

Free and Inexpensive Software Alternatives for X-ray Diffraction

(prepared by James R. Connolly, for EPS400-001, Introduction to X-Ray Powder Diffraction, Spring 2009)

Introduction

Sophisticated analytical software for X-ray Diffraction (like MDI's Jade or Bruker's Difrac^{Plus}) is very powerful, very flexible and very expensive. As an example, a single workstation installation of Jade+ software will cost at least \$5,000, and the ICDD Powder Diffraction file database on CD-ROM will cost \$3,000 to \$7,000 (depending on version purchased and other possible discounts). Addition of Rietveld-type modules for profile refinements will typically add \$3,000-\$5,000 to the cost of the "basic" software. This type of software provides a very high level of functionality in data processing and analysis, and is essential for anyone operating an XRD laboratory.

For those without large budgets who have X-ray data they need to display and analyze, there are free or inexpensive alternatives to these commercial packages. The purpose of this document is to introduce some of this software with which the author (who is admittedly spoiled by easy access to MDI's Jade) has had some experience. The programs are discussed briefly below in sections related to their function. Some software is also included for which the author has little or no experience, but that has a good reputation in the XRD community.

The programs discussed in this document are a small fraction of all that is available. By far the best source for free software (and information about commercial software packages) is the Collaborative Computational Project #14 (CCP14) for Single Crystal and Powder Diffraction. Their main address is hosted in the UK at: <http://www.ccp14.ac.uk/index.html> but mirrors of the site exist in the U.S., Canada and Australia. All of the software listed in the remainder of this document may be found (or linked) in the CCP14 archive. Subsidized funding of CCP14 ended in 2007, but as of this writing the information is still there and much of it is clearly updated regularly.

The CCP14 search interface to the site now entered using a Google JavaScript interface on the home page. The search window is a somewhat elusive popup, but it does work. For browsing the Site Map interface (<http://www.ccp14.ac.uk/sitemap.html>) might a be better choice than the search. Many programs are archived by CCP14 but the index also provides links to the most authoritative source (if there is one) so that the most recent versions may usually be downloaded directly from their author(s). CCP14 also includes links to quite a bit of free tutorial information for analyzing different materials including clays, thin-films, etc.

The IUCr (International Union of Crystallographers site at <http://www.iucr.org/iucr-top/> is also maintains an index (SInCris) of free software. The interface is not terribly friendly or easily searchable or as up-to-date as CCP14, but if you know the name of a program you are looking for, you can use their alphabetical index. Their site also includes links to lots of useful crystallographic information. The free "Teaching Pamphlets" can be useful self-tutorial resources.

Most of the software listed below is also available on our local FTP site at in the Department of Earth and Planetary Sciences at <ftp://eps.unm.edu/pub/xrd>. All the XRD programs available are indexed for easy access at <ftp://eps.unm.edu/pub/xrd/index.htm>. These programs are provided for convenience only and will frequently not be as up-to-date as the versions linked on the CCP14 index.

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Use of standard commercial web-crawling search engines (like Google.com, Ask.com, etc.) for keyword searches related to X-ray Diffraction is generally the first place to go to find what you are looking for. If working from a campus address, you may search a wide variety of academic databases from the UNM Libraries sites (<http://library.unm.edu>).

Data Conversion Tools

MDI Jade Export/Import

Many data exchange tools do not support the MDI data format as an import or export file format, although a bit of investigation reveals that the MDI data format is very close to the “standard” data interchange format or DIF. Jade includes a conversion program which exports Jade data as a simple two column ASCII (filename.txt) format and these files may be easily converted with a simple ASCII text editor to numerous other formats readable by other programs. The MDI ASCII file includes the sample description information in the first header line followed by two columns listing sequentially listing each 2θ value and counts for each “step” of the scan. Most programs discussed below require modification of the “header” portion of the file (i.e., deleting title information, adding total # of data points in a specific location, saving with a new filename extension, etc.) before it can be used. The format required for the program you are using will usually be part of the documentation or help information for the program. The actual editing can be done with Notepad, WordPad or any ASCII text editor.

PowDLL Converter

By far the most comprehensive file converter I have found is Nikos Kourkoumelis’ PowDLL Converter. It is a Windows program that requires installation of the (free) Microsoft .NET framework and converts the following file types:

Imports: Bruker/Siemens RAW Files (all versions plus V4 - XRD Wizard format from Bruker-AXS), STOE RAW Files, Scintag RAW Files, Rigaku RAW Files, Shimadzu RAW Files, Philips RD Files, Scintag RD Files, Panalytical XRDML Files, INEL CPS 120 Files, Scintag ARD Files, powderCIF Files, Sietronics CPI Files, Riet7 DAT Files, DBWS Files, GSAS Files (CW STD), Jade MDI Files, Rigaku RIG Files, Philips UDF Files, UXD Files, XDA Files, XDD Files, ASCII XY Files, EDX.

Exports: Bruker/Siemens RAW Files (versions 1,2), Philips RD Files, Scintag ARD Files, Sietronics CPI Files, Riet7 DAT Files, DBWS Files, GSAS Files (CW STD), Jade MDI Files, Rigaku RIG Files, Philips UDF Files, UXD Files, XDA Files, XDD Files, Panalytical XRDML Files, ASCII XY Files, MS-Excel Multiple X-Y, EDX.

The converter will show you your data before conversion, and batch-convert groups very nicely. In the newest version the filenames in conversion-batches are automatically incremented as to not overwrite existing files (a problem with early versions) and conversions for several new formats have been added. The newest release is always available on the authors site at <http://users.uoi.gr/nkourkou/powdll.htm>.

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ConvX

Simple but useful free program for converting between XRD data formats that can be very useful in translating a file that cannot be imported into a particular program into a format that can be imported. Supports conversion to/from the following data formats: Phillips RD and SD (PC and VAX versions), ASCII 2 θ -Intensity, Bruker/Siemens RAW formats (DiffracPlus, DiffracAT, DiffracV1), Sietronics GPI, GSAS, DBW-type and ScanPI. Jade ASCII *.txt files may be used, but may require removal of the first line (the File description information). Users will need to experiment with what works.

Other Data Conversion Programs

Two other simple windows-based data conversion programs are POWF 2.11 and CONV 3.01. Their function and capabilities are similar to ConvX.

All of these converters are available on our FTP site (<ftp://eps.unm.edu/pub/xrd/index.htm>).

Many of the other programs discussed below include modules for importing and exporting data files and can be used for that purpose exclusively if desired. These include PowderX, WinFit, and FullProf.

General Data Processing Software

PowderX

Powder X is a freeware program from Cheng Dong of the Institute of Physics at the Chinese Academy of Sciences in Beijing. A basic tutorial for the use of Powder X can be found at <http://www.ccp14.ac.uk/tutorial/powderx/index.html>.

If you have unlimited access to Jade to handle your data analysis, you will probably not need PowderX. PowderX can be used to easily export data to many other formats (including GSAS and FullProf), though not as many as the PowDLL converter. If you don't have Jade on your personal workstation (or the several thousand dollars needed to get it there) and want to work on your data outside of the lab, PowderX is free and can be installed where Jade is not available.

Powder X is basically a Windows-based pattern-processing program that operates under all versions of Windows. It has many useful functions such as data smoothing, background subtraction, $K\alpha_2$ elimination, peak search, and indexing. It imports and exports data in multiple data formats, and includes algorithms to correct for specimen displacement and zero-angle errors. Many of the output formats are those used by a variety of pattern refinement programs such as GSAS and FullProf. The program also includes a simple pattern calculation algorithm developed by the author (LAZY) that will generate a calculated pattern from input structural data.

Import of MDI data files requires starting with an ASCII export file and then editing that file to conform to the import requirements of the PowderX ASCII data¹. It is not difficult to do, but must be done correctly for the import to work.

¹ To be used in PowderX, MDI data must be saved in MDI ASCII Text format (with Jade) and edited: add a second header line consisting of the total number of data points, and saved with a *filename.xrd* extension.

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The software is available from the CCP 14 site as a single large ZIP file, or a series of 5 smaller ones. The archives are password protected. There is no charge for non-commercial use of the software, but to be “legal” users must send an Email to the author, Cheng Dong at chengdong@aphy.iphy.ac.cn including the following information: Your Full Name, Title, affiliations, mailing address, telephone and Fax numbers. He will then register you as an official user of the program and send you the password to unlock the archive.

WinFit

WinFit is a free peak-fitting program from Stefan Krumm of the Institute for Geology in Erlangen, Germany. Several years ago I used WinFit to successfully resolve overlapping peaks of multi-phase rock samples in Siemens (Brukker) .RAW data files. The latest update available is dated 1997 and it doesn't support long filenames (which can make navigating your file system a bit tricky) and it is somewhat crash prone in modern versions of Windows. It is instructive as a tool for learning about peak decomposition.

The menu lists the MDI data file as one of the formats (with ????) next to it), but my experience is that attempting this import will invariably crash the program. To successfully convert an MDI data file for input into WinFit you must first save it in Jade as an MDI ASCII file (*.TXT) then edit the file removing the first line (the sample title) leaving only the two-column 2 θ and counts data. That file then is saved with a *.ASC extension, and can be imported into WinFit. WinFit also supports direct input from Siemens/Brukker *.RAW and a variety of Phillips and Rigaku formats. PowDLL converter may also be used to convert what data you have into an importable format for WinFit.

Other available through Dr. Krumm is linked on his software page at <http://www.geol.uni-erlangen.de/index.php?id=58&L=3>. The other program include:

- **WinStruct:** a structure and pattern simulator for clays that is similar in some respects to NewMOD.
- **SediCalc:** a sedimentology lab toolbox for clays and other phases calculates suspension settling times and the Mg/Ca contents of dolomites from XRD data.

Powder Cell for Windows

W. Krause & G. Nolze's program for doing simple pattern comparisons is a kind of simple profile refinement tool. The program takes input structural data and creates a structural model and a calculated diffraction pattern that can then be compared with the experimental pattern to see how closely it matches the calculated pattern. Structural parameters can then be “tweaked” until the calculated pattern and experimental pattern match resulting in a kind of simple interactive profile refinement. Program is installed by running the executable installer, unzipping to a folder of your choosing and running the program (pcw25.exe) or making a program shortcut for it in a location of your choosing. The program includes extensive (if somewhat interestingly worded) program help, and is available on CCP14 archive; a copy is located on the <ftp://eps.unm.edu/pub/xrd> site.

Microsoft Excel

Microsoft Excel may be used for display and analysis of XRD data. The main issue is getting the data into spreadsheet format so that it can be used. Excel can be setup to import a

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variety of parsed data, and many ASCII formats may be read, although you may find yourself having to create a specialized import routine to do so. A two column 2θ vs Intensity format is easiest to import. The easiest way to do this with Jade is to save the file as an MDI ASCII Text format and use Excel's text import Wizard (under the Data menu). Patterns may be plotted as simple X-Y "Scatter" plots for presentation, and different data formats overlaid in a common environment fairly easily².

Excel is not commonly used for sophisticated data analysis, but it can be. A look at Dennis Eberl's Excel applications Mudmaster and RockJock (discussed below) demonstrate how the analytical power of Excel's solver and other mathematical functions can be used to create pretty amazing analytical tools. To tap some of the hidden data analysis power in Excel, you need to install the Solver and Analysis Toolpack "Add Ins" from the Tools menu.

For those wanting to pursue Excel as a serious analytical tool, there are a lot of fat computer books available about programming in VBA (Visual Basic Applications). Two highly regarded books that get high marks for readability and information are "Excel 2003 Power Programming with VBA" and "Microsoft Excel 2003 Formulas", both by John Walkenbach. Though some recent reviewers have decried the lack of the most up-to-date information (XML, SharePoint integration and InfoPath), they still are indispensable for the kind of programming done by Dennis Eberl in Mudmaster and RockJock. These are available from larger local bookstores (but not UNM's), or online from Amazon.com.

Specialized Data Analysis Tools

Mudmaster

Mudmaster is an Excel spreadsheet that is designed to determine particle size in fine-grained powders. Since it uses peak shape and size to evaluate peak broadening as related to "particle" size, it is actually measuring crystallite size rather than the actual of the particles. If each particle is a single crystal, then this is not an issue. The spreadsheets also can be used to examine peak asymmetry and evaluate strain in addition to crystallite size.

The crystallite size is equal to $(N - 1)d_{hkl}$, where N is the number of hkl planes responsible for a reflection. The program makes use of this to evaluate the crystallite size in a diffraction pattern. The program consists of a main workbook (MudMastr.xls) that includes the "Peak Picker" to select the peak to be analyzed, Sheet 1 where results are calculated and shown, and Sheet 2 containing all the macro bells and whistles that do the calculations. A few other spreadsheets perform specialized functions including editing data to remove minor peaks in the "tail" of the peak of interest (PkChopr), shifting of patterns using a standard to correct for linear offsets (PkSift), modifying data to change step size (Stepcon), estimate the layer scattering intensity Lorentz polarization factor and G^2 when this is not known (CALCLPG2), and a sample data set (Samp). The program include a detailed operations manual that "walks" you through the data entry and calculation process, and includes references to papers that discuss crystallite size and strain calculations.

² Note: The newest version of the PowDLL Converter program discussed earlier includes the ability to convert batches of diffraction data files to an Excel file that puts each data file into two-column angle-intensity data that can be stored or exported.

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Crysfire

One of the obstacles to using powder patterns in structural analysis programs such as GSAS or FullProf is an accurate determination of the unit cell parameters for input into the modeling program. Crysfire is a Windows interface to nine different computer programs that perform pattern indexing. In a simplistic way, you input your analytical peak data in one of a number of different formats, the interface “feeds” your data to the different indexing programs, calculates unit cell parameters by a variety of methods and returns the data to the Crysfire interface. Crysfire makes use of system environment variables to exchange information between the different indexing programs and the results module; this requires careful installation to make sure the data is exchanged successfully. As described by the authors, “Hopefully it all works seamlessly together, allowing non-specialist users to perform indexing operations on their datasets with a minimum of keystrokes and effort. By non-specialist I mean non-specialists in powder indexing - they are still assumed to have some crystallographic knowledge and are likely to be people engaged on structure determination from powder data, for whom indexing is simply a necessary but critical preliminary to the main show.”

The software may be download from <http://www.ccp14.ac.uk/tutorial/crys/index.html>. The page includes some online documentation and tutorial resources. Robin Shirley, the author of Crysfire, died unexpectedly in March, 2005. The most recent (and likely last) version is included in our XRD FTP archives at <ftp://eps.unm.edu/pub/xrd/index.htm>.

Quantitative Analysis Tools

GSAS

“Generalized Structural Analysis System” is a very mature Rietveld program, and comes in versions to run on Windows/DOS and Linux PCs and MacOSX.4 (or newer) systems. Written originally for UNIX, the “port” to the Windows platform essentially links a series of DOS command windows in which the actual work is done with command line modules. EXPGUI (Mac, Windows & Linux) is a graphical interface that is a bit friendlier than the command line interface. The latest version includes a windows installer (gsas+expgui.exe) that sets up most of the program for you (including, in most cases setting environment variables appropriately as described in the readme.txt in the c:\gsas folder). It has been developed as free (but not open source) software and is maintained by Allen C. Larson & Robert B. Von Dreele of Los Alamos National Laboratory. For the last few years, distribution has been handled by Brian Toby of NIST.

GSAS has a very good reputation and a large community that uses it, but it is an “expert’s” program in that the user really needs to know what they are doing to get good results. In popular terms, the learning curve is very steep. It comes with a 231 page manual which contains surprisingly little about Rietveld refinements and is chiefly concerned with how to interact with the 37 different program modules. Initial impressions are quite intimidating, but the software gets great reviews from those who learn to put it through its paces.

GSAS information and distribution has been assumed by the NIST Center for Neutron Research. The main page linking everything connected with GSAS is available at: <http://www.ncnr.nist.gov/programs/crystallography/software/gsas.html>. This page also

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includes links to all mirror sites for various versions of the program, and an excellent tutorial about how to use EXPGUI, the graphical interface to GSAS that allows you to do much (but not all) of what GSAS can do in a “friendlier” graphical environment. We have the most recent (Feb. 2005) distributions of EXPGUI and GSAS available on our FTP site at <ftp://eps.unm.edu/pub/xrd/index.htm>.

We have recently added an excellent tutorial for EXPGUI created by Lachlan Cranswick in 2005 to our FTP site. This 100+ page PDF document is part of a full CD-ROM with programs, tutorial exercises, and lots of other resources that can be freely shared; contact Jim Connolly if you are interested in obtaining a copy.

FullProf 2000

FullProf is another profile refinement (Rietveld) system produced by Juan Rodríguez-Carvajal at the Laboratoire Léon Brillouin (CEA-CNRS) in France. The software presents a friendlier GUI interface than GSAS (through the plotting Program WinPLOTR co-written by Thierry Roisnel and the author at the LLB) but is still a complicated analytical tool requiring good data input by a user who understands diffraction data, and crystal structure analysis, and is willing to master fairly complicated input data file structures.

Unlike the GSAS manual, the 139-page FullProf 2000 manual (in Acrobat PDF format) includes a good discussion of the Rietveld procedure and suggests the best sequence of steps to follow to produce a good refinement. It is still no substitute for the study required from the Rietveld literature referenced in the previous “Introduction to Quantitative X-Ray Diffraction” chapter. We have a recent version of FullProf on our ftp site at <ftp://eps.unm.edu/pub/xrd/index.htm>. The CCP14 source page for FullProf with tutorial information and links is at <http://www.ccp14.ac.uk/tutorial/fullprof/index.html>.

FULLPAT

Dave Bish and Steve Chipera's Excel-spreadsheet-based whole pattern fitting system uses the Excel solver functions to do a least squares refinement to fit whole-pattern data to standard pattern data to produce quantitative analyses. The program archive consists of two files -- the actual Excel spreadsheet used to do the calculations and a well written 23 page manual that explains the use of the program in sufficient detail to make it usable. It does require rather extensive development of in-house standard XRD patterns prepared using a suitable corundum standard as a "spike". This system was used routinely in Bish and Chipera's well respected LANL XRD lab. Available from CCP14 (<http://www.ccp14.ac.uk/ccp/web-mirrors/fullpat/>) or on our FTP site at <ftp://eps.unm.edu/pub/xrd/index.htm>.

RockJock

RockJock is a massive (40 MB) Excel spreadsheet that uses Excel (Visual Basic) Macros, Formulas and the (add-in) Solver function compare integrated intensities of phases identified in a whole-pattern with those of an internal standard to perform quantitative analysis on an XRD pattern. While not as precise as full-blown Rietveld refinements, the system holds promise for doing reasonable quantitative analyses since it does a least-squares fit on the intensities of the whole pattern that can reduce the effect of preferred orientation on the results.

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Written by Dennis D. Eberl, the software was published in 2003 as U.S.G.S. Open-File Report 03-78, "Determining Quantitative Mineralogy from Powder X-ray Diffraction Data" and modified in 2005. It is available through the CCP14 archive; search for RockJock on the CCP14 homepage. An updated archive is also available on the EPS FTP site. The 45 page manual is well written, easy to follow and includes appropriate literature references.

Data to be analyzed in RockJock must conform to certain conditions: An internal standard of 10% ZnO (by weight mixed as 9 parts sample to 1 part standard or 3.00 g to 0.333 g), 2θ range 5° to 65° with a 0.02 step size and a count time of at least 2 seconds per step. Specific methods of grinding (using a McCrone micronizing mill) and mounting (side-drifted against frosted glass) are also indicated. The data range may be modified by changing the spreadsheet, but is not recommended. A "Peak Chopper" spreadsheet is included to modify data collected with other step sizes, but this sort of conversion will invariably result in loss of data quality.

Your author's first impression of the program is that the least-squares refinements using Solver in Excel are extremely slow. Eberl recommends a 1GHz (or faster) processor, and your author's system ran at half of that speed. He states that calculation times can be $\frac{1}{2}$ hour or more for many samples. It took about 10 minutes each to do the initial tests on the "Full Pattern" and "Clays" sheets (recommended in the installation procedures) and the data presented in these is fairly simple. The program continues doing "trial" fits until you interrupt it, and during the first calculations the CPU was so busy that it was difficult interrupt it to stop the calculations. It is slow, but if it does decent quantitative analyses it could be worthwhile.

Mudmaster

Mudmaster is a group of Excel spreadsheets (from Dennis Eberl of USGS) that are designed to determine crystallite size in fine-grained powders by making use of Excel solver and math add-ins. The spreadsheets also can be used to examine peak asymmetry and evaluate strain in addition to crystallite size primarily in clay minerals (though the system has also been successfully applied to other non-clay phases). A detailed operations manual is included that "walks" you through the data entry and calculation process, and includes references to papers that discuss crystallite size and strain calculations. The CCP14 archive is the "authoritative" source for the latest versions of the spreadsheets. Also included in the Mudmaster archive on the EPS FTP site is a paper from a recent Clay Mineral Society workshop and the six spreadsheets that comprise the varied parts of the system and tutorials.

Sources of XRD Standard Data

The International Center for Diffraction Data (ICDD)

The ICDD, located in Newton Square, Pennsylvania (near Philadelphia) is the chief source for X-Ray powder diffraction data in the world. Founded in 1950, the ICDD database is the Powder Diffraction File (or PDF). It has grown from a few thousand patterns in its first years to almost 250,000 patterns in its current (2006) release. In 2005 after 20 years of evolution of the digital database, ICDD moved from a large flat-file (PDF2) format to a fully relational database (PDF4+) format. The change allowed for efficient expansion of the database to include data from several new sources and allows for the incorporation of structural data that

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was not possible in the old format. Virtually every XRD software vendor writes its Search-Match software to access the PDF, and this format change required a lot of labs (including ours) to upgrade their software to access the new file format.

The database is expensive. The older-format PDF-2 database for a first-time purchase will cost a commercial user close to \$7,000; a 20% academic discount reduces this cost to University labs (like ours) to under \$5,000. Annual updates are now required for the PDF2 and new PDF4 since the software is time-locked. This costs an academic user \$1,100 (including a 20% academic discount). The PDF4 includes some good relational software for data retrieval, draws real patterns instead of stick figures for comparison with your data and is generally a better product. High-cost analytical software (like Jade) can read and use either form of the database with equal functionality, but stand-alone retrieval functions require an add-on program to the PDF2 that is included with the PDF4. A side benefit of the PDF4 database is that the relational structure makes it a lot easier to create subsets of the PDF in Jade that can be used in search match operations.

Since ICDD is virtually the only source for XRD data, particularly that used by automated search/match programs, those who want to use the data have little choice but to purchase it (or work in an environment in which it has been purchased for you).

The Inorganic Crystal Structure Database (ICSD)

The ICSD is the premier source for inorganic crystal structure data. This data is the required starting point for use with Rietveld-type profile refinement method(s), and most Free and commercial Rietveld programs read Crystallographic Information Files (CIF) created by this database directly eliminating a lot of tedious manual entry of data. It currently contains about 97,000 entries of detailed structural data. Cost is considerably less than the ICDD products: A single commercial license is \$1,736 annually, but an individual at a University can license the data for \$450 annually, and academic departments can license site-wide use for \$950 annually. The database is priced in Euros, so the cost in dollars varies with the exchange rate. Current information are at <http://icsd.ill.fr/icsd/>. Purchases are handled through FIZ Karlsruhe at <http://www.fiz-karlsruhe.de/ecid/Internet/en/DB/icsd/index.html>. This is a bargain compared to the ICDD databases, but most search/match software cannot use ICSD data directly. Recent versions of Jade, however, can read the structural database automatically and create calculated patterns from the data making the need for the ICDD database not totally necessary.

Mineralogical Society of America

If you want structural data for minerals for your Rietveld refinements, this free online source has structural data for every experimentally determined structure published in the Journal of the Mineralogical Society of America (around 11,000 of them). The entire database is online at the following URL (including a link to a PDF of the article by Downs and Hall-Wallace (2003) that explains how to use it): http://www.minsocam.org/MSA/Crystal_Database.html. The database now includes the original text for retrieved data, plus two downloadable structure exchange formats (AMC and CIF), d-I diffraction data with peaks indexed, and the ability to view 3D structure within the database (cool, but functionally somewhat quirky). The visualization software (XtalDraw) that can be used to display the crystal structures from the CIF files is available on our FTP site at <ftp://eps.unm.edu/pub/xrd/index.htm>.

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Other Diffraction and Crystallographic Data Sources

The International Union of Crystallographers (IUCr) maintains an index page to sources of crystallographic and diffraction data at <http://www.iucr.org/iucr-top/data/>. There are some free sources listed here (the Mineralogical Society of America being by far the largest) but the ICDD and ICSD are clearly the dominant players in this area.