; c:\diffdat

Direct File Access:

1. On the D8 Discover instrument computer, using windows explorer, navigate to the data file directory **c:\frames**.
2. Copy the data files to the desired destination.

Network file sharing from compatible computer:

1. A "compatible computer" is one that:
   a. Has **Client for Microsoft Networks** over the **TCP/IP Protocol** enabled.
   b. Is a member of the **Physics & Astro** workgroup.
   ** Note all computers in the X-Ray lab are compatible computers.
2. **Go to START | Search | Computers or People | A Computer on the Network**. If a shortcut is already on the desktop, double-click it and go to step 4.
3. For computer name type **Bruker-xrd** and click **Search**.
4. When it finds the computer it will be listed in the search results pane. Double-click on **Bruker-xrd.**
5. In the connect login window enter *xrduser* for user and *xrd* for password.
6. If there are no networking problems, you should see a list of available shares on **Bruker-xrd**. Double click on **frames** or **diffdat**.
7. Copy the data files to the desired destination.

# X-Ray Diffraction Data file format conversion

When X-Ray diffraction scans are taken on the Rigaku D/Max-B and Bruker-AXS D8 Discover, the files are saved in a unique binary format that can be read directly only by software written by the manufacturer that created them.
If you wish to load or import this data into another program, (for example you wish to analyze data taken on the Rigaku diffractometer with Bruker-AXS software) you must first convert the file into a compatible format. **X-Ray data file conversion utilities are available on the x-ray facility computers (in the "XRD Applications" folder) and/or can be downloaded from the facility** [website](). You may encounter the following XRD file formats:

Rigaku Raw	Rigaku D/Max-B initial data file forma which can only be read by Rigaku software and Microcal Origin (with a special script). (e.g. *Z04500.raw*)
ASCII (2theta,Int)	Application XRD CONV.EXE can convert Rigaku Raw files into this ASCII file format. It contains 2 columns of data (2theta / Intensity pairs) and can be directly read and easily displayed by most applications. (e.g. *Z04500.dat*)
Diffrac Plus Raw	Bruker-AXS initial data file format which can only be read by Bruker-AXS software. (e.g. *Silicon.raw*)

Rigaku Raw → ASCII or Diffrac Plus Raw

Use the program **XRD CONV.EXE**. This file is available for download on the X-Ray facility web-site and is installed on all computers in the facility in the "XRD Applications" folder.

1. Run **XRD CONV.EXE** by double-clicking the icon.
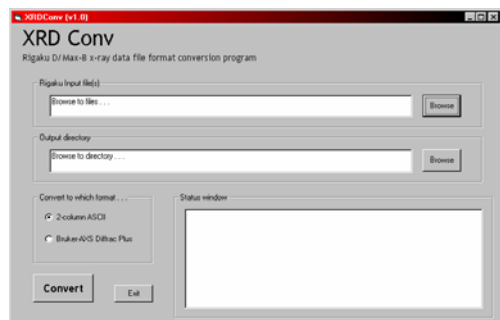
2. Browse to and select the Rigaku Raw files you wish to convert

   (* Note that you may select more than one file at a time by holding the CTRL button while you select with the mouse)

3. Browse to and select the directory where you would like to store the converted file. If it is the same as the input directory, no entry is required.

4. Choose the output format required.

5. Click the "Convert" button to begin the conversion. The status window will show conversion progress.

Diffrac Plus Raw → ASCII

Use the program **ConvX.EXE**. This file is available for download on the X-Ray facility web-site and is installed on all computers in the facility in the "XRD Applications" folder.

1. Run **ConvX.EXE** by double-clicking the icon.
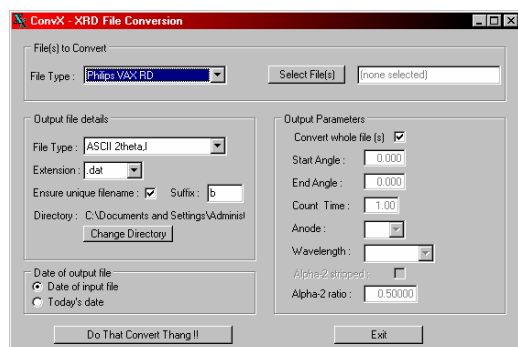
2. Under *File(s) to Convert*, set *File Type* to "DiffracPlus Raw" and select the Files for conversion.

3. Under *Output file Details* select *ASCII 2theta/I* and change any other values if desired.

4. Normally leave all *Output Parameters* alone

5. Click *Do That Convert Thing !!*